



NC-AFM 2026 Conference

The 27th International Conference on
Non-Contact Atomic Force Microscopy

Innsbruck, Austria

August 3–7, 2026

Program

The 27th International Conference on Non-Contact Atomic Force Microscopy Innsbruck, Austria

NC-AFM 2026 is the 27th of a series of conferences devoted to non-contact atomic force microscopy. The conference covers experimental, theoretical, and instrumental developments in frequency modulation and other dynamic modes of scanning force microscopy with particular emphasis on high-resolution imaging and force mapping.

Previous NC-AFM conferences were held in **Toyama**, Japan (2025), **Montréal**, Canada (2024), **Singapore** (2023), **Nijmegen**, Holland (2022), **Regensburg**, Germany (2019), **Porvoo**, Finland (2018), **Suzhou**, China (2017), **Nottingham**, UK (2016), **Cassis**, France (2015), **Tsukuba**, Japan (2014), **Maryland**, USA (2013), **Český Krumlov**, Czech Republic (2012), **Lindau**, Germany (2011), **Kanazawa**, Japan (2010), **New Haven**, USA (2009), **Madrid**, Spain (2008), **Antalya**, Turkey (2007), **Kobe**, Japan (2006), **Bad Essen**, Germany (2005), **Seattle**, USA (2004), **Dingle**, Ireland (2003), **Montreal**, Canada (2002), **Kyoto**, Japan (2001), **Hamburg**, Germany (2000), **Pontresina**, Switzerland (1999), **Osaka**, Japan (1998).

Contents

1	Committees	2
2	Sponsors	3
3	Venue	4
4	Social events	6
5	Technical Symposium	9
6	Session Schedule	12
7	Oral contributions	14
8	Posters	87
9	Conference Schedule	165

1 Committees

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2 Sponsors

The following sponsors support the conference:

- ScientaOmicron GmbH, Taunusstein (Germany)
- Zurich Instruments AG, Zurich (Switzerland)
- CreaTec Fischer & Co. GmbH, Erligsheim (Germany)
- SPECS Surface Nano Analysis GmbH, Berlin (Germany)
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- Park Systems Corporation, Gwacheon, (South Korea)
- NanoAndMore GmbH, Wetzlar (Germany)
- Beilstein Journal of Nanotechnology, Frankfurt (Germany)



3 Venue

Conference site: CCB

CCB Innsbruck
Innrain 80
6020 Innsbruck

[View on Google Maps](#)

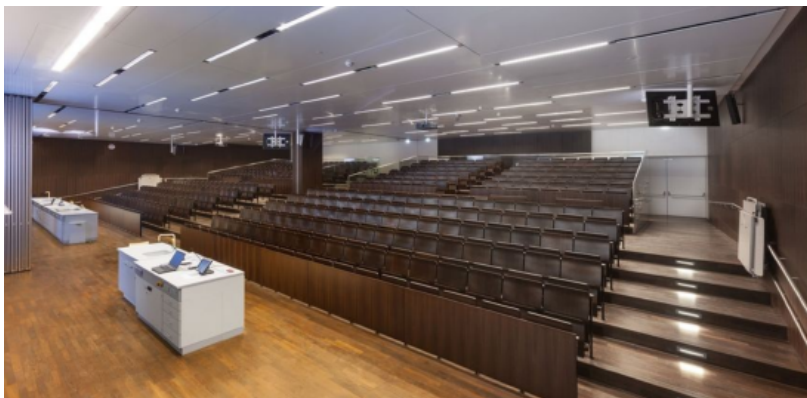
The Center for Chemistry and Biomedicine (CCB) is a modern venue designed for academic and professional events. It is conveniently situated approximately 15 minutes from Innsbruck's historic city centre.



The CCB features a lecture hall with seating for up to 400 participants and a 600 m² foyer, providing ample space for networking, exhibitions, and receptions. Its barrier-free design ensures full accessibility for all participants.

Oral sessions

All the oral presentations will take place in room M.EG.180.



Free Wi-Fi will be available at the venue, with the password announced on-site. Several Type F (230 V, 50 Hz, 16 A, Schuko) power outlets are available. Please note that power converters will not be provided, so attendees should bring their own if needed.

Poster and exhibition sessions

The exhibition and coffee breaks will take place on the same floor as the lecture hall (M.EG.180). The poster sessions will be held both on the same floor as the oral session hall and on the first floor. Free Wi-Fi will be available throughout the venue.

Lunch

Lunch will be provided each day and can be enjoyed at the UNI LOUNGE, a short 5-minute walk from the conference venue. Vouchers for lunch will be distributed to all participants and can be used at the following location:

UNI LOUNGE
Agnes Heller Haus
Innrain 52a
6020 Innsbruck

[View on Google Maps](#)
[View Menu \(DE\)](#)

4 Social events

The conference program includes three social events.

Welcome reception

The welcome reception will take place on Monday evening in the foyer of the CCB, directly in front of the M.EG.180 lecture hall. This informal get-together will provide participants with an opportunity to meet, reconnect, and begin the conference in a relaxed atmosphere.

Excursions

In addition to the scientific program, conference excursions starting at 11:00 on Thursday offer a choice of activities that combine informal scientific exchange with the opportunity to experience the region beyond the conference venue.

Participants will have the opportunity to join one of the following excursions, providing a more relaxed setting for scientific discussion:

- **Hikes to the Patscher Alm and Patscherkofel Schutzhaus**

This half-day hike explores the alpine landscape surrounding Innsbruck and offers a relaxed setting for informal discussions and networking amid the scenery of the Tyrolean mountains. Lunch will be provided at one of the alpine huts along the routes.

Difficulty: Easy | **Duration:** Approx. 1-1.5 hours | **Elevation gain:** Approx. 250 m

Options: Participants may choose between two walking options (first come, first serve): one group will walk uphill, while another group will walk downhill. Alternatively, participants may take the cable car uphill and join the group without any walking.

11:00: Meeting point in front of the CCB, followed by a bus transfer to the Patscherkofel cable car.

12:00: Start of the hikes.

16:00: End of the hikes and return transfer to the CCB.

DISCLAIMER: Participation in the excursion is voluntary and at the participant's own responsibility. Participants confirm that they are physically capable of taking part in an easy walking excursion and are responsible for wearing appropriate footwear and weather-appropriate clothing. Please note that the activity takes place outdoors and that natural risks may occur, including uneven terrain, changing weather conditions, and other circumstances associated with outdoor activities. The organizers do not assume liability beyond the scope of applicable law.

- **Guided tour of the city centre**

This walking tour introduces participants to Innsbruck's historic city centre, including renowned landmarks such as the Golden Roof and the Imperial Palace. In addition to learning about the

city's history and heritage, the tour provides a pleasant opportunity for continued scientific conversations and informal interaction in a more casual setting.

11:00: Meeting point in front of the CCB, followed by lunch at the UNI LOUNGE (Campus Innrain, Ágnes-Heller-Haus, Innrain 52a, 6020 Innsbruck).

13:00: Start of the tour.

15:00: End of the tour.

Conference dinner

*Weitsicht Restaurant
Brunecker Straße 1
6020 Innsbruck*

*[View on Google Maps](#)
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The conference dinner will take place on Thursday at the **Weitsicht** restaurant, located in the city center and only a few minutes' walk from Innsbruck main station. Participants will gather for an evening of informal exchange and networking while enjoying panoramic views over the rooftops of Innsbruck.

Following the dinner, participants will have the opportunity to experience a traditional Tyrolean cultural performance featuring *Schuhplattler* dancing. This traditional folk dance, characterized by rhythmic clapping, stamping, and lively movements, offers a glimpse into the cultural heritage of the region and will provide an entertaining conclusion to the evening.

Freedom to Innovate in SPM Ultimate Tip Control With the VHFLI Lock-in Amplifier



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5 Technical Symposium

Multifrequency and Adaptive Scanning Probe Microscopy

Multifrequency techniques applied to scanning probe microscopy (SPM) are rapidly expanding the capabilities of non-contact atomic force microscopy (nc-AFM) across a wide range of applications, from ambient conditions to ultra-high vacuum (UHV). By enabling simultaneous access to multiple interaction channels, these approaches enhance sensitivity, improve the discrimination between electrostatic and non-electrostatic contributions to normal and lateral tip-sample interactions, and enable more quantitative nanoscale analysis. Adaptive scan modes can further resolve heterogeneous surfaces.

This half-day symposium, jointly organized by **Zurich Instruments** and **Scienta Omicron** in the framework of NC-AFM 2026, will focus on recent advances in instrumentation and experimental applications of multimodal techniques.

The program will highlight state-of-the-art approaches to multifrequency excitation and detection (bimodal, heterodyne, and multi-harmonic), leveraging advanced lock-in amplification and feedback control, as well as their integration into ultra-stable SPM platforms operating down to 1 K temperature. Emphasis will be placed on practical applications, including high-resolution imaging, dissipation and lateral force mapping, Kelvin probe force microscopy and spectroscopy in demanding environments such as UHV and low temperature.

Through a combination of technical presentations and live demonstrations, the symposium aims to provide researchers and advanced users with actionable insights into implementing multifrequency methods and adaptive scan modes for optimizing performance on modern SPM systems.

Program overview

9:15-9:30 **Juergen Koeble and Romain Stomp**, Welcome and introduction.

Opening remarks, symposium orientation and a concise framing of why multifrequency and time-domain methods are becoming central to advanced non-contact AFM and SPM experiments.

9:30-9:50 **Juergen Koeble**, Stability, Low Noise, Resolution and Bandwidth: the ingredients for SPM

Low temperatures yield access to ultimate energy resolutions and stability but typically complicate the accessibility for external equipment to the tip-sample region. With the proper design of the SPM platform and modularity, this accessibility can be maintained. The talk highlights the role of high mechanical, thermal and electrical stability; dedicated cabling; precooling stages; low-noise preamplifiers and signal creation; and adequate data acquisition. It also discusses frequency-dependent measurement schemes such as bimodal AFM excitation and multi-harmonic detection, including IETS.

9:50-10:20 **PD Dr. Daniel Ebeling**, Tweaking the Bond Imaging Technique

With chemical bond imaging using CO-functionalized AFM tips, the chemical structure and orientation of individual organic molecules can be visualized. This invited talk presents approaches to enhance the method: constant-current AFM and adaptive feedback for imaging adsorption conformations and surrounding metal atoms in a single scan, lateral force microscopy through torsional eigenmodes of qPlus sensors, and active MEMS microcantilever concepts with integrated piezoelectric sensing for multifrequency AFM and higher throughput.

10:20-10:40 **Romain Stomp**, From Multifrequency to Time-Domain Measurements in SPM

This talk explores real-time data processing and signal generation for bridging multifrequency and timedomain measurements in scanning probe microscopy. It will provide concrete strategies to optimize SPM setups and enable new measurement methods through flexible detection, control and time-critical orchestration techniques.

10:40-11:10 **Coffee break**, Come and chat with the Scienta Omicron and Zurich Instruments teams

11:10-11:30 **Romain Stomp**, VHFLI Hands-on Tutorial: A New Standard for SPM

This tutorial will show how the VHFLI Lock-in Amplifier can serve demanding SPM applications, including time-resolved measurements in a single box. The new graphical workflow and complete time-frequency domain analysis toolbox illustrate how to build complex experiments from a bottom-up approach following the signal path.

11:30-12:00 **Dr. Marco Thaler**, Need for Speed: Dissipation-based Kelvin Probe Force Microscopy for Quartz Tuning Fork Sensors

Non-contact AFM with quartz tuning forks enables bond-resolved imaging and electrostatic probing at the atomic scale. Conventional Kelvin probe force spectroscopy grids can reach submolecular resolution but typically require several hours. This talk presents dissipation-based KPFM adapted to quartz tuning forks operated in UHV at 8 K, increasing LCPD map acquisition rates by more than an order of magnitude, and introduces a second bimodal heterodyne approach.

12:00-12:20 **Juergen Koeble**, Modular and cost-effective SPM Controller for state-of-the-art SPM experiments: a hands-on introduction

This tutorial will introduce the main features and some special modes of operation using its built-in lockin amplifiers with multifrequency operation in a live demonstration. Attendees will have the opportunity of getting hands-on experience with the core functionality and user interface.

Atomyx SPM Controller

Modular control platform for UHV Scanning Probe Microscopy

The new Atomyx SPM Controller is designed to integrate all functionality currently required for basic and advanced UHV Scanning Probe Microscopy in a single unit.

With its modular design and its industry-rated PC it is open for upgrades and simultaneously delivers long lifetime and best maintainability. The optical communication interface prevents noise introduction and ground loops.

The integrated fourfold Lock-in module not only supports standard operation modes like dI/dV and IETS but also allows for highest flexibility for custom experiments with its unmatched frequency range of up to 5 MHz. The integrated PLL and amplitude controller support all Non-Contact AFM modes including e.g. bimodal excitation schemes.

Finally, the user interface is optimized for UHV SPM experiments and yields easy access to all relevant parameters and workflows integrating the Atomix hardware components seamlessly



Atomyx SPM Controller

Technical Highlights

Architecture	Modular cardframe with plug-in modules for upgrades and easy maintenance
Low noise	Optical communication: galvanic isolation of high-voltage, low-voltage and PC components; short circuit-proof low noise power supplies
Scan generation	Advanced 32-bit high-resolution DACs for XY scan generation
Lock-in modules	4x fully featured dual-phase lock-in modules, up to 5 MHz, two reference channels
AFM support	Integrated PLL and amplitude controller for Non-Contact AFM/QPlus™ AFM, including bimodal excitation schemes and KPFM
PC and UI	Industry PC with Windows 11; comprehensible user interface for beginners and experts

Learn more at scientaomicron.com/AtomyxSPM



6 Session Schedule

Monday August 3rd, 2026

- 14:00 Welcome
- 14:20 Nanoscale Measurements of Charge and Work Function
- 16:00 Single-Molecule Studies

Tuesday August 4th, 2026

- 9:00 On-Surface Synthesis
- 11:00 Theory and Machine Learning 1
- 14:00 Structure and Growth of Interfacial Systems
- 16:00 Atomic-Structure Characterisation
- 17:20 Open-Access Publishing
- 17:30 Poster Session A

Wednesday August 5th, 2026

- 9:00 Magnetism
- 11:00 Characterisation of Molecular Systems
- 14:00 Novel Instrumentation and Techniques
- 16:00 High-Resolution Force Mapping
- 17:20 Poster Session B

Thursday August 6th, 2026

- 9:00 Lateral Forces, Friction, and Energy Dissipation

Friday August 7th, 2026

- 9:00 Theory and Machine Learning 2
- 11:00 Mineral and Oxides Surfaces
- 12:20 Closing Remarks

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7 Oral contributions

Monday August 3rd, 2026

14:00 **Welcome**

Nanoscale Measurements of Charge and Work Function

Chair **Thilo Glatzel**

14:20 **Yoichi Miyahara**, Scanning single-electron box probe for force-detected charge and potential sensing

14:40 **Brian Kiraly**, KPFM Imaging of Coulomb Confinement in Atomically Engineered Quantum Dots

15:00 **Ryota Fukuzawa**, Kelvin probe force microscopy with dual-bias modulation for frequency response analysis of surface band bending in semiconductors

15:20-16:00 **Coffee Break**

Scanning single-electron box probe for force-detected charge and potential sensing

Binod DC¹, Noah Austin-Bingamon², Md Mahamudul Hasan¹, and Yoichi Miyahara^{1,2*}

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Probing local electrical charge and electrostatic potential with high sensitivity at the nanometer scale is increasingly important for understanding and controlling quantum and nanoscale electronic devices. Random potentials arising from dopants, defects, and trapped charges can strongly affect device characteristics and limit coherence as device dimensions shrink.

Building on earlier atomic force microscopy (AFM)-based single-electron charging detection in self-assembled quantum dots [1], and inspired by scanned electrometers such as scanning single-electron transistor microscopy [2] and scanning quantum dot microscopy [3] for quantitative surface-potential imaging, we implement a Scanning Single-Electron Box (SSEB) probe within a low-temperature frequency-modulation noncontact AFM operated at 4 K for local charge and potential sensing. The SSEB probe integrates a metallic island at the apex of a cantilever-type AFM tip, tunnel-coupled to the conductive tip body and capacitively coupled to the sample, forming a single-electron box geometry. In this configuration, the sample acts as a gate electrode, and single electrons tunnel between the island and tip body in response to the cantilever oscillation, producing characteristic single-electron charging peaks in the resonance frequency-shift and dissipation signals of frequency modulation AFM.

We demonstrate reproducible single-electron charging peaks in the dissipation vs bias voltage curves of SSEB probes with metal-islands. We discuss how these features can be used to extract information about the local electrostatic environment. The simple fabrication process without multi-electrode nanolithography on the tip, makes the SSEB concept broadly accessible for investigating charge distribution and potential landscapes in nanostructures and quantum devices.

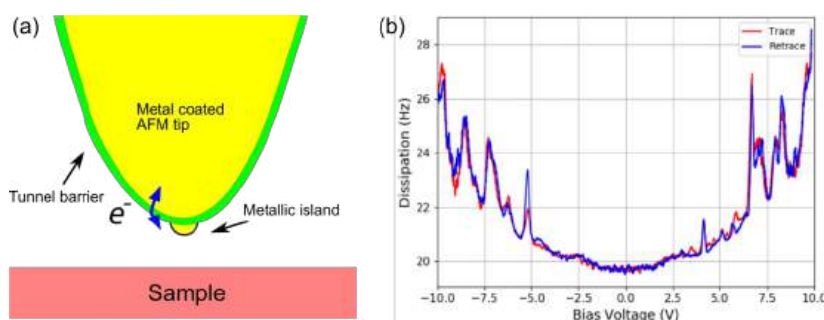


Figure 1: (a) Schematic of SSEB probe. (b) Single-electron tunneling peaks in dissipation vs bias voltage curve.

- [1] L. Cockins, Y. Miyahara, S. D. Bennett, A.A. Clerk, S. Studenikin, P. Poole, A. Sachrajda and P. Grutter, Proc. Natl. Acad. Sci. U.S.A. **107**, 9496 (2010).
- [2] M. J. Yoo, T. A. Fulton, H.F. Hess, R.L. Willett, L.N. Dunkleberger, R.J. Chichester, L.N. Pfeiffer and K.W. West, Science **276**, 579 (1997).
- [3] C. Wagner, M.F.B. Green, M. Maiworm, P. Leinen, T. Esat, N. Ferri, N. Friedrich, R. Findeisen, A. Tkatchenko, R. Temirov and F.S. Tautz, Nat. Mater. **18**, 853 (2019)

KPFM Imaging of Coulomb Confinement in Atomically Engineered Quantum Dots

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Quantum simulation based on atomically engineered structures on surfaces has been explored since the earliest demonstrations of atomic manipulation, yet only recently have atomically precise semiconductor platforms emerged [1]. These systems diverge from traditional scattering approaches by utilising adatoms to sculpt electrostatic landscapes, which define quantum dots and produce localised electronic states [2]. Using these systems, researchers have observed the emergence of atomic-like orbitals, hybridisation, chemical bonding, and extended molecular structures [3]. However, a direct experimental observation of the underlying electrostatic confinement potential has remained elusive.

Here, we measure the electrostatic potential of a single quantum dot in the Cs/InSb(110) platform using Kelvin probe force microscopy (KPFM). We observe a smooth confinement potential closely resembling an unscreened Coulomb well (fig. 1b), directly revealing the electrostatic origin of the artificial atomic states. We further map the spatially varying ground-state charge density, demonstrating the exponential decay expected for a two-dimensional artificial atom (fig. 1c). Using this tool, we demonstrate a method to control the depth of this electrostatic potential via the local atomic arrangement, effectively mimicking distinct atomic species within the artificial lattice. Finally, we construct heterogeneous atomic pairs and observe signatures of emergent electronegativity through the formation of polar bonding and antibonding states. These results substantially expand the capability of semiconductor-based quantum simulators and establish a route toward engineering increasingly complex and chemically-analogous quantum matter in two dimensions.

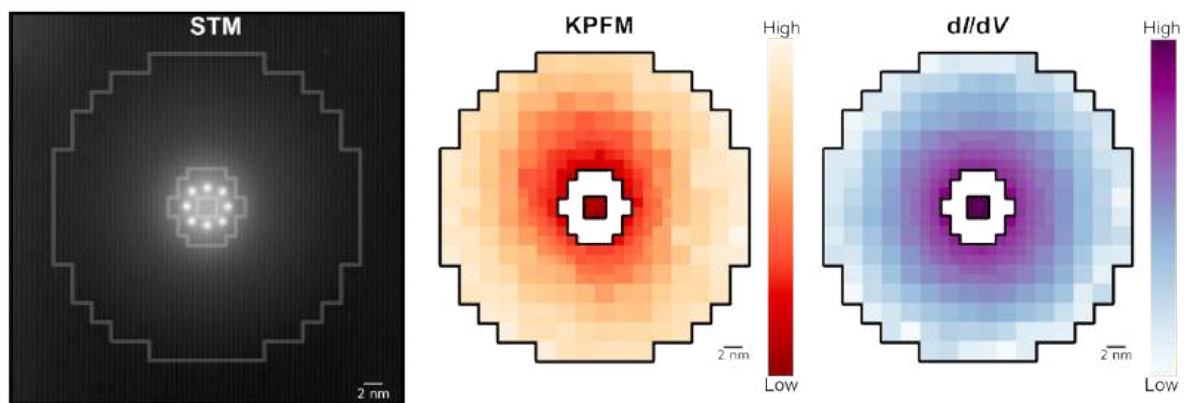


Fig 1. (a) Constant current STM image of the artificial atom, with the sampling grid overlaid. (b) constant height contact potential difference (CPD) map measured with KPFM. (c) Constant height differential conductance map at the bound state's energy.

References:

- [1] A.A. Khajetoorians, *et. al.*, *Nat. Rev. Phys.* **1**, 703 (2019).
- [2] S. Fölsch, *et. al.*, *Nat. Nanotech.* **9**, 505 (2014).
- [3] E. Sierda, *et. al.*, *Science* **380**, 1048 (2023).

Kelvion probe force microscopy with dual-bias modulation for frequency response analysis of surface band bending in semiconductors

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Kelvin probe force microscopy (KFM) is a powerful technique for measuring surface potential with high spatial resolution, which is crucial for understanding the electronic properties of semiconductor materials and devices. Although, conventional KFM typically measures the contact potential difference (CPD) under static conditions, some modulation techniques enabling the analysis of carrier dynamics such as photo-assisted KFM and pump-probe KFM [1,2]. In electrostatic force microscopy, surface/interface states in semiconductors can be analyzed by dual-bias modulation techniques by measurement of the frequency response of the electrostatic force [3]. However, in KFM, such dual-bias modulation techniques have not been developed, and the frequency response of surface band bending in semiconductors has not been analyzed using KFM. To address this limitation, we have developed a novel KFM technique called dual-bias modulation KFM (D-KFM), which allows for the analysis of the frequency response of surface band bending in semiconductors.

Figure 1 illustrates the operating principle of D-KFM. In this method, an AC voltage, $V_{\text{KFM}} \cos \omega_{\text{KFM}} t + V_{\text{bm}} \cos \omega_{\text{bm}} t$, is applied between the tip and sample, where $\omega_{\text{KFM}} < \omega_{\text{bm}}$. The semiconductor surface potential is periodically modulated by $V_{\text{bm}} \cos \omega_{\text{bm}} t$, and the time-averaged contact potential difference, $\bar{V}_{\text{cpd}}$, depends on V_{bm} and ω_{bm} because of the asymmetric behavior between accumulation and depletion, together with carrier trapping at surface states. Under the surface potential modulation induced by V_{bm} , $\bar{V}_{\text{cpd}}$ is detected using $V_{\text{KFM}} \cos \omega_{\text{KFM}} t$ through conventional frequency-modulation KFM.

To verify the validity of D-KFM, we performed $\bar{V}_{\text{cpd}}$ measurements on n- and p-type Si substrates with native oxide layers. Figure 2 shows the dependence of $\bar{V}_{\text{cpd}}$ on V_{bm} and ω_{bm} . Although $\bar{V}_{\text{cpd}}$ shows a strong dependence on both V_{bm} and ω_{bm} , the direction of the shift is opposite for the n- and p-type substrates. This behavior can be attributed to the opposite directions of band bending in the two substrates. In the frequency response of $\bar{V}_{\text{cpd}}$, a larger shift in $\bar{V}_{\text{cpd}}$ is observed at higher ω_{bm} , which is attributed to interface traps at the SiO_2/Si interface. These results suggest that D-KFM can be used to analyze the frequency response of surface band bending in semiconductors, which is crucial for understanding the electronic properties of semiconductor materials and devices.

This work was partially supported by JST PRESTO (Grant No. JPMJPR20A3) and ACT-X (Grant Number JPMJAX24DI), Japan.

- [1] M. Takahara *et al.*, *Appl. Phys. Lett.* **93**, 021902 (2008).
- [2] J. Murawski *et al.*, *J. Appl. Phys.* **118**, 154302 (2015).
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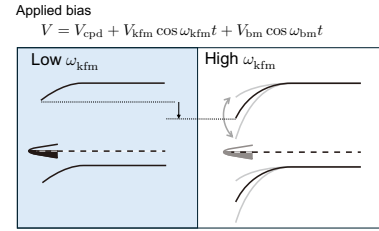


Figure 1: Schematic of the frequency response of surface band-bending.

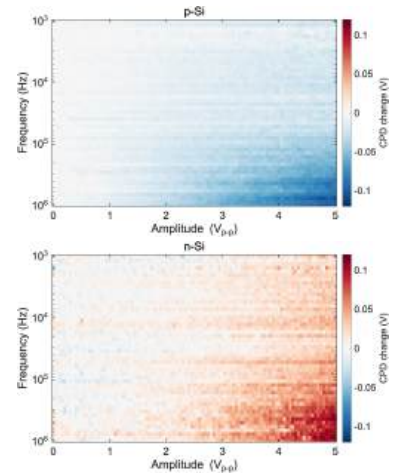


Figure 2: Dependence of time-averaged potential CPD ($\bar{V}_{\text{cpd}}$) on V_{bm} and ω_{bm} .

Monday August 3rd, 2026

Single-Molecules Studies

Chair **Jay Weymouth**

16:00 **Leo Gross**, A molecule with half-Möbius topology

16:20 **Xinnan Peng**, Breaking Peierls' theorem in polyacetylene chains via lattice-topology design

16:40 **Shijing Tan**, Interpolating delocalized topological solitons in single conjugated polymers

17:00 **Percy Zahl**, A hybrid workflow for molecular identification: Application to complex extraterrestrial organic mixtures

A molecule with half-Möbius topology

Leo Gross^{1*}, Igor Rončević^{2,3}, Fabian Paschke¹, Yuezhe Gao³, Leonard-Alexander Lieske¹, Lene A. Gödde³, Stefano Barison¹, Samuele Piccinelli¹, Alberto Baiardi¹, Ivano Tavernelli¹, Jascha Repp⁴, Florian Albrecht¹, Harry L. Anderson³

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Stereoisomers of $C_{13}Cl_2$ exhibiting helical orbitals were synthesized by atom manipulation on bilayer NaCl on Au(111) [1,2]. We resolved the enantiomeric geometries of the singlet states by AFM and mapped their helical orbital densities by STM. A π -orbital basis of the helical, non-planar singlets that twists by 90° in one circulation is consistent with a half-Möbius topology. In such a topology, the π -orbital basis changes sign with respect to two circumnavigations and is periodic with respect to four circumnavigations. We demonstrate reversible switching of the topology, between the two singlets of oppositely threaded half-Möbius topology, and the planar, topologically trivial, triplet state (see Figure). Multireference calculations, including large-scale sample-based ab initio calculations executed on quantum hardware, reveal that the switching is associated with a helical pseudo Jahn-Teller effect. [2]

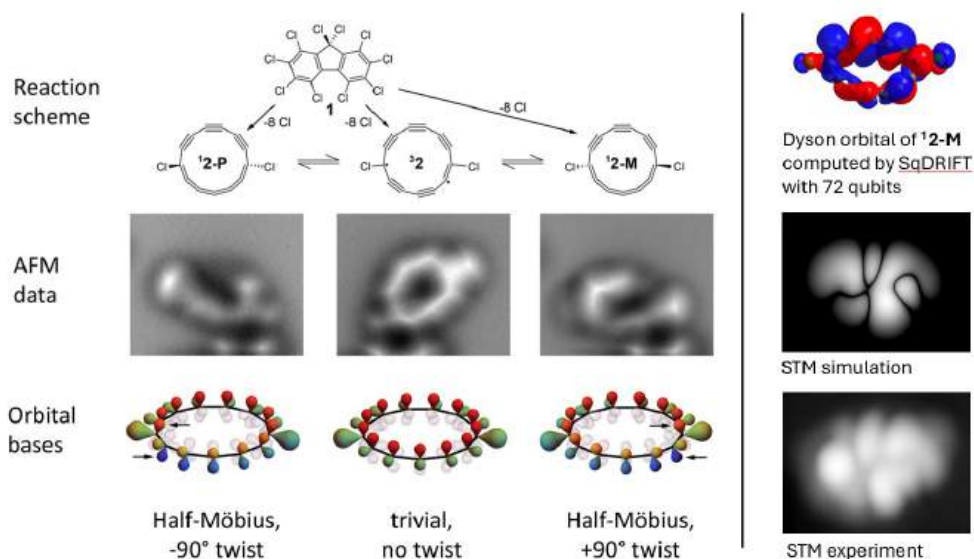


Figure 1: Compound **2** was generated by atom manipulation from precursor **1**. The topology can be controllably switched between the left-handed half-Möbius singlet ^12-P , the topologically trivial triplet excited state ^{32} and the right-handed half-Möbius singlet ^12-M . Observables of the topology are the molecular geometries (by AFM) and the orbital densities (by STM). The experimental STM data match the simulation based on the Dyson orbital calculated on quantum hardware in an active space of 36 electrons in 32 orbitals [2].

[1] F. Albrecht *et al.*, *Science*, **384**, 677–682, (2024). DOI: 10.1126/science.ado1399

[2] I. Rončević *et al.*, *Science*, **392**, eaea3321 (2026). DOI: 10.1126/science.aea3321

Breaking Peierls' theorem in polyacetylene chains *via* lattice-topology design

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Peierls' theorem postulates that a one-dimensional (1D) metallic chain must undergo a metal-to-insulator transition *via* lattice distortion, resulting in bond length alternation (BLA) within the chain¹. The validity of this theorem has been repeatedly proven in practice, as evidenced by the absence of a metallic phase in low-dimensional atomic lattices and electronic crystals, including π -conjugated polymers^{2,3}, artificial 1D quantum nanowires⁴⁻⁶, and anisotropic inorganic crystals^{7,8}. Overcoming this transition enables realizing long-sought organic quantum phases of matter, including 1D synthetic organic metals and even high-temperature organic superconductors⁹⁻¹¹. Herein, we demonstrate that the Peierls transition can be globally suppressed by employing lattice-topology design of classic trans-polyacetylene chains connected to nanographene terminals, that are open-shell in their isolated form. The appropriate topology connection enables an effective interplay between the singly occupied states of terminals and the finite odd-membered polyacetylene chain. This creates a critical topology-defined highest occupied molecular orbital that compensates for bond density variations, thereby suppressing BLA (Figure 1) and reestablishing their metallic-like character. Moreover, it also causes the formation of an unconventional *boundary-free resonance state*, being delocalized over the entire chain with non-decaying spectral weight, distinguishing them from traditional solitons observed in polyacetylene. Our finding sets the stage for pioneering the suppression of material instability and the creation of synthetic organic quantum materials with unconventional quantum phases previously prohibited by the Peierls transition.

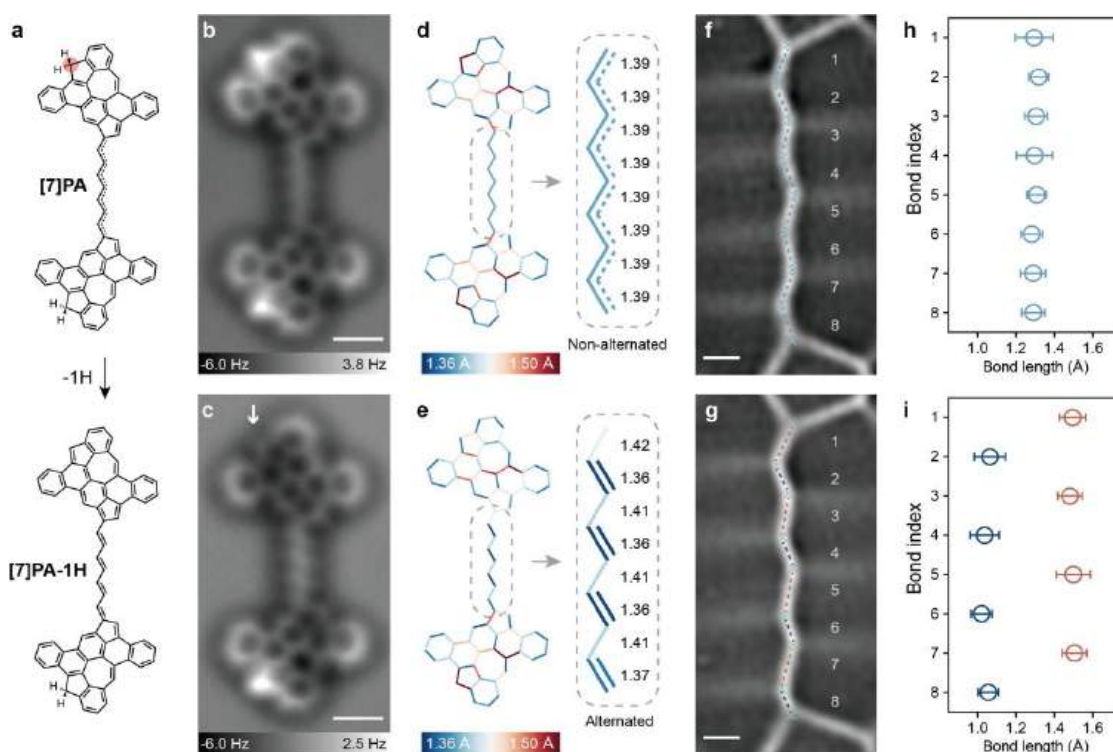


Figure 1: Measuring the bond lengths of C-C bonds in polyacetylene chains. **a**, Reaction scheme illustrating tip-induced dehydrogenation. **b,c**, Constant-height AFM images of **[7]PA** (**b**), and **[7]PA-1H** (**c**) ($V = 2$ mV, $\Delta z = -1.6$ Å (**b**) and -1.8 Å (**c**); set point prior to turning off feedback: $V = 20$ mV, $I = 30$ pA). **d,e**, DFT-calculated bond lengths of **[7]PA** (**d**) and **[7]PA-1H** (**e**), plotted in the selected color range, with zoomed-in views of the central OPA chains exhibiting either identical (**d**) or alternated (**e**) bond lengths. **f,g**, Laplace-filtered AFM images of the central OPA chains in **[7]PA** (**f**) and **[7]PA-1H** (**g**), highlighted with dashed lines ($V = 2$ mV, $\Delta z = -2.4$ Å; set point prior to turning off feedback: $V = 20$ mV, $I = 30$ pA). **h,i**, Plots of the measured bond lengths of the indicated bonds in (**f,g**). The values are obtained by averaging measurements from multiple images. Scale bars: 0.5 nm (**b,c**) and 0.1 nm (**f,g**).

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Interpolating delocalized topological solitons in single conjugated polymers

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The well-developed on-surface synthesis provides a powerful means for the accurate bottom-up design and on-site characterization by combining multimodal tip-based techniques for designer carbon-based quantum nanostructures. Here, I will introduce our recent advances of the joint tip-based STM-AFM-TERS techniques in characterizing the topological solitons in single structurally-engineered ethynylene-bonded ($-C\equiv C-$) polypentacene (EBPP). The bridging bond orders can be engineered through tuning the amount of charge transfer by leveraging workfunctions of distinct metal substrates from Ag(111)/Ag(100) to Au(111) [1]. The cumulene-bonded ($=C=C=$) polypentacene (CBPP) with both termini anchored to the Au surface atoms were achieved when grown on Au(111) [2]. This is well understood by the negligible doping on Au(111) both experimentally and theoretically, which well suppresses the Peierls transition. More interestingly, by transforming one of the terminals into the CH_3 configuration that locally induces the structural transition into EBPP, topological solitons are introduced at the EBPP and CBPP domain walls. The spatially extended characteristics of the solitonic properties are revealed with both the electronic zero-modes and multiple vibration modes. Our findings can well advance the field of carbon-based quantum materials in the way of both the mythology and high-quality data that can benchmark the theoretical modeling of the intricate quasiparticles.

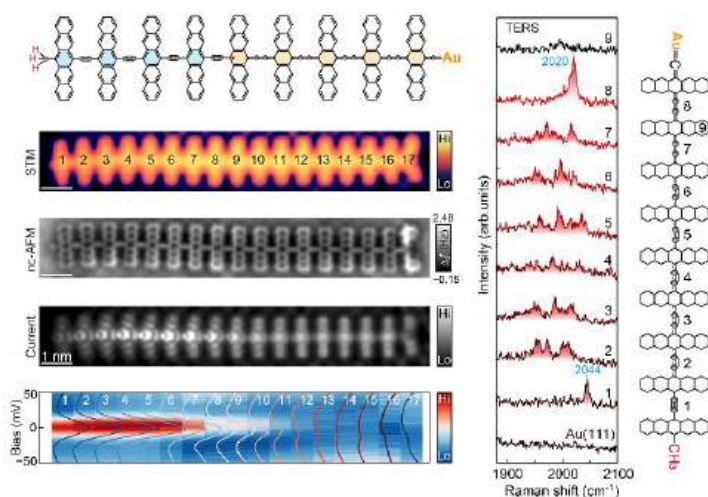


Figure 1: Multimodal characterization of topological solitons in single conjugated polymers, using scanning tunnelling microscopy (STM), non-contact atomic force microscopy (nc-AFM), and tip-enhanced Raman spectroscopy (TERS).

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A hybrid workflow for molecular identification: Application to complex extraterrestrial organic mixtures

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High-resolution non-contact atomic force microscopy (HR-AFM) enables direct imaging of individual molecules in complex organic mixtures, but robust structure assignment — particularly of peripheral functional groups — remains a major challenge. Current approaches rely on ab initio full density-based model (FDBM) simulations [1,2] and machine learning (ML) models trained on these data; however, their performance is limited by incomplete training sets, insufficient surface-relaxed structures, and discrepancies arising from experimental artifacts and other factors.

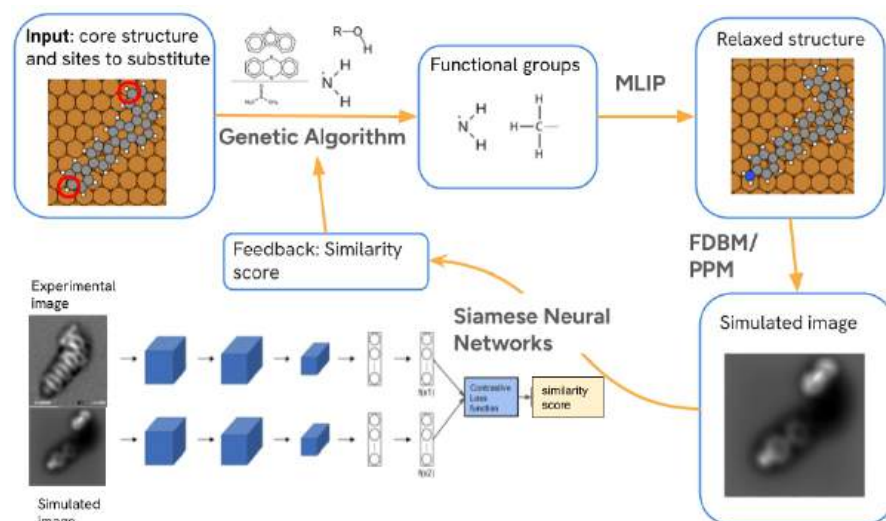


Figure 1:

Semi automatic work flow for best match molecule structure evaluation.

Here, we introduce a hybrid, stepwise (Figure 1) workflow that combines human expertise with computer- and AI-assisted analysis to improve structure determination from HR-AFM data. The approach first focuses on reliable identification of the aromatic carbon backbone, which can be robustly extracted from experimental images. Based on this core structure, candidate side groups are systematically introduced from a chemically informed library, followed by surface relaxation using ML interatomic potentials [3]. Simulated AFM images are then generated and quantitatively compared to experimental data using dedicated chemical fingerprint metrics that capture both local contrast features and global structural consistency. This iterative procedure enables ranking and refinement of candidate structures toward the most probable solutions.

This framework addresses key limitations of current automated approaches and provides a scalable pathway toward more reliable molecular structure elucidation from HR-AFM data. It further establishes a foundation for future integration with fully data-driven methods, advancing toward comprehensive, high-throughput structure determination of complex organic mixtures as for example in meteoritic or environmental samples.

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[2] M. Ellner, P. Pou, and R. Pérez, ACS Nano **13**, 786 (2019).

[3] M.G. Lastre, J.S. Jestilä, R. Pérez and A.S. Foster, arXiv:2601.18852 [cond-mat.mtrl-sci]



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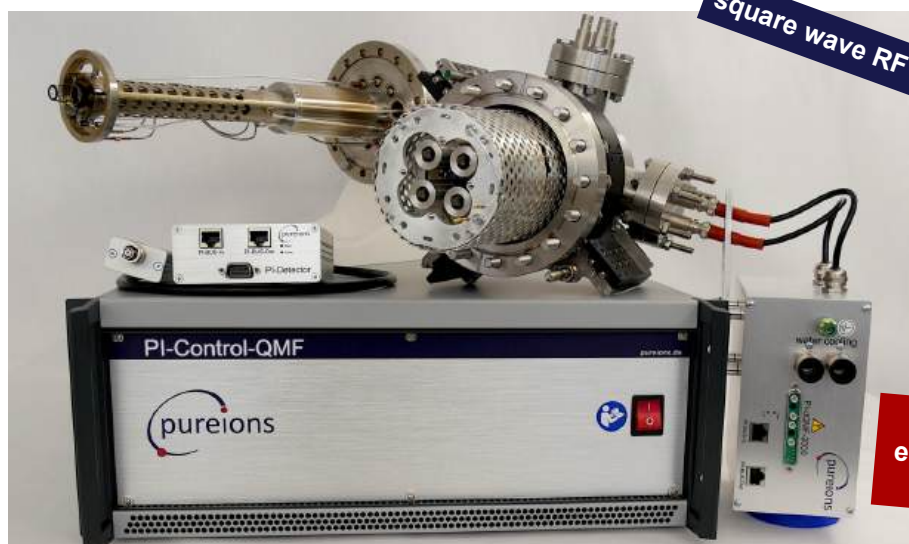
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deposition rates: ~ 1 ML/h
vacuum level: ~ 10^{-10} mbar
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PI-Quad

Mass-spec electronics and vacuum hardware

performance boost for quadrupoles, RGAs, traps, guides... no mass limit



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- fits to all quadrupole sizes and standard RGAs
- replacements for performance limited and defect electronics
- optional: ion source supplies, detectors, quadrupole rods

Applications: probe your thermal evaporators for the intact molecule's mass and more, record TDS/TPD

Tuesday August 4th, 2026

On-Surface Synthesis

Chair **Daniel Rothhardt**

- 9:00 **Amogh Kinikar**, On-surface synthesis of edge extended zigzag graphene nanoribbons
- 9:20 **Ye Liu**, On-surface synthesis of a free-base [3]triangulene-fused porphyrin and its chirality-dependent electronic configuration
- 9:40 **Lisanne Sellies**, On-surface synthesis and aromaticity of large cyclocarbons
- 10:00 **Yuejian Zhang**, Experimental realization of a two-dimensional clathrate hydrate

On-surface synthesis of edge extended zigzag graphene nanoribbons

Amogh Kinikar,^{1,2*} Feifei Xiang,¹ Xiushang Xu,^{3,4} Yanwei Gu,⁴ Akimitsu Narita,^{3,4} Pascal Ruffieux,¹ Klaus Müllen,⁴ Roman Fasel^{1,5}

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Surface-catalyzed chemical reactions leading to the formation of covalent bonds between and within surface-adsorbed molecular building blocks have allowed for the on-surface synthesis of graphene nanoribbons (GNRs). The properties of GNRs can be widely tuned by their width and edge structure, and the GNRs that can be achieved—and the properties they can exhibit—depend critically on the available design motifs. Homocoupling by forming a single C-C bond between molecular precursors leads to polymerization in the armchair direction. Consequently, most of the GNRs that have been synthesized to date are armchair graphene nanoribbons (AGNRs). However, zigzag graphene nanoribbons (ZGNRs) are highly desirable as they can host strongly interacting electronic states localized on their edges. Here, we present a versatile design motif based on surface-catalyzed debromination and subsequent polymerization of 2,7-dibromo-9-R₁-10-R₂-anthracene to synthesize structurally diverse GNRs along the zigzag direction. This design motif entails the incorporation of edge extensions fused onto the zigzag edge at alternating sides of the backbone, providing a platform for synthesizing several different types of edge-extended ZGNRs due to the simplicity and versatility of the design motif. These GNRs are thus a platform for realizing strongly interacting 1D Hamiltonians.

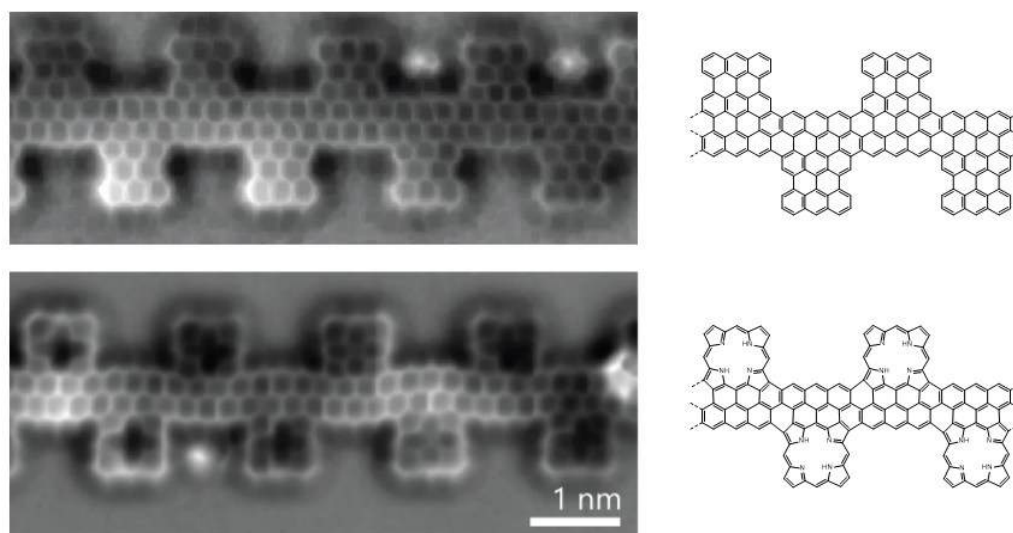


Figure 1: nc-AFM images and corresponding chemical structures of two atomically precise edge-extended ZGNR.

[1] Xiang, F.*, Gu, Y.*, Kinikar, A.* et al. *Nature Chemistry* **17**, 1356–1363 (2025)

[2] Xu, X.*, Kinikar, A.* et al. *Precision Chemistry* **2**, 81–87 (2024)

[3] Kinikar, A.*, Xu, X.* et al. *Advanced Materials* **35**, 23063–2306311(2024)

On-surface synthesis of a free-base [3]triangulene-fused porphyrin and its chirality-dependent electronic configuration

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Molecular architectures hosting delocalized π -radicals with tunable electronic structures are highly attractive for spintronics applications [1]. The porphyrin (Por) macrocycle, featuring an 18 π -electron conjugated framework, provides a versatile platform for engineering π -magnetism systems through fusing organic substituents with unpaired π -electrons to the periphery, for example triangulenes [2,3]. Free-base porphyrins fused with two and four [2]triangulenes have been reported to exhibit diradicals in gas phase with planar and slightly bent geometries, respectively. More recently, a zinc-Por fused with four [3]triangulenes (Zn-Por-T4) was prepared. It was shown to preserve the diradical nature in the gas phase while adopting a chiral configuration [4].

To explore the fascinating interplay of chirality and π -magnetism in more detail, we realized free-base 2H-Por-T4 on Au(111) by means of on-surface synthesis from suitable precursor molecules. Nc-AFM reveals that the steric hindrance between adjacent [3]triangulene moieties gives rise to several symmetry-distinct configurations. Despite the geometric differences being largely limited to a bending distortion, the electronic structures differ significantly, with a near-degeneracy between singlet and triplet ground states. A chiral configuration with D_2 symmetry and an achiral configuration with C_i symmetry differ dramatically in the localization of their frontier orbitals. Specifically, in the C_i -symmetric structure the frontier orbitals are selectively delocalized over two diagonally opposing triangulene moieties. Even more surprisingly, this selective delocalization depends on the multiplicity. These results demonstrate a direct correlation between molecular chirality and electronic delocalization in triangulene-fused porphyrins, providing a promising platform for chirality-dependent spintronics and studying phenomena related to chirality-induced spin selectivity (CISS).

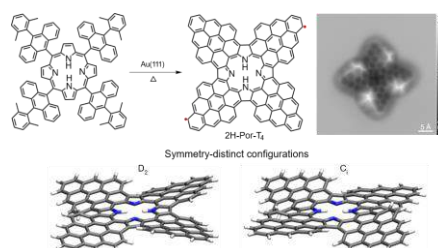


Figure 1: On-surface synthesis of 2H-Por-T4 on Au(111) and its symmetry-distinct configurations.

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On-surface synthesis and aromaticity of large cyclocarbons

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Cyclocarbons, molecular rings of carbon atoms, have been synthesized on surface using tip-induced chemistry [1-3], and the formation of larger cyclocarbons by dimerization of precursors was shown [3,4]. Because of their monocyclic geometry, cyclocarbons are fundamentally important for testing theoretical models of aromaticity. In this talk, I will show that we can synthesize large cyclo[*N*]carbons, C_N , with *N* up to 88, on a monolayer NaCl on Au(111) by fusing multiple cyclocarbons using atom manipulation with a scanning tunnelling microscope (STM) [5]. Using atomic force microscopy (AFM), we identified the intermediates and products, see Fig. 1. We studied the aromaticity of the formed cyclocarbons by measuring their transport gaps using scanning tunnelling spectroscopy. Our experimental results show that aromaticity persists at *N* = 42, and theory predicts ring currents comparable in magnitude to that of benzene in cyclocarbons of this size [5].

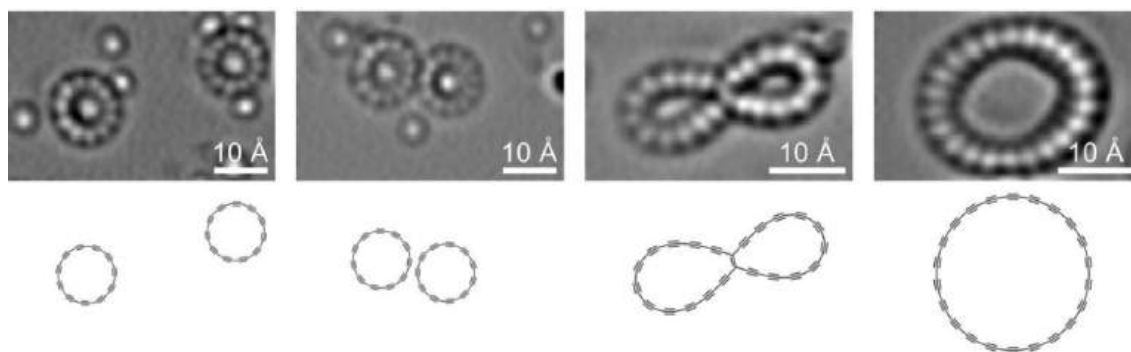


Figure 1: On-surface synthesis of C_{44} . Laplace-filtered AFM data and chemical structures. By applying voltage pulses, two C_{22} were moved adjacent to each other and then fused into an intermediate where the carbon rings share a C=C bond, which after ring-opening resulted in C_{44} .

[1] K. Kaiser[#], L. M. Scriven[#] et al., Science **365**, 1299-1301 (2019).

[2] L. Sun[#], W. Zhen[#] et al., Nature **623**, 972-976 (2023).

[3] F. Albrecht[#], I. Rončević[#], Y. Gao[#], F. Paschke[#] et al., Science **384**, 677-682 (2024).

[4] Y. Guo et al., Nat. Commun. **16**, 11507 (2025).

[5] L. Sellies[#], M. Vitek[#], Y. Gao[#], F. Paschke[#] et al., arXiv arXiv:2603.02040 (2026).

Experimental realization of a two-dimensional clathrate hydrate

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Clathrate hydrates are guest–host compounds in which small molecules are encapsulated within hydrogen-bonded water cages. Owing to their porous structures, they are of interest for applications such as energy storage, gas separation, and water desalination. However, hydrate formation in bulk generally requires high pressures, which limits both practical applications and microscopic understanding of nucleation and growth processes. Nanoscale confinement, frequently encountered in natural and interfacial environments, has been proposed as an effective means to facilitate hydrate formation under milder conditions. Despite this, the structural characteristics of clathrate hydrates in reduced dimensions remain poorly understood. Here we report the first realization of a two - dimensional (2D) clathrate hydrate using cryogenic atomic force microscopy under ultrahigh vacuum. In contrast to crystalline bulk clathrate hydrates, the 2D hydrate lacks long-range order and exhibits rich phase coexistence. Combined with calculations, we reveal two fundamentally distinct growth pathways at two extreme guest concentrations and demonstrate that the formation of the two-dimensional clathrate hydrate is governed by the local guest–water concentration. These findings provide an atomic-scale picture of how non-equilibrium kinetics stabilize unconventional hydrate phases and govern guest dynamics.

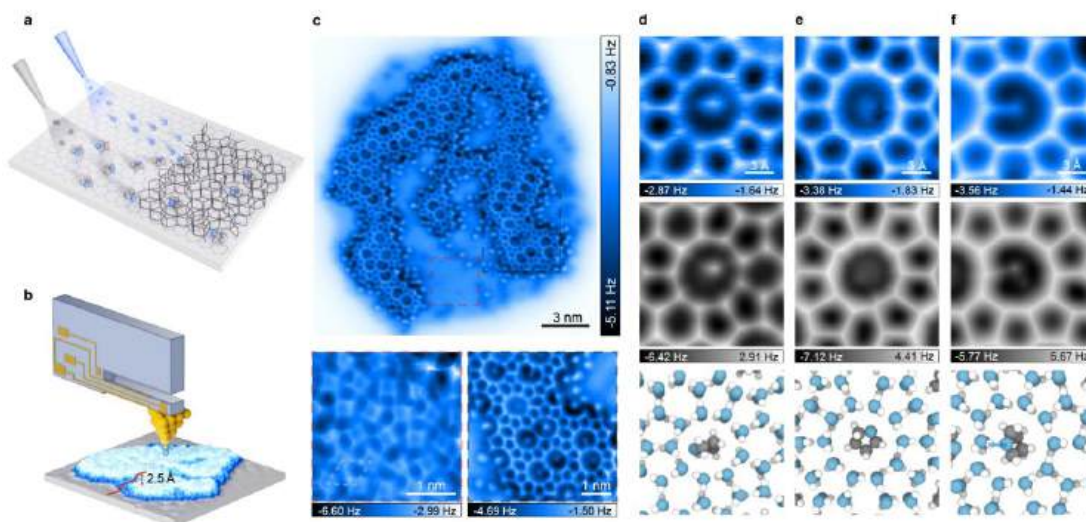


Figure 1: Experimental setup and AFM images of 2D bilayer clathrate hydrate.

Tuesday August 4th, 2026

Theory and Machine Learning 1

Chair **Martin Ondráček**

- 11:00 **Mithun Manikadan**, Which Molecules Make Good AFM Tips?
- 11:20 **Manuel González Lastre**, MAD-SURF: a general machine-learning interatomic potential for molecular adsorption on metal surfaces
- 11:40 **Prokop Hapala**, High-throughput integrated SPM simulation platform FireCore
- 12:00 **Farzin Irandoost**, Tip recognition in NC-AFM images in liquid via pattern analysis and machine learning

Which Molecules Make Good AFM Tips?

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Atomic force microscopy (AFM) with CO-terminated tips has become a key enabler of submolecular resolution because it produces intuitively interpretable images in which chemical bonds, lone electron pairs, Kekulé structures, and other regions of enhanced electron density appear as bright protrusions [1]. Although bond resolution has also been achieved with several alternative terminations (e.g. Xe, Cl-, CuO), it remains unclear whether CO is uniquely suited for high-resolution AFM imaging and which other molecules could serve as effective or even superior tip terminations. To address these questions, we performed systematic PPAFM simulations of flat heterocyclic samples with tip modeled by small molecules including CO, H₂O, HF, HCN, NH₃, NO, CH₄, and C₂H₂, considering different orientations (e.g. H or N end of HCN). To obtain predictive results in the absence of experimental reference, we employed innovative approach where the grid-based force field central to PPAFM simulations is constructed by kernel interpolation of interaction-energy profiles $E(z)$ calculated above atoms, bond centers, and other positions using B3LYP-D3 in the Psi4 package [2–4]. This eliminates uncertainties in parameter selection required by both classical force-field and full-density-based PPAFM approaches [5,6]. Our results show that intuitively interpretable contrast is obtained primarily with electronegative terminating atoms (e.g. O, N), while the exceptional performance of CO arises from its small dipole moment, which minimizes electrostatic image distortions despite the low lateral stiffness. Increasing tip stiffness is crucial for suppressing these unwanted effects enabling use of other terminations. H-terminated molecules, in particular, may provide a sensitive probe of lone electron pairs through hydrogen-bond formation. We believe that this study, comprising approximately one hundred tip-sample combinations and tens of thousands of interaction-energy calculations, provides both insight for the future design of optimized AFM tips and a practical reference for interpreting AFM images obtained with unknown or contaminated tip terminations.

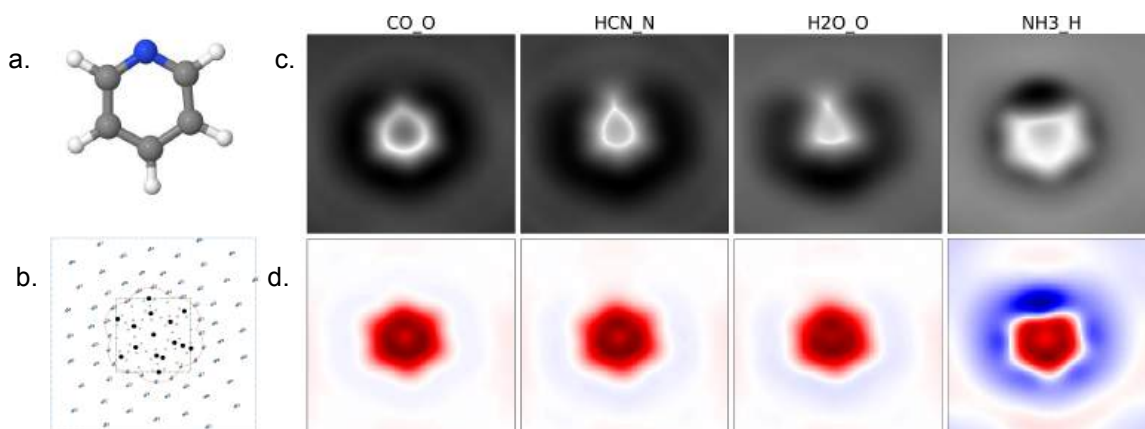


Fig.1. a. Ball and stick model of pyridine. b. Sampling points considered for $E(z)$ calculations. c. PPAFM simulated images with tip bending stiffness 1.0 N/m. d. The interpolated Interaction potential (eV) used for the simulations with different tip terminations.

- [1] L. Gross *et al.*, *Science*, **325**, 1110 (2009).
- [2] A. D. Becke, *J. Chem. Phys.*, **98**, 5648 (1993).
- [3] S. Grimme *et al.*, *J. Chem. Phys.*, **132**, 154104 (2010).
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- [5] M. Ellner *et al.*, *Nano Lett.*, **16**, 1974 (2016).
- [6] N. Oinonen *et al. Comput. Phys. Commun.*, **305**, 109341 (2024).

MAD-SURF: a general machine-learning interatomic potential for molecular adsorption on metal surfaces

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Predicting how organic molecules adsorb, assemble, and interact on metal surfaces is central to surface chemistry and scanning probe microscopy, but first-principles simulations of metal–organic interfaces remain limited by the cost of density functional theory, which restricts accessible system sizes and configurational sampling [1]. Machine-learning interatomic potentials can approach first-principles accuracy at much lower cost, enabling large-scale simulations of surfaces and interfaces [2]. Here we present **MAD-SURF** [3], a general machine-learning interatomic potential for molecular adsorption on coinage-metal surfaces. The model is trained on a chemically diverse dataset calculated at the PBE+vdWsurf level, covering adsorption motifs generated via Bayesian optimization structure search, intramolecular flexibility sampled through normal-mode sampling, non-covalent interactions, and finite-temperature *ab initio* molecular dynamics on Cu(111), Ag(111), and Au(111). MAD-SURF achieves near-DFT accuracy for energies, forces, and adsorption geometries while providing speedups of several orders of magnitude over density functional theory. We demonstrate the generality of the potential across experimentally relevant systems of increasing complexity, including ordered pentacene and PTCDA monolayers, thermally generated polycyclic aggregates, flexible biomolecules such as β -cyclodextrin, and the long-range herringbone reconstruction of Au(111), reproduced without Au-specific active learning [4,5]. These examples span molecular adsorbates and surface structures routinely studied by high-resolution scanning probe microscopy. By combining accuracy, efficiency, and chemical generality, MAD-SURF provides a

practical framework for predictive atomistic modelling of complex molecular adsorption phenomena.

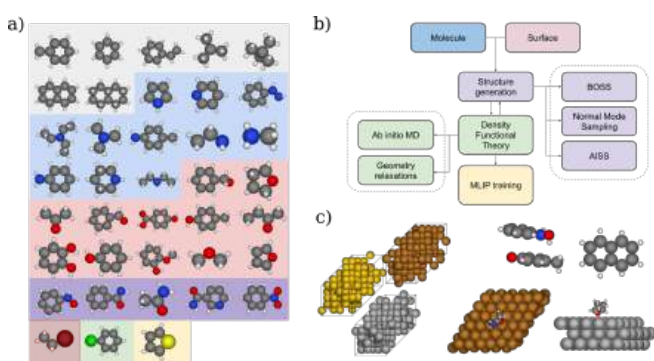


Figure 1: Dataset construction pipeline. (a) Representative molecules relevant to on-surface chemistry. (b) Dataset-generation workflow combining BOSS, NMS, AIMD, and AISS, followed by DFT reference calculations for MLIP training. (c) Representative gas-phase, adsorbed, and metal-only configurations.

[1] W. Liu, A. Tkatchenko, and M. Scheffler, *Acc. Chem. Res.* **47**, 3369 (2014).

[2] I. Batatia et al., *Adv. Neural Inf. Process. Syst.* **35**, 11423 (2022).

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[5] P. Li and F. Ding, *Sci. Adv.* **8**, eabq2900 (2022).

High-throughput integrated SPM simulation platform FireCore

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Over the last decade, the probe-particle model (PPM) and full-density-based model (FDBM), combined with Chen's derivative rules applied to molecular orbitals, have become established tools for the simulation of bond-resolved atomic force microscopy (BR-AFM) and scanning tunneling microscopy (BR-STM) [1,2]. GPU-accelerated implementations can produce hundreds of simulated AFM data volumes per second and provide an efficient source of data for training machine-learning models and other high-throughput applications. Nevertheless, the preparation of the inputs — namely DFT calculations of electron density, molecular orbitals, and structural relaxation of molecules on substrates — still poses a significant bottleneck. This may result in a laborious workflow especially when molecular structure on the surface is not known *a priori*. To address these limitations, we developed an integrated QM/MM SPM simulation platform that combines fast local-orbital DFT(B) methods [3] with classical grid-projected force fields (GridFF) [4] within a unified framework. The platform, which can be accessed either through an interactive GUI or via Python scripting, enables rapid end-to-end simulation workflows comprising not only AFM and STM imaging, but also molecular structure design and relaxation on surfaces. Powerful GPU-parallelized engine further enables autonomous searches for AFM manipulation trajectories and polymorph adsorption structures on surfaces via global optimization algorithms sampling millions of molecular geometries per second [3]. Furthermore, the framework also supports simulations of scanning probe imaging of coupled excitonic and charged states in molecular assemblies [5,6].

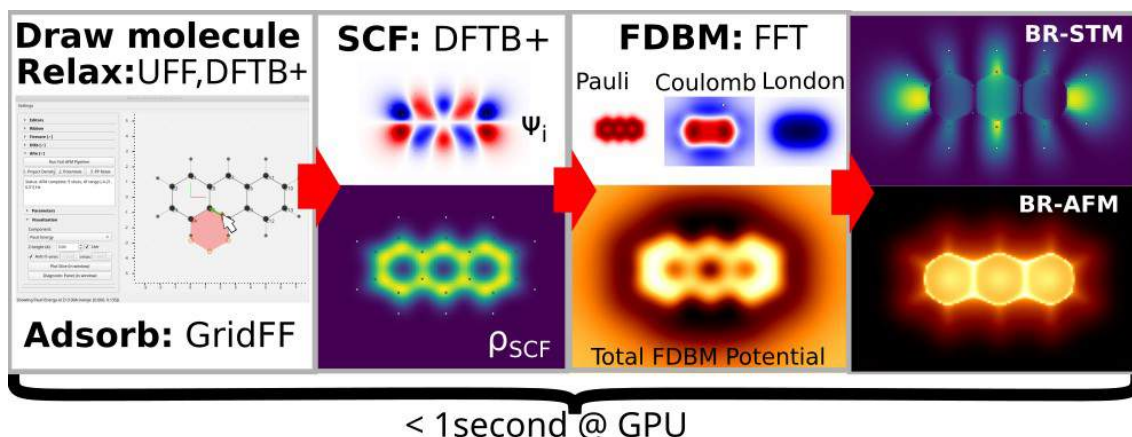


Figure 1: Integrated SPM simulation pipeline from molecular design to BR-AFM/STM images.

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- [3] B. Hourahine et al., J. Phys. Chem. A 129, 5373–5390 (2025).
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Tip recognition in NC-AFM images in liquid via pattern analysis and machine learning

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Tip control and identification remains a significant challenge for in-liquid NC-AFM imaging [1,2]. While expert eyes can recognize different hydration patterns, a systematic and quantitative methodology has been lacking either for pattern recognition or comparison with simulations.

In the current study, we first developed an algorithm based on Fourier transforms (FT) to extract high resolution features from a vast range of experimental data. While FT offers a robust mathematical framework to analyze ideal periodic patterns, it often fails to describe fine details required for clear characterisation in NC-AFM due to noise in the data and/or low resolution. After establishing our own FT-based descriptors, we built an automated pattern recognition workflow integrated with Equivariant Steerable CNNs [3] and clustering algorithms to process large-scale experimental datasets.

We apply this method to characterize calcite hydration patterns in large experimental NC-AFM datasets, first establishing “good” and “bad” data, before identifying contrast patterns characteristic of different tips and comparing them to existing simulated patterns. Our tool offers comprehensive processing utilities giving experimentalists the flexibility to tailor the analysis to their specific data, while enabling efficient automated recognition of patterns in large datasets.

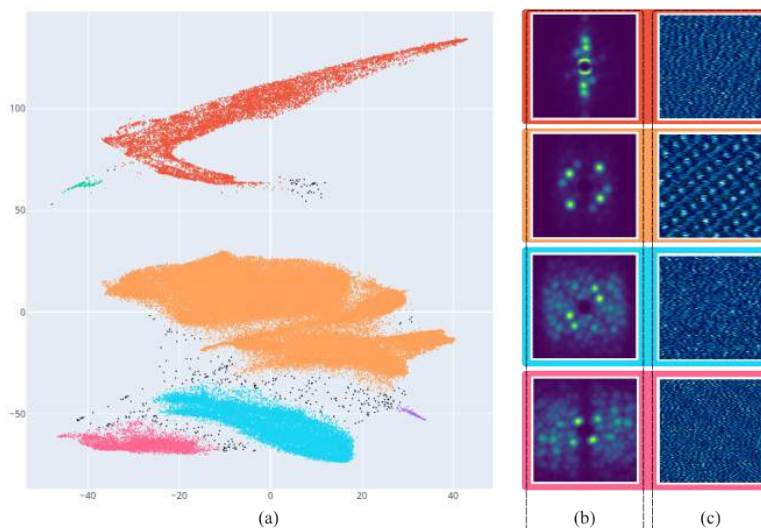


Figure 1: Result for a clustering on calcite datasets. (a) Trimap embedding of the distance matrix of the latent space. This map shows that all the data can be divided into four prominent groups. (b and c) Representative Fourier maps and patterns belonging to each cluster.

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Tuesday August 4th, 2026

Structure and Growth of Interfacial Systems

Chair **Tobias Dickbreder**

- 14:00 **Rémy Pawlak**, Revealing the Atomic Structure of Blue Phosphorus Phases on Au(111) with Non-Contact Atomic Force Microscopy
- 14:20 **Jie Huang**, High-Resolution AFM and Simulation of THF Clathrate Hydrate Growth and Structure
- 14:40 **Daniel Rothhardt**, From Dehalogenation to Stoichiometric NiBr_2 through Ordered Non-Stoichiometric Phases on Au(111)
- 15:00 **Jonas Heggemann**, Ice structures on $\text{CaF}_2(111)$ and $\text{BaF}_2(111)$ surfaces

Revealing the Atomic Structure of Blue Phosphorus Phases on Au(111) with Non-Contact Atomic Force Microscopy

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Blue phosphorene (BlueP), a two-dimensional phosphorus allotrope with a buckled honeycomb lattice, has attracted significant interest for its semiconducting properties that extend beyond graphene. Yet, its growth on Au(111) remains debated, with structural phases highly discussed due to possible incorporation of substrate adatoms into the phosphorus adlayer [1]. Here, we present a general methodology combining low-temperature non-contact atomic force microscopy (nc-AFM) and force spectroscopy to unambiguously discriminate between competing structural models of BlueP/Au(111) obtained by density functional theory (DFT) [2]. Each phosphorus phase is resolved at the atomic scale by nc-AFM imaging, while site-dependent force spectroscopy probes local atomic corrugations within the structure (Figure 1). Comparison with probe-particle simulations [3] using DFT coordinates reveals that all structural phase on Au(111) consists of an assembly of BlueP₉ or BlueP₁₆ units stabilized by Au adatoms [4]. These results not only solve the long-standing debate over the phosphorus-Au(111) interface but also provide an experimental strategy for identifying atomic structures of epitaxial Xenes.

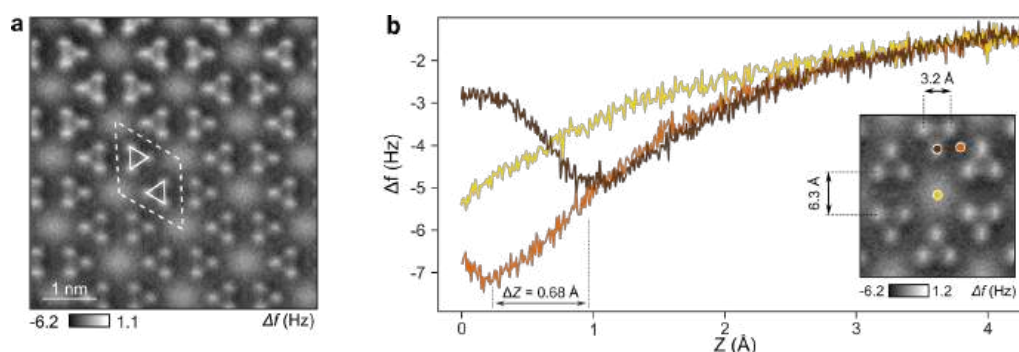


Figure 1: **a**, Experimental nc-AFM image with a CO-functionalized tip. **b**, $\Delta f(Z)$ spectra acquired above the upmost P atoms of a triangle (brown), at the center of the pore (yellow) and in the gap between neighboring triangles (orange), as shown in the inset.

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High-Resolution AFM and Simulation of THF Clathrate Hydrate Growth and Structure

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² International Center for Quantum Materials, Peking University, Beijing, China

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Clathrate hydrates are crystalline host–guest materials in which hydrogen-bonded water frameworks form cages that encapsulate guest molecules. Their growth mechanisms and nanoscale structural organisation are central in the development of new clean energy storage materials and suppression of gas emissions during mining. In this study, we combine non-contact atomic force microscopy (NCAFM) using CO-functionalised tips with molecular simulations to characterise the growth and structure of tetrahydrofuran (THF) clathrate hydrates.

High-resolution imaging of THF clathrate surfaces reveal structural motifs associated with the clathrate lattice, including repeated characteristic clusters which likely play a critical role in the nucleation and decomposition process. Complementary quantum and classical simulations were used to interpret the NCAFM contrast and relate observed surface patterns to the underlying arrangement of water cages and encapsulated THF molecules. The predicted structures and their energetic hierarchy provides a clear understanding of the crystallisation process, and its temperature dependence. The results provide new insight into the mechanisms controlling THF clathrate hydrate growth and demonstrate the capability of CO-functionalised AFM to resolve complex hydrogen-bonded host–guest materials.

From Dehalogenation to Stoichiometric NiBr₂ through Ordered Non-Stoichiometric Phases on Au(111)

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Two-dimensional transition-metal dihalides are promising van der Waals magnets, yet their epitaxial growth on noble metals is frequently governed by substrate-induced dehalogenation that precedes stoichiometric film formation. Such behavior has been reported for NiBr₂,¹ CoBr₂,² FeBr₂,^{3,4} MnBr₂,⁵ and MnI₂,⁶ in which precursor structures form before the stoichiometric layers develop.

Here, we study coverage-dependent NiBr₂ growth on Au(111) by combining scanning tunneling microscopy, non-contact atomic force microscopy with site-resolved $\Delta f(z)$ spectroscopy, X-ray photoelectron spectroscopy, and density functional theory. At low coverage, where the Au(111) surface is largely exposed, dehalogenation produces ordered buffer layers, bromine-rich structures, and metallic Ni⁰ clusters pinned to herringbone elbows (Fig. 1a). These buffer layers are non-stoichiometric Ni–Br phases with distinct atomic arrangements and rotational alignments relative to the substrate.

With increasing coverage, these dehalogenated species reorganize, and the growth evolves from coexisting buffer layers and emerging NiBr₂ islands at intermediate coverage (Fig. 1b) into multilayer stoichiometric NiBr₂ at high coverage (Fig. 1c).

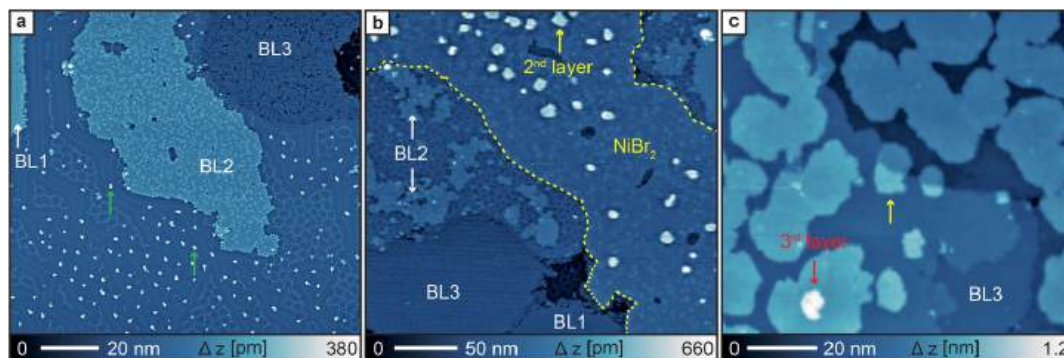


Figure 1. STM overview of NiBr₂ growth on Au(111) at low (a), intermediate (b), and high coverage (c). At low coverage, the buffer layers BL1–BL3, the bromine mesh, and metallic Ni⁰ clusters at herringbone elbows (green arrows) coexist. At intermediate coverage, the first NiBr₂ layer (yellow dashed outline) and a nucleating second layer (yellow arrow) grow alongside the remaining buffer layers. At high coverage, third-layer islands are indicated by red arrows.

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Ice structures on $\text{CaF}_2(111)$ and $\text{BaF}_2(111)$ surfaces

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Wolf Gero Schmidt,² Philipp Rahe,¹

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Mineral-water interfaces are ubiquitous in nature and host to several key processes in geological and biological systems on earth [1,2]. Minerals furthermore act as agents in heterogeneous ice nucleation; yet, with the underlying molecular mechanisms still being intensively discussed and studied [3,4]. Interestingly, substrates whose surface structure matches the dimensions of ordinary ice (ice I_h) faces are known to not necessarily express favourable nucleation ability [5].

Here, we investigate ice structures on two chemically comparable but structurally distinct model surfaces, namely on the (111) faces of CaF_2 and BaF_2 . The key difference are the lattice dimensions compared to ice I_h : While a mismatch of 17% to $\text{CaF}_2(111)$ renders ice nucleation as unfavourable, a close match of better than 3% on $\text{BaF}_2(111)$ suggests ice nucleation ability [6].

By combining experimental non-contact atomic force microscopy (NC-AFM) measurements using CO terminated tips with density functional theory (DFT) and molecular dynamics (MD) calculations, the structures evolving after dosing water at sub-monolayer coverage are investigated. On $\text{CaF}_2(111)$, individual hexagonal ring structures are a common observation, see Fig. 1(a), while extended network structures are identified on $\text{BaF}_2(111)$, see Fig. 1(b). These findings are in full agreement with the DFT and MD analysis, where a closed ice layer is found to be energetically unfavourable on $\text{CaF}_2(111)$, but possible on $\text{BaF}_2(111)$.

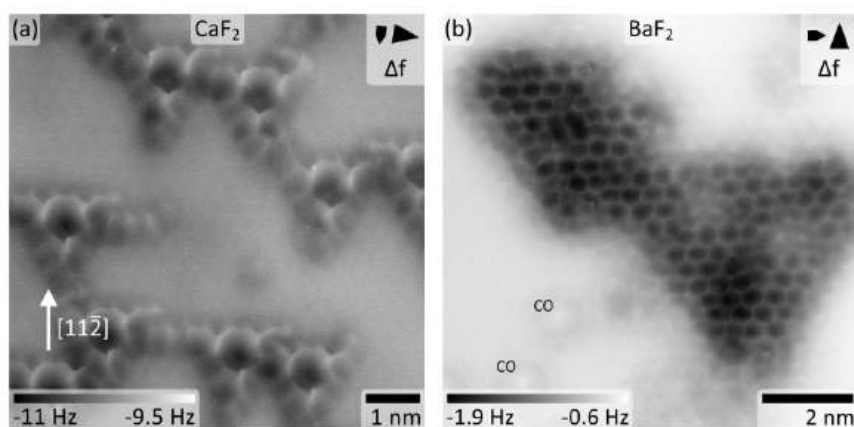


Figure 1: NC-AFM images after sub-monolayer deposition of water on (a) $\text{CaF}_2(111)$ and (b) $\text{BaF}_2(111)$ surfaces. Images acquired at 5K with CO-functionalised tips.

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Tuesday August 4th, 2026

Atomic-Structure Characterisation

Chair **Philipp Rahe**

- 16:00 **Jing Guo**, Visualizing alkali metal aggregation-induced coordination in CO₂ activation on copper
- 16:20 **Paul Laubrock**, Chiral water structures on dolomite(104) surfaces
- 16:40 **Davoud Pourzadeh**, Atomic-Scale Characterization of Annealing Effects on Hydrogenated Diamond (100) Surface with Non-Contact Atomic Force Microscopy
- 17:00 **Jara Trujillo-Mulero**, Resolving Graphene Defects at the Single-Bond with NCAFM

Open-Access Publishing

Chair **Jan Balajka**

- 17:20 **Barbara Hissa**, A true open-access route: how to go diamond in the nanoscience field?

Visualizing alkali metal aggregation-induced coordination in CO₂ activation on copper

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Alkali metals are widely recognized as promoters in CO₂ activation and conversion. However, how the alkali metals activate CO₂ molecules and stabilize the reaction intermediates remains controversial due to the lack of atomic-scale characterization. Here, using scanning tunneling microscopy and non-contact atomic force microscopy, we directly visualized the coordination structure of alkali metal cations and CO₂ reaction intermediates on copper surfaces. At the initial step, we find the aggregation of alkali ions into trimers to facilitate the activation of CO₂. Subsequently, the activated CO₂^{δ-} undergoes C-C coupling to form oxalate on Cu(100), that is coordinated with four alkali ions. Density functional theory calculations reveal the cooperative role of alkali trimers in stabilizing key intermediates, overcoming Coulomb repulsion, and significantly lowering the reaction barrier for CO₂ conversion [1]. Higher CO₂ pressure promotes the production of two-dimensional ordered alkali carbonate films.

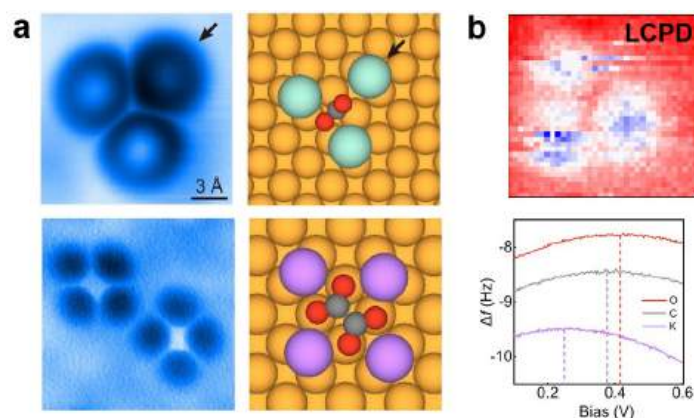


Figure 1: Activation of CO₂ on alkali metal modified copper surfaces and the formation of oxalate that is coordinated with four alkali ions.

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Chiral water structures on dolomite(104) surfaces

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Despite dolomite ($\text{CaMg}(\text{CO}_3)_2$) being an abundant rock-forming mineral on earth, the formation pathways of this carbonate mineral are not fully understood and an explanation of the particular distribution along the geological timescale is still lacking [1]. In addition, the growth of dolomite under geological conditions is still a challenge in a laboratory setting – even reaction experiments prolonging over 32 years failed to precipitate crystalline dolomite [2]. Attempts to find explanations and models addressing this so-called “dolomite-problem” range from kinetic factors setting constraints for dolomite growth [3] to microbe-facilitated pathways. In the latter model, decomposition of organic matter into extracellular polymeric substances is suggested to provide favourable environments for dolomitization [4]. Within these approaches, consensus has been reached that mineral formation requires the presence of fluid phases [5].

Here, we use non-contact atomic force microscopy with CO-terminated tips to disclose chirality of the most stable surface planes of dolomite [6], namely the (104) surfaces. Combined with density functional theory calculations and probe-particle model simulations, two surface enantiomers are identified (see Fig. 1(a)). We furthermore investigate the adsorption of water on this chiral surface with coverage ranging from isolated molecules to a full water layer. A preferential adsorption at the surface calcium and magnesium sites is identified (see Fig. 1(b)) and the adsorbed water structures show a clear chiral character. Thus, the dolomite(104) surface transfers chirality to the intrinsically achiral water molecules with widespread implications in the fields concerned with dolomite and its formation.

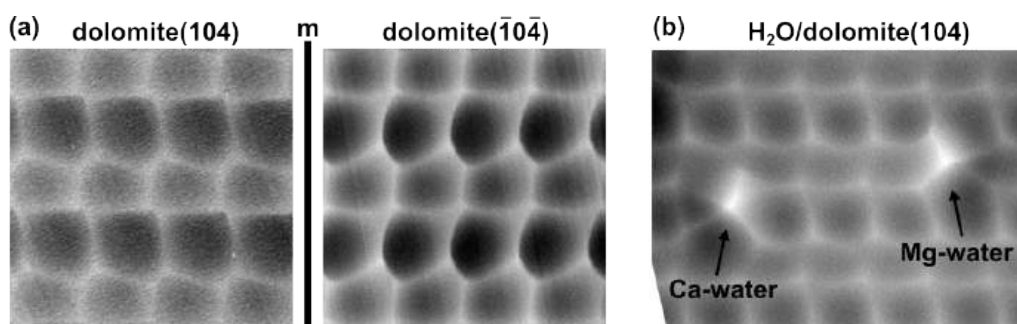


Figure 1: High-resolution frequency shift images acquired with CO tips (a) of the two dolomite(104) surface enantiomers with the indicated mirror plane **m** and (b) of two single water molecules on dolomite(104) adsorbed at calcium and magnesium surface sites.

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Atomic-Scale Characterization of Annealing Effects on Hydrogenated Diamond (100) Surface with Non-Contact Atomic Force Microscopy

Davoud Pourzadeh,¹ Andrew Mayne,² Michael Reichling,¹ Bob Kyeyune^{1,*}

¹ Institut für Physik, Universität Osnabrück, Barbarastrasse 7, 49076 Osnabrück, Germany

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Diamond surfaces have attracted significant interest due to diamond's unique properties, making it a promising material for next-generation electronic devices. The hydrogenated diamond surface exhibits p-type surface conductivity relevant for device applications. However, such surfaces become unstable at elevated temperatures. Therefore, understanding the effect of annealing on the hydrogenated diamond surfaces at the atomic-scale is of fundamental importance. The atomic structures of clean and hydrogenated diamond surfaces have recently been demonstrated using the non-contact atomic force microscopy (NC-AFM) at room temperature (RT) [1]. In this work, we use the NC-AFM operated in the quasi-constant height mode at RT to investigate the influence of annealing temperature on the atomic structure of a high-purity hydrogenated (100) diamond surface. At an annealing temperature of 780 K, the frequency shift (Δf) data in Figure 1(a) reveals a (2×1) reconstruction, with lattice parameters consistent with previous studies [1, 2]. At annealing temperatures of 837 K, the Δf data in Figure 1(b) reveals a (2×1) reconstruction with lattice parameters, characteristic of the clean diamond surface [1, 2]. These results suggest hydrogen desorption at annealing temperatures as low as 837 K. This observation is consistent with recent reports of hydrogen desorption signatures at annealing temperatures of 823 K [3] and underscores the sensitivity of H-termination to preparation conditions and operation temperature in electronic devices. Furthermore, we characterize the features observed on the hydrogenated surface including, vacancies V, adatoms A, and subsurface anti-phase boundaries P (Figure 1(a)). In addition, both buckled and unbuckled dimmers are observed on the clean diamond surface, with the buckled dimmer being the more prevalent configuration (Figure 1(b)).

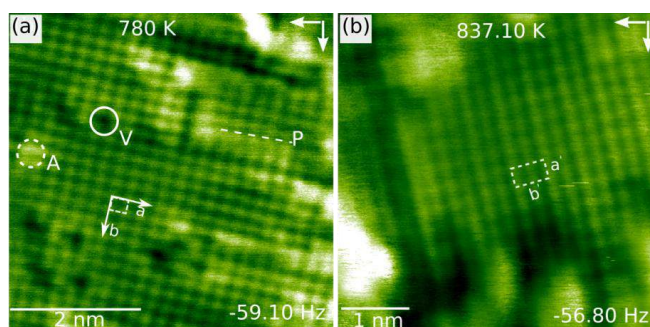


Figure 1: (a) NC-AFM image of diamond (100)-(2×1):H acquired at $\Delta f_{\text{set}} = -59.10$ Hz after annealing at 780 K. (b) Δf image of clean diamond (100)-(2×1) acquired at $\Delta f_{\text{set}} = -56.80$ Hz after annealing at 837 K.

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Resolving Graphene Defects at the Single-Bond with NCAFM

Jara Trujillo-Mulero¹, Haojie Guo², Pablo Pou^{1,3}, Julio Gómez-Herrero^{3,4}, Iván Brihuega^{3,4} and Rubén Pérez^{1,3*}

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Building upon our previous work resolving the atom-by-atom structural configurations of graphene grain boundaries [1], we extend our investigation to isolated point defects and complex topological reconstructions. In this study, we focus on the precise structural mapping and theoretical replication of four defect archetypes within the graphene lattice: the flower, the Stone-Wales, the reconstructed double-vacancy (DV 5555-6-7777), and the classic single-vacancy defect.

Experimentally, low-temperature non-contact atomic force microscopy (ncAFM) functionalized with copper oxide tips yielded images of these configurations with exceptional, sub-chemical spatial resolution, clearly resolving the non-hexagonal ring layouts and localized lattice distortions. To interpret the underlying contrast mechanisms, we performed numerical simulations utilizing the Full-Density-Based Model (FDBM) [2,3]. The FDBM simulations faithfully reproduce the experimental features across all four defect classes. Crucially, by mapping the Pauli repulsion forces arising from the probe-sample electronic charge density overlap, we establish a direct correlation between the observed ncAFM contrast and the local carbon-carbon bond order. This joint experimental and theoretical approach clarifies how structural disruptions alter chemical bonding at the single-bond scale.

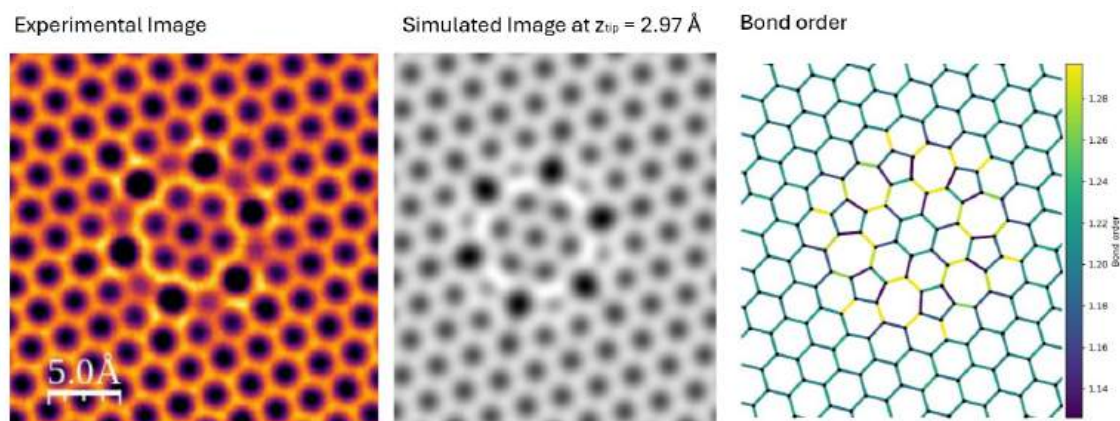


Figure 1: Flower defect. From left to right: experimentally obtained frequency shift image, simulated frequency shift image and bond order map

[1] Guo H., Ventura-Macías E., Jiménez-Sánchez M. D., Nicoara N., Mallet P., Veuillen J.-Y., Renard V. T., Martínez-Galera A. J., Pou P., Gómez-Herrero J., Pérez R., and Brihuega, I. Adv. Mater. e10899 (2025).

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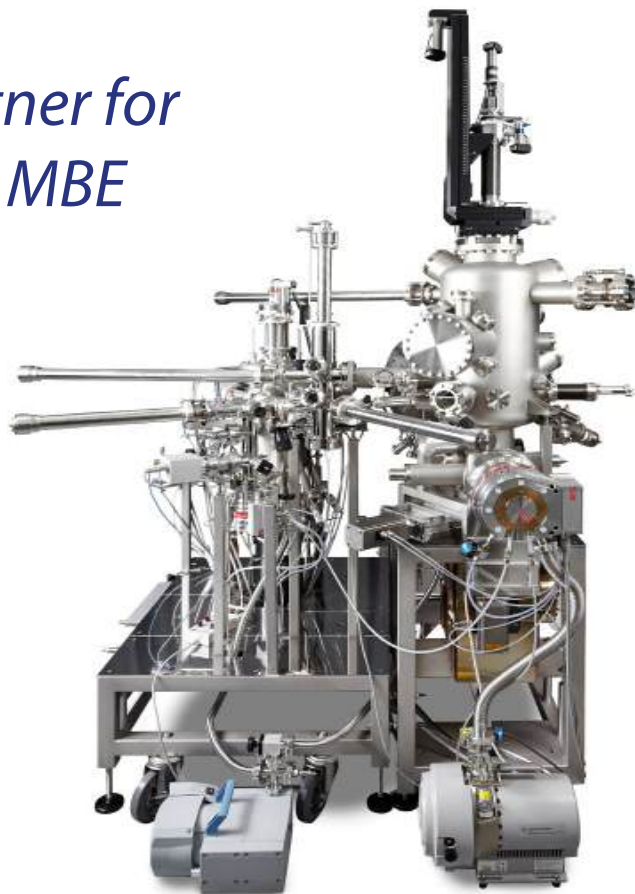
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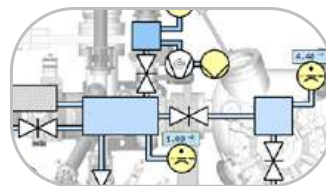
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Wednesday August 5th, 2026

Magnetism

Chair **Nadine Hauptmann**

- 9:00 **Alexander Schwarz**, Magnetically Sensitive Force Microscopy - What to Do Next?
- 9:20 **Aris Lafranca**, Magnetic Susceptibility Imaging of a 2D van der Waals Magnet with Nanowire Magnetic Force Microscopy
- 9:40 **Yuuki Adachi**, Probing a Single Co Atom on MgO Using Magnetic Exchange Force Microscopy
- 10:00 **Susanne Baumann**, Time-resolved energy transfer between a single magnetic adatom and the AFM cantilever

Magnetically Sensitive Force Microscopy - What to Do Next?

Alexander Schwarz^{1*}

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Magnetically sensitive force microscopy, namely Magnetic Force Microscopy (MFM) and Magnetic Exchange Force Microscopy (MExFM), operates in the non-contact regime and can resolve magnetic structures ranging from micrometer-sized domains down to atomic-scale spin textures [1]. In this sense, everything that a scientist interested in surface magnetism can ask for has been accomplished – a statement that raises the question: what to do next?

Using MFM, a spatial resolution below 10 nm has been demonstrated. This is close to the limit attainable at with realistic tip-sample separations and sharp tips that exhibits laterally very confined emanating magnetic stray field [2]. However, such performance is usually achieved only in specialized laboratories. To address this limitation, I will discuss two technical aspects: optimized magnetically sensitive tips and a broader range of dedicated data-acquisition schemes. Both could help make high-resolution MFM imaging more accessible to a wider user community, including users performing experiments under ambient conditions.

For MExFM, the situation is somewhat different. It is a powerful method and, for many sample systems, the only technique capable of revealing spin textures with atomic resolution. It does not require a dedicated imaging mode beyond standard NC-AFM operation. However, the tip must not only terminate in a single atom, it also must also possess a stable magnetic moment. As with NC-AFM in general, MExFM has its greatest impact when applied to non-conductive sample systems. Nevertheless, apart from NiO(001) [3], all sample systems investigated so far have been conductive. Moreover, their magnetic structure was revealed previously using Spin-Polarized Scanning Tunneling Microscopy (SP-STM). While this is understandable as a starting point and could reveal additional information, this strategy offers limited prospects for the future. I will therefore address the challenges associated with imaging non-conductive samples, particularly with respect to in-situ tip preparation, and discuss potential sample systems that are difficult or impossible to investigate using other techniques.

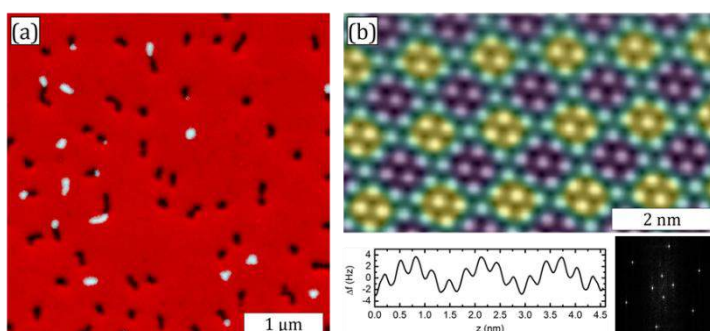


Figure 1: (a) An LSMO/LAO thin film imaged with MFM in vacuum at 5.2 K. The smallest features in the composite image exhibit true diameters below 10 nm. (b) MExFM image of the an Fe monolayer on Ir(111) recorded at 10 K. The composite color scales reveal the hexagonally arranged Fe atoms (grey) and the spin texture of a squarely nano-

skyrmion lattice (color). The line profile shows that the magnetic contrast is superimposed on the chemical contrast. The Fourier transform of the real-space data demonstrates that the atomic lattice (outer peaks) and magnetic structure (inner peaks) are incommensurate.

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Magnetic Susceptibility Imaging of a 2D van der Waals Magnet with Nanowire Magnetic Force Microscopy

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Nanowire Magnetic Force Microscopy (NW-MFM) employs nanowires as cantilevers with hard-magnetic tips, combining exceptional force sensitivity on the order of a few aN Hz^{-1/2} [1] with sub-100 nm spatial resolution [2]. Resonance frequency shifts encode magnetic force gradients from the sample's stray field, while changes in oscillation amplitude reflect energy dissipation. Near a magnetic phase transition both quantities can be linked to the complex magnetic susceptibility of the sample [3], and rather than treating this invasiveness as a limitation, we leverage it to probe the local susceptibility response.

We use the 2D van der Waals ferromagnet Cr₂Ge₂Te₆ (CGT) as a test platform. CGT is a soft 2D ferromagnet with a bulk Curie temperature of around 62 K and uniaxial anisotropy. In exfoliated flakes, T_c decreases with layer number [4]. By mapping frequency-shift and dissipation contrasts across a single CGT flake containing regions of 8 to 16 atomic layers, we observe a sequential onset of magnetic response as the temperature is lowered from above T_c toward 5 K. Thicker regions develop contrast first, followed successively by thinner ones. Notably, the dissipation signal resolves transition temperatures between regions differing by only single atomic layers separated by only a few degrees in temperature.

These results demonstrate that NW-MFM provides spatially resolved maps of the local magnetic susceptibility in 2D van der Waals magnets with single-layer sensitivity, establishing it as a powerful tool for nanoscale studies of weakly magnetic and few-layer systems.

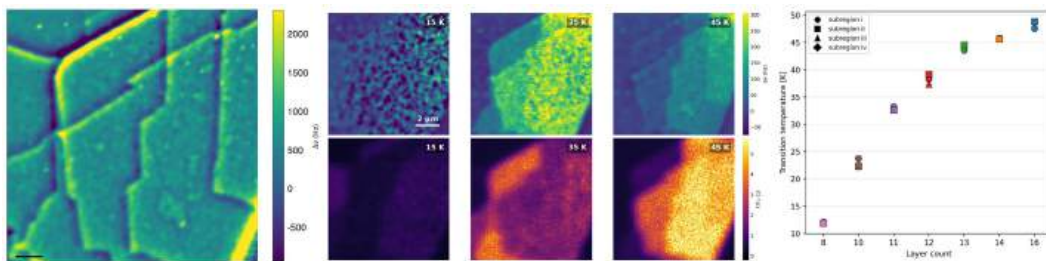


Figure 1: Left: Force-gradient image of CGT at 200 mT and 4.5 K, with layer edges clearly visible; scale bar 2 μm. Center: Temperature-dependent imaging at zero field. Top row shows frequency-shift contrast (f^+), bottom row shows dissipation contrast (Γ^+), recorded at 15, 35, and 45 K. Regions of different layer thickness develop contrast at distinct temperatures, reflecting their layer-dependent Curie transitions. Right: Extracted T_c as a function of physical layer number, with different symbols (i, ii, iii, iv) denoting measurements at distinct spots within the same layer region, showing that T_c increases with layer thickness.

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[3] Mattiat et al., Nanoscale 16, 5302 (2024)

[4] Gong et al., Nature 546, 265 (2017)

Probing a Single Co Atom on MgO Using Magnetic Exchange Force Microscopy

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Magnetic excitations, such as magnons, have been studied in bulk compounds for spintronic applications [1]. Recently, significant progress has been made in the study of spin excitations at the single-atom level [2]. However, it is the elusive non-equilibrium properties of these excited states that govern the temporal evolution of such systems [3]. Probing spins at the single-atom level has been performed using magnetic exchange force microscopy (MExFM), but to date, this has only been applied to the equilibrium states of surface atom spins [4,5].

Here, we demonstrate the use of MExFM to probe single cobalt (Co) atoms on MgO thin films at 4.5 K under external magnetic fields. The Co atoms and a holmium (Ho) atom were identified using scanning tunneling microscopy (STM), as shown in Fig. 1. Co atoms were picked up from the MgO surface to fabricate the magnetic tip. To characterize the fabricated magnetic tip, we measured the exchange interaction between the fabricated magnetic tip and a single Ho atom [5]. We pumped the electron spins of a Co atom on the surface into excited states and probed the interaction between the excited Co atom and the magnetic tip. We found that the force between the Co atom and the magnetic tip differs between the ground and excited states. Our findings open the possibility of measuring nonequilibrium spin-excited states of a single atom using MExFM.

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- [2] C. F. Hirjibehedin, C. Lin, A. F. Otte, M. Ternes, C. Lutz, B. Jones, and A. J. Heinrich, *Science* **317**, 1199–1203 (2007).
- [3] S. Loth, K. von Bergmann, M. Ternes, A. F. Otte, C. P. Lutz, and A. J. Heinrich, *Nat. Phys.* **6**, 340–344 (2010).
- [4] U. Kaiser, A. Schwarz, and R. Wiesendanger, *Nature* **446**, 522–525 (2007).
- [5] Y. Adachi, K. Ueda, Y. Yasui, and Y. Sugimoto, arXiv: 2511.03413 (2025).

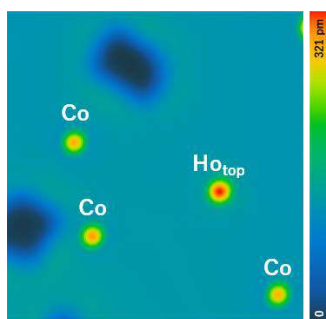


Figure 1: STM image of cobalt atoms and a holmium atom on MgO/Ag(001). Imaging condition: Constant current mode. $V = 200$ mV, $I = 1.0$ nA, $T = 4.5$ K and $B = 3.0$ T. Both Co and Ho_{top} atoms adsorb on top of the oxygen site of the MgO surface.

Time-resolved energy transfer between a single magnetic adatom and the AFM cantilever

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The dissipation signal of the oscillating cantilever in an atomic force microscope (AFM) time-averages atomic-scale dynamics over many oscillation cycles. We use fast time-resolved detection of the tunnel current in a combined AFM/STM to resolve the microscopic mechanism of magnetically induced dissipation at the level of individual quantum jumps of a magnetic atom.

A single Fe adatom on MgO/Ag(100) couples to the tip via magnetic exchange interaction and its stochastic dynamics can be tuned by applying a voltage across the tunnel junction. We track each individual switching event with timing precision below the cantilever oscillation period, which reveals that the phase relationship between spin switches and cantilever motion determines the sign and magnitude of the time-averaged dissipation signal – energy flows into or out of the cantilever depending on switching rate and phase.

Exploiting this mechanistic understanding, we demonstrate that synchronized spin switching generates an alternating exchange force that rectifies energy transfer from the quantum spin to the macroscopic cantilever. The Fe atom functions as a single-atom electric motor: current-driven spin excitations sustain free-running mechanical oscillations of the cantilever. This bridges the quantum-classical divide and establishes exchange force spectroscopy as a tool for studying energy transfer in hybrid quantum-classical systems.

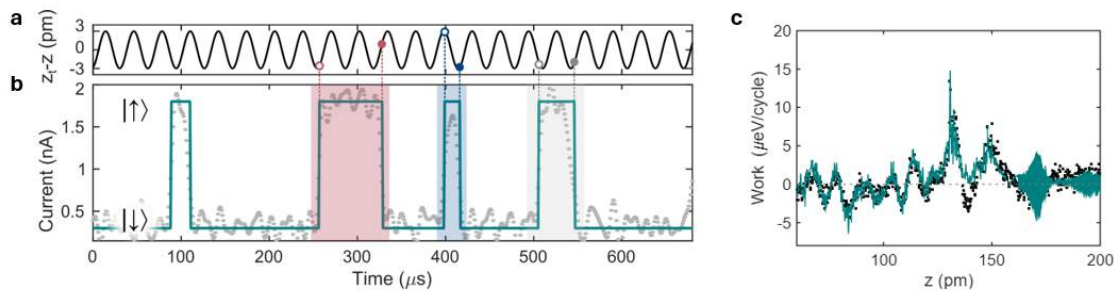


Figure 1: (a) AFM cantilever oscillation and (b) simultaneously recorded quantum jump trajectory (teal) in the STM current on a single Fe atom. (c) Spin-induced work per cycle (teal) extracted from the quantum jump trajectories agrees with the independently measured AFM dissipation (black) as a function of tip-atom distance z . ($V = -11.8$ mV, $A = 3$ pm, $B = 1$ T)

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Wednesday August 5th, 2026

Characterisation of Molecular Systems

Chair **Shigeki Kawai**

11:00 **Jascha Repp**, Atomic-scale sensing of photoexcitation processes

11:20 **Christian Loppacher**, Reversible Radical Formation of Naphthalene Diimide Adsorbed on KCl in the Monolayer Regime

11:40 **Indranil Mal**, Framework for simulation of coupled excitons in molecular aggregates

12:00 **Antoine Hinaut**, Solution synthesized macrocycles: Investigation with AFM in UHV after electrospray deposition

Atomic-scale sensing of photoexcitation processes

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Atomic-scale insights into light-matter interaction can be obtained using various light-assisted scanning probe microscopy techniques. Recently, photoexcited charge carriers have been detected by means of scanning tunneling microscopy (STM), enabling the study of photo-induced charge transfer with atomic-scale spatial resolution [1]. Here, we propose an approach based on atomic force microscopy (AFM) to detect photoexcitation in single molecules adsorbed on non-conductive dielectric films. Synchronizing laser pulses to the oscillation of the tip of an AFM enables the detection of electron tunnelling events that follow photoexcitation. We demonstrate this photoexcitation AFM technique for individual copper phthalocyanine molecules and achieve photoexcitation-driven AFM contrast with ångström spatial resolution, see Fig. 1. The observed sub-molecular contrast suggests the involvement of a long-lived quadruplet excited state. When combined with the recently developed AFM excited-state spectroscopy [2] including lifetime measurements [3], photoexcitation AFM enables comprehensive characterization of electronic states involved in photoexcitation and subsequent intersystem crossing, establishing a powerful platform for investigating photophysical processes at the single-molecule level.

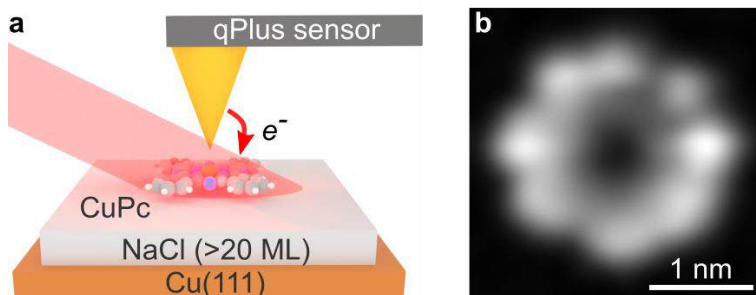


Figure 1: **a)** Schematic of the photoexcitation AFM measurement scheme. Nanosecond laser pulses are phase-locked to the AFM cantilever oscillation and photoexcite charge carriers that subsequently tunnel between molecule and AFM tip. **b)** Constant-height AFM dissipation signal upon photoexcitation close to the neutral-to-cationic transition of the molecule.

- [1] H. Imada, K. Miwa, M. Imai-Imada, S. Kawahara, K. Kimura, Y. Kim, *Nature* **538**, 364 (2016).
- [2] L. Sellies, J. Eckrich, L. Gross, A. Donarini, J. Repp, *Nat. Nanotechnol.* **20**, 27 (2025).
- [3] J. Peng, S. Sokolov, D. Hernangómez-Pérez, F. Evers, L. Gross, J. Lupton, J. Repp, *Science* **373**, 452 (2021).

Reversible Radical Formation of Naphthalene Diimide Adsorbed on KCl in the Monolayer Regime.

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Aromatic diimide moieties have been reported to undergo electrochemical reduction (in solution) to form relatively stable radical anions.¹ Besides electrochemical reduction, diimides also show photochemical reduction, in particular a photoinduced intramolecular electron transfer (PIET) has been observed for naphthalene diimides in the form of powder and crystals.²

In this work, we present the deposition of naphthalene diimides consisting of two donor and one acceptor (the diimide) group on bulk and thin films of KCl under ultrahigh-vacuum conditions. Combined ncAFM and STM measurements show that the molecules form an highly-ordered monolayer with planarly adsorbed molecules on KCl. Differential Reflectance Spectroscopy (DRS, reflects the optical absorption spectra) during the deposition of the organic layer confirms the formation of a radical species upon illumination. The radical is stable over hours and can be reversibly excited after relaxation.

These results are compared with DFT calculations, EPR (Electron Paramagnetic Resonance) spectra of thin films and powder, and UV-vis spectroscopy in solution to understand the formation of the radical and its magnetic and optical properties. These results indicate the potential use of these molecules as organic Spin-State Photoswitches.

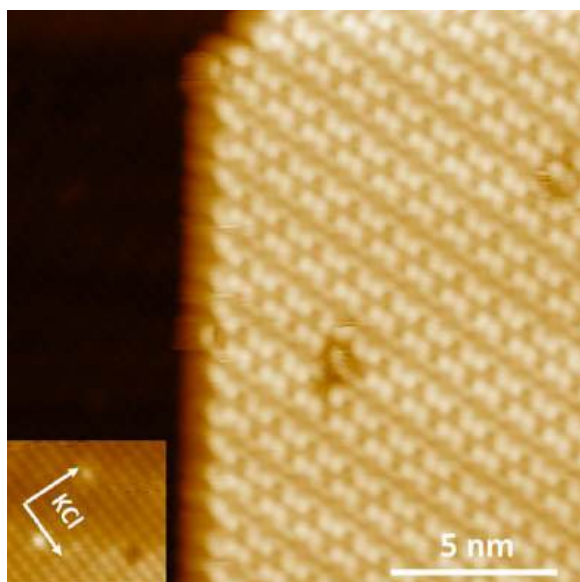


Figure : Topography image (STM) of a monolayer of naphthalene diimide adsorbed on a thin film of KCl on Au(111). Lower left part, contrast highlighted to show the KCl substrate periodicity. A point-on-point epitaxy of planarly adsorbed molecules is observed.

- [1] A. Viehbeck et al., J. Electrochem. Soc. **137**, 1460 (1990);
S.K. Lee et al., J. Am. Chem. Soc. **121**, 3513 (1999).
- [2] Y. Matsunaga et al., Chem. Eur. J. **20**, 7309 (2014).

Framework for simulation of coupled excitons in molecular aggregates

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Tip-enhanced photoluminescence (TEPL) and STM-induced luminescence (STML) allows the study of emission of light from molecules and their assemblies with sub-nanometre resolution and study processes which are dark in far field[1]. While optical response of individual molecules can be simulated efficiently ab-initio (e.g. by TDDFT), for molecular clusters on the surface this is difficult and computationally expensive. To address this challenge we developed an open-source package which efficiently simulates exciton coupling between molecule aggregates via Frankel hamiltonian and the resulting photon maps. The code also computes spectral shifts due to the Stark-effect induced by the electric field of the tip and neighbouring molecules. The parameters including diagonal stark-shift and off-diagonal exciton coupling are computed from ab-initio input as coulomb integrals over transition density resp. electron density difference exported as cube files. The photon-emission intensity map of coupled excitons is obtained in one step by convolution of linear combination of molecular transition densities projected on a common grid using FFT. Integrated grid-projected forcefield (GridFF)[2] allows rapid global optimization of molecular adsorption geometries on insulating substrates (e.g. NaCl films) and their self-assembly into aggregates. We validate the code against recent TEPL experiments on PTCDA anion assemblies [3] and demonstrate the pipeline from a single-monomer $D_0 \rightarrow D_1$ transition density through to a multi-molecule excitonic photon map of a large cluster (Fig. 1).

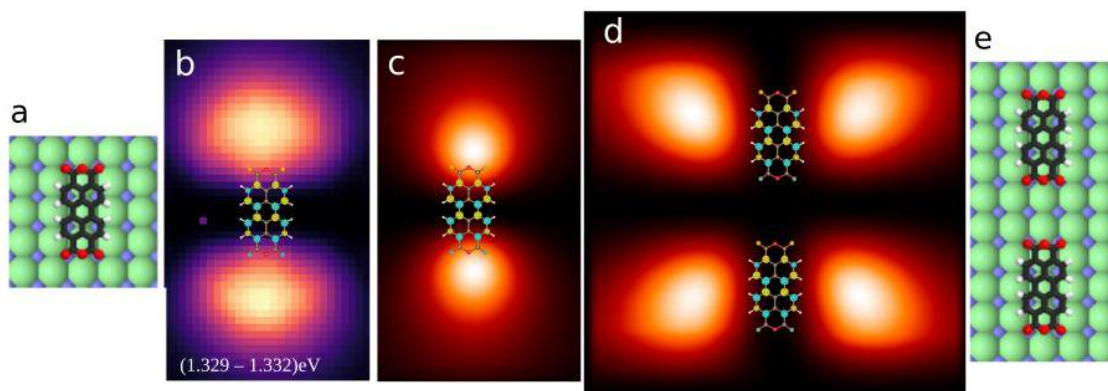


Figure 1: (a) TD-DFT $D_0 \rightarrow D_1$ transition density of the PTCDA anion. (b) Photon map simulated by Light-PPSTM. (c) Experimental TEPL map from Ref. [3] integrated over 1.329–1.332 eV. The two-lobed pattern with a central node reflects the spatial structure of the $D_0 \rightarrow D_1$ transition density.

[3] de Campos Ferreira, Sagwal, Doležal, Neuman, Švec, Nat. Commun. 16, 61296 (2025).

[5] Mal, I., Kočí, M., Nicolini, P. & Hapala, P. J. Chem. Theory Comput. 21, 12214–12226 (2025).

[6] Sagwal et al., arXiv:2605.05872 (2026).

Solution synthesized macrocycles : Investigation with AFM in UHV after electrospray deposition

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Macrocycles, organic molecules with large ring-like architectures, are promising candidates for supramolecular and host-guest chemistry due to their flexible shape and tunable chemical composition. A clean transfer from solution to surfaces is crucial to bridge the gap between solution-phase and surface-confined chemistry. Electrospray deposition (ESD) techniques enabled the safe deposition into UHV environments of large organic molecules and their investigation on various surfaces [1,2,3].

Here [4], we investigate two crown ether macrocycles, with identical ether chains but different linkers (Figure left), on Ag(111) surface in UHV conditions. Using low-temperature scanning tunneling microscopy (STM) (Fig center) and CO-functionalized atomic force microscopy (CO-AFM) (Figure right), we compare the molecular assemblies formed by the two macrocycles on the surface. We show that the linker type modifies the adsorption geometry of macrocycles allowing the formation of open or closed ring conformations.

We further explore the coordination properties of the macrocycle by taking advantage of the ESD technique to directly deposit host-guest complexes pre-formed in solution. We observe ion incorporation within the macrocycle cavity and reveal conformational changes together with their effect on supramolecular assemblies.

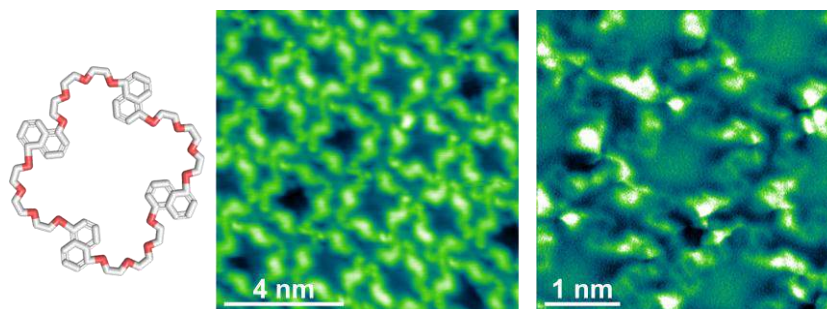


Figure 1: Macrocycle on Ag(111). Left: Macrocycle structure with naphthalene linker. Center: STM topography of the molecular assembly. Right: CO-AFM imaging of the structure.

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- [2] A. Hinaut et al., *Beilstein J. Nanotechnol.* **12**, 552–558 (2021).
- [3] S. Scherb et al., *ACS Nano* **17**, 597–605 (2023).
- [4] A. Hinaut et al., *submitted* (2026).

Wednesday August 5th, 2026

Novel Instrumentation and Techniques

Chair **Christian Loppacher**

- 14:00 **Peter Grutter**, AFM excess noise measures electrochemical reaction rates
- 14:20 **Yuto Nishiwaki**, Long-Range Order and Superstructure on Molten Metal/Solid Interfaces Imaged by Three-Dimensional Force Spectroscopy
- 14:40 **Yasuhiro Sugawara**, Nanosecond measurement of charge emission from interface states to bulk states in Si by pump-probe heterodyne FM-KPFM
- 15:00 **Vijayalaxmi Sankeshwar**, Low-Temperature Beam Deflection Atomic Force Microscope

AFM excess noise measures electrochemical reaction rates

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About 20% of global CO₂ emissions are due to energy intensive processes needed to manufacture steel, concrete and fertilizer. Carbon can be recycled sustainably and stored at high energy densities via the electrocatalysis of CO₂ into hydrocarbon products – precisely as needed for scalable industrial decarbonization. Moreover, the energy required to recycle carbon in this manner can be taken from waste heat or renewables. Hence, CO₂ recycling can act as crucial bridge technology to decarbonize key industrial infrastructure. It is important to note that rebuilding all industrial infrastructure to be carbon-neutral could take more than 50 years, whereas CO₂ electrocatalysis technologies can be retrofitted onto existing infrastructure to offer immediately needed steep emissions reductions. Though innovation gains have been made in CO₂ electrocatalysis, it still does not have the stability and energy efficiency required to make it a commercially viable technology.

Electrocatalytic processes occurring at a heterogeneous interface are complex, and their understanding at the molecular level remains challenging and often requires non-electrochemical approaches. Atomic force microscopy (AFM) can detect force interactions down to the atomic level, but so far it has been mainly used to obtain in situ structural images of electrocatalysts, down to the atomic scale [1]. We are developing AFM methods to measure electrocatalytic activity with the aim of understanding structure-property relations on an atomic scale. We have demonstrated how excess force noise can be quantitatively correlated with electrochemical activity (Figure 1). Specifically, for the first time, we employed AFM to investigate the hydrogen evolution reaction (HER) at a platinum ultramicroelectrode (Pt UME) under actual electrochemical reaction conditions using force noise measurements. We detect excess force noise when individual H₂ gas bubble nucleation, growth, and detachment events occur, allowing us to develop a mechanistic understanding of this key process [2]. Similarly, we have also studied the oxygen evolution reaction (OER) [3]. We find that O₂ gas bubbles nucleate at Pt UME step-edge sites and interact with catalytically active sites. This interaction between primary catalytic sites and bubble nucleation sites is the main reason for a decrease in the current density at a given high overpotential of the OER, limiting the reaction rate. As an outlook, I will report our latest result on investigating CO₂ electrocatalysis using AFM noise spectroscopy on copper surfaces.

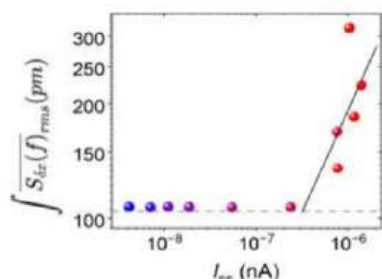


Figure 1: Log-log plot of the correlation of integrated AFM deflection noise versus electrochemical steady-state current for hydrogen evolution reaction on a Pt Ultramicroelectrode. The dashed line is the AFM noise floor.

[1] A. Labuda, et al., Rev. Sci. Instr. **81**, 083701 (2010).

[2] N. Bodappa, et al., J. Phys. Chem. Lett. **16**, 6015 (2025).

[3] N. Bodappa, et al., J. Phys. Chem. Lett. **17**, 1815 (2026).

Long-Range Order and Superstructure on Molten Metal/Solid Interfaces Imaged by Three-Dimensional Force Spectroscopy

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¹ Department of Materials Science and Engineering, Kyoto University, Yoshida Honmachi, Sakyo, Kyoto 606-8501, Japan

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The interfaces between molten metals and solids are crucial in metallurgy. Since modeling non-classical liquids at finite temperatures remains computationally challenging, experimental investigation and the formulation of interfacial liquid structures and their relationship with the solid structure are essential. Atomic force microscopy (AFM) and its force spectroscopy technique on liquid/solid interfaces are powerful tools for visualizing the interfacial structures and mechanical responses with high spatial resolution. We have previously demonstrated the effectiveness of qPlus-sensor-based AFM in molten metals [1], as it is applicable to opaque liquids where conventional Si-microcantilever-based AFM is unsuitable. In this study, we extend this approach to three-dimensional (3D) force spectroscopy to reveal how the solid surface structure determines the interfacial (solvation) structure at the molten metal/solid interface.

3D force mapping requires high throughput to achieve adequate pixel resolution within a minimum timeframe, ensuring robustness against thermal drift and interfacial dynamics. To address this, we have developed a high-speed AFM using a qPlus sensor [2], which incorporates a Quadpod high-speed tip scanner designed to drive the heavy mass of the qPlus sensor. This system is further equipped with a Hybrid-loop wideband frequency demodulator, which maximizes the force detection bandwidth despite the low f_0 of the qPlus sensor, thereby increasing the throughput of intermittent height feedback during 3D mapping.

Figure 1 displays 3D frequency shift (Δf) maps obtained on (a) molten Ga/AuGa₂ and (b) molten Ga/PdGa₅ interface at room temperature, alongside their respective topographic images obtained by separate topographic scans. For the Ga/AuGa₂ interface (Figure 1(a)), the 3D Δf map showed a slanted lattice-like Δf distribution extending over seven atomic layers, with a lattice spacing comparable to the atomic diameter of Ga ($2r_{\text{Ga}} \sim 0.27$ nm). This suggests that the structural templating of the liquid Ga phase on the AuGa₂(111) surface, with its simple sixfold atomic arrangement in the topographic image, introduced long-range order to the liquid phase. In contrast, at the Ga/PdGa₅ interface (Figure 1(b)), the 3D Δf map showed a lattice-like structure with a spacing of about twice as long as $2r_{\text{Ga}}$. The topographic and corresponding energy dissipation image for a topographic scan showed a long-period superstructure attributed to the PdGa₅(211) surface. The correlation between the liquid/solid structure suggests that structural templating on a complex surface can induce long-range, long-period order in the liquid, forming an “interfacial superstructure”. Since such long-range order at liquid/solid interfaces is not observed in most classical liquids but aligns with emerging reports of first-principles molecular dynamics simulations of the molten metal/solid interface [3], these findings likely reflect the unique, non-classical behavior of molten metals at the solid/liquid interface.

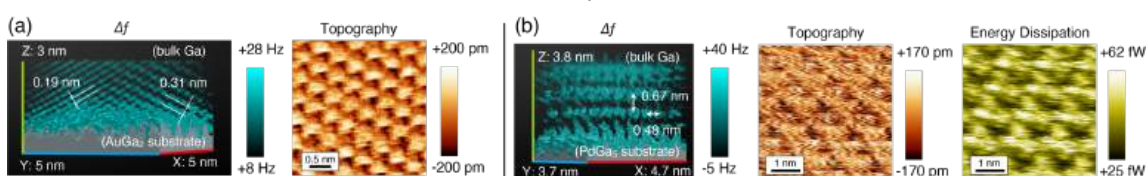


Figure 1: The 3D frequency shift (Δf) maps and the topographic (with energy dissipation) images obtained on the interface of (a) molten Ga/AuGa₂ and (b) molten Ga/PdGa₅ at room temperature.

[1] T. Ichii, M. Murata, T. Utsunomiya, H. Sugimura, J. Phys. Chem. C **125**, 26201–26207 (2021).

[2] Y. Nishiwaki, T. Utsunomiya, T. Ichii, arXiv (preprint) 2604.04970 (2026).

[3] C. M. Fang, H. Men and Z. Fan, Metall. Mater. Trans. A **49**, 6231–6242 (2018).

Nanosecond measurement of charge emission from interface states to bulk states in Si by pump-probe heterodyne FM-KPFM

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¹ The University of Osaka, 2-1 Yamada-oka, Suita 565-0871, Japan

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Understanding the temporal evolution of surface potential is crucial for understanding the fundamental nanoscale electrodynamics of nanomaterials and nanodevices. Pump-probe KPFM is an intriguing technique for performing time-resolved surface potential measurements [1]. Its operating principle involves limiting the application of the modulated bias voltage used for electrostatic measurements in KPFM to a finite time window.

In this study, we propose a pump-probe heterodyne FM-KPFM using high frequency AC bias voltage to improve the temporal resolution and the sensitivity of surface potential measurement. In pump-probe heterodyne FM-KPFM, the heterodyne (frequency conversion) technique was used and AC bias voltage with a frequency $2f_0 + f_m$ was applied (f_0 and f_m are the resonance frequency of the cantilever and the modulation frequency, respectively) [2, 3].

For impurity-doped Si samples, we have successfully observed surface potentials that change rapidly on a timescale of the order of 100 ns and those that change slowly on a timescale of the order of μ s in response to a square-wave pump voltage (Fig. 1A). The rapid change in the surface potential is attributed to changes in the band structure in response to the square-wave signal, while the slow change in the surface potential is attributed to the thermal emission of electrons from the interface states into the conduction band states (Fig. 1B). This success is a promising development in the exploration of atomic-scale physical and chemical interactions at surfaces and provides greater insight into the various functions of surfaces and catalytic processes.

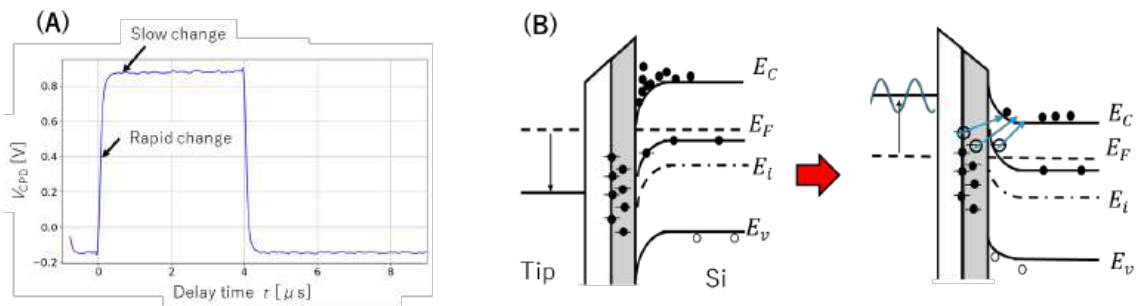


Figure 1: (A) Surface potential as a function of time for square-wave signal of the pump voltage with amplitude of 1.5V, repetition frequency of 100 kHz, duty ratio of 40 %, and probe voltage width of 100 ns. Experimental parameters: PtIr-coated Si cantilever, $k = 45$ N/m, $f_0 = 285$ kHz, $2f_0 + f_m = 571.6$ kHz, and $f_m = 150$ Hz. (B) Energy band diagram of the metal-gap-semiconductor sample showing electron emission from interface states to conduction band states.

- [1] J. Murawski *et. al.*, J. Appl. Phys. **118**, 154302 (2015).
- [2] Y. Sugawara, M. Miyazaki, Y. J. Li, J. Phys. Communications, **4**, 075015 (2020).
- [3] R. Izumi, M. Miyazaki, Y. J. Li, Y. Sugawara, Beilstein J. Nanotechn., **14**, 175 (2023).

Low Temperature Beam Deflection Atomic Force Microscope

Vijayalaxmi Sankeshwar*, Antoine Hinaut, Yves Pellmon, Andreas Tonin, Ernst Meyer and Thilo Glatzel

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We present a newly developed home-built optical beam deflection microscope designed for high-bandwidth multimodal measurements at cryogenic temperatures. The beam-deflection detection system consists of a photoluminescent diode, two alignment mirrors, and a four-quadrant photodiode, all mounted on linearly stepped piezoelectric motors for precise positioning and alignment. A custom preamplifier positioned in close proximity to the beam-deflection unit, approximately 30 cm from the quadrant photodiode, enables a detection bandwidth approaching 2 MHz. To ensure stable low-temperature operation, the preamplifier is thermally insulated using chrome-steel wiring and includes an optional self-heating capability.

The microscope further incorporates four electrical contacts at the sample stage, allowing simultaneous electrical characterization during scanning probe measurements. The entire microscope assembly is mechanically isolated from external vibrations by a spring suspension system combined with eddy-current damping inside a liquid nitrogen–helium bath cryostat, enabling operation down to 4 K. In addition, two integrated heaters allow temperature-dependent investigations over a wide range of operating conditions.

The large detection bandwidth enables simultaneous multimodal operation, including normal force, torsional force, and Kelvin probe force microscopy. The capabilities of the instrument were evaluated on benchmark systems such as $C_{60}/KBr(001)$ and $C_{60}/Au(111)$, demonstrating high spatial resolution and stable multimode imaging performance.

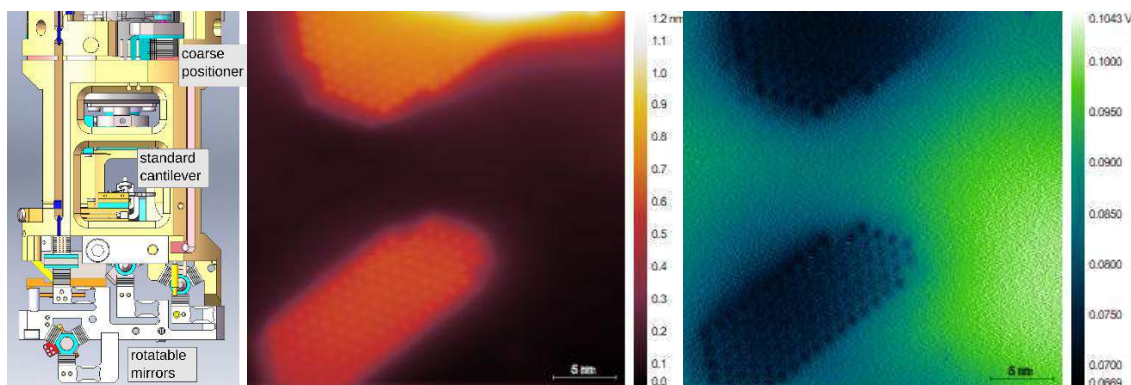


Figure 1: LT- Beam Deflection Microscope (left); Topography of C_{60} islands on $Au(111)$ ($\Delta f = -162$ Hz, $A = 2.4$ nm) (middle); and simultaneously measured KPFM ($f = 1.028$ MHz; $V_{ac} = 100$ mV) (right)

Wednesday August 5th, 2026

High-Resolution Force Mapping

Chair **Harry Mönig**

- 16:00 **Daniel Martin-Jimenez**, Bimodal atomic force microscopy with a torsional eigenmode for highly accurate imaging of grain orientation in organic thin films
- 16:20 **Omur Dagdeviren**, Quantifying the Site-Resolved Energy Landscape of Au(111) Herringbone Reconstruction via Three-Dimensional Non-contact Atomic Force Microscopy
- 16:40 **Udo Schwarz**, Expanding 3D-AFM To Enable the Mapping of Quantitative Molecule-Molecule Reactivity Landscapes
- 17:00 **Daniel Ebeling**, Probing weak chemical interactions of metal surface atoms with CO-terminated AFM tips identifies molecular adsorption sites

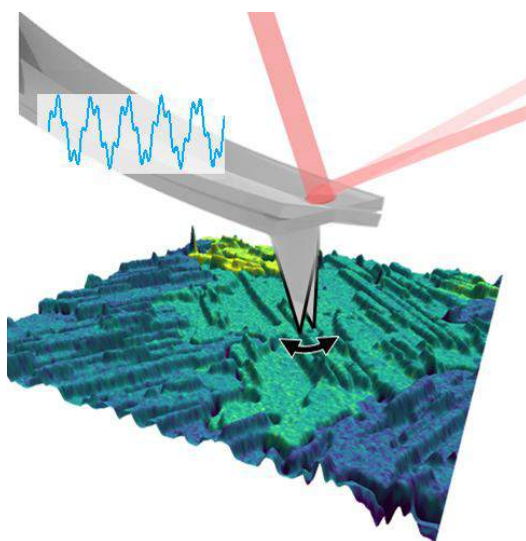
Bimodal atomic force microscopy with a torsional eigenmode for highly accurate imaging of grain orientation in organic thin films

R. Arilla, E. Barrena, C. Ocal, **D. Martin-Jimenez***

Institut de Ciència de Materials de Barcelona (ICMAB), CSIC, Campus Bellaterra 08193, Barcelona, Spain

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In organic electronics, the nature and spatial distribution of grains in polycrystalline thin films of small organic semiconductor molecules greatly impact the electronic properties of devices. Therefore, tools that accurately characterize organic films at the mesoscopic level are essential. To this end, we demonstrate here the power of a bimodal Atomic Force Microscopy (AFM) with a torsional eigenmode for highly accurate imaging grain orientations in organic thin films. The energy dissipated between tip and sample during scanning depends on the in-plane crystalline orientation of each grain. This fact alters the cantilever torsional observables, allowing grain orientation recognition. Remarkably, bimodal AFM with the torsional eigenmode has important advantages, such as high sensitivity in the applied forces, true molecular resolution, and multiple parameters for regulating the image contrast, making it competitive with other well-established AFM methods for grain detection in organic thin films, namely Friction Force Microscopy and Transverse Shear Microscopy.



[2] R. Arilla, E. Barrena, C. Ocal, D. Martin-Jimenez, *Nano Lett.* **25**, 3597 (2025).

Quantifying the Site-Resolved Energy Landscape of Au(111) Herringbone Reconstruction via Three-Dimensional Non-contact Atomic Force Microscopy

Nuray Basaran,¹ Bugrahan Guner,^{1,2} and Omur E. Dagdeviren^{1,*}

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² Department of Mechanical Eng., Yale University, New Haven, Connecticut, 06520, USA

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Reconstructed metal surfaces provide chemically inequivalent adsorption environments; however, their local interaction potentials are not directly quantified in most cases. The Au(111) herringbone reconstruction is a typical example. Alternating face-centered cubic (FCC) and hexagonal close-packed (HCP) domains, soliton walls, elbows, and junction motifs generate a nanoscale template that can modify adsorption, molecular assembly, and diffusion. Despite the significance and wide use of Au(111), its energetic corrugation across the full reconstructed surface has not been quantitatively resolved with site-specific resolution. Here, we use three-dimensional non-contact atomic force microscopy to map the interaction landscape of Au(111) under low-temperature ultrahigh vacuum conditions. Atomically defined Au-terminated and CO-functionalized tips were used to acquire volumetric $\Delta f(x, y, z)$ datasets across the herringbone reconstruction. At each lateral position, $\Delta f(z)$ curves were fitted, and the long-range tip-background contribution was subtracted, enabling reconstruction of the short-range tip-apex/surface interaction potential, $U^{\text{tip-apex}}(x, y, z)$, and the corresponding vertical and lateral force fields. As Figure 1 shows, this method resolves the interaction-energy landscape across FCC and HCP domains, ridges, elbows, and junction structures with picometer-scale spatial precision.

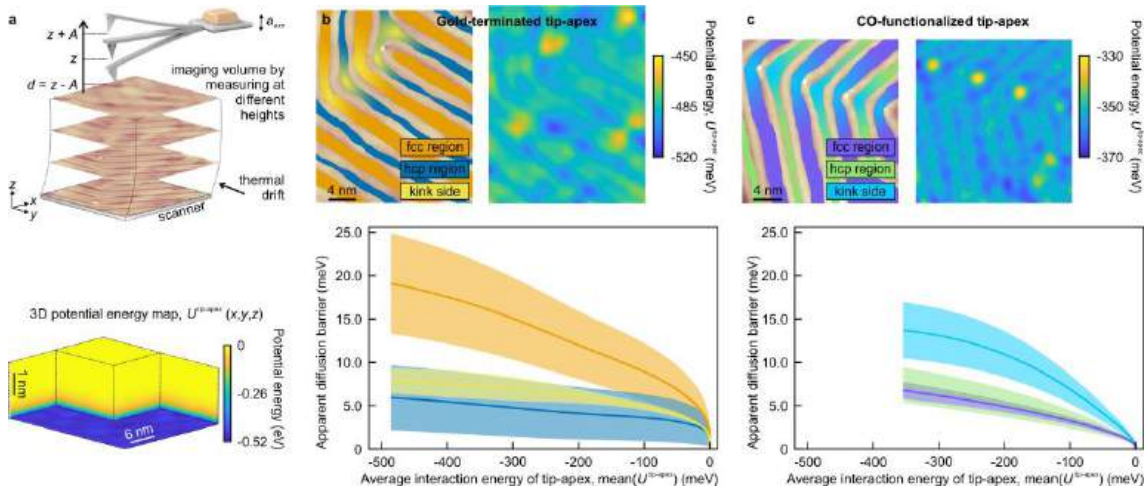


Figure 1. Three-dimensional mapping of tip-sample interaction energy. (a) Three-dimensional non-contact atomic force microscopy measurements were performed at different tip-sample heights to calculate the corresponding interaction energy map. (b, c) Potential energy corrugation measured with Au-terminated and CO-functionalized probes.

The reconstructed maps reveal that, with an Au-terminated tip, the apparent diffusion barrier is highest over FCC domains (18.7 ± 5.7 meV), while HCP and kink-side regions remain lower (5.8 ± 3.7 and 7.9 ± 1.5 meV, respectively). In contrast, with a CO-functionalized tip, the FCC and HCP barriers become comparable (6.6 ± 1.0 and 7.3 ± 2.0 meV), whereas the kink-side region exhibits the higher barrier (13.7 ± 3.2 meV). Thus, the Au(111) reconstruction does not define a single universal barrier landscape; instead, the measured interaction landscape depends on both local surface registry and the chemical identity of the interacting apex.

Expanding 3D-AFM To Enable the Mapping of Quantitative Molecule-Molecule Reactivity Landscapes

Xinzhe Wang,^{1,2} Percy Zahl,³ Jara Trujillo-Mulero,⁴ Emiliano Ventura-Macias⁴, Yunus Dogan,⁵ Bugrahan Guner,¹ Rubén Pérez,^{4,6} Eric I. Altman,^{5,7} and **Udo D. Schwarz**,^{1,5,7*}

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Studying molecular interactions at surfaces is crucial for advancing catalytic technologies and addressing numerous challenges in materials science. While three-dimensional atomic force microscopy (3D-AFM), which has been introduced in 2009 [1], is able to measure forces between a tip and a sample with sub-angstrom spatial and piconewton force precision, quantitative site-specific information on molecule-molecule interactions was thus far not available. This is because the total tip-sample force recovered includes contributions from the substrate (labeled as F_1 and F_2 in the inset of Fig. 1b) and the back part of the tip (F_4), which typically dominate the total interaction. Here, we show how a novel post-processing correction framework can eliminate these unwanted F_1 , F_2 , and F_4 contributions using the interaction between cobalt phthalocyanine (CoPc), a prototypical CO₂ reduction catalyst that we deposit on Ag(111), and CO that is attached to the end of the tip to provide the CoPc-CO force F_3 only (Fig. 1a), revealing site-specific reactivity landscapes and their modulation through -NH₂ substitution. This advance transforms 3D-AFM into a chemically specific, quantitative tool for probing interaction forces between complex molecules, with an accuracy previously accessible only in theoretical models (Fig. 1b).

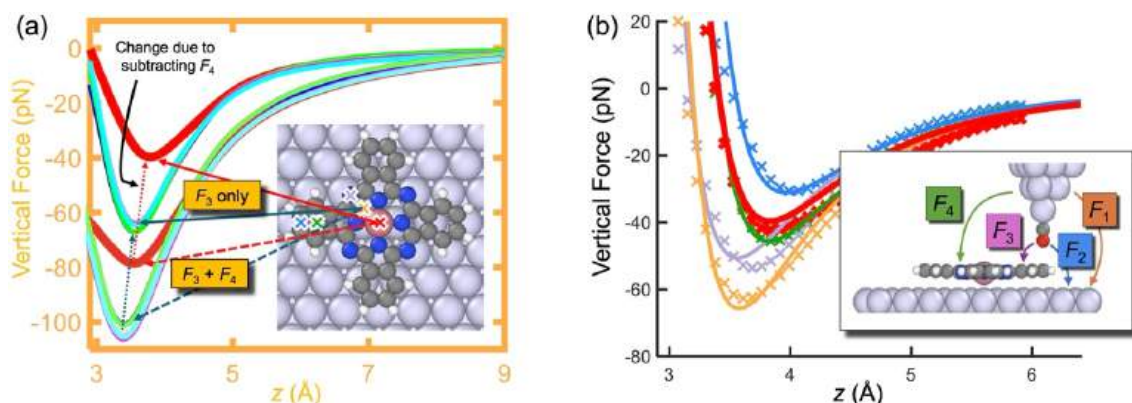


Figure 1: (a) Illustration how the tip-CoPc forces $F_3 + F_4$ (dashed arrows), recovered at the locations marked using a previous procedure [2], change when isolating the CO-CoPc force F_3 (solid arrows). (b) Comparison between the CoPc-CO forces F_3 extracted from experiment (solid lines) and simulations (x), revealing a close match. Colors reflect the locations marked in (a).

[1] B. J. Albers et al., Nature Nanotechnology **4**, 307 (2009).

[2] Xinzhe Wang et al., ACS Nano **18**, 4495 (2024).

Probing weak chemical interactions of metal surface atoms with CO-terminated AFM tips identifies molecular adsorption sites

Jalmar Tschakert¹, Qigang Zhong¹, Alexander Sekels¹, Pascal Henkel^{2,3}, Jannis Jung², K. Linus H. Pohl², Hermann A. Wegner⁴, Doreen Mollenhauer⁵, André Schirmeisen¹, **Daniel Ebeling^{1,*}**

¹ Institute of Applied Physics (IAP), Justus Liebig University Giessen, Germany

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Metal surfaces are pivotal in on-surface synthesis because they provide a two-dimensional catalytic environment that facilitates the activation, diffusion, and coupling of molecular reactants. A fundamental understanding of the interactions between surface atoms and reactants is still limited, but such knowledge would enable control of self-assembly and reaction processes, thereby allowing the rational design of functional nanomaterials. Building on our recent finding that surface-induced charge redistribution can steer two-dimensional molecular assemblies by reversing the selectivity of intermolecular halogen bonds, [1] we investigated the interactions between CO-terminated tips and Cu(111), Ag(111), and Au(111) surface atoms in all spatial directions. [2] Using low temperature atomic force microscopy with picometer resolution, we achieved site-specific quantification of the weak chemical forces acting between densely packed metal atoms and CO-terminated tips (Fig. 1). Complementary density functional theory calculations reveal a small orbital overlap between the *p*- and *d*-states of the CO tip and the metal surface atoms as the cause of these site-specific interactions. This approach allows a more reliable determination of molecular adsorption sites, essential for deciphering on-surface reaction pathways and validating theoretical studies. In future work, this methodology could be extended to halogen-functionalized tips, enabling direct probing of the metal–halogen interactions that trigger surface-catalyzed dehalogenation—a key step in on-surface Ullmann-type coupling.

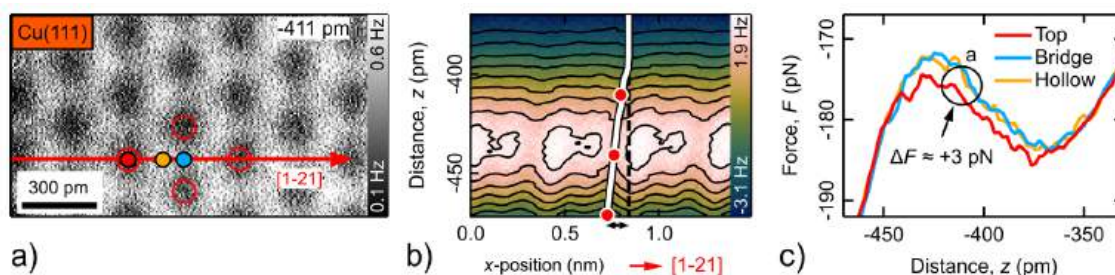


Figure 1: Site-specific tip-surface interactions measured with a CO-terminated tip. (a) Constant-height frequency shift AFM image of Cu(111) surface. (b) 2D frequency shift vs. distance map measured along red arrow in (a). (c) Force vs. distance curves measured above top (red), bridge (blue), and hollow sites (orange) revealing Cu surface atoms as most attractive sites.

[1] J. Tschakert et al., Nature Communications **11**, 5630 (2020)

[2] J. Tschakert et al., Nature Communications **16**, 7874 (2025)

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Thursday August 6th, 2026

Lateral Forces, Friction, and Energy Dissipation

Chair **Peter Grutter**

- 9:00 **Akash Gupta**, Mechanical detection of sub-band mobilities of two dimensional electron gas on reduced SrTiO_3 surface
- 9:20 **Shuyu Huang**, Vibration-induced dynamic superlubricity on $\text{MoS}_2/\text{Au}(111)$ under ultra-high vacuum
- 9:40 **Jay Weymouth**, A direct measurement of weak lateral trapping over a C_6 ring
- 10:00 **Sophia Schweiss**, Atomic scale energy dissipation over copper oxide studied with lateral force microscopy
- 10:20 **J. G. Vilhena**, Quantifying Irreversibility (Dissipation) in Single-Molecule Nanomanipulation
- 10:40 **Mengxi Liu**, Interplay of Backbone Rigidity and Side-Group Flexibility in One-Dimensional Structural Superlubricity

Mechanical detection of sub-band mobilities of two-dimensional electron gas on reduced SrTiO3(001) surface.

Akash Gupta^{1,*}, Marcin Kisiel¹, Rémy Pawlak¹, Ernst Meyer¹

¹ Department of Physics, WSS-Research Center for Molecular Quantum Systems, University of Basel, Klingelbergstrasse 82, Basel, CH-4056, Switzerland.

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The two-dimensional electron gas (2DEG) in reduced strontium titanate offers a versatile platform for oxide electronics, yet its dissipation mechanism under field driven charge fluctuations remains poorly understood. Here, we combine low-temperature atomic force microscopy with scanning tunneling spectroscopy to probe the force and dissipation responses of a mechanical oscillator interacting with the STO 2DEG. The observation of Rydberg-like image potential states by tunneling experiments confirm the 2DEG formation, while dissipation spectroscopy reveals bias-dependent peaks linked to local electrostatic gating and charge redistribution within the 2DEG energy sub-bands. These features are quantitatively explained by variations in quantum capacitance as carrier density is tuned by electric fields. Under magnetic fields, dissipation peaks obey the Kohler's rule, allowing extraction of carrier mobilities in each sub-band. Our results establish a non-invasive AFM-based methodology for quantifying energy losses in quantum oxides, providing new insights into charge dynamics relevant for spintronic applications.

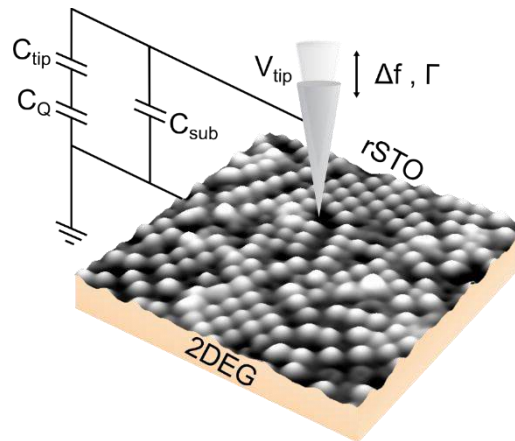


Figure 1: A capacitively coupled AFM tip to the 2DEG of reduced STO surface with quantum capacitance of C_Q .

Vibration-induced dynamic superlubricity on MoS₂/Au(111) under ultra-high vacuum

Shuyu Huang,¹ Yiming Song,¹ Antoine Hinaut,¹ Gema Navarro-Marín,¹ Antonio Cammarata,² Ernst Meyer¹ and Thilo Glatzel^{1*}

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² Department of Control Engineering, Faculty of Electrical Engineering, Czech Technical University in Prague, 16627 Prague, Czech Republic

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Achieving rapid and flexible control of friction across different material surfaces is of great significance and remains a longstanding challenging goal in modern tribology. Here, we demonstrate dynamic superlubricity on monolayer MoS₂-coated gold surfaces induced by external mechanical actuation. By tuning the excitation frequency to the cantilever resonance, stick-slip motion is effectively suppressed, leading to a significant reduction in friction even under high-load conditions. Experimental results, supported by a modified phononic friction model, reveal that torsional vibrations reduce energy barriers and promote transitions between atomic sites. This strategy provides a universal and reversible approach for active friction control at the nanoscale.

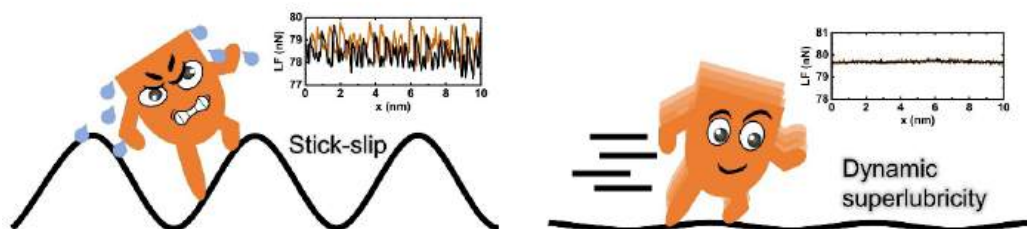


Figure 1: Dynamic superlubricity on monolayer MoS₂/Au(111).

A direct measurement of weak lateral trapping over a C₆ ring

Alfred J. Weymouth,^{1*} Maximilian Titl,¹ Shinjae Nam¹, Lukas Hörmann², Franz J. Giessibl¹

¹ University of Regensburg, Regensburg, Germany

² University of Vienna, Vienna, Austria

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Six-membered carbon rings (C₆ rings) can be found in a multitude of systems from graphite to organic molecules. Graphitic surfaces are so flat that they have been used to explore superlubricity, where one important aspect of their frictional response is the trapping of a single atom in an individual C₆ ring.

While we have previously concentrated on energy dissipation as the tip passes over chemical bonds [1, 2], in this work we concentrate on trapping within one C₆ ring. This trapping also plays a role in the lateral movement of adsorbates on these surfaces. However, studies investigating trapping on these surfaces often focus only on strongly-bound adsorbates.

We experimentally measure the trapping of a weakly-bound single atom asperity using lateral force microscopy with a CO-tip and simulate this system with DFT-based methods. Surprisingly, we observe a uniform lateral spring constant within individual C₆ rings over heights of tens of picometers for a range of systems. To precisely determine the surface trapping, we re-evaluate the lateral spring constant of the CO at the tip apex. With this value, we determined a very weak lateral spring constant of a particle within a C₆ ring.

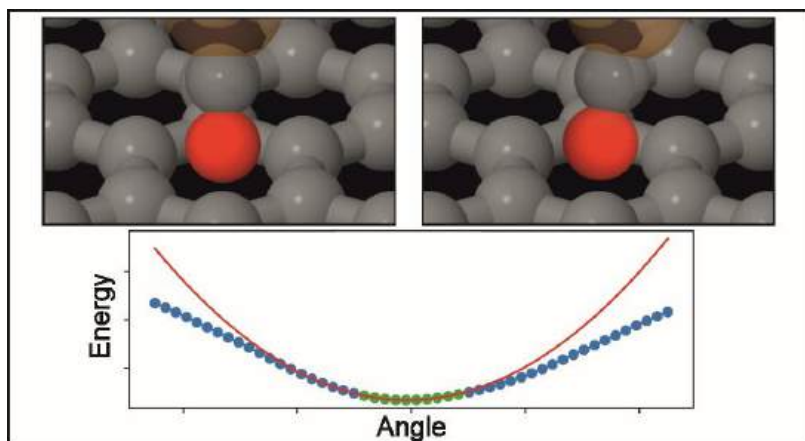


Figure: Above, trapping is measured by lateral force microscopy measurements with a CO tip within a C₆ ring. Below, DFT calculations show that this can be understood by a Hookian model.

- [1] A.J. Weymouth, E. Riegel, O. Gretz and F.J. Giessibl. *Strumming a single chemical bond*. Phys. Rev. Lett. **124**, 196101 (2020)
- [2] S. Nam, L. Hörmann, O. Gretz, O. T. Hofmann, F. J. Giessibl, and A. J. Weymouth. *Sliding friction over individual aromatic bonds correlates with bond order*. Nat. Comm., **17**, 3694 (2026)

Atomic scale energy dissipation over copper oxide studied with lateral force microscopy

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Lateral force microscopy (LFM) can be implemented by rotating the quartz oscillator of a qPlus sensor so that the tip oscillates laterally with respect to the surface [1]. LFM can be performed in frequency-modulation mode, similar to normal-force FM-AFM, in which energy dissipation (E_{diss}), as well as frequency shift (Δf) are recorded. The tip apex can be functionalized with a CO molecule [2], providing an inert and well characterized tip. The enhanced flexibility of this CO tip means it can strum over potential energy barriers. If the CO snaps over such a barrier and energy is dissipated with each oscillation, E_{diss} can be recorded [3].

Here, a partially oxidized Cu(110) with the (2x1)O added row reconstruction is studied with LFM. Lennard-Jones based simulations recreate the data well and aid the understanding of the CO snapping mechanism. DFT-based calculations support the Lennard-Jones parameters and give further insight into the dominant tip-sample interaction.

We propose that the well-defined atomic rows can be used in the future as standards for evaluating friction at the atomic scale. Moreover, measurements of Δf and E_{diss} both show a clear difference between metal and oxygen sites, whereas normal-force FM-AFM measurements with a CO-tip cannot clearly identify the sites [4]. This highlights the potential of LFM for future applications in oxides and ionic crystals.

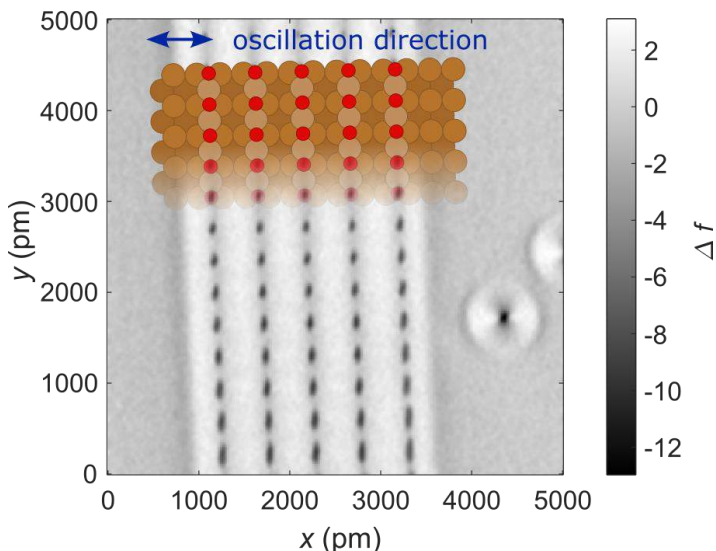


Figure 1: LFM frequency shift (Δf) measurement of partially oxidized Cu(110) in (2x1)O AR-reconstruction. The oscillation direction is indicated, as well as the atomic positions of the surface. A CO molecule is present on the bare Cu(110).

- [1] F. Giessibl et al., Proc. Natl. Acad. **99**, 12006 (2002).
- [2] L. Gross et al., Science **325**, 1110 (2009).
- [3] A.J. Weymouth et al., Phys. Rev. Lett. **124**, 196101 (2020).
- [4] B. Lammers et al., Nanoscale **13**(32), 13617 (2021).

Quantifying Irreversibility (Dissipation) in Single-Molecule Nanomanipulation

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An atomically detailed understanding of friction and dissipation requires submolecular resolution and exceptional control over the molecule-substrate contact. On-surface synthesis offers both: it produces atomically defined covalent chains that can be imaged and lifted individually with cryo-AFM, and it gives access to molecular architectures unavailable in solution chemistry, such as sterically frustrated atropisomers [1]. We have studied polyaromatic CPAA chains on Au(111), in which contiguous monomers adopt parallel or antiparallel arrangements [1]. Cryo-AFM lifting yields a frequency-shift trace whose periodic dips correspond to monomer detachments, with a detachment length systematically shorter than the monomer size. All-atom molecular dynamics with quantum-derived force fields traces this anomaly to tethering of the chain end, distinguishing two peeling regimes, sliding exfoliation and delamination, and validating the analytical model of Silva *et al* for tethered chains.

Additional, we use this same platform to address a complementary question: how much of the lifting process is actually irreversible? The tuning-fork amplitude ($A \approx 0.1$ nm) is an order of magnitude smaller than the monomer size, so each lifting step is sampled by many cantilever cycles. From the per-cycle work integral, computed in simulations that explicitly resolve the tip oscillation, we obtain a dissipation trace in one-to-one correspondence with the experimental Δf signal. The result is striking: most of the lifting is essentially dissipationless, and irreversibility is sharply concentrated in a small alphabet of elementary events (monomer detachments, semi-redepositions, and slips of the still-adsorbed segment), resolved through two reaction coordinates tracking the free (head) and tethered (tail) ends of the chain. Cryo-AFM thus emerges as a quantitative probe of irreversibility at the single-molecule level, with direct bearing on friction and adhesion at the nanoscale.

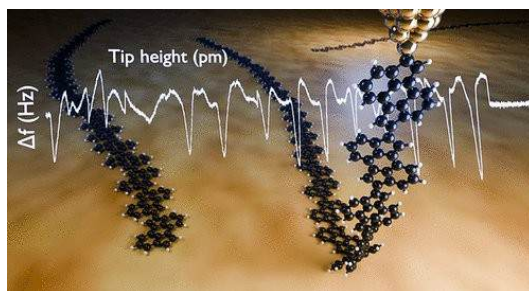


Figure 1: Cryo-AFM lifting of a single CPAA polymer on Au(111) with the overlaid Δf trace (white). Most of the lifting is dissipationless; irreversibility is concentrated in discrete monomer-scale events. Adapted from Ref. [1].

[1] P. D'Astolfo, J. G. Vilhena et al., ACS Nano **19**, 13805 (2025).

Interplay of Backbone Rigidity and Side-Group Flexibility in One-Dimensional Structural Superlubricity

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National Center for Nanoscience and Technology, Beijing, China

*liumx@nanoctr.cn

Structural superlubricity emerges at incommensurate interfaces, where lateral forces cancel collectively across the contact and suppress static friction. In finite systems, however, this cancellation becomes incomplete at the boundaries, leaving residual friction dominated primarily by edge contributions. As the dimensionality is reduced from 2D to 1D systems, edge effects become increasingly important because the boundaries constitute a dominant fraction of the entire interface. Theoretical studies predict several competing frictional regimes depending on the interplay among structural rigidity, interfacial commensurability, and molecular flexibility. In rigid graphene nanoribbons adsorbed on metal surfaces, superlubricity originates from the preservation of long-range incommensurability enabled by the stiff π -conjugated backbone and weak vdW interaction with the substrate.^[1] In contrast, flexible polymer chains may locally adapt to substrate corrugation, potentially destroying collective force cancellation. Nevertheless, recent experiments revealed a distinct regime of flexible superlubricity, in which sidewinding molecular motion reduces diffusion barriers through conformational adaptation, local strain redistribution, and the generation of transient metastable configurations.^[2] These studies suggest that molecular flexibility may either destabilize or promote superlubricity depending on how elastic relaxation couples to interfacial pinning.

Here, we investigate this intermediate regime using dimethyl ladder phenylene (DM-LP) nanoribbons, which combine a rigid backbone with flexible methyl side groups. DM-LP nanoribbons adsorbed on Au(111) are vertically lifted and laterally manipulated while recording the frequency-shift signal using nc-AFM. By systematically varying the lifting height, we construct two-dimensional $\Delta f(x,z)$ maps that directly visualize the evolution of the sliding process under partial suspension conditions. The lateral friction response exhibits weak dependence on the adsorbed ribbon length, indicating suppression of collective interfacial pinning and providing a characteristic signature of structural superlubricity. Our analysis further suggests that the flexible methyl groups near the dynamic contact edge dominate the local stick-slip instability, whereas interactions from methyl groups within the adsorbed interior are largely compensated through collective force cancellation. These results reveal a hybrid superlubric regime in which long-range incommensurate sliding is preserved by the rigid molecular backbone while local adaptive depinning is mediated by flexible side groups, establishing molecular nanoribbons as a model system bridging rigid structural superlubricity and flexible conformational lubricity.

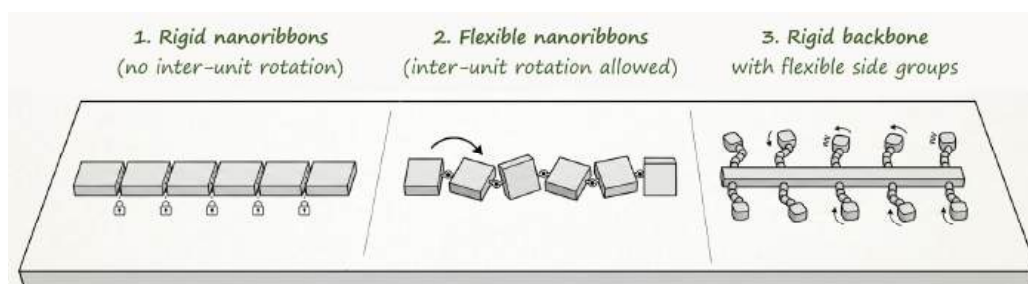


Figure 1: Schematics illustrating three cases of one-dimensional structural superlubricity.

[1] S. Kawai, et al. Science **351**, 6296 (2016)

[2] J. G. Vilhena, et al. Phys. Rev. Lett. **351**, 216102 (2022)

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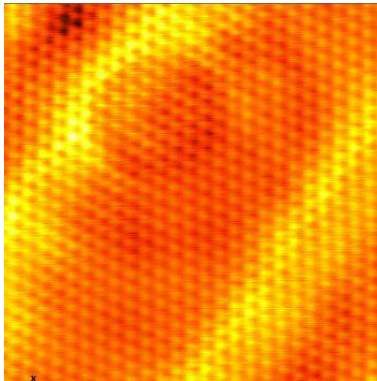
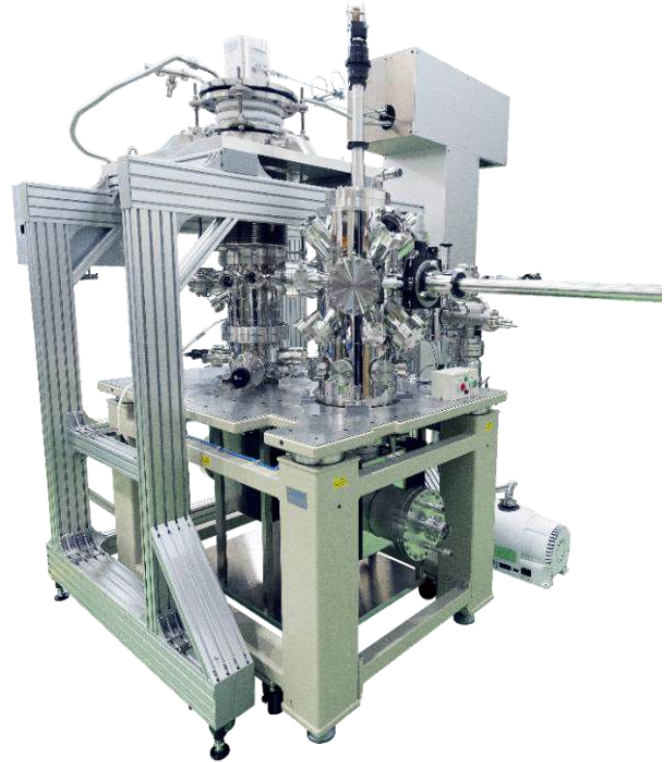
USM1500 2K & affordable magnets

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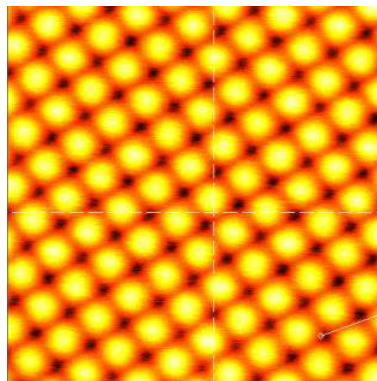
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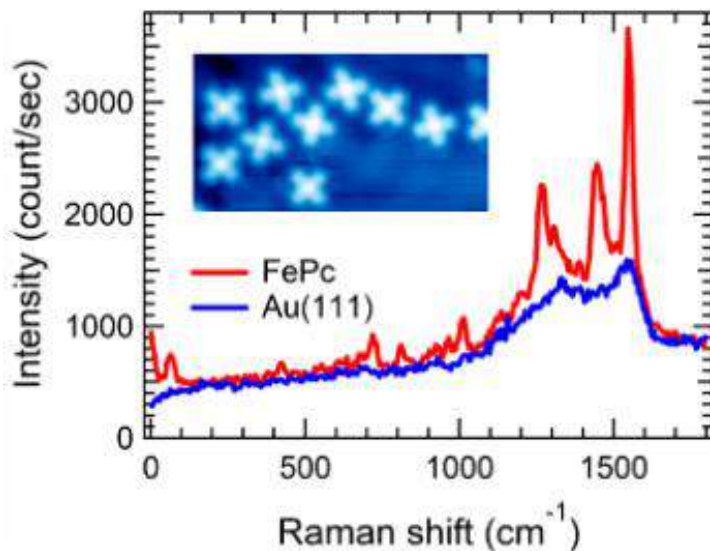
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Friday August 7th, 2026

Theory and Machine Learning 2

Chair **Prokop Hapala**

- 9:00 **Mong-Wen Gu**, Configuration monitoring of a molecular junction and its applications
- 9:20 **Orlando Jose Silveira Junior**, Automated structure discovery for Tip Enhanced Raman Spectroscopy
- 9:40 **Ondrej Krejci**, Accelerating Atomic Configuration Identification on Reconstructed Surfaces with Machine Learning
- 10:00 **Martin Ondráček**, Atomic-scale Kelvin probe force microscopy on Ho atoms on the MgO surface

Configuration monitoring of a molecular junction and its applications

Joshua Scheidt,¹ Jonas Lederer,² **Mong-Wen Gu**,¹ Hadi Arefi,¹ Jose M. Guevara,¹ Amin Karimi,¹ Rustem Bolat,¹ Marvin Knol,¹ Klaus-Robert Müller,² F. Stefan Tautz,¹ and Christian Wagner^{1,*}

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² Institut für Softwaretechnik und Theoretische Informatik, Technische Universität Berlin, *Berlin, Germany*

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Understanding the structure-property relationships of nanoscale structure is essential to developing molecular devices. The scanning probe microscope (SPM) enables molecules to be manipulated with nanoscale precision, however, accessing the real-time configuration of a metal-molecule-metal junction remains challenging. Here, we present an experimental protocol for manipulating a single PTCDA (3,4,9,10-perylene tetracarboxylic dianhydride) molecule on Ag(111) by using NC-AFM/STM. We compare one of the monitored observables, the force gradient, with a DFT-trained machine learning model [1] and obtain a sequence of molecular configurations by solving an inverse problem via search through configuration space. We explore the correlation between the junction configurations and the current passing through the molecule. Then, we employ this approach to analyze the process of vertically manipulating a single PTCDA molecule and to investigate the impact of the junction configuration on abrupt changes in junction conductance. Furthermore, this approach also provides insights into leveraging the junction configuration for the fabrication of artificial nanostructures.

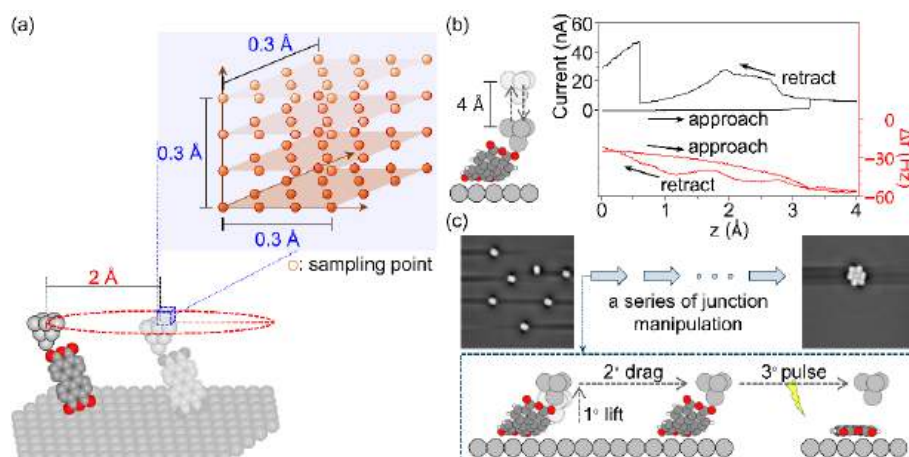


Figure: (a) The illustration of the experimental protocol for manipulating a molecular junction to move along alternating cube (blue) and circular (red) trajectories. The simultaneously recorded tunnelling current and frequency-shift serve as the fingerprint to reconstruct the junction configuration. (b-c) Applications of the protocol in (b) the analysis of a vertical manipulation process and (c) the fabrication of artificial nanostructures.

[1] J. Scheidt et al., J. Phys. Chem. C **127**, 13817 (2023).

Automated structure discovery for Tip Enhanced Raman Spectroscopy

Harshit Sethi,¹ Markus Junttila,¹ Orlando J. Silveira,¹ and Adam S. Foster^{1,2}

¹Department of Applied Physics, Aalto University, Espoo, 02150, Finland

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Presenting author's e-mail: harshit.sethi@aalto.fi

Tip-Enhanced Raman Spectroscopy (TERS) provides nanoscale chemical fingerprints alongside high-resolution topographic mapping of molecules, offering a powerful tool for materials discovery [1]. However, TERS images are challenging to interpret and typically demand time-consuming, computationally intensive quantum-chemistry calculations [2]. To overcome this problem, we present an encoder-decoder model trained and evaluated on simulated TERS images of molecules [3]. Our approach demonstrates high accuracy for molecular structure and chemical identification from simulated TERS images. These findings provide a foundation for extending machine learning methods to experimental TERS datasets, potentially accelerating molecular discovery by integrating nanoscale spectroscopy with automated computational analysis.

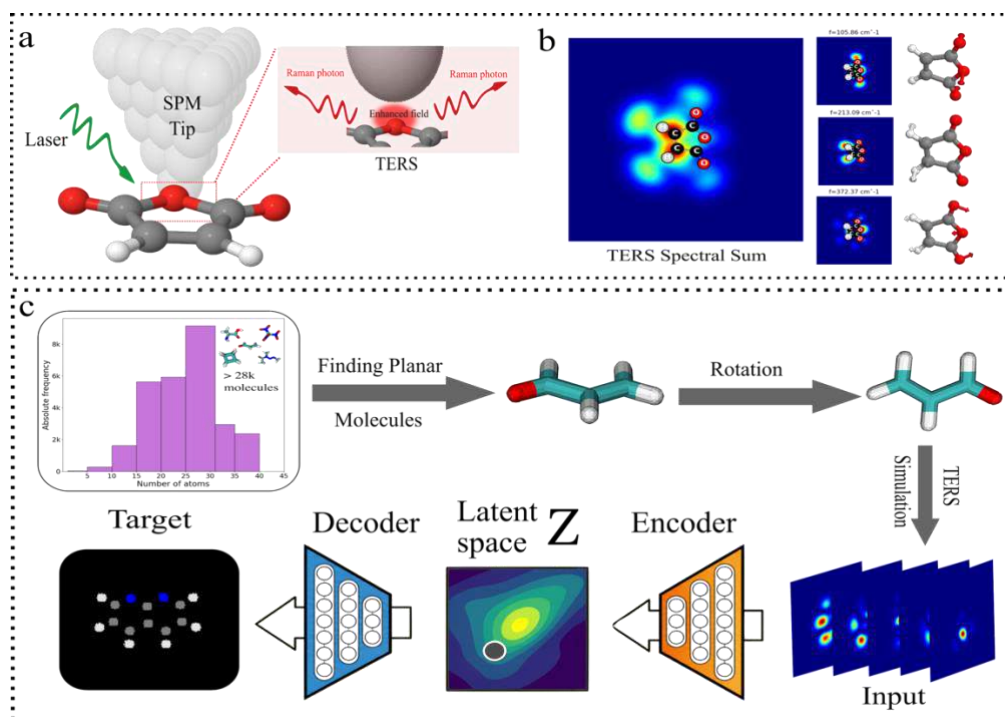


Figure: (a) Schematic representation of a tip-enhanced Raman spectroscopy (TERS) setup. (b) Schematic depiction of molecular vibrational modes probed in TERS. (c) Machine learning workflow for structure and chemical property prediction using TERS image data.

Reference

- [1] T. Itoh et al. Chemical Reviews, 123(4):1552–1634, 2023.
- [2] Y. Zhang, et al. Journal of Raman Spectroscopy, 52(2), 296–309, 2020.
- [3] H. Sethi et al., arXiv:2602.19932, 2026.

Accelerating Atomic Configuration Identification on Reconstructed Surfaces with Machine Learning

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Nc-AFM has played a crucial role of revealing of atomic structure of molecules, for example asphaltenes [1], as well as reconstructed surfaces, like calcite [2] or silver iodide [3]. Recent advances in theory and computation have enabled substantial progress in the automated identification of molecular structures from nc-AFM data. These include usage of convolutional neural networks [4] or machine-learned interatomic potentials (MLIPs) [5]. In contrast, comparatively limited progress has been made in the automation of the identification of surface reconstructions using nc-AFM and computational modeling.

In this work, I will introduce my current work on building automatized workflow for predicted surface reconstructions: Starting from automatized tool for passivation of bottom side to reinforcement learning agent able to build few top layers of reconstructed surface, enhancing the original strategy by [6]. To speed-up and computationally cheapen the workflow, I will be employing already pre-trained ML interatomic potentials, like MACE-MP [7], and fine-tuning it for surface applications. Finally, the workflow is using Probe-Particle Model [8] based simulations for comparison with experiment, as illustrated in Figure 1.

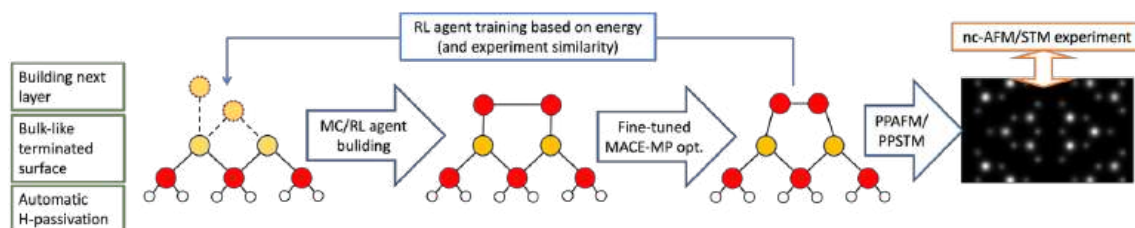


Figure 1: The automatized workflow is using building final layer(s) of the surface reconstruction using Monte Carlo sampling (MC) or reinforcement learning (RL) agent for placing atoms to the new layer. Fine-tuned MLIP, like MACE-MP, will be used for intermediate optimizations and final energy estimation for training of the RL agent and selection of candidates. The most promising once will be then calculated on full density functional theory level and their PPAFM or PPSMT simulations will be compared with SPM experiments.

- [1] B. Schuler et al., J. Am. Chem. Soc. **137**, 9870 (2015).
- [2] J. Heggemann et. al., J. Phys. Chem. Lett. **14**, 1983 (2023).
- [3] Johanna I. Hütner et al., Sci. Adv. **11**, eaea2378 (2025).
- [4] B. Alldritt et al., Sci. Adv. **6**, eaay6913 (2020).
- [5] M. G. Lastre et al., arXiv:2601.18852v2 (2026).
- [6] X. Du et al., Nat. Comput. Sci **3**, 1034 (2023).
- [7] I. Batalia et al. J. Chem. Phys **163**, 184110 (2025).
- [8] N. Oinonen et al. Comput. Phys. Commun. **305**, 109341 (2024)

Atomic-scale Kelvin probe force microscopy on Ho atoms on the MgO surface.

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Although Kelvin probe force (KPFM) microscopy enables imaging of charge states and distributions at the atomic level, determining the sign and magnitude of the charge of the investigated entity remains problematic.

We have performed KPFM measurements on individual Ho atoms on oxygen and in the bridge position on a thin MgO layer grown on Ag(100) surface, which show a different local contact potential difference (LCPD) curve as the tip approaches than measurements on the MgO surface, suggesting a different sign of charge on the Ho atoms.

However, in both cases, both chemical intuition and DFT calculations indicate that the Ho atoms are positively charged due to charge transfer from Ho to the substrate. We show that this apparent discrepancy in the LCPD curves can be attributed to the combined effects of Ho atom charges and polarizabilities in interaction with the KPFM probe. (See [1] for the theoretical description of the two KPFM components related to static charge and polarizability.)

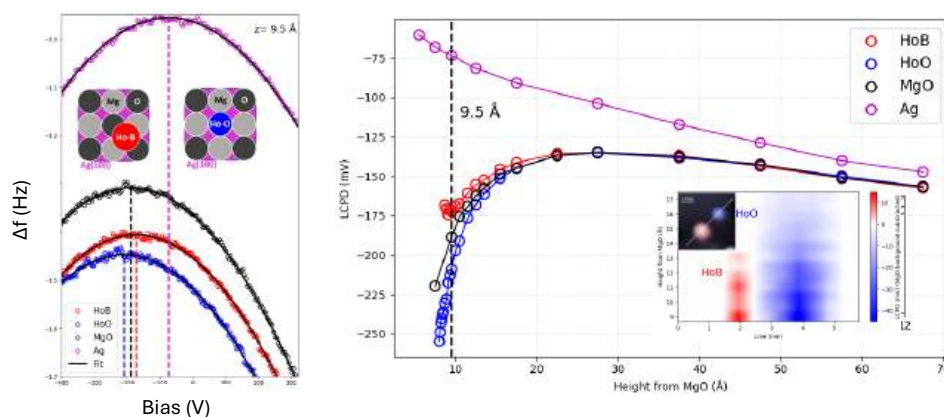


Figure 1: KPFM on Ho/MgO/Ag(100) comparing LCPD over oxygen-site Ho atom, bridge-site Ho atom and LCPD away from Ho.

[1] B. Mallada *et al.*, Science **374**, 863 (2021).

Friday August 7th, 2026

Mineral and Oxides Surfaces

Chair **Franz Giessibl**

- 11:00 **Ruben Perez**, Atomic-scale reactivity of the $\text{CeO}_2(100)$ surface reconstructions by scanning probe microscopy
- 11:20 **Tobias Dickbreder**, K-feldspar microcline (001): Atomic structure of nanoscopic feldspar islands
- 11:40 **Sarah Tobisch**, Cooperative CO_2 adsorption on In_2O_3
- 12:00 **Ulrike Diebold**, Mineral Surfaces– Opportunities and Challenges for ncAFM
- 12:20 **Closing Remarks**

Atomic-scale reactivity of the CeO₂(100) surface reconstructions by scanning probe microscopy

Rubén Pérez,^{1,2,*} Manuel González Lastre,^{1,2} Kyungmin Kim,³ Estefanía Fernández-Villanueva,^{1,4,5} Pablo Pou,^{1,2} Hossein Sepehri-Amin,⁶ Masayuki Abe,³ Shigeki Kawai,⁶ M. Verónica Ganduglia-Pirovano,⁴ Oscar Custance⁶

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⁴ Instituto de Catálisis y Petroleoquímica (CSIC), 28049 Madrid, Spain

⁵ Universitat Politècnica de València, Camí de Vera s/n, 46022 València, Spain

⁶ National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba, 305-0047, Japan

*Corresponding authors: ruben.perez@uam.es

Cerium dioxide (CeO₂) is a benchmark redox catalyst. While the CeO₂(111) surface has been extensively studied, the polar CeO₂(100) facet remains less understood due to its intrinsic instability that leads to complex reconstructions [1, 2]. Building on recent STM/AFM studies showing that site-specific force spectroscopy can reveal local reactivity, defects, and adsorbates on CeO₂(111), including Ce³⁺ sites identified through individual water molecules [3], we apply this combined experimental-theoretical approach to reconstructed CeO₂(100) thin films grown on Cu(111). Using oxygen-terminated probes at 4.8 K, we provide a direct atomic-scale assignment of the two dominant CeO₂(100) reconstructions: the CeO₄-pyramid-terminated CeO₄-t(100) p(2×2) phase and the oxygen-terminated O-t(100) c(2×2) phase. Constant-height AFM imaging and site-specific Δf(z) spectroscopy reveal the exposed atomic species beyond the periodic information accessible by STM alone. On CeO₄-t(100), both cerium and oxygen sites are resolved, whereas on O-t(100) the contrast is assigned to top-layer oxygen atoms. In parallel, simulated STM images show that STM contrast alone is not a reliable fingerprint of the local reduction state, since oxidized and reduced CeO₄-t(100) surfaces, as well as different Ce³⁺ distributions in O-t(100), can produce very similar apparent corrugations. Finally, we observe anomalous features on CeO₄-t(100), characterized by an asymmetric single-lobed AFM contrast and a distinct force response. These signatures are inconsistent with a pristine lattice configuration and are compatible with an adsorbate-induced perturbation. Overall, this work establishes combined STM/AFM imaging, force spectroscopy, and first-principles simulations as a robust framework to connect surface reconstruction, local chemical interaction, and adsorbate sensitivity on polar wide-band-gap oxide surfaces.

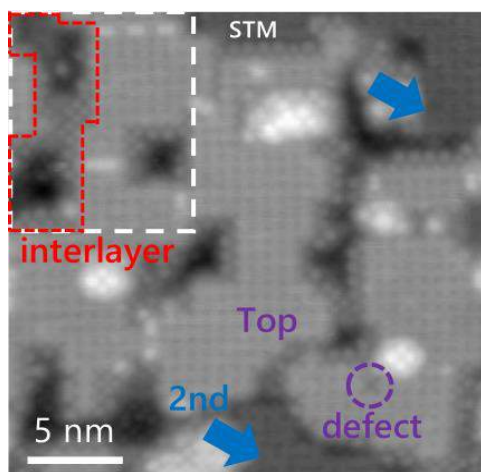


Figure 1: Topographic STM image of the top and second terraces of the island showing the predominance of the CeO₄-t(100) reconstruction.

[1] O. Stetsovych et al., Appl. Surf. Sci. 285, **766** (2013).

[2] Y. Pan et al., Adv. Mater. Interfaces 1, **1400404** (2014).

[3] O. Custance et al., Commun. Mater. 7, **39** (2026).

K-feldspar microcline (001): Atomic structure of nanoscopic feldspar islands

Tobias Dickbreder,^{1,*} Franziska Sabath,² Florian Schneider,² Uwe Güth,³ Adam S. Foster,^{4,5} Ralf Bechstein,² Angelika Kühnle²

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² Physical Chemistry I, Faculty of Chemistry, Bielefeld University, 33615 Bielefeld, Germany

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As the most abundant rock-forming minerals in Earth's crust, feldspar minerals play an important role in a variety of environmental processes such as silicate weathering and ice nucleation in mixed-phase clouds. Since many of these processes take place at the feldspar surface, an in-depth understanding requires elucidating the micro- and nanoscopic surface topology. However, especially in the field of ice nucleation on feldspar surfaces, most experimental studies are limited to the micrometer scale, while insights on the nanometer scale are still sparse. The latter are of importance especially in the view of identifying active sites for ice nucleation.

Here, we report on an intrinsic island structure observed on K-feldspar microcline (001). High-resolution atomic force microscopy (AFM) images taken in ultra-high vacuum show nanometer-sized islands on the terraces and at the step edges [1]. Atomic scale images on the islands reveal an atomic contrast and lattice parameters consistent with the hydroxyl terminated surface structure previously observed on the microcline (001) terrace [2], suggesting that the islands are an intrinsic feature of the microcline surface. This hypothesis is corroborated by the atomic structure revealed by AFM images taken at the microcline-water interface. Furthermore, solid-liquid AFM demonstrates that the observed nanostructure is stable in water on the timescale of our experiments. As the existence of islands significantly increases the density of edge and kink sites, the observed nanostructure might have important implications for surface reactivity and potentially ice nucleation efficiency.

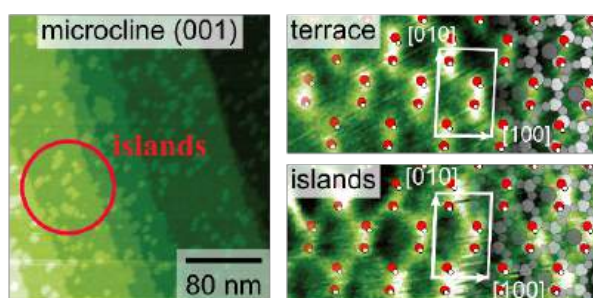


Figure 1: left: Overview image of a microcline (001) sample covered with islands. Right: High resolution NCAFM images of the atomic structure on the terraces (top) and islands (bottom). All images were taken on a cleaved microcline sample kept under UHV conditions at 305 K. Adapted from [1,2].

[1] T. Dickbreder, F. Sabath, F. Schneider, U. Güth, R. Bechstein, A. Kühnle, PCCP, **27**, 23574 (2025).

[2] T. Dickbreder, F. Sabath, B. Reischl, R. Nilsson, A. Foster, R. Bechstein, A. Kühnle, Nanoscale, **16**, 3462 (2024).

Cooperative CO₂ adsorption on In₂O₃

Sarah Tobisch,^{1,*} Andreas Ziegler,² Marco Knapp,¹ Sarah Horak,¹ Hao Chen,¹ Matthias Blatnik,¹ Michele Riva,¹ Jiri Pavelec,¹ Michael Schmid,¹ Gareth Parkinson,¹ Ulrike Diebold,¹ Bernd Meyer,² Margareta Wagner,¹

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² Interdisciplinary Center for Molecular Materials (ICMM) and Computer Chemistry Center (CCC), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Germany

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CO₂ reduction to methanol is a promising pathway towards a more sustainable and circular economy, converting CO₂ into valuable fuels and feedstock for the chemical industry. In₂O₃ has been identified as a promising catalyst material with high selectivity towards methanol [1].

In this work, the adsorption of CO₂ molecules was studied on three different In₂O₃(111) surfaces with non-contact atomic force microscopy (nc-AFM): the stoichiometric, the reduced [2] and the hydroxilated surface [3]. Strong cooperative effects were observed for the adsorption of CO₂ on In₂O₃(111) by probing multiple adsorption configurations and studying individual molecule-substrate and molecule-molecule interactions via density functional theory (DFT). The CO₂ adsorption configurations were probed for different temperatures with atomic precision using nc-AFM and show excellent agreement with theoretical predictions. Contrast inversion in nc-AFM makes it possible to distinguish different geometric orientations of physisorbed CO₂ as well as chemisorbed carbonate species. Out of the twelve molecules that fit within the unit cell, only two were identified to adsorb as carbonates, leading to a breaking of the three-fold symmetry of the surface.

In comparison, the In adatoms of the reduced surface are partially displaced by the CO₂ molecules but show similar features to the stoichiometric case, whereas CO₂ blocks adsorption sites on the hydroxilated surface with no long-range order.

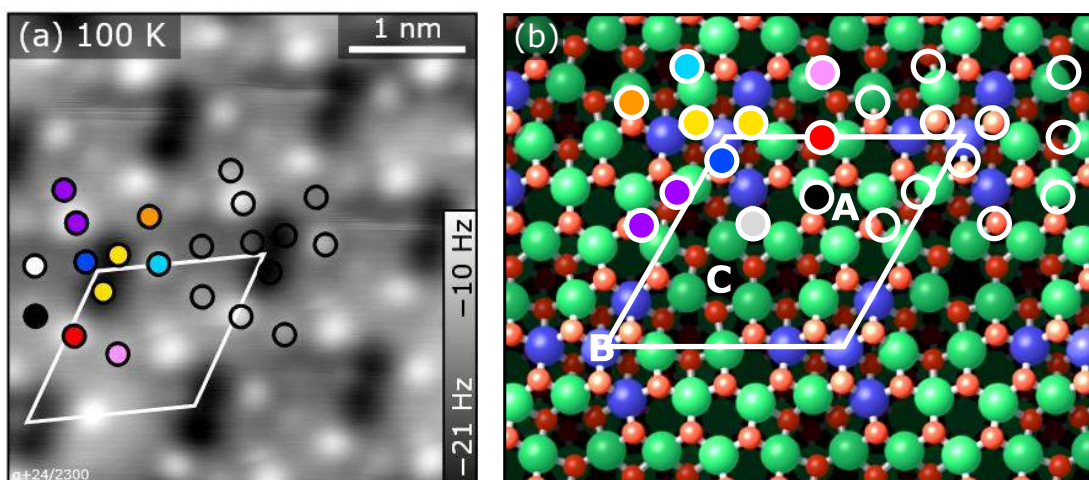


Figure 1: (a) CO₂ adsorption configuration observed at 100 K. 11 CO₂ species, two of which form carbonates (yellow), breaking the threefold symmetry of the surface. (b) Adsorption sites with respect to the In₂O₃(111) unit cell.

- [1] O. Martin et al., Angew. Chem. **128**, 6369–6373. (2016)
- [2] M. Wagner et al., Adv. Mater. Interfaces, **1**, 1400289 (2014).
- [3] H. Chen et al., ACS Nano. **16**, 21163–21173, (2022)

Mineral Surfaces – Opportunities and Challenges for ncAFM

Ulrike Diebold,^{1*} Andrea Conti,¹ Luca Lezuo,¹ Johanna I. Hütner-Reisch,¹ David Kugler,¹ Florian Mittendorfer,¹ Jan Balajka,¹ Giada Franceschi,¹ Michael Schmid,¹ Rainer Abart²

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² Department of Lithospheric Research, University of Vienna, Austria

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With its capability to provide atomically resolved images of highly insulating surfaces [1, 2], ncAFM opens new research avenues. The investigation of minerals is particularly interesting; they are all around us in the Earth's crust, and their surfaces regulate many natural and technological processes. Yet, at the fundamental, atomic scale, little is known about the surface structure of these materials and how they interact with abundant molecules.

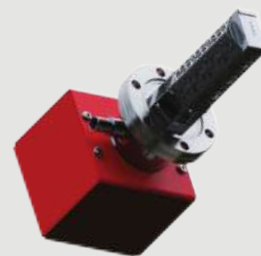
In the talk, we will discuss recent results on the aluminosilicate feldspar microcline [3, 4] and the calcium silicate wollastonite surface [5, 6]. We will discuss experimental challenges, such as sample charging, optimal tip termination, and the limited information available in constant-height imaging, and we will highlight opportunities to broaden the scope of ncAFM research across other research communities.

- [1] J. I. Hütner, et al., *Science*, **385**, 1241 (2024).
- [2] G. Franceschi, et al., *Nature Commun.*, **14**, 208 (2023).
- [3] G. Franceschi, et al., *J. Chem. Phys.*, **160**, 164312 (2024)
- [4] G. Franceschi, et al., *J. Phys. Chem. Lett.*, **15**, 15 (2024)
- [5] L. Lezuo, et al., *Nanoscale*, accepted doi:10.1039/d6nr01063f
- [6] A. Conti, et al., *ACS Nano*, **20**, 10456 (13) (2026)

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8 Posters

Poster Session A

Candidates for the Student Poster Award

- P1 **Yukun Zhang**, Beyond Imaging: Atomic-resolution Scanning Probe Microscopy Uncovers Nanometer-scale Substrate-mediated Interactions in CO/Cu(111)
- P3 **Walburga Freyja Bischofberger**, Annealing-Induced Morphological and Photophysical Changes of PTCDA on NaCl/Ag(111)
- P5 **Antonia Köhler**, Implementation of a Setup for Three-Dimensional Atomic Force Microscopy under Electrochemical Conditions
- P7 **Mona Mona**, Atomic-Scale Identification of Surface Reconstructions on LaAlO₃ (001) and (111)
- P9 **Sreehari Sreekumar**, Temperature and Electric Field Dependent Migration of Polarons in Hematite Fe₂O₃
- P11 **Hsiang-Ling Chuang**, Hadamard-Enhanced AFM Imaging of Ligand-Triggered Membrane Raft Dynamics in Live MCF-7 Cells
- P13 **Henry Rodriguez**, Force to Spin a Molecular Rotor
- P15 **Nazanin Poursheikhali**, Atomic scale characterization of the reconstructed anatase TiO₂(001) surface using non-contact atomic force microscopy
- P17 **Sandhya Anchamkudy**, SQDM Investigation of Orientation-Dependent Electrostatics in Single PTCDA Molecules
- P19 **Lisanne Sellies**, Excited-state spectroscopy of individual molecules by means of atomic force microscopy
- P21 **Benjamin Scheffel**, Exploring the Binding Configurations of Functional 3D Molecules Chemisorbed on Si(100)
- P23 **Fabian Schulz**, Characterization of interfacial charge transfer between graphene nanoribbons and a 2D ferromagnet by STM/ncAFM
- P25 **Zuned Ahmed**, Playing 'Hide & Seek' at Atomic-scale
- P27 **Yasuo Cho**, Non-Contact Writing and Reading in Ultra-High Density Ferroelectric HDD Based on NC-SNDM

- P29 **Franz J. Giessibl**, A Commercial Version of Orpheus II Using Si Cantilevers and qPlus Sensors
- P31 **Qitang Fan**, Intercalation-based decoupling method for graphene nanoribbons on metal surfaces
- P33 **David Kugler**, Atomically Resolved Imaging of Crystal and Adsorbed Water on Gypsum (010) Surface
- P35 **Aji Alexander**, Investigating the growth mechanism of KBr on glass by nc-AFM.
- P37 **Ing-Shouh Hwang**, Comparative Study of Alkane Derived and Gas Hydrate Stripe Structures on HOPG
- P39 **Alice Kern**, Surface Structure of $\text{Cu}_2\text{O}(110)$
- P41 **Olga Artemyeva**, Chemical reactivity of Pd (111) surface
- P43 **Fabian Stilp**, Ring Features of Single Adatoms Investigated with a CO Tip
- P45 **Callum Hayward**, On the origin of divergences in quantitative lateral force recovery in bimodal NC-AFM
- P47 **Ryota Fukuzawa**, AC voltage measurement in atomic force microscope potentiometry
- P49 **Jonathan Hein**, On-Surface Synthesis of Kagome Metal-Organic Frameworks
- P51 **Christoph S. Setescak**, High Resolution Imaging of KBr with CO Functionalized Tips
- P53 **Rick Kort**, Understanding how Electrochemical Atomic Force Microscopy Can Reveal the Potential of Zero Charge
- P55 **Himani Malik**, Towards the Largest Starphene: [22]Starphene
- P57 **Milan Koci**, Fast SPM simulation with complex molecular attachment
- P59 **Johanna Schnorrenberg**, Automatic tip functionalization with CO on Ag(111) using machine learning
- P61 **Philipp Rahe**, Upcycling a commercial scan controller for scanning probe microscopy with the GXSM4 OpenSource system
- P63 **Gilbert Lamtecson Pado**, Noncontact AFM Potentiometry for Nanoscale Potential Imaging via Distance-Derivative Capacitance Analysis

- P65 **Thilo Glatzel**, Kelvin Probe Force Microscopy of Mixed Monolayer Doping of Silicon
- P67 **Toyoko Arai**, Challenge toward high-resolution infrared spectroscopy based on frequency modulation AFM
- P69 **Yuta Okabe**, Spectral response of a tuning-fork sensor to a pulsed infrared irradiation detected via a dissipation channel of FM-AFM

Beyond Imaging: Atomic-resolution Scanning Probe Microscopy Uncovers Nanometer-scale Substrate-mediated Interactions in CO/Cu(111)

Pengcheng Chen,¹ Dingxin Fan,¹ **Yukun Zhang**,^{1,2} Nan Yao^{1,*}

¹ Princeton Materials Institute, Princeton University, Princeton, New Jersey 08540, USA

² Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA

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Recent advances in scanning probe microscopy (SPM) have enabled the direct, real-space visualization of adsorbates at atomic resolution [1]. Here we show that, beyond structural imaging, such capability allows fundamental surface physics to be uncovered through statistical analysis of real-space distributions [2].

Using combined STM/AFM measurements of CO adsorption on Cu(111), we analyze over 3,400 atomic-resolution images and identify an anomalous saturation coverage of ~26%, significantly below the expected 33% for the canonical $\sqrt{3} \times \sqrt{3}/R30^\circ$ structure [3]. This saturation limit is robust across a wide range of temperatures and dosing conditions, indicating an intrinsic thermodynamic origin rather than kinetic effects.

Statistical analysis reveals that each CO molecule influences adsorption within a radius of ~5.3 nm, far exceeding the length scale of chemical bonding and nearest-neighbor interactions. This nanometer-scale interaction leads to spatial correlations that suppress further adsorption and impose a collective self-limiting density. Density functional theory calculations show that this behavior arises from substrate-mediated electronic and elastic interactions, which progressively weaken CO binding with increasing coverage.

These results demonstrate that atomic-resolution SPM can serve as a quantitative probe of emergent, long-range interactions at surfaces, enabling direct access to fundamental collective interactions at surfaces.

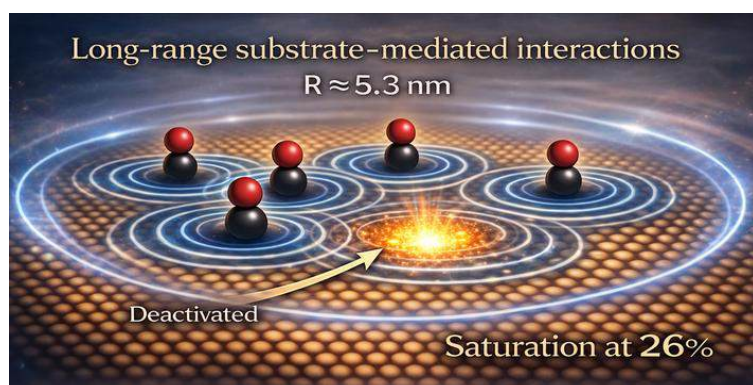


Figure 1: Long-range interaction-induced surface deactivation behind the 26% saturation limit of CO on Cu(111).

[1] D. Fan, Y. Zhang, Z. Tang, J. R. Chelikowsky, and N. Yao. *J. Chem. Phys.* **164**, 021002 (2026).

[2] P. Chen, D. Fan, A. Selloni, J. Fan, and N. Yao. *J. Am. Chem. Soc.* **148**, 1, 360-367 (2026).

[3] J. Kessler and F. Thieme, *Surf. Sci.* **67**, 405-415 (1977).

Annealing-Induced Morphological and Photophysical Changes of PTCDA on NaCl/Ag(111)

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Organic molecular thin films on insulating surfaces provide an ideal platform for disentangling the interplay between nanoscale structures and excited-state dynamics, which is central to the design of future optoelectronic devices. Perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA) is a prototypical π -conjugated organic semiconductor whose optical response is highly sensitive to intermolecular packing and molecule-substrate interactions [1,2]. When adsorbed on NaCl films grown on Ag, the electronic decoupling from the metallic substrate enables direct access to intrinsic photophysical properties.

Here, we report on the temperature-driven evolution of submonolayer and monolayer PTCDA films on NaCl/Ag surfaces. Using a combination of atomic force microscopy (AFM), photoluminescence (PL) spectroscopy, and time-correlated single photon counting (TCSPC), we investigated how controlled annealing between 78 and 323 K modifies molecular ordering, surface morphology, as well as fluorescence behaviour. Through analysis of topographic images, emission spectra, and decay times, we reveal coverage-dependent thermally activated reorganisation processes, accompanied by distinct changes in spectral shape, and exciton lifetimes (Figure 1). While submonolayer films are dominated by more weakly interacting molecular species, monolayer films exhibit stronger collective effects. These results demonstrate that thermal annealing can be used to steer structural rearrangement and tune the optical functionality of organic adsorbate layers on insulating surfaces.

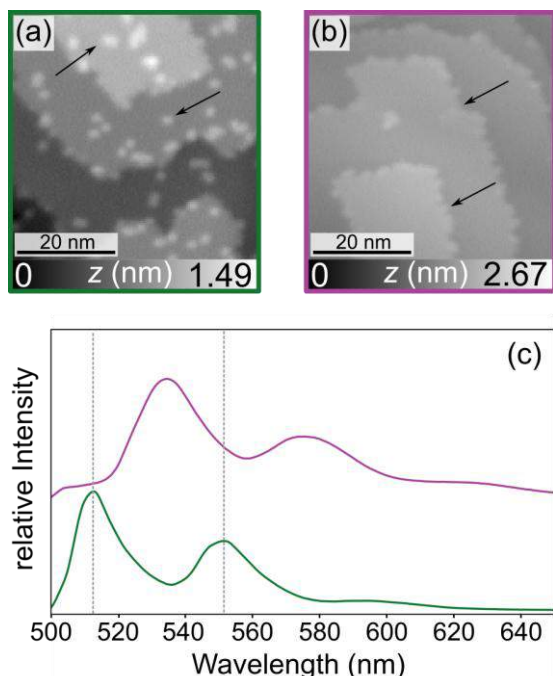


Figure 1: AFM images of the temperature-induced redistribution of PTCDA molecules on NaCl/Ag and respective PL spectra – submonolayer coverage. Arrows indicating PTCDA molecules. (a) PTCDA deposited on NaCl/Ag at 78 K, showing a dispersed molecular distribution. (b) PTCDA after post-annealing to 270 K, showing pronounced accumulation at step edges. (c) PL spectra of PTCDA deposited at 78 K (green) and PTCDA post-annealed at 270 K (purple).

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Implementation of a Setup for Three-Dimensional Atomic Force Microscopy under Electrochemical Conditions

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Electrochemical processes are of importance in a wide range of fields such as energy storage, sensors and electrocatalysis. However, many fundamental processes at the electrode-electrolyte interface are still poorly understood [1]. It is widely known that the presence of an applied electric field has a significant influence on the structure at the interface, including the hydration structure [2, 3]. In this context, the Au(111)-water interface constitutes a prototypical model system as gold is believed to be a relatively inert and well-characterized sample material. So far, however, little is known about the hydration structure at the Au(111)-water interface at the molecular level. Here, we present the implementation of a setup for three-dimensional atomic force microscopy under electrochemical conditions. For this, the original AFM is further equipped with a three-electrode setup. A gold wire serves as the counter electrode and a palladium wire, charged with hydrogen, as the reference electrode. All three electrodes (including the gold crystal acting as the working electrode) are connected to a potentiostat. With this instrument, we are able to control the surface potential of the working electrode. Here, we show the technical implementation of such a setup for an existing AFM, and our first proof-of-principle measurements to demonstrate the feasibility of our system.

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Atomic-Scale Identification of Surface Reconstructions on LaAlO_3 (001) and (111)

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Lanthanum aluminate (LaAlO_3 , LAO) is an insulating perovskite oxide widely used as a substrate for the growth of functional oxide thin films. It combines a relatively high dielectric constant with a wide band gap, making it a versatile dielectric material [1]. In addition, its small pseudo-cubic lattice constant makes LAO an important template for strain engineering in perovskite oxides. Because LAO is intrinsically polar, its surface structure plays a critical role in determining electrostatic boundary conditions that can influence the growth and properties of epitaxial films. However, achieving and maintaining well-defined surface terminations is challenging and atomic-scale investigations of reconstructed LAO surfaces remain incomplete [2,3]. In this contribution, we aim to address a systematic investigation of surface terminations on LAO (001) and (111) surfaces prepared under different sample preparation conditions (temperature range 800-1200°C). Atomic-scale imaging of the reconstructed surfaces is achieved using qplus noncontact atomic force microscopy (nc-AFM) under cryogenic ultrahigh vacuum conditions. The structural observations are corroborated with low-energy electron diffraction (LEED) and x-ray photoelectron spectroscopy (XPS) studies. This approach enables access to distinct surface reconstructions and their comparative analysis for varying surface stoichiometry.

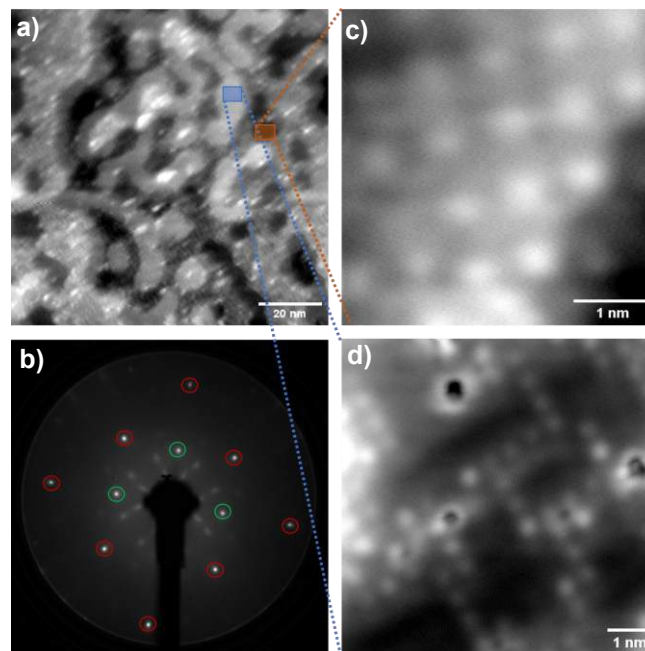


Figure 1: (a) Constant-frequency AFM image of the LAO (001) surface morphology prepared by annealing sample in 10^{-6} mb O_2 upto 1200°C. (b) corresponding LEED pattern (acceleration voltage is 77[eV]). (c, d) Constant-height AFM images of the indicated regions showing atomic-scale structure of two distinct surface terminations.

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Temperature and Electric Field Dependent Migration of Polarons in Hematite Fe_2O_3

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The non-contact atomic force microscopy (nc-AFM) technique has recently enabled precise manipulation of single charges [1,2]. In this work, we exploit this capability to investigate polaron dynamics at the single-quasiparticle limit. Polarons are self-localized charge carriers arising from strong electron-lattice interactions in ionic crystals and they play a central role in determining key material properties, including conductivity, catalytic activity, and emergent phenomena such as high-temperature superconductivity and colossal magnetoresistance [3].

This work presents a methodology for controlled charge injection, localization, and quantification on insulating surfaces, enabling direct investigation of polaron behavior in hematite (Fe_2O_3). Systematic experiments performed under varying tip-sample conditions demonstrate how mobility depends on the local electric field and temperature, establishing a pathway for quantitatively probing polaron transport at the atomic scale.

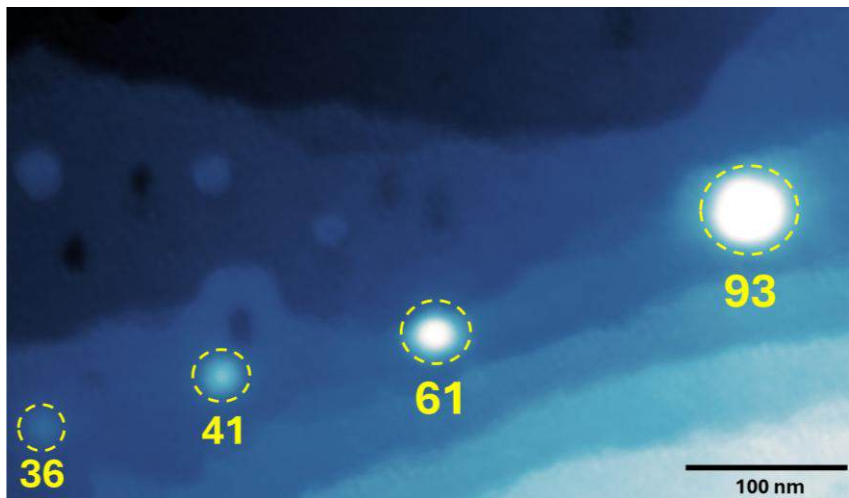


Figure 1: Constant-frequency nc-AFM image showing charge clouds at injection sites, with the injected charge count indicated.

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Hadamard-Enhanced AFM Imaging of Ligand-Triggered Membrane Raft Dynamics in Live MCF-7 Cells

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Membrane rafts are highly dynamic, sterol- and sphingolipid-enriched nanodomains (10–200 nm) that play an essential role in cell signaling by interactions between transmembrane proteins and extracellular ligands. It remains a challenge to observe the membrane rafts due to the required spatiotemporal resolution. This study employs Atomic Force Microscopy (AFM) to investigate the dynamic remodeling of membrane microdomains in live MCF-7 cells stimulated by fibrinogen and resveratrol—ligands for the raft-associated receptor integrin $\alpha\beta_3$ which is embedded in membrane rafts. Herein we implement a Hadamard product-based image processing that effectively suppresses background and amplifies raft-specific features in AFM images. After introducing fibrinogen, the sizes of membrane rafts evolved from 60–380 nm to coalesced into $\sim 1.8\text{-}\mu\text{m}$ features. For resveratrol cases, the features remained isolated and they protruded by ~ 15 nm with a nominal size of ~ 400 nm. The observed dynamics and biological pathways of stimulation are consistent with established theoretical models. The study offers a new way to visualize signaling cascades and decipher the biochemical and cellular functions.

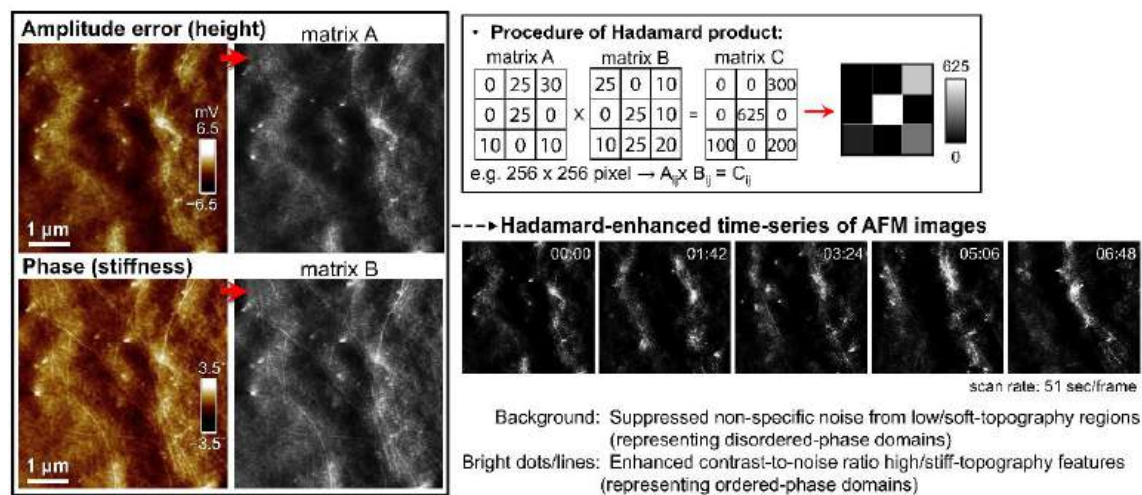


Figure 1. Visualization of membrane-raft dynamics via Hadamard product enhanced AFM imaging. Left box: Original AFM images showing Amplitude error (topography) and Phase (stiffness), which are converted into matrix A and matrix B respectively. Top-right: The Hadamard product procedure, where the corresponding elements are multiplied ($A_{ij} \times B_{ij} = C_{ij}$) is applied to suppress background noise from disordered-phase regions (e.g., high/soft, low/stiff or low/soft features) and effectively amplify high/stiff features (membrane rafts). Bottom-right: A time-lapse sequence of Hadamard product enhanced images revealing the dynamic behavior of membrane rafts on live MCF-7 cells. scan rate: 51 sec/frame.

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Force to Spin a Molecular Rotor

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Frequency-modulated atomic force microscopy (fm-AFM) is well suited to probe forces between the tip and surface. Vertical forces can be inferred by sampling the frequency shifts while varying the tip-sample distance above a point on the sample. In our work, we explore a custom-synthesized molecule: tetrakis(iodomethyl)germane ($\text{Ge}(\text{CH}_2\text{I})_4$; TIme-Ge), which consistently presents a near-normal-facing $-\text{CH}_2\text{I}$ group upon deposition on depassivated Si(100). At 4 K, the normal-facing $-\text{CH}_2\text{I}$ group remains stationary in one of three energy-minimized rotamers. The group can be manipulated into each of the three rotamers by using the attractive force between the tip and the $-\text{CH}_2\text{I}$.

We employ the methodology used by Ternes et al.[1] to measure the horizontal force required to switch between rotamers. In this work, we iteratively took frequency shift measurements along lines parallel to the sample surface at sequentially smaller tip-sample separations. The line direction is off-center from the TIme-Ge molecule, such that the normal-facing $-\text{CH}_2\text{I}$ group is manipulated into a new rotamer. The frequency shift data can then be used to determine the potential energy landscape at each point along this line. By taking a partial derivative along the direction of the horizontal line, horizontal forces can be inferred at each point, including the point at which the $-\text{CH}_2\text{I}$ group rotates. Varying the distance of the horizontal line from the rotamer's axis of rotation provides a straightforward way to measure the torque needed to switch between rotamer positions. By demonstrating the ability to measure this force for a single bond, this work highlights the utility of fm-AFM as a technique to investigate molecular rotors and other simple molecular machines.

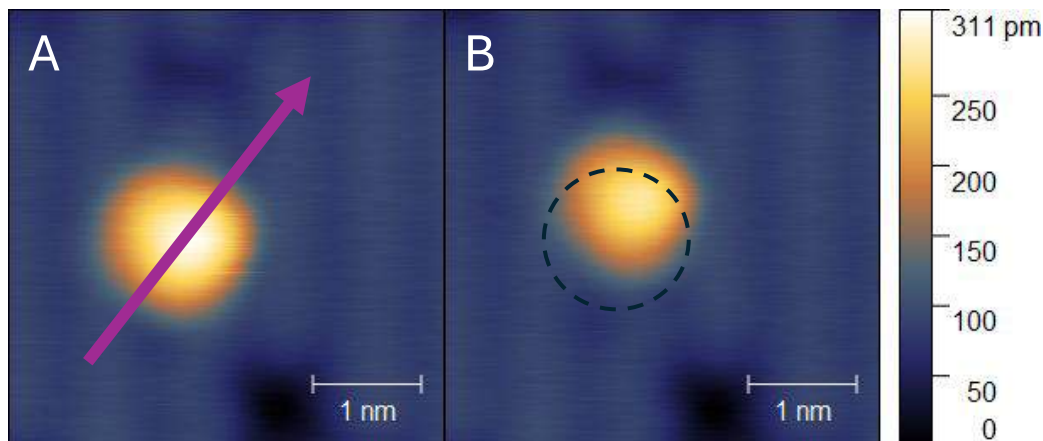


Figure 1: Constant current STM images of a TIme-Ge molecule. Frequency shift measurements are iteratively collected along the path shown in panel A at 0V at sequentially smaller tip-sample separations. At small enough separations, attractive forces between the tip and molecule cause a reversible rotation into the rotamer configuration in panel B (previous configuration indicated by a dashed circle.)

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Atomic scale characterization of the reconstructed anatase $\text{TiO}_2(001)$ surface using non-contact atomic force microscopy

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The reconstructed anatase $\text{TiO}_2(001)$ surface of a natural titanium dioxide crystal is investigated using non-contact atomic force microscopy (NC-AFM). Following repeated sample preparation cycles of sputtering and annealing at temperatures around 800°C , the characteristic (1×4) surface reconstruction is observed.[1,2]

Three distinct topographic NC-AFM imaging modes are identified, differing in the apparent contrast formation of the topmost atoms of the reconstructed surface as shown in figure 1. In contrast I, pronounced bright protrusions are resolved along the (1×4) reconstruction rows, yielding a strongly corrugated row-like appearance. This contrast matches the so called “neutral mode” which has been observed before.[3,4] Contrast II exhibits broader atomic rows in which pairs of atoms within the topmost row appear as double-feature structures. In contrast III, additional protrusions are observed as bright spots located between the atomic rows. These protrusions exhibit an ordered arrangement, in some regions occupying every lattice site, while in others partially vacant sites are observed. Transitions between the three contrast modes are frequently observed when scanning across surface defects or step edges, leading to tip changes inducing a flip in the imaging contrast.

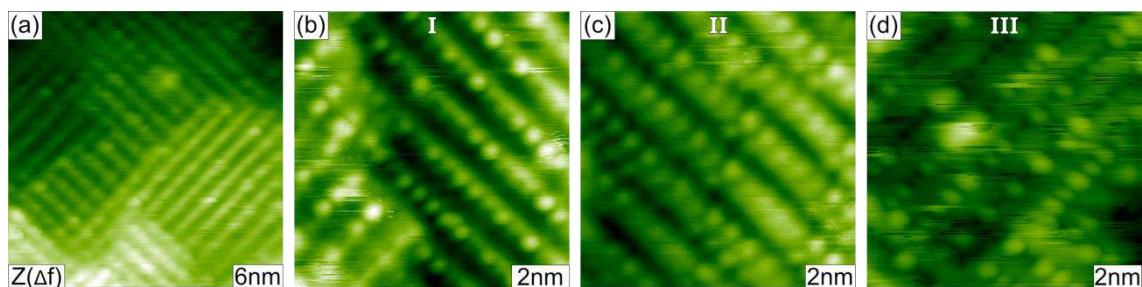


Figure 1: NC-AFM topography images of the anatase $\text{TiO}_2(001)$ -(1×4) reconstructed surface. (a) Overview image of the reconstructed surface. (b-d) Distinct atomic contrast modes observed on the surface: (b) localized protrusions along the reconstruction rows (contrast I), (c) double-feature row contrast (contrast II) and (d) inter-row protrusions (contrast III).

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SQDM Investigation of Orientation-Dependent Electrostatics in Single PTCDA Molecules

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Amongst the scanning probe techniques, Scanning Quantum Dot Microscopy (SQDM) offers very high sensitivity for electrostatic surface potentials, enabling quantitative imaging of surface dipoles [1]. SQDM has been applied to molecular adsorbates, adatoms, defects, and atomic assemblies on the Ag surface [2,3] - and provided valuable benchmarks for theory where metal-organic hybrid systems are particularly challenging. Here, we investigate the subtle effects that adsorption geometry has on the electric properties of isolated perylene tetracarboxylic dianhydride (PTCDA) molecules on Ag(111). We could identify two preferred adsorption orientations of PTCDA which differ by 30 degrees from each other showing distinctly different surface dipoles. Considering the three-fold symmetry of the Ag(111) surface, possible positioning of PTCDA molecules on the silver surface can be categorized into $\langle 1-10 \rangle$ and $\langle 11-2 \rangle$ respectively yielding dipole moments -0.51 D and -0.65 D with the SQDM measurement.

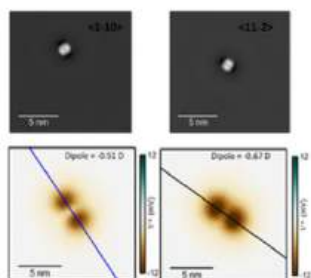


Figure 1: SQDM PTCDA dipole on Ag(111) showing orientation dependence. Top two STM images of PTCDA molecules orient $\langle 1-10 \rangle$ and $\langle 11-2 \rangle$. Bottom panel show corresponding surface potential map with the dipole values mentioned on the upper right corner.

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Excited-state spectroscopy of individual molecules by means of atomic force microscopy

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The combination of scanning probe microscopy with an increasing number of spectroscopic techniques, such as Raman and luminescence, provides unprecedented microscopic understanding. Despite its very direct access to well-defined single-molecule model systems, the unambiguous assignment of observations to specific quantum transitions is not always straightforward [1,2], and typically only a small fraction of all transitions can be studied. Here, we demonstrate a novel type of single-molecule spectroscopy based on atomic force microscopy (AFM) that enables access to many quantum transitions of different types, including radiative, non-radiative and charge-related transitions [3]. The molecules are deposited on thick insulating films, preventing electron tunneling to and from the underlying support (see Fig. 1a). By controlled charge exchange between the conductive tip of an AFM and a molecule, we bring the molecule into different electronic configurations. The population of the states is read-out by mapping the populated states onto two charge states, which can be distinguished in the AFM signal. In this way, quantum transitions can be mapped out in energy, enabling access to the energies of the ground and low-lying excited electronic states of individual molecules. We demonstrate our technique by applying it to pentacene and PTCDA (see Fig. 1b), shedding light on recent scanning tunneling microscopy luminescence experiments on PTCDA [1,2].

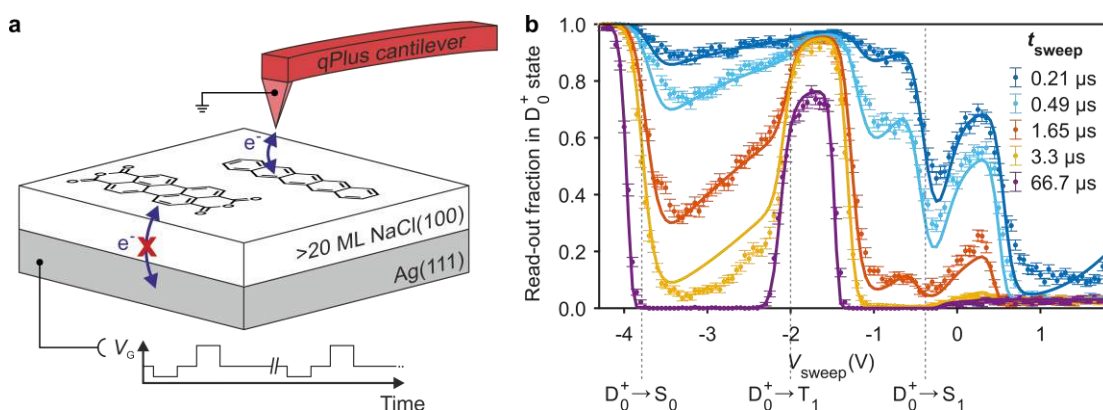


Figure 1: **a**, Sketch of the experimental set-up. Molecules were deposited on a thick NaCl film that prevents electron tunnelling to the underlying metal substrate. Single electron tunnelling between tip and molecule was steered using a pump-probe voltage pulse sequence. **b**, Measured AFM excited-state spectrum (subset of full dataset) of a single PTCDA molecule, enabling extraction of the voltages at which transitions into electronic states open or close (three examples are indicated).

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Exploring the Binding Configurations of Functional 3D Molecules Chemisorbed on Si(100)

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The characterization of functional 3D molecules is a longstanding challenge in scanning probe microscopy (SPM). Recent advances towards atomically precise fabrication (APF) have been made through the use of inverted-mode scanning tunneling microscopy (IM-STM) [1] and 3D surface-bound molecules that can be “activated” in situ to present an out-of-plane radical [2-3]. This approach, which we term positionally controlled mechanosynthesis (PCM), enables chemical reactions to be performed with precisely positioned reagents. Understanding how these molecules are bound to the sample surface and how different configurations of the molecules present could lead to more reliable PCM processes. Here, we present an SPM study of a group of functionalized adamantane molecules chemisorbed on Si(100)-2x1. Automated acquisition workflows enabled the collection of hundreds of high-resolution SPM images of each of the four molecules examined in this work and allowed for a statistical assessment of the common binding configurations. X-ray photoelectron spectroscopy (XPS) was used to confirm the proportion of molecules bound to the surface in the desired “feedstock-up” configuration, and to verify the activation of molecules through dehalogenation after UV exposure.

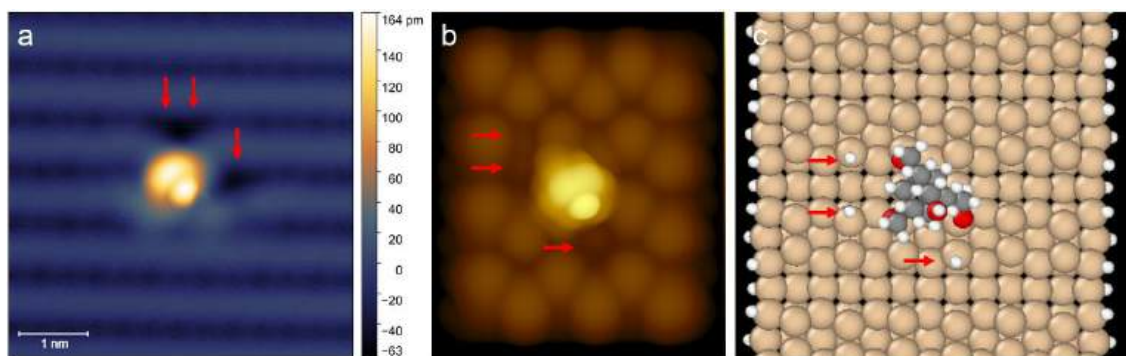


Figure 1: Example of sub-molecularly resolved STM of a 3D molecule on Si(100)-2x1 at 4 K. (a) Experimental STM scan ($V_s = -2.0$ V, $I_T = 50$ pA) of an adamantane-1,3,5,7-tetrayltetramethanol (MAOC-CH₂OH) molecule bound to Si(100)-2x1. (b) STM simulation of a MAOC-CH₂OH molecule in an (c) inter-row geometry. Hydrogens from the legs are bound to adjacent Si dangling bonds and result in depressions in the STM image. Red arrows highlight the depressions in the experimental and simulated images, as well as the surface-bound H in the optimized geometry. The out-of-plane CH₂OH “leg” appears as a secondary bright lobe.

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[3] T. McCallum, et al., chemRxiv.15002728/v1 (2026).

Characterization of interfacial charge transfer between graphene nanoribbons and a 2D ferromagnet by STM/ncAFM

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Chiral graphene nanoribbons (chGNRs) can exhibit symmetry-protected electronic states at their zigzag termini. At half-filling, each of these end states hosts a highly localized spin-1/2 magnetic moment. Owing to their topological protection, these spins are promising candidates for future applications in spintronics and quantum information technology. chGNRs can be grown on various substrates by on-surface synthesis from suitable precursor molecules. However, on electronegative substrates these states are found to be fully depleted, while they are fully occupied on electropositive substrates. In both cases, this leads to closed-shell electronic configurations and quenching of the magnetic moments in the end states.

Using scanning tunneling and noncontact atomic force microscopy, we show that chGNR synthesis on the rare earth surface alloy GdAu₂ enables recovering the magnetic moment of their end states [1], by virtue of its work function matching with graphene. Due to the work function modulation along the GdAu₂ moiré superstructure, the nanoribbons can be found either in a diradical neutral ground state or a singly anionic doublet. In addition, the exchange field of the ferromagnetic GdAu₂ substrate can stabilize a triplet state in neutral chGNRs. Our results demonstrate a route to local control of pi-radical systems adsorbed on metallic substrates.

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Playing ‘Hide & Seek’ at Atomic-scale

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The layered transition-metal telluride compound TaCo_2Te_2 has attracted growing attention because of its fermionic band degeneracy, air-stability, and low-dimensional crystal structure [1,2]. In this work, we investigate the structural, electronic, and magnetic properties of TaCo_2Te_2 using a combination of experimental characterization techniques and density-functional theory calculations. TaCo_2Te_2 possesses a distorted crystal structure in which the top Te atoms occupy three nonequivalent positions, leading to distinct structural appearances depending on the scanning probe technique employed. In particular, constant-current scanning tunneling microscopy (STM) images reveal a square-like surface structure, whereas constant frequency-shift atomic force microscopy (AFM) images display a pseudohexagonal arrangement. Furthermore, the electronic properties of TaCo_2Te_2 is examined using scanning tunneling spectroscopy (STS), and the obtained results are consistent with complementary angle-resolved photoemission spectroscopy (ARPES) measurements.

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Non-Contact Writing and Reading in Ultra-High Density Ferroelectric HDD Based on NC-SNDM

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It is expected that in the near future all information in physical space will be recorded and that this information will be analyzed by advanced artificial intelligence. To realize such data collection and analysis, it is essential to develop next-generation ultrahigh-density recording devices that can record and reproduce information at much higher densities and speeds than those of current magnetic hard disk drive (HDD).

Against this background, we have been conducting research and development on next-generation ultra-high-density ferroelectric HDD (Fe-HDD; SNDM Probe memory).[1][2] While data from SNDM probe memory has traditionally been acquired with the tip in contact, the practical realization of Fe-HDDs requires non-contact writing and reading, just as with conventional magnetic HDDs. Therefore, in this study, we applied a non-contact SNDM (NC-SNDM) method with atomic resolution [3][4] to conduct experiments on non-contact writing and reading in Fe-HDDs.

Figure 1 shows the one dimensional NC-SNDM of polarization-reversed ferroelectric nano domain dots formed in a non-contact state, as observed in a non-contact state.

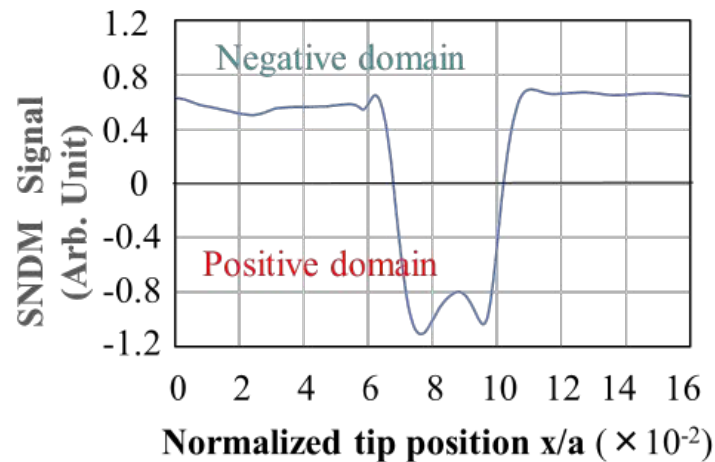


Figure 1: NC-SNDM signal profile of polarization-reversed ferroelectric nano domain dots formed in a non-contact state (tip height is $0.00255a$, a denotes tip radius).

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A Commercial Version of Orpheus II Using Si Cantilevers and qPlus Sensors

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The conference series of Noncontact Atomic Force Microscopy was launched in 1998 by Seizo Morita after true atomic resolution by noncontact AFM was achieved [1] and confirmed by several groups [2,3]. Those first atomic resolution results were obtained with soft cantilevers with a stiffness of about 20 N/m and oscillation amplitudes of about 10 nm.

The qPlus sensor is about 100 times stiffer and enables oscillation amplitudes of about 1/1000 of the previous values, increasing signal-to-noise ratio and spatial resolution [4]. The introduction of the Orpheus II platform [5], based on our experience with compact low temperature microscopes and the compact coarse motor introduced by Shuheng Pan [6], allowed stable imaging with atomic resolution at ambient conditions. Andrea Auer et al. could even demonstrate that the Orpheus II can operate in an electrochemical environment [7].

Two reasons speak for a commercialization of the design ideas behind the Orpheus II. First, it is desirable to provide wide access to ambient studies with atomic resolution AFM. Second, the best results of low temperature qPlus AFM are obtained by groups with a profound knowledge behind the operation of the sensors but many students never get to see and work on the sensors as they are hidden in inaccessible LT-AFMs. For this reason, the NX1 was created (see Fig. 1), a new ambient AFM that allows to use both standard Si cantilevers and qPlus sensors.

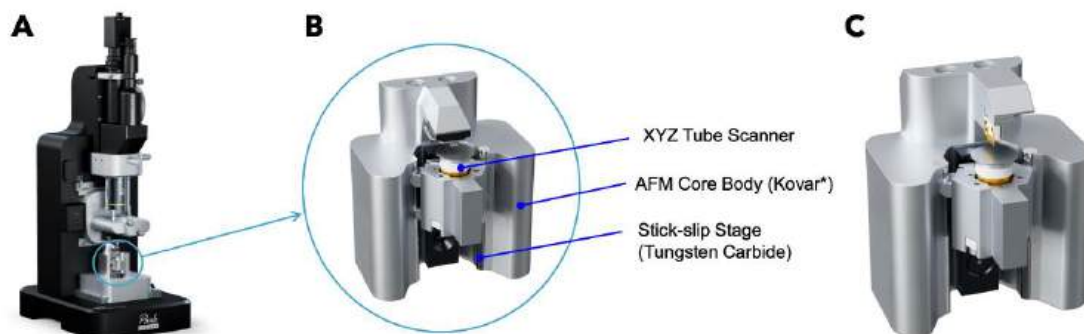


Figure 1: A Microscope setup consisting of body (bottom), optical stage (center) and optical microscope (top). B Microscope body configured for Si cantilever operation with optical detection. C Microscope body configured for qPlus operation.

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Intercalation-based decoupling method for graphene nanoribbons on metal surfaces

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Atomically precise graphene nanoribbons (GNRs) and nanographenes synthesized on surfaces host a variety of emergent electronic properties, such as magnetism. However, most of these carbon nanostructures are grown on metal substrates, where charge transfer and strong electronic screening can obscure their intrinsic correlated electronic behavior, making faithful characterization challenging. Here we use tetrabromocyclooctane as a bromine source to realize a mild and substrate-compatible Br intercalation strategy. This approach can “lift” pre-grown GNRs onto a Br interlayer, and further lift them onto another GNR supported by the Br layer, yielding a doubly intercalated Br/graphene decoupling architecture (Figure 1). Scanning tunneling spectroscopy reveals that the intercalation markedly suppresses metallic screening, allowing Coulomb-driven correlation effects to re-emerge, while the double-intercalation configuration effectively eliminates charge transfer between the metal substrate and the GNRs. Our method provides a versatile and efficient decoupling platform for probing the intrinsic properties of on-surface synthesized carbon-based nanostructures.

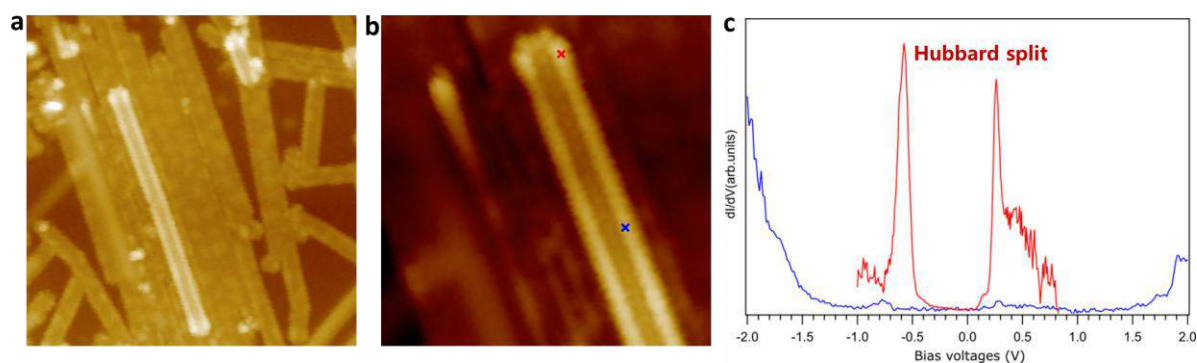


Figure 1: Doubly intercalated 7-AGNR.

Atomically Resolved Imaging of Crystal and Adsorbed Water on Gypsum (010) Surface

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Gypsum ($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$), the dihydrate of calcium sulfate, is the most abundant sulfate mineral in Earth's crust and is widely used in agriculture and construction. Its bulk crystal structure contains calcium sulfate (CaSO_4) bilayers alternating with bilayers of crystal water. While water in the gypsum bulk has been studied [1], a comprehensive understanding of the surface is still missing. Water is present on all surfaces in ambient environment and influences surface chemistry of mineral surfaces. Due to weak interlayer hydrogen bonding, gypsum cleaves readily along the (010) plane, exposing large, atomically flat terraces [2]. In this work, noncontact atomic force microscopy (nc-AFM) with a qPlus sensor was used to resolve the atomic structure of the cleaved gypsum (010) surface and to visualize the configuration of adsorbed water. We find that instead of a simple bulk-terminated surface, every second surface water molecule reorients into a lower-energy configuration, forming an additional hydrogen bond with a neighboring surface water molecule within the unit cell. This modified configuration of the surface water molecules has been previously proposed based on molecular dynamics calculations [3]. Our *ab-initio* modelling suggests that the first adsorbed water layer preserves the periodicity of the surface, consistent with preliminary experimental results. In contrast, subsequent water layers contain water molecules in two different configurations, resulting in a (2×1) superstructure.

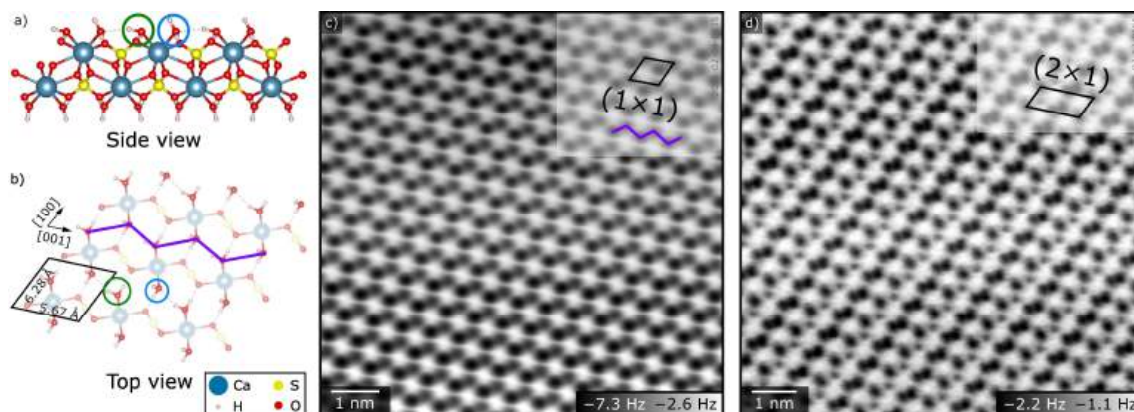


Figure 1: a) Side view of a DFT-relaxed cleaved gypsum (010) surface terminated by a layer of crystal water. b) Top view of the DFT-relaxed surface. The unit cell and a characteristic zig-zag pattern reflecting two different orientations of water molecules within the unit cell are indicated. c) nc-AFM image of the cleaved gypsum (010) surface, cleaved at 105 K, measured at 78 K with a tip modified on gypsum surface, $U_s = -5.4$ V, oscillation amplitude = 300 pm. d) nc-AFM image of the adsorbed multilayer (≈ 5.4 ML) of water on gypsum (010) dosed at 105 K, measured at 78 K with a tip modified on gypsum surface, $U_s = -4.6$ V, oscillation amplitude = 300 pm.

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Investigating the growth mechanism of KBr on glass by nc-AFM.

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Scanning probe microscopy is used to study the surface morphology of alkali halides [1,2], a model system for their importance as insulators and as insulator/semiconductor interfaces. Advances in nc-AFM have enabled high-resolution studies of such insulating surfaces.

In this work, we discuss the thermal deposition and growth of potassium bromide (KBr) on an insulating glass substrate. The nc-AFM technique is used to demonstrate temperature- and coverage-dependent morphological changes of the deposited KBr surface and to compare its tendency to form atomically flat surfaces with that of freshly cleaved KBr single-crystal surfaces. In addition, we discuss the potential to grow an atomically thin gold layer on the optimized KBr/glass substrate to develop a platform for on-surface synthesis and laser-coupled molecular excitation studies.

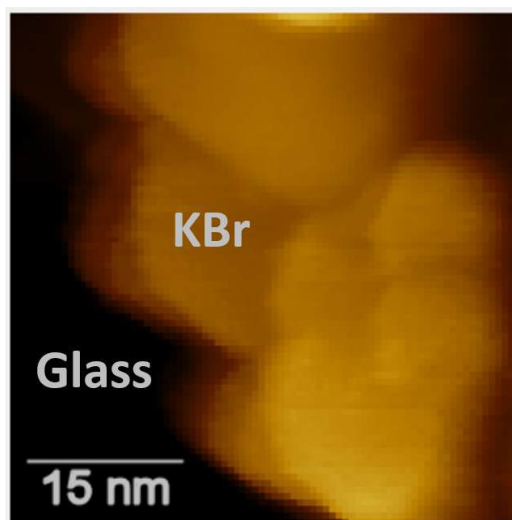


Figure 1: Constant frequency AFM image of the KBr island formed on the glass substrate.

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Comparative Study of Alkane-Derived and Gas Hydrate Stripe Structures on HOPG

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Using frequency-modulation atomic force microscopy (FM-AFM), we observed the formation of two-dimensional stripe domains on highly ordered pyrolytic graphite (HOPG) immersed in DI water [1]. These domains, with heights of ~ 0.5 nm and row separations of 4–6 nm, aligned along the zig-zag direction and gradually nucleated and expanded laterally over several hours. Their nucleation and growth were promoted in a nitrogen gas environment. Importantly, the stripe domains play a key role in the formation and stabilization of surface nanobubbles, frequently appearing at the nanobubble–water–graphite contact line and pinning nanobubble motion (Fig. 1a) [2,3]. Similar stripe structures have also been reported in AFM studies of aged graphitic samples, including HOPG and graphene exposed to ambient air for several days [4–6]. In 2022, Pálincás et al. demonstrated that these aged sample stripes originate from the adsorption and self-assembly of mid-length normal alkanes (C20–C26) present in the environment [7]. They further showed that the molecules align parallel to the HOPG zig-zag axis, producing stripes oriented along the arm-chair direction. For many years, the similarity of AFM images led to the assumption that stripe structures observed in water shared the same origin as those on aged van der Waals materials. Our recent study, combining AFM, X-ray photoemission spectroscopy, and thermal desorption spectroscopy, revealed instead that the stripes formed on HOPG in water consist of $\sim 90\%$ water and $\sim 10\%$ nitrogen molecules [8]. In this work, we compare the morphology and behavior of stripe structures formed by alkane self-assembly with those of interfacial nitrogen gas hydrate overlayers. To probe the former, we exposed freshly cleaved HOPG surfaces to vapors of mid-length normal alkanes and imaged the resulting stripe domains in both air and water using AFM (Fig. 1b,c).

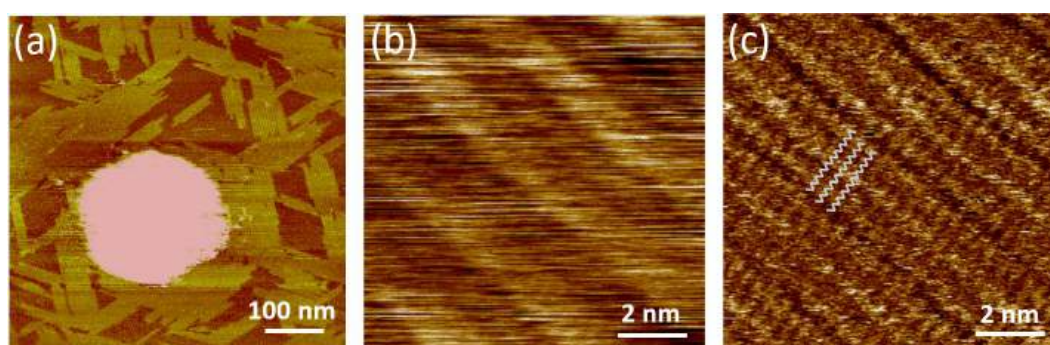


Figure 1: (a) Height image of a surface nanobubble confined by stripe domains. (b) Height image of $C_{20}H_{42}$ on HOPG acquired by lateral-resonance mode. (c) Corresponding phase image of (b).

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Surface Structure of Cu₂O(110)

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Cuprous oxide (Cu₂O) is an earth-abundant, non-toxic p-type semiconductor with a direct band gap of approximately 2 eV. Due to its favorable band-edge alignment, Cu₂O has been proposed as a promising material for photocatalytic water oxidation and the reduction of CO₂ to products such as methanol [1]. Despite its potential, there remains a limited understanding of Cu₂O surfaces under different conditions, ranging from ultrahigh vacuum (UHV) to ambient and liquid environments. In recent years, structural models have been proposed for the major facets of Cu₂O – (111), (100), and (110). Among these, the Cu₂O(110) surface has been identified as especially interesting due to its potentially enhanced photoactivity. In particular, the oxidation state of active sites has been reported to reversibly change from Cu⁺ to Cu²⁺ upon co-adsorption of CO₂ and H₂O, and to revert back to Cu⁺ under visible light illumination [2]. Nevertheless, Cu₂O(110) remains the least understood low-index facet [3]. For computational modelling, most studies relied on a simplified bulk-truncated (1 × 1) termination. However, experimental confirmation of this structure is lacking.

The primary goals of this work are to experimentally validate the existence of a (1 × 1) structure for Cu₂O(110) in UHV, to find reproducible procedures to prepare it, and to develop quantitative structural models by combining scanning tunneling microscopy (STM), non-contact atomic force microscopy (nc-AFM) at cryogenic temperatures, low-energy electron diffraction intensity–voltage analysis (LEED-IV), and density functional theory (DFT). During room-temperature LEED and STM measurements, a (1 × 1) structure is observed. However, nc-AFM data acquired at 78 K reveal a different structure with a larger unit cell and two coexisting domains. A low-temperature phase transition is currently hypothesized.

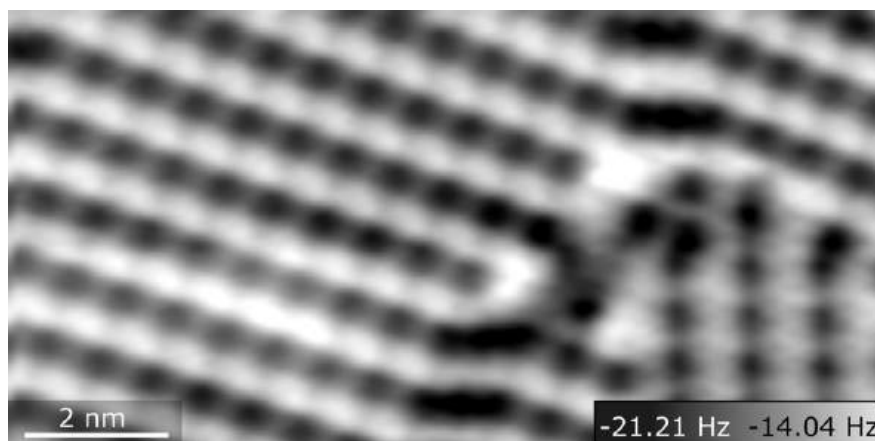


Figure 1: Constant-height nc-AFM image of Cu₂O(110) (1 × 1) structure as beforehand determined by LEED. The image was acquired at 78 K with a Cu-terminated tip.

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Chemical reactivity of Pd (111) surface

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Palladium (Pd) is widely known as a catalyst. Its exact catalytic mechanisms and surface still require more research. Typically, Pd surfaces are studied with STM methods [1, 2]. We have studied the Pd (111) surface with FM-AFM in UHV. This method consistently showed quasi regular island structures along the edge of terraces in several areas of the sample. STM was not sensible to these structures. The islands typically have a size of 50 nm and less in both directions. Some islands were strongly elongated growing up to 100 nm along the terrace edge while staying short in perpendicular direction. The islands were absent on non-edge areas.

The structures imply significant surface charge. We intend to explore further how Pd steps influence chemical reactivity on its surface.

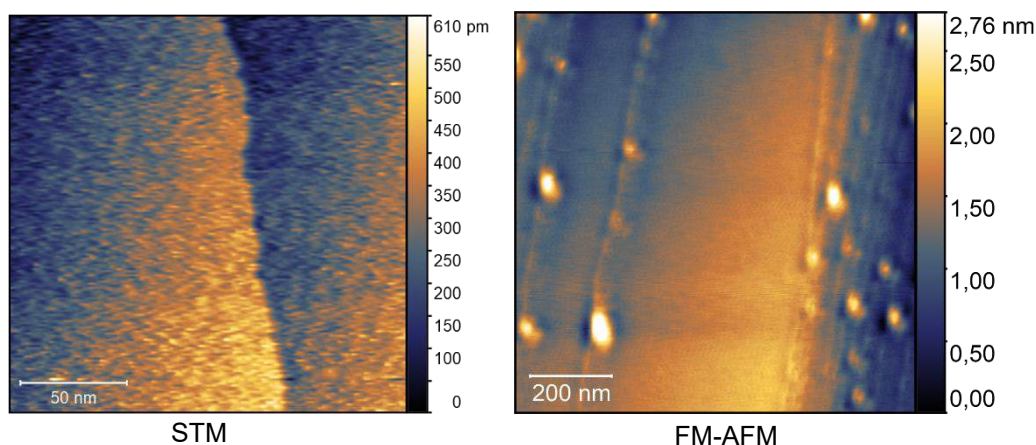


Figure 1: Structures on the edge of terraces always appeared along the terrace edge when measured in FM-AFM. STM wasn't sensitive to them.

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Ring Features of Single Adatoms Investigated with a CO Tip

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When a CO-functionalized tip approaches single atoms adsorbed on Cu(111), five interaction regimes can be distinguished: an initial electrostatic repulsion, followed by van der Waals attraction, an interaction barrier, chemical attraction, and finally Pauli repulsion (see left Figure). The latter four regimes were identified in [1] as the transition from physisorption to chemisorption.

If all five interactions were radially symmetric, several characteristic ring-like features would be expected in constant-height images. At larger tip-sample distances, an electrostatic ring surrounding a van der Waals minimum should appear, as observed for Gd (top Figure). At closer distances, a van der Waals ring around a central Pauli repulsion is expected, as observed for Au (middle Figure). Finally, at even smaller separations, a repulsive ring surrounding a chemically attractive center emerges, as reported for Fe and explained in [1] (bottom Figure).

However, the experimental observations deviate significantly from this simplified picture, as some of the expected rings are absent. This discrepancy arises from variations in the relative strengths of the individual interaction regimes for different atomic species, as well as from the angular dependence of the underlying forces.

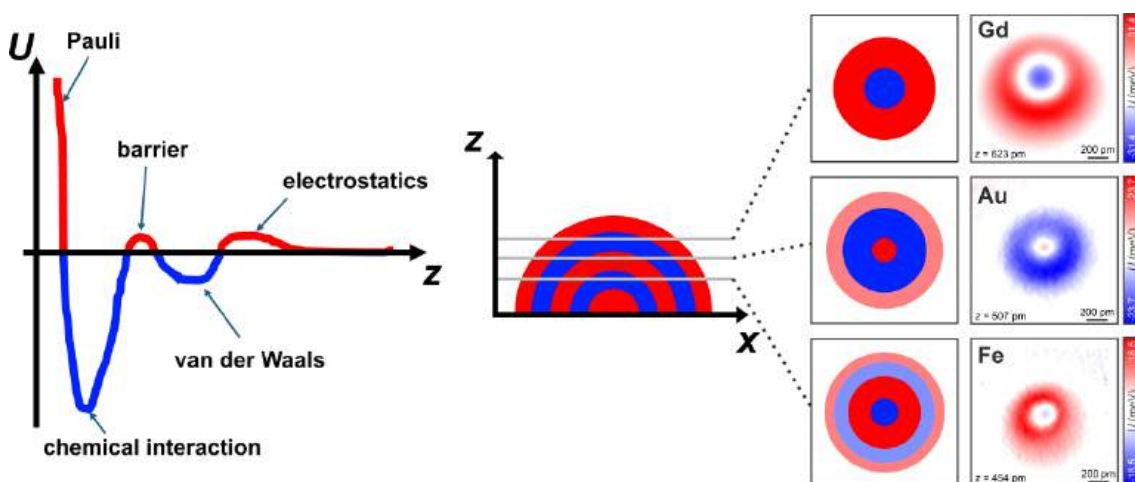


Figure 1: Schematic z -spectrum on single adatom with CO tip. Schematic x - z map with radially symmetric interactions. Schematic constant height images. Measurement for Gd, Au and Fe. Fe data from [1].

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On the origin of divergences in quantitative lateral force recovery in bimodal NC-AFM

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Bimodal non-contact atomic force microscopy (NC-AFM), with simultaneous excitation of the first flexural and torsional eigenmodes of the cantilever, enables the simultaneous measurement of normal and lateral tip-sample interactions via decoupled frequency shifts of both modes [1]. The high sensitivity of the torsional oscillation to short-range interatomic forces makes it attractive for imaging systems with small potential corrugations [1] or where long-range background forces are large.

Several approaches have been proposed for the quantitative recovery of lateral forces from torsional frequency shift measurements, though implementation of these methods is complicated by physical assumptions and numerical complexity [1,2,3].

Notably, for a physically consistent conservative interaction potential, lateral forces recovered directly from torsional frequency shift measurements should quantitatively converge with forces independently derived via lateral differentiation of the interaction potential obtained from integration of the flexural mode frequency shifts, at least within the small lateral oscillation amplitude regime.

Here, we perform a quantitative comparison of these methods using two separate bimodal NC-AFM systems on both the Si(111)-7×7 and KI surfaces. Significant quantitative divergence is observed between direct torsional force recovery methods and forces derived from the measured interaction potential in some inversions, despite qualitative similarity in the spatial features of the recovered force fields. We investigate the origin of these discrepancies, including the role of oscillation amplitude, cantilever geometry, calibration uncertainties, and the physical assumptions underlying each inversion formalism. These results highlight the challenges associated with quantitative lateral force recovery in bimodal NC-AFM and establish a framework for assessing the validity and uncertainty of atomic-scale lateral force inversion methods.

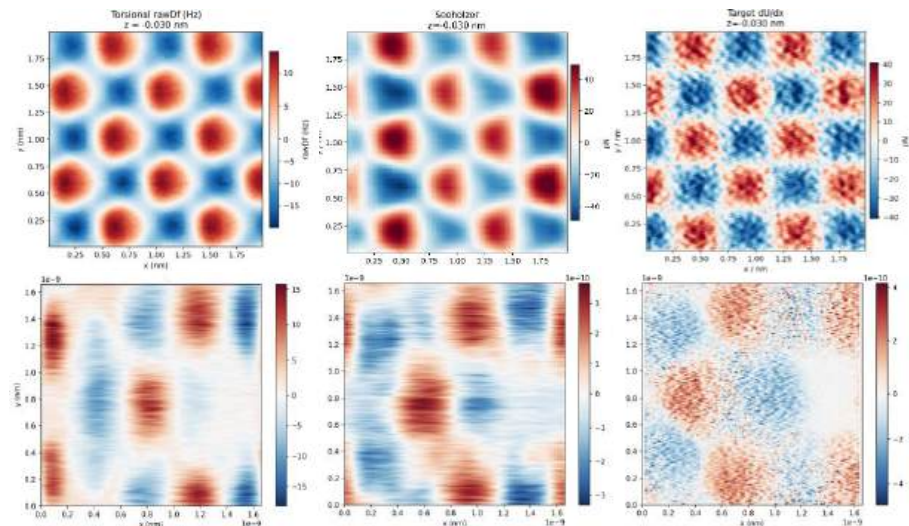


Figure 1. Constant-height bimodal NC-AFM measurements and reconstructed lateral forces on two surfaces. **Top:** KI lattice. **Bottom:** Si(111)-7×7 cornerhole region. For each row: torsional frequency shift map (left), lateral force reconstructed from torsional frequency shift using modified Fourier decomposition (centre), and lateral force obtained simultaneously from lateral differentiation of the flexural-mode interaction potential, $F_x = -dU/dx$ (right). KI forces shown in pN; Si forces shown in N.

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AC voltage measurement in atomic force microscope potentiometry

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Atomic force microscope potentiometry (AFMP) is a powerful technique for measuring the voltage distribution of electronic devices under operation [1]. In AFMP, the sample voltage is detected as the cantilever voltage using a voltage-follower circuit while the tip is in contact with the sample, and the technique can be operated in either contact or tapping mode. Although AFMP is suitable for DC voltage measurements, measuring AC voltages is challenging because of the contact resistance and input capacitance of the measurement circuit; typically, the time constant is on the order of 0.1 s, limiting the measurement frequency to relatively low values. Under non-contact or tapping-mode operation, AC voltages can be detected through the capacitive coupling between the tip and sample. However, the contributions from the tip cone and cantilever are dominant, making local voltage measurements difficult. In this study, we achieved high-resolution AC voltage measurements by detecting the amplitude-modulated signal induced by tip oscillation in FM-AFM.

Figure 1 shows a schematic of the AFMP system. When an AC voltage is applied to the sample, an AC current flows through the tip-sample junction, and the resulting voltage is detected using a voltage-follower circuit. The tip oscillation (A) modulates the tip-sample capacitance, leading to amplitude modulation of the AC voltage, ΔV , which can be approximated as

$$\Delta V \approx V_s \frac{C_i}{(C_{\text{stray}} + C_i)^2} \frac{dC(z)}{dz} A. \quad (1)$$

Equation (1) suggests that the spatial resolution of the amplitude-modulated signal (ΔV) is comparable to that of the dC/dz image. Furthermore, higher-harmonic components of the amplitude modulation may enable further improvement of the spatial resolution[2,3].

Figure 2 shows the results of AC voltage measurements on a carbon nanotube (CNT) transistor. An AC voltage was applied to the drain electrode, while the gate and source electrodes were grounded. By comparing the amplitude signal and the amplitude-modulated signal in Fig. 2, it can be seen that the amplitude-modulated signal exhibits much higher spatial resolution than the amplitude signal, which is consistent with the theoretical prediction. These results demonstrate that the proposed method enables high-resolution AC voltage measurements in AFMP. Furthermore, as shown in Fig. 2, a phase difference ($\Delta\theta$) between the amplitude-modulated signal and the applied AC voltage was clearly observed, suggesting that the proposed method can be extended to local impedance analysis in AFMP.

This work was partially supported by JST PRESTO (Grant No. JPMJPR20A3) and JST NEXUS (Grant Number JPMJNX25D3), Japan.

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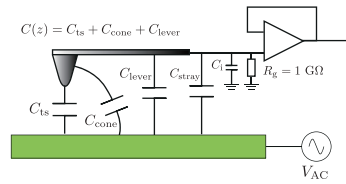


Figure 1: Schematic of the AFMP system.

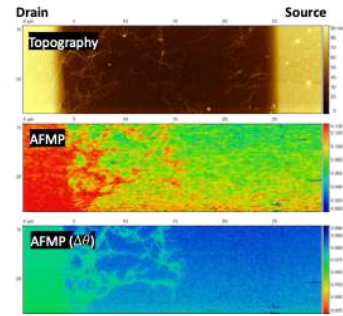


Figure 2: Topography and amplitude-modulated signal (ΔV) of AFMP.

On-Surface Synthesis of Kagome Metal-Organic Frameworks

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Two-dimensional metal-organic frameworks (2D-MOFs) with Kagome lattice symmetry are known to host exotic electronic structures, such as flat bands and ferromagnetic ordering [1,2]. However, the experimental realization of 2D Kagome MOFs exhibiting flat-band ferromagnetism remains challenging [3-5].

Here, we report the surface-assisted synthesis of a 2D Kagome MOF on Ag(111) using custom-designed precursor molecules, achieving highly ordered domains exceeding 200 nm in lateral size. Low-temperature scanning tunneling microscopy (STM) and atomic force microscopy (AFM) with a CO-functionalized tip provide insights into the electronic and structural properties of the Kagome lattice, while Kelvin Probe Force Spectroscopy (KPFS) has been exploited to elucidate the degree of charge transfer. Furthermore, we demonstrate doping strategies to influence the electronic structure of the framework. These modifications provide a versatile route to tune electronic coupling and band filling, highlighting the system's potential as a highly tunable platform for engineering correlated electronic phases.

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High Resolution Imaging of KBr with CO Functionalized Tips

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The first AFM image with true atomic resolution was obtained on the KBr(001) surface. In 1991, Franz J. Giessibl and Gerd Binnig achieved atomic-resolution on KBr(001) in contact-mode AFM under low-temperature and ultra-high-vacuum conditions. Their measurements resolved both ionic species, and the observation of step-like features interrupting the lattice periodicity confirmed the genuine atomic nature of the contrast.

More than three decades later, we revisit the KBr(001) surface using non-contact AFM with CO-terminated tips. Due to the ionic charges and differing ionic radii, the two ionic species are observed at different tip-sample distances. The imaging properties are strongly influenced by the flexibility and lateral bending of the CO molecule at the tip apex, which plays a central role in the observed contrast formation.

As in the original experiment, we resolve point defects and atomic step edges on the surface. In 1991, the experiment pushed AFM to the limits of what was technically possible, and even the original researchers doubted whether the measurement could be reproduced reliably. More than three decades of advances in AFM instrumentation and methodology have since transformed this into an almost routine measurement, while it continues to be highly relevant and intriguing, still yielding new insights.

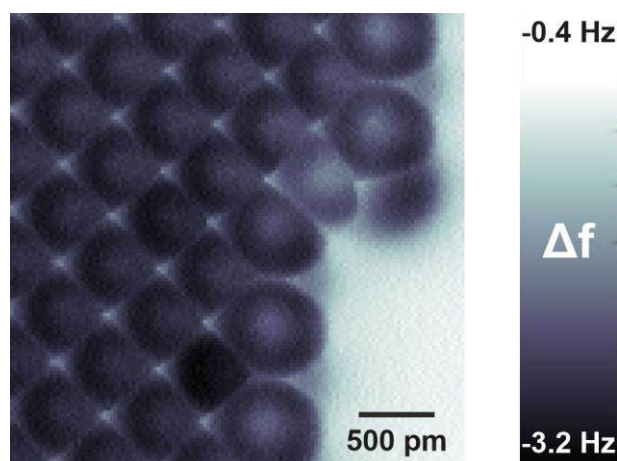


Figure 1: Atomic step edge on KBr. The Bromide ions appear as sharp repulsive features, whereas the Potassium Ions appear as broad repulsive features in this imaging height.

Understanding how Electrochemical Atomic Force Microscopy Can Reveal the Potential of Zero Charge

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The potential of zero charge (PZC) is the electrode potential at which the net surface charge density is zero. Around this potential, the interfacial electric field changes sign, which strongly affects the orientation of water in the electrical double layer. Electrochemical atomic force microscopy (EC-AFM) force-distance curves are sensitive to this interfacial water structure and may therefore contain signatures of the PZC. However, the microscopic origin of the measured force remains difficult to interpret, because the total force contains multiple coupled contributions from water layering, ion effects, electrostatics, and tip-surface interactions.

A useful description separates the AFM force-distance curve into two main contributions [1]. The first is an oscillatory contribution, which reflects the layered solvent density near the electrode. The second contribution is a monotonic background force, which decays approximately exponentially with distance. The physical origin of this monotonic contribution is less clear, but we hypothesize that it is strongly connected to the relative orientation of water at the AFM tip and at the electrode surface [1].

Here, we propose an AIMD-based framework to interpret EC-AFM force-distance curves at electrified metal-water interfaces. From the water density, an approximate free-energy profile can be constructed through a potential-of-mean-force relation. However, density alone cannot correctly describe the monotonic background force, because it neglects water orientation. To include orientational effects without explicitly simulating the AFM tip in the same system, we use AIMD to simulate a water orientation profile near an amorphous SiO₂ surface as a physically motivated weighting factor for the tip-side water orientation distributions. This allows the electrode-side AIMD data to be reweighted according to whether interfacial water is aligned or oppositely oriented with respect to tip-side water. In this picture, aligned water orientations may lead to attraction, whereas opposite orientations may lead to repulsion. The sign and magnitude of the resulting monotonic background force can then be related to the surface charge and to the water orientation induced by the electrode potential.

This workflow aims to connect AIMD-derived interfacial water structure directly to experimentally measured EC-AFM force-distance curves. If the monotonic force background follows the orientational change described, EC-AFM may provide a direct experimental signature of the PZC in realistic electrolyte environments.

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Towards the Largest Starphene: [22]Starphene

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Starphenes are trigonal polycyclic aromatic hydrocarbons composed of three acene-like arms connected through a central aromatic core, giving rise to extended π -conjugation and threefold-symmetric electronic structures.[1,2] Their unique topology and tunable electronic properties make them attractive platforms for molecular electronics, spintronics, and quantum materials research.[1,3]

Here, we report the on-surface synthesis of [22]starphene on Ag(111) via thermally induced surface-assisted coupling reactions under ultra-high vacuum conditions. The structure extends the size of previously reported starphenes, including the recently described [19]starphene. High-resolution scanning probe microscopy and spectroscopic measurements confirm the formation of the trigonal π -conjugated framework and allow characterization of its electronic structure. The synthesized [22]starphene exhibits a bandgap of approximately 0.4 eV, lower than those reported for smaller starphenes, consistent with the increased conjugation length of the system.

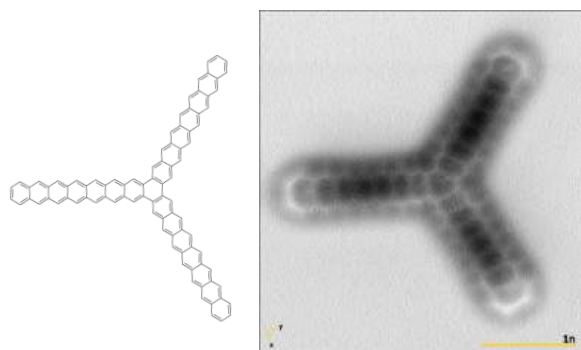


Figure 1: Molecular structure and non-contact atomic force microscopy (nc-AFM) image of [22]Starphene on Ag(111).

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Fast SPM simulation with complex molecular attachment

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AFM and STM images obtained with simple single-particle tip terminations such as CO or Xe are easily interpretable considering isotropic tip-bending and efficiently simulated within the probe-particle model [1,2], providing intuitive insight into the submolecular structure of the sample. More complex molecular tip attachments, such as PTCDA, introduce additional degrees of freedom that can enable advanced functionalities including scanning quantum dot microscopy (SQDM) [3] or electron spin resonance imaging (ESR-SPM)[4], but also make image interpretation substantially more challenging. To address this problem, we employ GPU-accelerated classical and grid-projected force fields within the GridFF framework [5] to rapidly simulate molecular relaxation in the combined tip-sample potential independently for each AFM image pixel in parallel. Combined with parallel evaluation of hopping integrals between the tip, attached molecule, and sample, this approach enables near-interactive simulations of AFM and STM images involving complex molecular junctions.

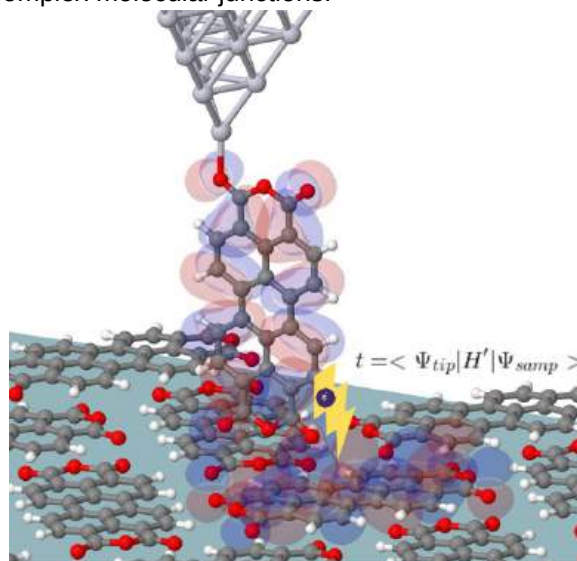


Figure 1: Parallel calculation of tip-sample orbital overlap for current and conductance evaluation.

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Automatic tip functionalization with CO on Ag(111) using machine learning

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Functionalization of scanning probe microscopy tips with CO molecules enables both high-resolution imaging with sub-molecular contrast and a reliable interpretation of experimental data [1, 2].

However, the manual functionalization procedure is time-consuming and limits experimental throughput. To address this, tip functionalization can be automated [3].

The crucial part of the automation process is assessing the properties of the tip after CO pick-up. Along this line, inverse imaging of a CO molecule with the functionalized tip is commonly used [4]. Fig. 1 shows an example of imaging surface-bound CO molecules on Ag(111) with two tips of different qualities.

Here, we implement a full pipeline for CO tip functionalization on Ag(111) as shown in Fig. 2. The process includes localizing a CO molecule during scanning the surface, performing the pick-up of this CO molecule, and evaluating the resulting tip condition. Tip quality is assessed by imaging CO molecules on the substrate and by classifying the achieved resolution as "bad" or "good" for a CO-tip using a convolutional neural network (CNN). The CNN performance is compared to a conventional image analysis algorithm based on template matching.

We expect this automated approach to significantly improve the efficiency of AFM experiments and thereby enabling faster and more systematic data acquisition on molecular systems.

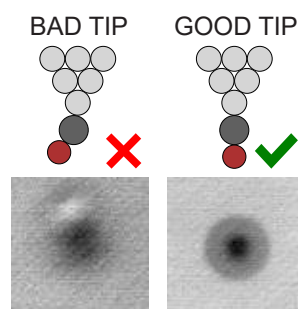


Figure 1: Inverse imaging of surface-bound CO molecules on Ag(111) with a "bad" and a "good" tip.

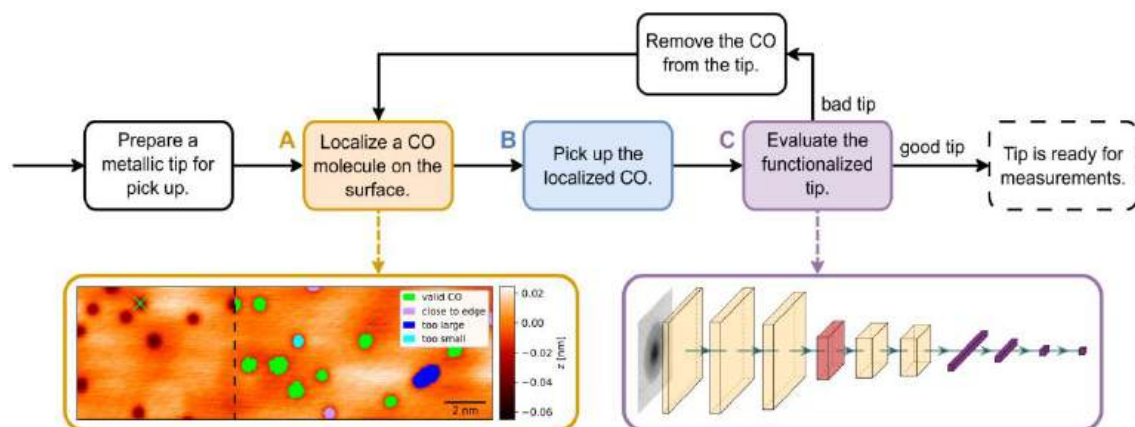


Figure 2: Pipeline of the automated CO functionalization process.

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Upcycling a commercial scan controller for scanning probe microscopy with the GXSM4 OpenSource system

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The complexity of scanning probe microscopy experiments, in particular when using the non-contact atomic force microscopy variant, requires a flexible, performant, and intelligent control system [1]. At the same time, the current drive to implement methods of machine learning in the whole scientific process including the experiment design and execution [2,3] leads to further requirements such as a flexible programming interface – or ideally an open source code base of the scan control system.

Here, an interface board to re-use components of a commercial scan controller (Omicron SCALA) for state-of-the-art SPM operation by the Open Source GXSM4 system with the new RPSPMC hardware [4] is presented, see Fig. 1 for a system overview. The original units for the tip coarse control as well as the high-voltage piezo amplifiers of the commercial system are reused, while all further logic and analog control including feedback loop, scan generator, and AFM detection are removed. The interface board directly connects to the signal bus of the commercial scan controller, providing both analog signals for the piezo scan movement from RPSPMC and digital signals for the coarse approach. Based on a careful analysis of the original coarse control signal timing, a state machine is implemented with an on-board Teensy 4.0 microcontroller. Fast interface to GXSM4 is realized via a shared-memory module in GXSM4.

The performance assessment from measurements on the Si(111)-(7×7) surface at room temperature clearly highlights the superior capabilities of the GXSM4 system.

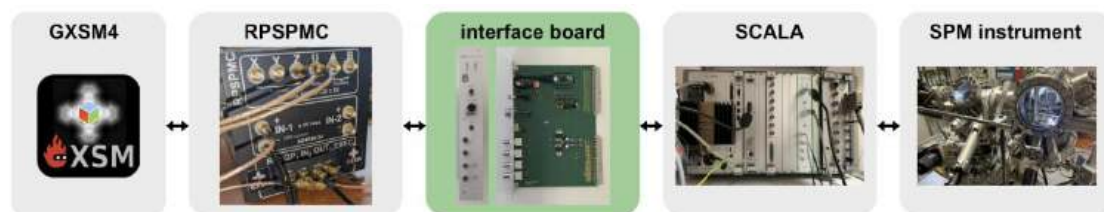


Figure 1: Interface board as central component to control the coarse control and piezo amplifier units of a commercial scan controller via GXSM4 with the RPSPMC hardware.

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Noncontact AFM Potentiometry for Nanoscale Potential Imaging via Distance-Derivative Capacitance Analysis

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Atomic force microscope potentiometry (AFMP) enables nanoscale potential imaging in operating electronic devices using a high-input-impedance voltage follower circuit [1]. However, conventional AFMP operates in contact or intermittent-contact modes, making it unsuitable for characterization of fragile samples such as carbon nanotube transistors. To address this limitation, we developed noncontact AFM potentiometry (NC-AFMP) based on frequency-modulation AFM, where electrical measurements are performed without direct tip-sample contact [2]. Under noncontact operation, AC potentials are detected through capacitive coupling between the tip and sample; however, the spatial resolution is severely degraded by parasitic capacitance contributions from the tip cone and cantilever beam (Fig. 1).

In this study, nanoscale potential imaging of carbon nanotube field-effect transistors (CNT-FETs) was performed with an AC voltage applied to the drain electrode while FM-AFM was operated in the attractive noncontact regime. To improve the spatial resolution, distance-derivative analysis of the potential was introduced based on an analytical apex-cone-lever capacitance model [3-4]. While the raw potential image is dominated by the cantilever beam contribution, which fatally degrades spatial resolution (Fig. 2b), the first and second derivatives of the potential with respect to the tip-sample distance selectively enhance the apex contribution, revealing detailed structures that are not discernible in the raw potential image (Figs. 2c,d). This approach effectively suppresses capacitance components with weak distance dependence while selectively enhancing localized electrostatic signals, significantly improving the spatial resolution of noncontact potential imaging. These results demonstrate that distance-derivative capacitance analysis is an effective approach for enhancing spatial resolution in NC-AFMP and for nanoscale electrical characterization.

This work was partially supported by JST NEXUS (Grant Number JPMJNX25D3) and JST PRESTO (Grant Number JPMJPR25J7), Japan.

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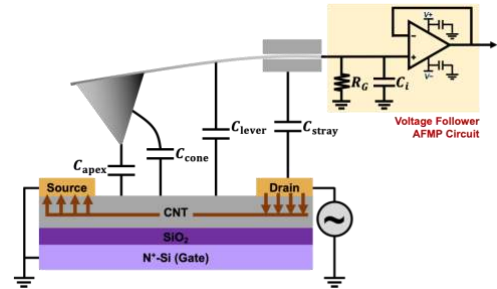


Figure 1: Schematic of NC-AFMP on a CNT-FET showing apex, cone, and cantilever capacitance contributions.

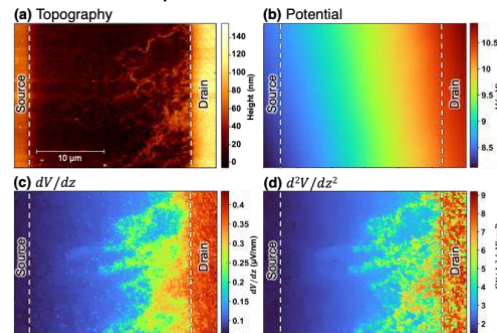


Figure 2: (a) Topography image, (b) raw potential image, and (c,d) first- and second-order distance derivatives of the measured potential obtained by NC-AFMP on a CNT-FET.

Kelvin Probe Force Microscopy of Mixed Monolayer Doping of Silicon

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Mixed monolayer doping (MMLD) is a surface-chemistry-based approach for low-damage silicon doping, in which a phosphorus-containing molecule in our case allyldiphenylphosphine (ADP) is co-grafted with a non-doping spacer (1-undecene) on hydrogen-terminated silicon [1,2]. The ADP molar fraction controls the surface phosphorus density and thus the dopant dose. After monolayer formation, samples undergo O₂ plasma ashing, SiO₂ capping, and rapid thermal annealing at 1050 °C to drive phosphorus into the silicon lattice.

Amplitude-modulation KPFM (AM-KPFM) at the second cantilever resonance was used to map the work function (WF) after capping-layer removal by HF. To preserve the oxide-free silicon surface, all measurements were performed inside a nitrogen glovebox (O₂, H₂O < 0.1 ppm). Using PtIr-coated cantilever with HOPG as a WF reference, we observe a systematic decrease in WF with increasing ADP fraction, from values consistent with the p-type substrate (~4.8 eV) toward the conduction band edge (~4.2 eV), indicating increasing n-type doping. Samples treated with O₂ plasma prior to evaporated SiO₂ capping show lower WF values than untreated counterparts, consistent with enhanced phosphorus activation due to reduced carbon contamination. In contrast, sputtered SiO₂ capping leads to strong Fermi-level pinning near ~4.1 eV, independent of ADP concentration, masking the doping signal entirely [3].

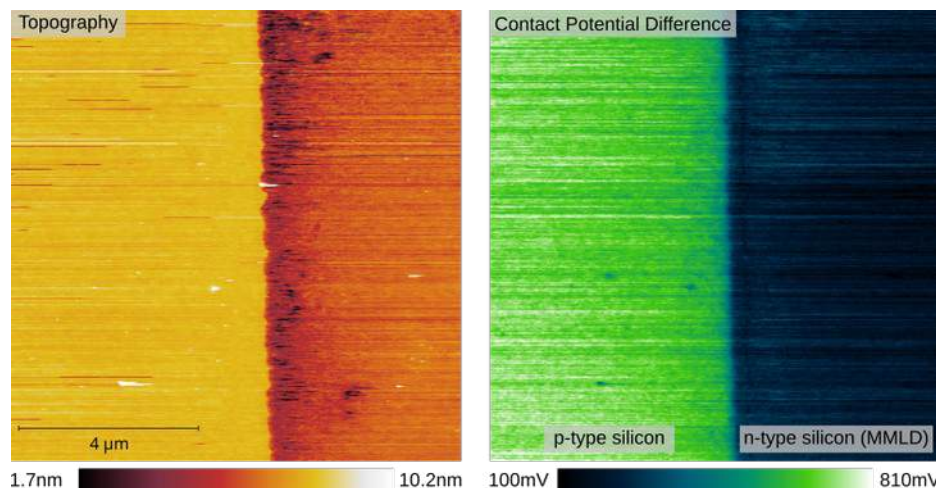


Figure 1: Topography (left) and KPFM contact potential difference map (right) of a one sided MMLD-processed silicon surface.

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Challenge toward high-resolution infrared spectroscopy based on frequency modulation AFM

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Infrared spectroscopy (IR) is remarkably powerful for analyzing the chemical composition and molecular structure of samples, leveraging the vast IR database. However, its spatial resolution is limited to 3–10 μm due to its optical wavelength. Meanwhile, the AFM offers significantly higher resolution, though its chemical analysis capabilities are limited. Recently, the combination method of IR and contact- or tapping-mode AFM, known as AFM-IR, has been developed and is attracting considerable attention. On the other hand, we develop an infrared spectroscopy method based on frequency-modulation (FM) AFM to achieve higher spatial resolution in non-contact mode, which we refer to as tip-oscillation-synchronized detection of infrared spectroscopy (TS-IR).

In TS-IR, the sample surface under the oscillating tip in FM-AFM mode is irradiated with a tunable infrared pulsed laser beam; the irradiation timing is synchronized with the tip oscillation with a variable phase shift and additional pulse modulation, as shown in the block diagram (Fig. 1). The irradiation alters the electric dipoles at the sample's specific wavelengths, leading to a change in the interaction force between the tip and the sample. The change results in a hysteresis in the force-distance curve, and the area of the hysteresis loop can be evaluated by detecting the change in dissipation energy. To reduce the fluctuations, including thermal drift, and noise in the dissipation signal using a lock-in amplifier, the tunable infrared pulsed laser is triggered with modulated pulses synchronized to the tip oscillation at the resonance frequency of the force sensor, which is modulated by multiplication with a low-frequency rectangular pulse at frequency f_M (e.g., 1 Hz). The f_M rectangular pulse serves as a reference signal for a lock-in amplifier, which extracts the differential signal between laser-on and laser-off states. This approach has enabled the acquisition of highly reproducible TS-IR spectra.

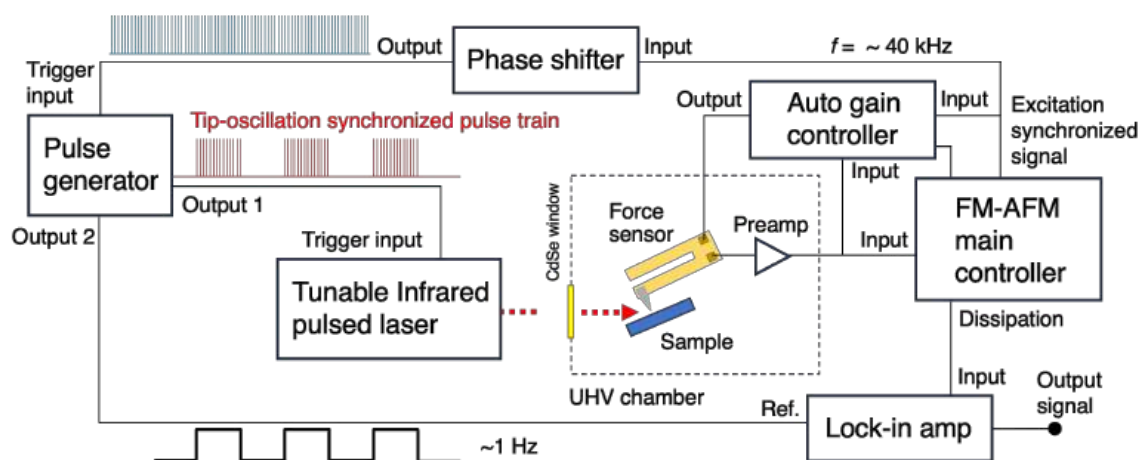


Figure 1: Block Diagram of TS-IR.

Spectral response of a tuning-fork sensor to a pulsed infrared irradiation detected via a dissipation channel of FM-AFM

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Infrared spectroscopy (IR) is a powerful technique for identifying functional groups and molecular structures of materials. However, the spatial resolution of IR is limited to several μm . Thus, combination of IR and AFM, such as AFM-IR and PiFM, has attracted considerable attention owing to their high spatial resolution. In our group, we are developing tip-oscillation synchronized infrared spectroscopy (TS-IR), in which a wavelength-tunable pulsed infrared laser is integrated into ultrahigh-vacuum (UHV) FM-AFM, enabling simultaneous surface imaging and IR measurements with atomic-scale spatial resolution.

In TS-IR, the sample is irradiated with a single infrared pulse in one oscillation cycle of the AFM tip, and the induced change in the tip-sample interaction force is detected as an energy dissipation signal. By sweeping the infrared wavenumber, the chemical species in the illuminated region can be identified. The force sensor used in this study is a retuned fork (RTF) force sensor based on a quartz tuning fork [1]. Recently, we found that intentional irradiation of infrared light onto the RTF sensor itself produces a dissipation response that depends on the irradiation wavelength. This finding provides insight into the integration of AFM and IR spectroscopy using quartz tuning-fork-based sensors and suggests a novel application of quartz tuning-fork force sensors.

Here, two types of RTF sensors were prepared. One had no tip attached, while the other had a small amount of conductive silver epoxy applied at the tip-mounting position. These sensors were installed in a room-temperature UHV chamber. To enhance the sensitivity of dissipation signal detection, the sensors were heated by blue-laser irradiation (~ 1.5 W for 1 s), resulting in an increase of the quality factor to $\sim 30,000$. Figure 1 shows the IR spectra obtained by sweeping the infrared laser wavenumber. For the untreated RTF sensor, a peak was observed at 1160 cm^{-1} , which is attributed to the Si-O vibrational mode of quartz. In contrast, when the infrared laser was irradiated onto the region coated with silver epoxy, multiple peaks attributed to the epoxy resin were detected. These results suggest that materials on the sensor surface can be detected and spectroscopically analyzed through dissipation measurements. Applications, including photoacoustic spectroscopy using variously treated RTF sensors, will also be discussed.

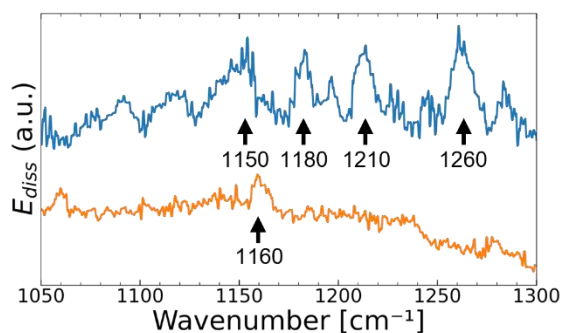


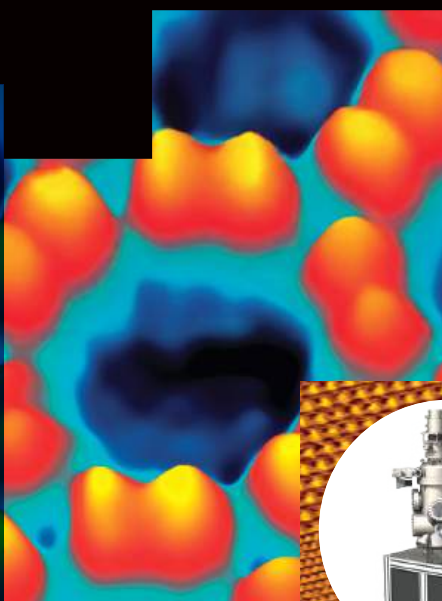
Figure 1: IR spectra of the untreated RTF sensor (quartz) and the silver epoxy coated RTF sensor, denoted by orange and blue curves, respectively. The possible assigned peaks are marked with the arrows with the wavenumbers.

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DOI: 10.1016/j.susc.2024.122589

Poster Session B

Candidates for the Student Poster Award

- P2 **Rajan Adhikari**, R10: From Bits to Bonds–An Advanced SPM Platform
- P4 **Kim Noelle Dreier**, No Indication for a Reconstruction of Silver Iodide (0001) in Various Liquids
- P6 **Florian Schneider**, Chiral multilayer structures on dolomite (10.4)
- P8 **Matthias Zeilerbauer**, Investigation of well-defined donor-acceptor interfaces by non-contact atomic force microscopy and photoluminescence
- P10 **Jinhui Guo**, Simulations of the optical near-field enhancement for tip-enhanced photoexcitation on non-conductive layers
- P12 **Marie Luigs**, Atomic-scale insights into the selenite incorporation mechanism at the calcite-water interface
- P14 **Lorena Niggli**, Nanowire magnetic force microscopy for imaging vdW magnets in the 2D limit
- P16 **Noah Wulforst**, Self-Assembly of Benzoic Acid Derivatives on Calcite (10.4)
- P18 **Benjamin Achatz**, Implementation of Dissipation-based Kelvin Probe Force Microscopy for Quartz Tuning Fork Sensors
- P20 **Janine Lorenz**, Quantitative imaging of the surface potential of a single PTCDA molecule on Pb(111)
- P22 **Marco Thaler**, From Inert Nitrogen to Reactive Metal Nitrene: An On-Surface Route to N-Heterocycles
- P24 **Marion A. van Midden Mavrič**, Upgrading an STM to STM/ncAFM using a qPlus sensor
- P26 **Martin Setvin**, AFM Imaging of Electrochemically Grown Metal Sulphides
- P28 **Llorenç Albons Caldentey**, Unravelling the ferroelectric behaviour and atomic structure of cleaved BaTiO₃(001) surfaces with nc-AFM and PFM.
- P30 **Faith Lewis**, Structural Insights into Metal Coordination on Au(111) Supported Melem Networks

- P32 **Massimiliano Labardi**, Relaxation Kinetics of Thin Film Ultrastable Glasses via Frequency-Modulated Kelvin Probe Force Microscopy
- P34 **Zheng Rong Guo**, Development of a High-Bandwidth Low-Noise AFM with Optical Beam-Deflection Detection and Photothermal Excitation
- P36 **Harry Mönig**, Tip functionalization with oxygen-terminated copper probes
- P38 **Fabian Fleidl**, Probing Interfacial Water organization on In_2O_3
- P40 **Furkan Ruhi Özyigit**, First steps with a qPlus-based ultrafast mid-infrared AFM
- P42 **Ajay Kumar**, Modeling and Measurement of Distance-Dependent Electrostatic Interactions on Pb Islands
- P44 **Haruka Tsuji**, Development of UHV-LT qPlus AFM/STM System for On-Surface Synthesis @ NIMS
- P46 **Callum Hayward**, Quantifying lateral and normal threshold forces during room-temperature manipulation of C_{60} on $\text{Si}(100)\text{-}2\times 1$
- P48 **Nadine Hauptmann**, Influence of the surface corrugation to the charge density wave contrast of 2H-NbSe_2 in SPM images
- P50 **Martin Kronberger**, Automated, reproducible conditioning of SPM tips
- P52 **Ing-Shouh Hwang**, Laser Annealing for Reliable Preparation of Noble Metal-Covered $\text{W}(111)$ Single-Atom Tips in UHV
- P54 **Viktoria Waidbacher**, Adsorption of Phthalocyanine on Indium Oxide: Influence of the Metal Ions
- P56 **Freddie Carlisle**, Invasive and non-invasive probes of sub-K molecular diffusion
- P58 **Tzu-Chao Hung**, Adsorption geometry determination of three-dimensional molecular architectures
- P60 **Nikhil Seeja Sivakumar**, Metallic Longitudinal Electrostatic Screening in a Type-I Superconductor
- P62 **Voni Fulitasari**, Molecular Resolution Imaging of Trisodium Citrate Cluster on $\text{NaCl}(001)$ in Air Using Frequency Modulation Atomic Force Microscope
- P64 **Oliver Phillips**, Force-Based Characterisation of Bond Formation in Coupled Artificial Atoms

P66 **Lucas Andreas Scheibel**, Force Microscopy at the Electrified Solid-Liquid Interface with Tip Apex Modification

P68 **Philipp Rahe**, qAFM: A Python toolbox for quantitative analysis in NC-AFM

R10: From Bits to Bonds–An Advanced SPM Platform

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RHK Technology presents the R10 controller, an advanced scanning probe microscopy (SPM) platform designed for high-performance imaging, spectroscopy, and force-based experiments. It combines time-based data acquisition with a fully digital AFM/STM architecture and large FPGA-based processing to enable flexible multi-probe, multi-frequency operation and complex measurement workflows.

The improved hardware and software architecture enhances performance, signal bandwidth, and data throughput while maintaining long-term compatibility through a modular, upgradeable structure. A platform-independent Inventor SDK with Python, Matlab, or Labview support enables automated workflows and machine learning-driven upgrade paths.

These capabilities enable quantum-scale investigations, including scanning tunneling spectroscopy, single-atom or single-molecule manipulation, as well as spin- or charge-sensitive measurements. Complementary advanced AFM modalities such as multifrequency AFM, KPFM, MFM, and time-resolved AFM, extend the system's reach to nanoscale electrical, magnetic, and dynamical characterization. Together, they support the study of quantum materials, qubit systems, and atomic-scale transport and coherence phenomena.

The system is complemented by an intuitive control environment designed to ensure stable, efficient, and reproducible experimental operation across a wide range of applications.



Figure 1: R10 SPM Controller (top) and R10 HV Amplifier (bottom).

No Indication for a Reconstruction of Silver Iodide (0001) in Various Liquids

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Silver iodide (AgI) has long been known as a material that induces precipitation in clouds. The superior ice nucleation ability is commonly explained by the close lattice match between β -AgI(0001) and the basal plane of ice. However, this surface is polar, indicating that a stabilization mechanism should be present. Here, we investigate the Ag-terminated β -AgI(0001) and the I-terminated β -AgI(000 $\bar{1}$) surfaces in water, *n*-dodecane, 0.1 M NaCl, and 0.1 M KI aqueous solutions [1]. In contrast to measurements under ultra-high vacuum conditions [2], our high-resolution images recorded in liquids consistently reveal a bulk-truncated structure [1,3]. These findings and observations at a larger scale indicate the absence of any surface reconstruction. Although the observed structures reveal a variety of features and depend on the surface termination, some general conclusions can be drawn. First, in solvents with poor AgI solubility, only minor changes are observed. Second, even in KI solution where AgI can and does dissolve, no indication for a surface reconstruction can be found. These results shed new light onto the surface structure of β -AgI(0001), challenging the expectation that a surface reconstruction is present under ambient conditions.

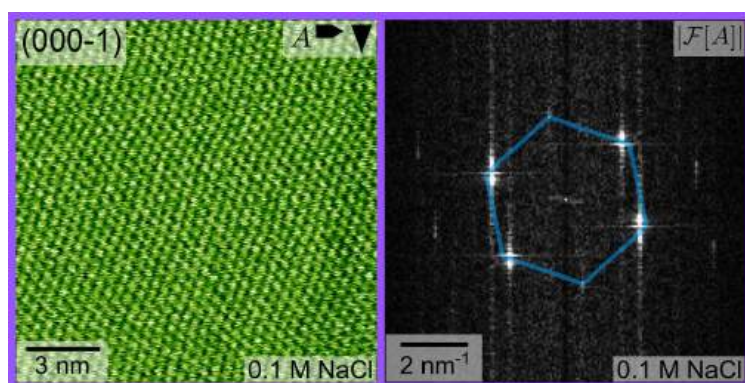


Figure 1: High-resolution AFM image of the AgI(000-1) plane in a 0.1 M NaCl aqueous solution with the corresponding fast Fourier transform. The spot positions in the FFT excellently match with XRD values for the bulk unit cell (blue hexagon). Figure taken and adapted from [1].

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Chiral multilayer structures on dolomite (10.4)

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Homochirality is a universal property of life on Earth, suggesting that it was initiated at the origin of life. To arrive at a homochiral state, a symmetry-breaking event has to create a chiral bias that can be amplified. However, the physical nature of this symmetry-breaking agent is still disputed. Chiral mineral-water interfaces might provide a simple and potentially ubiquitous symmetry-breaking mechanism as they can create enantioselective microenvironments. A promising candidate is the mineral dolomite ($\text{CaMg}(\text{CO}_3)_2$), whose most stable (10.4) surface is intrinsically chiral. Dolomite is reported to form in alkaline hydrothermal vent systems [1], which are a highly discussed plausible environment for life's emergence [2]. Here, we present high-resolution atomic force microscopy images of multilayer water structures grown on dolomite (10.4) in an ultra-high vacuum environment at 120 K. We observe the formation of chiral island borders and domain boundaries of the second water layer, clearly demonstrating a chirality transfer from the mineral surface to interfacial water structures. These findings support that chiral mineral surfaces might act as symmetry-breaking settings for prebiotic molecules.

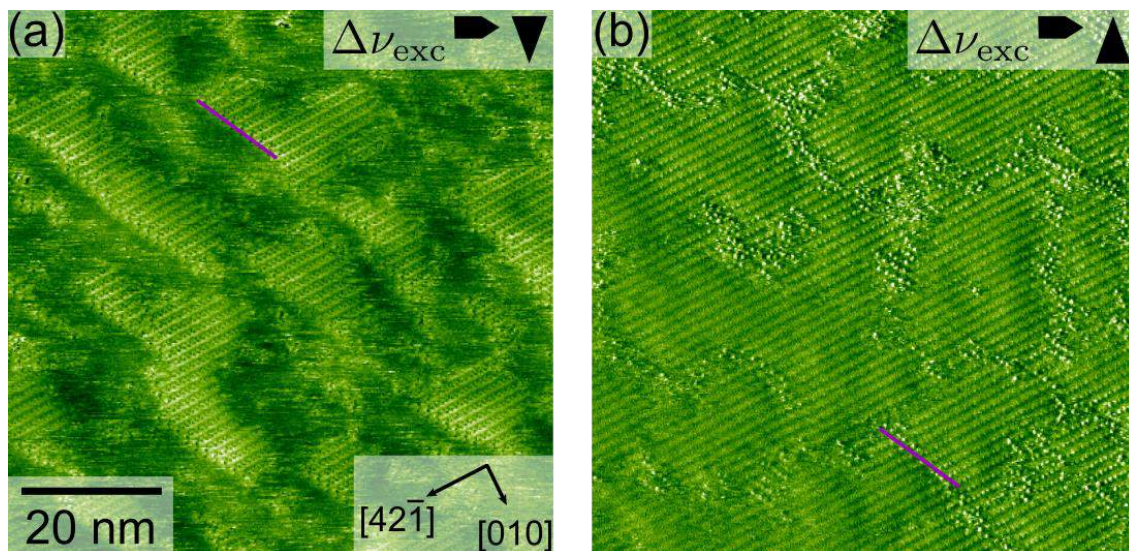


Figure 1: AFM images of the second water layer on dolomite (10.4): (a) Sub-monolayer coverage featuring several islands. (b) Full second-layer coverage with several domain boundaries. One direction of island and domain boundaries is predominantly expressed (violet lines). The direction arrows and scale bar apply to both images.

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Investigation of well-defined donor-acceptor interfaces by noncontact atomic force microscopy and photoluminescence

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Donor-acceptor model interfaces are essential for elucidating molecular-scale charge transfer, a fundamental process in organic solar cells [1]. Zinc tetraphenylporphyrin (ZnTPP) and perylenetetracarboxylic dianhydride (PTCDA) constitute a prototypical donor-acceptor pair ([3], [4]). Crystalline ZnTPP thin-films have been previously grown on Au(111) [2] and for film thicknesses above approximately 5 monolayers (ML) their photoluminescence (PL) becomes observable, consistent with electronic decoupling of the upper layers from the metal substrate and suppression of exciton quenching.

Here, we demonstrate the growth of PTCDA islands on top of ordered ZnTPP multilayers. The highly periodic ZnTPP donor film serves as an effective template for PTCDA adsorption, yielding well-defined PTCDA islands with lateral sizes up to ~10 nm under our preparation protocol (Figure 1). Non-contact atomic force microscopy (NC-AFM) at each stage provides topographic characterization. High-resolution images resolve the lattice periodicity of the flat, highly ordered films and quantify island height distributions, offering insight into interfacial ordering and interactions.

The photophysical properties of the donor thin-film and the combined donor-acceptor system were investigated by means of PL. From the layer thickness-dependent PL spectra of the ZnTPP donor-system we could determine an optimal multilayer-thickness for effectively decrease the exciton quenching, opening up a pathway to a long-lived charge-transfer state at the D-A interface.

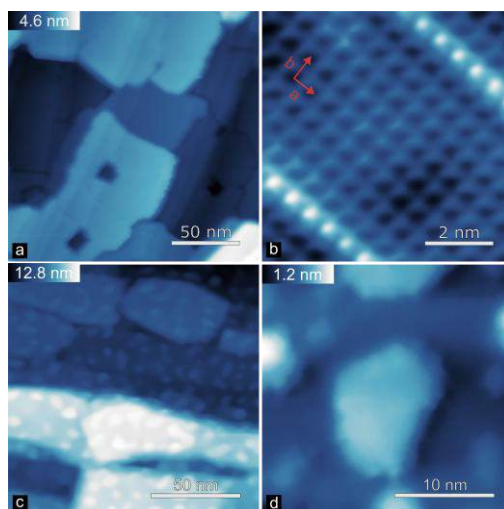


Figure 1: NC-AFM images of a) ZnTPP-multilayer (~20 ML)/Au(111) substrate b) Detail image on the multilayer, where the lattice vectors are indicated. c) Overview image of PTCDA islands on top of a ZnTPP-multilayer (~20 ML)/Au(111) substrate and d) Detail image of the PTCDA islands.

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Simulations of the optical near-field enhancement for tip-enhanced photoexcitation on non-conductive layers

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In tip-enhanced Raman spectroscopy (TERS), excitation of localized surface plasmons at the junction between a sharp metal tip and a substrate produces a strongly local enhancement of the optical electromagnetic field [1]. The near-field enhancement (NFE) further enables tip-enhanced photoluminescence (TEPL) in scanning tunneling microscopy (STM)-based setups for molecules deposited on two to four monolayers (ML) of NaCl on Ag substrates [2]. However, nonradiative quenching given by charge tunnelling through the insulating layer typically shortens the exciton lifetime [3]. Using sufficiently thick insulating layers (> 14 ML) strongly suppresses electron tunnelling [4], thereby minimizing the quenching of the photoexcitation. While such thick insulating layers preclude the use of STM, atomic force microscopy (AFM), in contrast, maintains stable feedback via force gradients [5].

Here, to elucidate the field enhancement in AFM-based TEPL experiments, we performed three-dimensional finite element method (3D-FEM) simulations [6] for various AFM-tip geometries and Cu substrates, with and without NaCl layers up to 20 ML. Our results confirm that a blunt tip with an atomic-scale protrusion realistically models the experimental tip. Under p-polarized illumination, where the electric field of the incident light is predominantly aligned along the z-axis, a highly localized in-plane NFE is surprisingly observed (see Figure 1a), resulting in a pronounced enhancement of approximately fivefold at the molecular adsorption plane (see Figure 1b). This enables efficient coupling to the transition dipole moments of planar organic molecules. Notably, this enhancement persists for NaCl films up to 20 ML, consistent with the reduced screening of in-plane fields in NaCl compared with metallic Cu, which yields an in-plane enhancement of about sevenfold. These findings motivate the use of nonconductive spacer layers for tip-enhanced photoexcitation experiments.

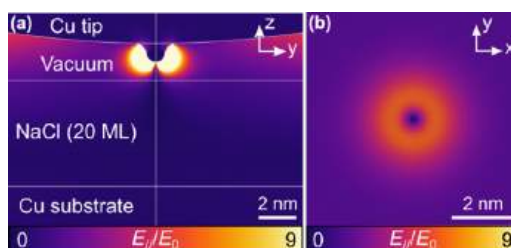


Figure 1: Simulated in-plane NFE ($E_{||}/E_0$) plots under p-polarized light. (a) NFE distribution in the y-z plane for the Cu tip-NaCl (20 ML)-Cu substrate system. (b) NFE distribution in the x-y plane 3 Å above the NaCl surface, for the same system. The incident light propagates along the x-direction with an angle of 5° .

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Atomic-scale insights into the selenite incorporation mechanism at the calcite-water interface

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Sequestration through incorporation into minerals represents a significant sorption mechanism for pollutants. Selenium is an essential trace element vital for human health, however, the margin between its required and toxic intake is exceedingly narrow [1]. Moreover, selenium ^{79}Se is a fission product of uranium ^{235}U , turning this long-lived radioisotope into an isotope of concern for the long-term safety of nuclear waste repositories. In this context, calcite, an abundant mineral in the Earth's crust, is interesting as a possible sorption material. Due to the structural similarity, selenite (SeO_3^{2-}) can replace carbonate (CO_3^{2-}) in the calcite crystal [2,3]. Regarding the molecular-level incorporation mechanism, however, different scenarios can be envisioned. Besides incorporation during growth, a possible incorporation mechanism is ion exchange, i.e., a carbonate group exposed at the surface is exchanged by a selenite group. Here, we present atomically resolved atomic force microscopy images collected at the interface of calcite and solutions with different selenite concentrations. Our data reveal distinct differences in the surface structure of terraces grown in the presence of selenite compared to those grown without it. In contrast to these findings, no change could be observed for surfaces exposed to selenite-rich solutions in the absence of growth. Our results thus confirm incorporation of selenite during growth, while the incorporation through ion exchange appears to be either absent or a mechanism, which is too slow to be observed.

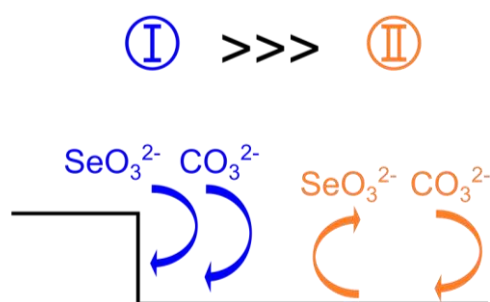


Figure 1: Schematic of selenite incorporation into the calcite surface via growth (I) or ion exchange (II).

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Nanowire magnetic force microscopy for imaging vdW magnets in the 2D limit

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Magnetic force microscopy (MFM) using a nanowire (NW) cantilever as the scanning probe allows for the imaging of especially weak magnetic field patterns on the nanometer scale [1, 2]. Compared to conventional MFM, such NW transducers result in a higher sensitivity due to their reduced size and high aspect ratios, making them ideal probes to study the behavior of van der Waals (vdW) magnets in the two dimensional limit. Here, we demonstrate the fabrication of NW-MFM probes using a combination of metal-assisted chemical etching of silicon to produce the NWs, followed by focused-electron-beam-induced deposition (FEBID) of cobalt to form the magnetic tips. We characterize the mechanical and magnetic properties of such NWs and show their use as MFM probes through stray field imaging at variable magnetic fields and temperatures.

In addition, we demonstrate that NW-MFM is capable of imaging the local magnetic susceptibility near magnetic phase transitions through spatially-resolved dissipation measurements [3]. This allows not only to investigate the layer number dependence of the magnetic phase transition temperature of 2D vdW magnets, but can also be applied to systems where different magnetic orders coexist [3].

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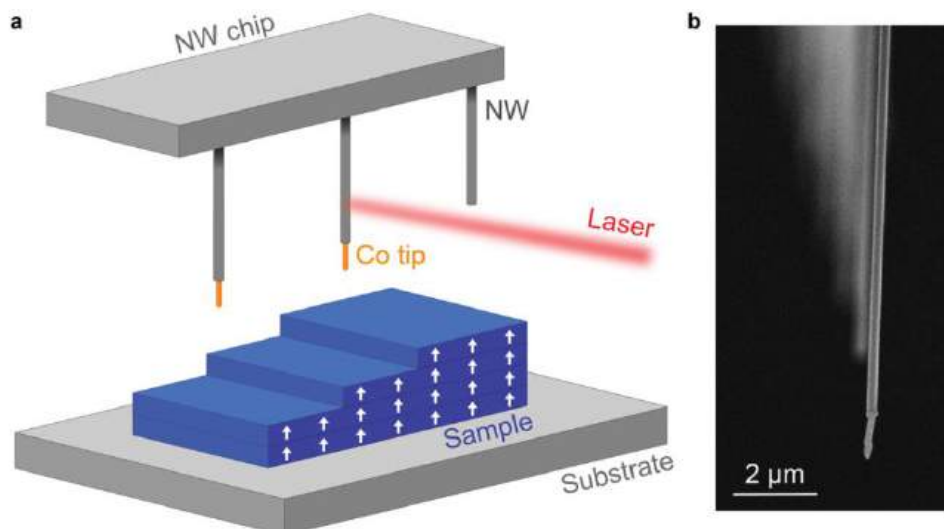


Figure 1: (a) Schematic of nanowire magnetic force microscopy employing a magnet-tipped nanowire as a scanning probe, whose flexural motion is detected interferometrically using focused laser light. (b) SEM micrograph of a Co-tipped Si nanowire grown by FEBID.

Self-Assembly of Benzoic Acid Derivatives on Calcite (10.4)

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Self-assembly of molecules on surfaces offers significant potential for building complex functional structures at the molecular level. Such structures have become increasingly relevant in recent years with the rising demand for smaller and ever more efficient electronic components. Here, we explore the influence of small functional groups on molecular self-assembly. We investigate a set of benzoic acid derivatives on the calcite (10.4) surface by atomic force microscopy under ultra-high vacuum conditions. The benzoic acid derivatives chosen for this study feature an additional substituent, an alteration of the carboxy group or both. The resulting self-assembled structures can be divided into three categories based on their unit cell dimensions and the proposed binding motif towards calcite. The various binding schemes are explored by comparison with previously published structures of other benzoic acid derivatives [1,2]. Our study highlights the decisive influence of small functional groups on molecular self-assembly and presents a promising approach for developing tailored structures through the targeted design of building blocks.

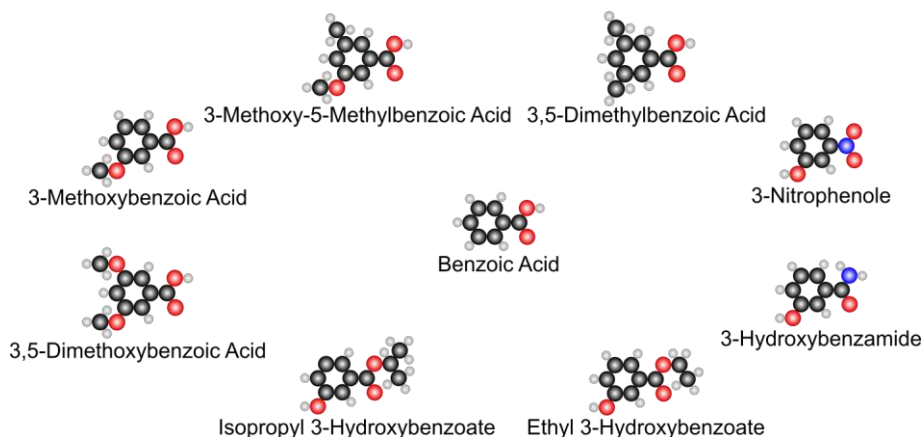


Figure 1: Overview of benzoic acid derivatives investigated in this study.

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Implementation of Dissipation-based Kelvin Probe Force Microscopy for Quartz Tuning Fork Sensors

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Kelvin probe force microscopy (KPFM) is a powerful tool for probing local variations of surface dipoles [1]. For quartz tuning forks [2], the spatial distribution of the local contact potential difference (LCPD) is commonly mapped by acquiring grids of frequency shift (Δf) versus bias (V) spectra [3]. Although this approach enables resolving charge distribution with sub-molecular resolution [3,4,5], it suffers from long acquisition times (typically several hours for an image).

Here, we implement dissipation-based KPFM (D-KPFM), previously introduced for silicon cantilevers by Miyahara et al. [6], for quartz tuning forks operated in ultra-high vacuum at low-temperatures (≈ 8 K). In this method, electrostatic forces are continuously minimized during scanning, enabling the simultaneous acquisition of LCPD and electrostatically compensated Δf images. Furthermore, we introduce a novel heterodyne KPFM approach that operates the sensor in bimodal mode. We demonstrate that both methods reduce the acquisition time by more than an order of magnitude compared to spectroscopy-based KPFM, without compromising lateral resolution. This advance enables rapid acquisition of three-dimensional KPFM datasets, in which the LCPD is mapped not only laterally but also as a function of tip-sample separation, yielding volumetric reconstructions of surface potential.

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Quantitative imaging of the surface potential of a single PTCDA molecule on Pb(111)

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Scanning quantum dot microscopy (SQDM) uses a low-temperature, non-contact atomic force microscope to map electrostatic potentials with unprecedented nanometer resolution [1]. From such electrostatic potential maps, the quantitative surface dipole of e.g., a molecule on a metal surface can be obtained by integrating over the measured electrostatic potential map. Measurements of a single organic PTCDA molecule adsorbed on an Ag(111) surface yield an experimental dipole moment of -0.65 Debye [2]. We now experimentally measure how the dipole of PTCDA changes when deposited on Pb(111). Interestingly, we find that the PTCDA molecule has a more than five times larger dipole when adsorbed on Pb(111), compared to Ag(111). This can be attributed to a significantly different charge transfer and adsorption height. Comparing the dipole of PTCDA on Pb(111) in the superconducting and non-superconducting state, we observe no significant change.

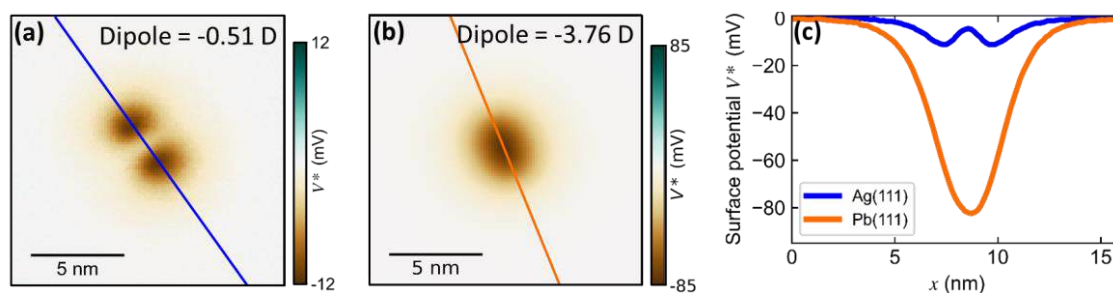


Figure 1: Electrostatic potential maps of a single PTCDA molecule in (a) on Ag(111) and in (b) on Pb(111). (c) Direct comparison of the surface potential extracted along the marked lines in (a) and (b).

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From Inert Nitrogen to Reactive Metal Nitrene: An On-Surface Route to N-Heterocycles

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Nitrenes are highly reactive intermediates in organic chemistry and play a key role in the synthesis of nitrogen containing compounds. In solution, nitrenes are typically generated from chemically activated precursors (e.g., azides), whereas direct conversion of primary amines remains challenging due to the inherent strength of N-H bonds. On surfaces, reactive nitrenes have likewise been formed from organic azides [1]; however, azides are thermally and photochemically labile and can decompose violently upon exposure to heat, light, or mechanical shock, posing safety risks. Here, using combined scanning tunneling microscopy (STM), non contact atomic force microscopy (nc-AFM), and density functional theory (DFT), we demonstrate the thermally activated formation of a surface stabilized metal-nitrene intermediate from a chemically inert amine, which mediates the on-surface formation of a nitrogen-containing heterocycle. Our findings establish non activated nitrogen functionalities as viable nitrene precursors and reveal new mechanistic pathways for on-surface synthesis of N-heterocyclic compounds.

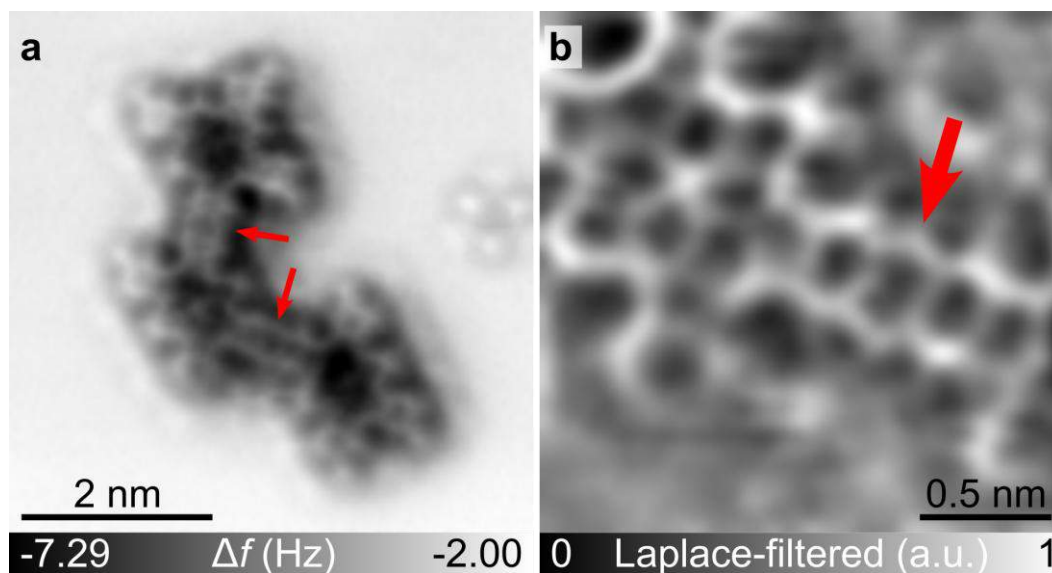


Figure 1: a) Bond-resolved constant-height nc-AFM image acquired with a CO-functionalized tip, showing the on-surface reaction product. b) Laplace-filtered close-up of the newly formed N-heterocyclic ring (see red arrows).

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Upgrading an STM to STM/ncAFM using a qPlus sensor

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Combining STM with ncAFM enables simultaneous measurements of the tunneling current and force between the tip and the sample, making it possible to disentangle topography and electronic contributions on the atomic scale. We report on the implementation and operation of a commercially available qPlus sensor [1] upgrade for a Besocke type Createc low-temperature scanning tunneling microscope (STM).

While the hardware integration itself is straightforward in principle, reliable ncAFM performance requires addressing several practical challenges related to mechanical stability, electrical noise, sensor wiring, resonance characterization, and controller integration.

We discuss the modifications performed on the microscope head and electronics. Particular attention is given to sample holder modifications to facilitate the measurements of quasi-low-dimensional materials which are well known to sometimes have unstable or flaky surfaces. We also discuss our strategies to reduce vibration coupling and how we optimized the grounding and minimized cross-talk between the different signals. By presenting our experiences we hope to open a discussion about the different strategies and solutions which would be beneficial for groups using similar setups.

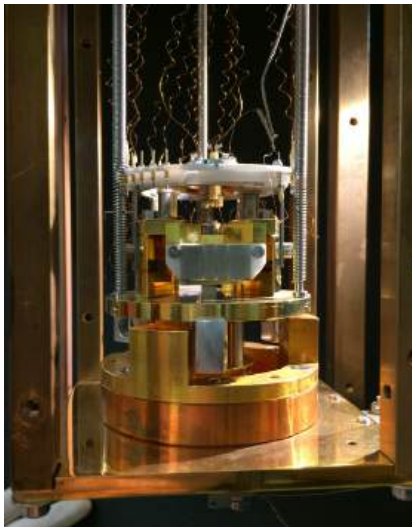


Figure 1: Modified Createc low-temperature STM head which will be used for combined STM/ncAFM operation.

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AFM Imaging of Electrochemically Grown Metal Sulphides

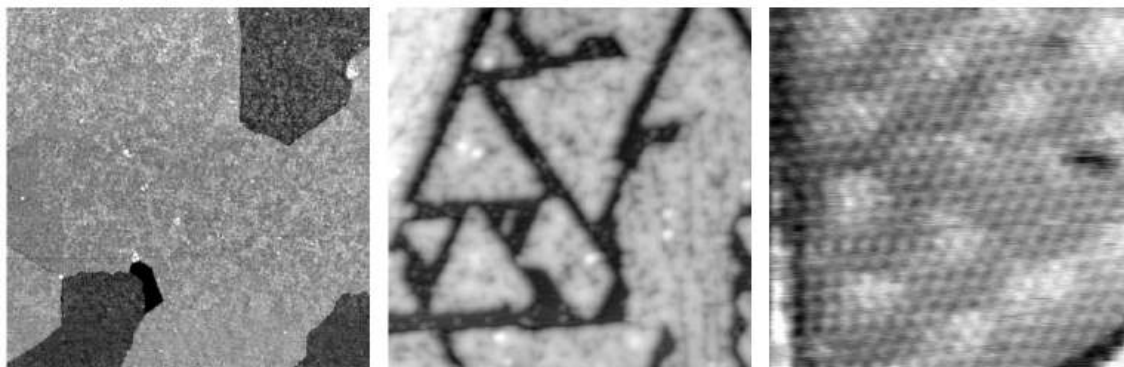
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Noncontact AFM in the q-Plus setup is typically used to provide atomically resolved images of various surfaces prepared under UHV conditions. However, the technique turns out to be powerful also for resolving the structure of surfaces exposed to harsher conditions such as liquid or ambient environment. Here we focus on imaging transition metal sulphides prepared electrochemically under liquid environment, namely Ag_2S and Cu_2S films grown on single crystals of the respective metals. These sulphides can be prepared in various thicknesses, ranging from a layer of adsorbed sulphur, through a trilayer sulphide sheet, up to bulk sulphide. The general morphology, atomically resolved imaging, and the structure of these films is discussed.



Left: Overview STM morphology image of a thick Cu_2S film, $500 \times 500 \text{ nm}^2$. **Middle:** Morphology of a submonolayer film of Ag_2S , $80 \times 80 \text{ nm}^2$. **Right:** Atomically resolved AFM image of the Ag_2S trilayer, $6 \times 6 \text{ nm}^2$.

Unravelling the ferroelectric behaviour and atomic structure of cleaved BaTiO₃(001) surfaces with Nc-AFM and PFM.

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Ferroelectric polarization can be used to dynamically modify the surface structure and electronic properties of ferroelectric catalysts and enhance their efficiency and selectivity [1]. However, the lack of understanding of the effects of bulk polarization on the surface's atomic and ferroelectric structure is a major roadblock towards the improvement of such catalysts [2]. BaTiO₃ is not only a model system for investigating fundamental properties and phenomena that manifest at the surface of ferroelectric materials, but also a promising material for prospective use as a ferroelectric catalyst.

In this work we demonstrate that one can prepare a pristine BaTiO₃ (001) surface by cleaving single crystals in UHV and characterize it with atomic resolution using the qPlus nc-AFM/STM. Poling the crystals at 70°C before cleaving induces a strong preferential polarization, which we successfully use to obtain either a BaO or TiO₂ terminated surface. We prove that the ferroelectric structure of the bulk crystal plays a dominant role in determining not only the structure, but also the properties of the cleaved surfaces. Moreover, we explore the surface structure and polarization at different temperatures and show that the 1×1 bulk-terminated surface persists upon transitions between different ferroelectric phase transitions but is destroyed if brought to the paraelectric phase.

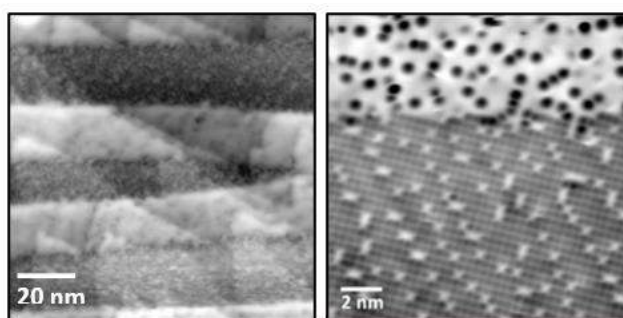


Figure 1: Constant frequency AFM image of the BaTiO₃ (001) two-terminated surface (left) and constant height AFM image of the surface's atomic structure (right).

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Structural Insights into Metal Coordination on Au(111) Supported Melem Networks

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Single-atom catalysis (SAC) is a rapidly growing field of research that combines the advantages of solid supports from heterogeneous catalysis with the tunability of active sites in homogeneous catalysis. SACs also lead to well-defined single-atom centers which can achieve high selectivity. Recently, graphitic carbon nitride (g-C₃N₄) has been identified as a framework to stabilize SACs that facilitate reactions such as the ORR and HER. The precursor, melem (2,5,8-triamino-heptazine) is typically polymerized, and the resulting structure features a network of 6-fold nitrogen pockets which stabilize the single atoms. The g-C₃N₄ framework is a common conceptual baseline for these catalysts, yet its structural specifics are increasingly debated, with recent studies directly challenging the prevailing model.¹ X-ray absorption spectroscopy (XAS) suggests a 4-fold metal coordination with equal bond lengths, a geometry that cannot exist within the often-proclaimed 6-fold pocket of g-C₃N₄.

In this work, we use the surface science approach to reconcile this contradiction through scanning probe microscopy (SPM) and X-ray photoelectron spectroscopy (XPS). On an Au(111) single crystal, melem forms a honeycomb overlayer that is stabilized through hydrogen bonding of the amino groups on the corners with the pyridinic nitrogens on the sides of the triangular molecule. When melem and metals, specifically Ni and Fe, were co-deposited at various temperatures onto Au(111), different overlayers formed. At lower temperatures, more densely packed regions of the same triangular features form next to the honeycomb structure. At higher temperatures, two different motifs form depending on the metal. With Fe, the densely packed regions observed at lower temperatures dominate, while for Ni a new structure appears in which the triangular melem molecules are no longer recognizable on the surface. We conclude this is the result of polymerization and formation of a 2D layer.

Our results indicate that, under these conditions, the Fe-melem species forms dimeric complexes centered by a metal atom. The resulting square-planar coordination environment aligns closely with recent XAS observations, offering a structural explanation for the 4-fold coordination.

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Relaxation Kinetics of Thin Film Ultrastable Glasses via Frequency-Modulated Kelvin Probe Force Microscopy

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Vapor-deposited organic glasses transform via a liquid front that propagates from free surfaces at a constant velocity. However, this can be suppressed by capping the free surface with other organic materials that have a higher glass transition temperature, leading to an anomalous transformation dynamics through the formation of isolated liquid-like regions that grow consuming the remaining glass by kinetic facilitation. AFM can follow transformation kinetics by detecting small surface wrinkles that form in liquid-like regions, serving as a reliable proxy for dynamic analysis [1]. We have applied FM-KPFM to detect changes in surface potential due to the transformation into supercooled liquid below the capping layer [2]. We assessed the dependence of both sensitivity and resolution of this method on the capping layer thickness.

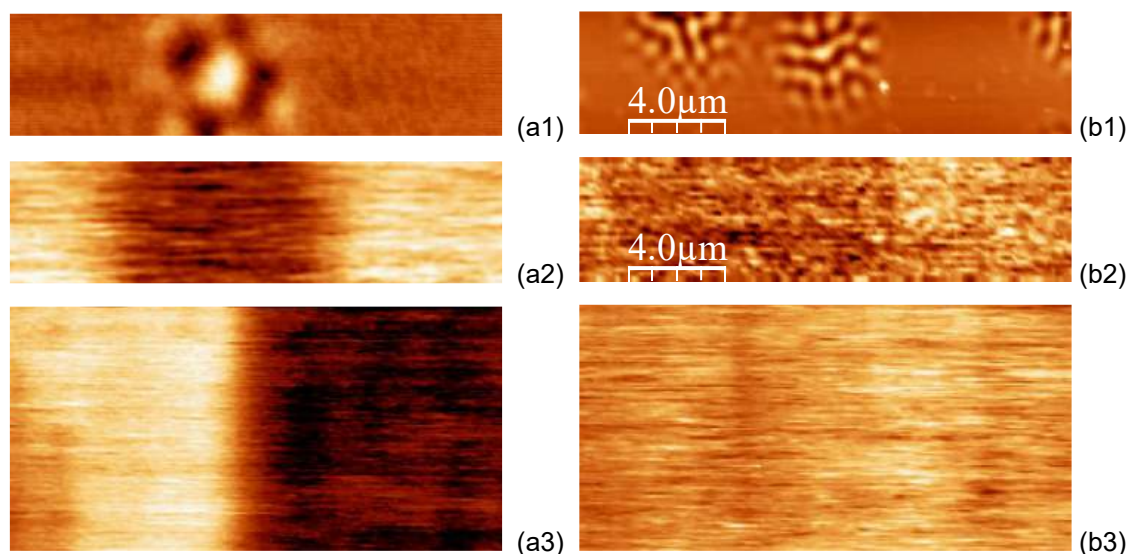


Figure 1: Topography scans of an ultrastable glass after nucleation of liquid domains, for samples with (a1) 13 nm and (b1) 25 nm capping layer thickness. (a2) and (b2): corresponding Kelvin potential maps. Width of images (a1) and (a2) is 5 μm . (a3) and (b3): repeated Kelvin potential profiles (128 scans) across the interface (image width 1 μm). Boltzmann fitting of averaged profiles provides interface width of (a3): 19 ± 2 nm, (b3): 27 ± 9 nm.

Acknowledgements. Partially supported by ONR Global NICOP N62909-23-1-2003 research grant. M. R.-R. acknowledges CEX2021-001214-S/MICIU/AEI/10.13039/501100011033 grant.

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Development of a High-Bandwidth Low-Noise AFM with Optical Beam-Deflection Detection and Photothermal Excitation

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Achieving high-resolution atomic force microscopy (AFM) necessitates displacement detection systems that exhibit both low noise and high sensitivity, while measurements exploiting higher-order cantilever eigenmodes additionally require a broad detection bandwidth. These specifications are particularly critical for advanced, high-performance AFM measurements. To meet these demands, we developed a high-bandwidth AFM platform that combines low-noise optical beam-deflection (OBD) detection with high-bandwidth photothermal cantilever excitation, enabling both conventional dynamic-mode and higher-eigenmode AFM operation. The system incorporates a custom-designed OBD detector and a self-developed blue-laser excitation module for photothermal actuation of AFM cantilevers. The detection system attains an OBD bandwidth of approximately 25 MHz, whereas the blue-laser excitation module provides a modulation bandwidth exceeding 10 MHz, with a laser-driver current noise of approximately $1 \text{ nA}/\sqrt{\text{Hz}}$. The platform further supports stable deflection-signal acquisition under high-gain dynamic-mode conditions, allowing the deflection signal to be used for accurate reconstruction of the true surface topography. Using standard dynamic-mode cantilevers, the system achieves a deflection sensitivity of 0.98 V/nm and a deflection noise density below $4.5 \text{ fm}/\sqrt{\text{Hz}}$, approaching the theoretical shot-noise limit of optical detection. Thermal noise spectra acquired in both air and liquid clearly resolve the thermal vibrations of higher-order resonances. The performance of the platform was validated through high-resolution AFM imaging experiments in air and in aqueous environments, including investigations of interfacial water-layer structures. These results demonstrate the capability of the proposed system to enable low-noise, high-bandwidth AFM measurements and to facilitate quantitative studies involving higher cantilever eigenmodes.

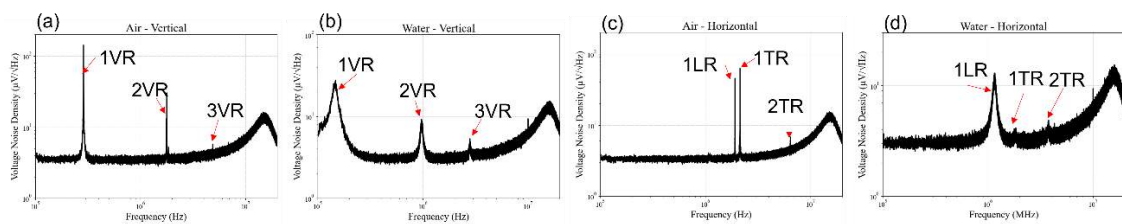


Figure 1: Thermal noise spectra of a NCH cantilever recorded with 2.5 mW incident power on the QPD. (a) VRs measured in air: 1VR (287 kHz), 2VR (1.78 MHz), 3VR (4.87 MHz). (b) VRs measured in water: 1VR (0.15 MHz), 2VR (0.97 MHz), 3VR (2.81 MHz). (c) Horizontal channel measured in air: 1LR (1.91 MHz), 1TR 2.14 MHz, 2TR (6.44 MHz). (d) Horizontal channel measured in water: 1TR (1.16 MHz), 1LR (1.82 MHz), 2TR (3.76 MHz). Vertical resonances (VRs), Torsional resonances (TRs), Lateral resonances (LRs).

Tip functionalization with oxygen-terminated copper probes

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NC-AFM imaging with atomically defined tip terminations in conjunction with the qPlus force sensor technology have led into a new era in surface science [1,2]. Tip functionalization with carbon monoxide molecules is by far the mostly utilized approach in the field [2]. The use of oxygen-terminated copper tips (CuOx-tips) constitutes an alternative approach, which not only provides sub-molecular resolution with reduced imaging artefacts [3], but also a robust chemically selective contrast on metal oxide- [4], ionic- [5], and heterogeneous 2D material surfaces. Furthermore, in direct comparability to other tips, CuOx-tips showed superior performance in atom manipulation experiments [6].

On the present poster I will give an overview of the recent progress in CuOx-tip functionalization and discuss future challenges and perspectives.

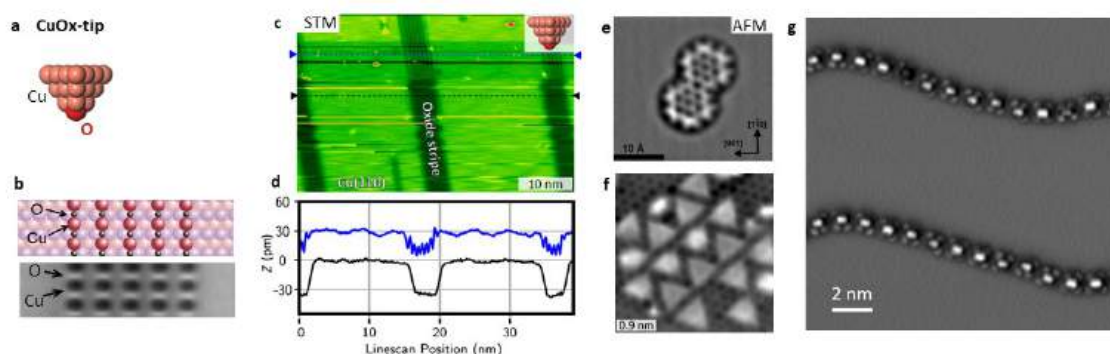


Figure 1: a) O-terminated copper tip (CuOx-tip). b) Constant-height AFM image recorded with a CuOx-tip on an oxide stripe of a partially oxidized (2x1)O Cu(110) surface serves as an unambiguous fingerprint for a CuOx-tip termination [7]. c,d) STM data recorded during CuOx-tip preparation [7]. After successful functionalization, CuOx-tips can be transferred to other substrate for imaging and force spectroscopy experiments [3]. e-g) Constant height AFM on a dicoronylene molecule [3], deprotonated and chemisorbed melamine [8], and polymerized N-heterocyclic carbenes [9].

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Probing Interfacial Water Organization on In_2O_3

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Indium(III) oxide (In_2O_3) is a well-established transparent conductive oxide with widespread applicability across diverse technological domains, including electrochemical catalysis, photoelectronic devices, and gas-sensing platforms.

Prior investigations of the $\text{In}_2\text{O}_3(111)$ surface under ultra-high vacuum (UHV) conditions combining noncontact atomic force microscopy (nc-AFM), scanning tunneling microscopy (STM), and density functional theory (DFT) calculations, have revealed a pronounced chemical heterogeneity within the large (1×1) unit cell.¹ Water dissociates and adsorbs selectively in specific regions of the unit cell, while an adjacent nanoscopic pocket remains water-free at all coverages. The first water layer thus organizes into nanoclusters separated by hydrophobic domains, revealing an amphiphilic character of the surface at the nanoscale.

Here, we employ in-liquid qPlus AFM/STM² surface imaging and z-spectroscopy³ to probe this system at the solid-liquid interface in the presence of bulk water. Surface imaging resolves the lateral organization of the solvated surfaces in situ, while z-spectroscopy captures normal density fluctuations in the near-surface region. Together, these complementary techniques enable us to assess whether the nanoscopic hydrophilic-hydrophobic heterogeneity identified under UHV conditions persists and influences the structural organization of interfacial water layers at the fully solvated interface.

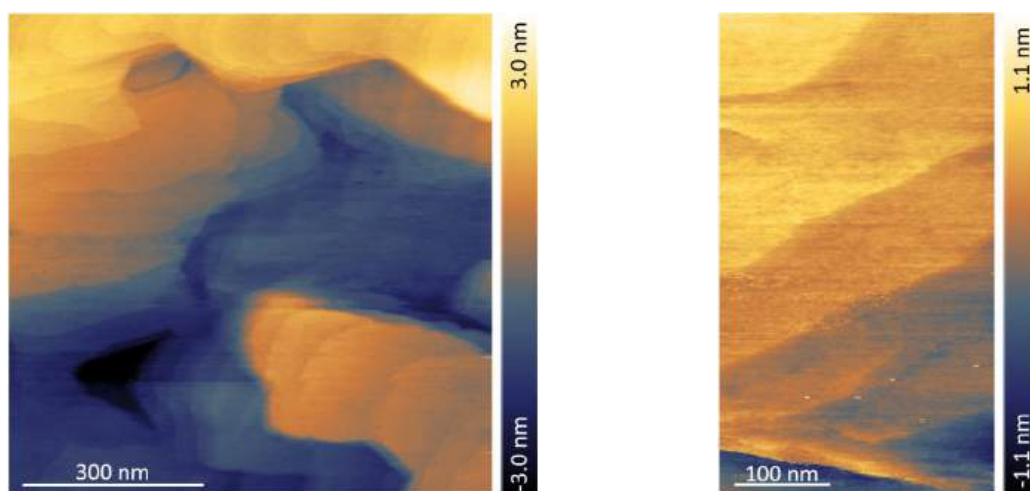


Figure 1: In-situ STM images of $\text{In}_2\text{O}_3(111)$ in ultra-pure bulk water ($V_{\text{bias}} = -50$ mV; $I_T = 100$ pA)

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First steps with a qPlus-based ultrafast mid-infrared AFM

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We report initial progress on an ultrafast non-contact atomic force microscopy/scanning tunneling microscopy (NC-AFM/STM) platform based on qPlus sensors, integrated with a carrier-envelope phase stabilized sub-cycle mid-infrared (MIR) pump-probe system. In first experiments, MIR pulses successfully induced transient tunneling currents on Cu(111) (Fig. 1 b), marking the first step toward controlled ultrafast electronic excitation in the tunneling junction.

While the tunneling current captures the underlying electronic dynamics, the qPlus sensor provides complementary force detection, enabling access to subsequent structural and electrostatic responses such as charge redistribution and lattice relaxation. This combined approach allows simultaneous probing of electronic and mechanical dynamics with femtosecond temporal and sub-nanometer spatial resolution.

The current focus is on tunneling current modulation of the electrostatic force, the so called phantom force effect, with the aim of resolving single-electron force dynamics on the Si(111) 7×7 surface using optical pump-probe techniques [1].

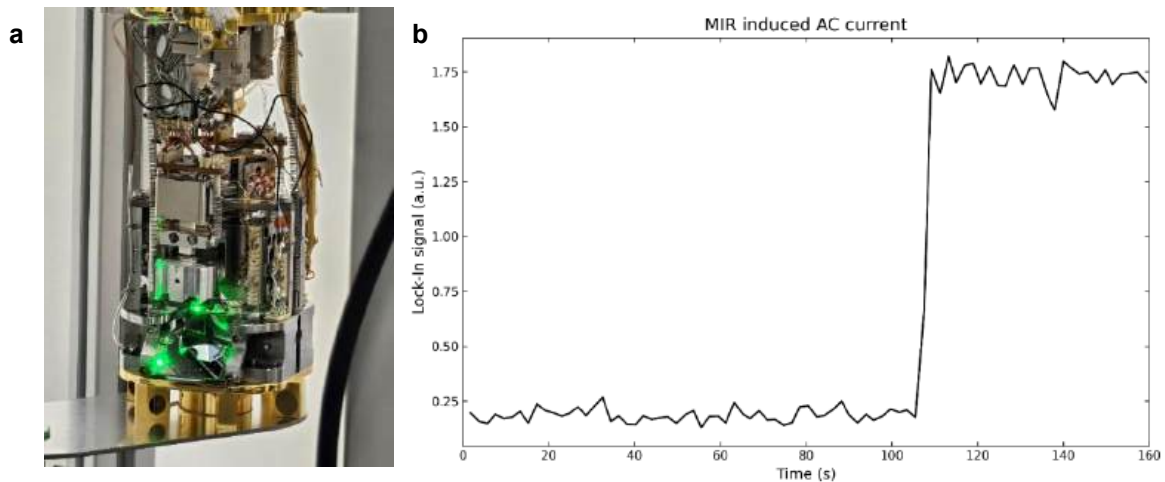


Figure 1: **a** STM/AFM head outside of its UHV chamber during adjustment of the optical pathway to the tip. **b** Chopped MIR pulses are focused on the tip-sample junction on a Cu(111) surface at 0 V applied bias revealing a clear AC signal in the Lock-In Amplifier that indicates MIR induced tunneling current between tip and sample serving as a first milestone of the ultrafast AFM setup.

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Modeling and Measurement of Distance-Dependent Electrostatic Interactions on Pb Islands

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Understanding the dependence of interactions between a tip and the sample with varying separation is essential for quantitative Kelvin probe force microscopy (KPFM), in particular for revealing electrostatic interactions including the underlying contact potential difference (CPD), at the nanoscale. In this study, Pb islands on the Si (111)-7×7 reconstructed surface serves as a model system of metallic islands on a semiconducting substrate. Using frequency modulation scanning force microscopy at 120 K, we performed frequency-shift bias spectroscopy during tip approach measurements to investigate the distance-dependent CPD. Furthermore, the electrostatic interaction at Pb island edges was analyzed using a two-charge-stripe model based on a corresponding solution of Poisson's equation. This approximate model is intended to study the impact of lateral symmetry breaking due to the diffusion of charges across the metal-semiconductor interface similar to Schottky junctions. Analytical and numerical results are compared with experimental data, providing insight into the force-distance behavior and edge-related electrostatic effects.

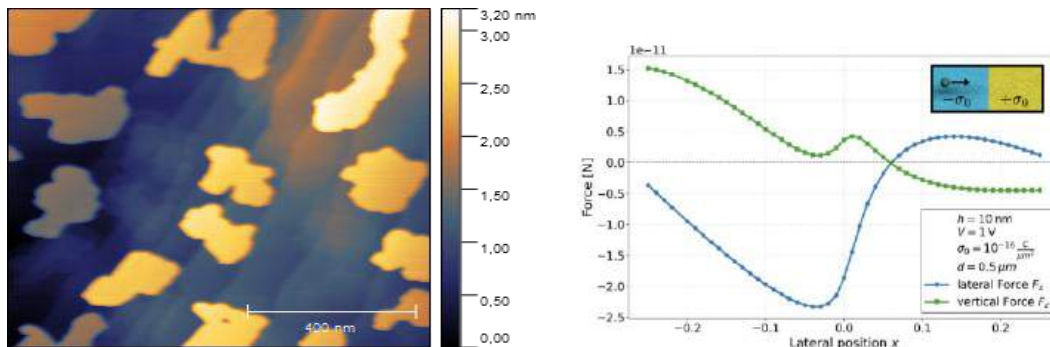


Figure: Topography and force vs lateral position plot of Pb on Si (111).

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Development of UHV-LT qPlus AFM/STM System for On-Surface Synthesis @ NIMS

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On-surface synthesis is a synthetic method in which molecular precursors are deposited and reacted on well-defined solid surfaces, offering a powerful approach to constructing nanostructures. One of the advantages of on-surface synthesis is precise elucidation of reaction mechanisms through structural analysis of precursors, intermediates, and products. To date, the development of various on-surface reactions has enabled the construction of a variety of nanoarchitectures.^[1]

The qPlus sensor^[2] has been widely used as a force sensor for high-resolution non-contact atomic force microscopy (nc-AFM). High-resolution qPlus nc-AFM with a CO-terminated tip enables direct visualization of chemical structures^[3], and therefore plays an important role in identifying products obtained by on-surface synthesis and investigating reaction mechanisms.

Recently, we developed an AFM/STM system by integrating a microscope head specially designed by UNISOKU into our home-built UHV system, employing an 8.5 L Cryovac bath cryostat (Figure 1a). The holding time of liquid helium at 4.5 K is approximately 190 hours, and the temperature can be lowered by pumping the cryostat down to about 2.0 K. The preamplifier for the qPlus sensor was installed at the bottom of the microscope at 4.5 K, following the procedure described in a previous article (Figure 1b)^[4].

To evaluate the system's performance, we first conducted STM experiments. Through on-surface synthesis, hexabenzocoronene and its derivatives were obtained. Using a CO-functionalized tip, we achieved chemical structure visualization (Figure 1c). AFM mode is currently under preparation. We have confirmed that the Q-factor reaches up to 60,000 at 4.5 K. However, we noticed significant variation in this value and encountered noise during the tip approach using the piezo motor. We are currently optimizing the tip holder and piezo motor to improve the AFM operation performance.

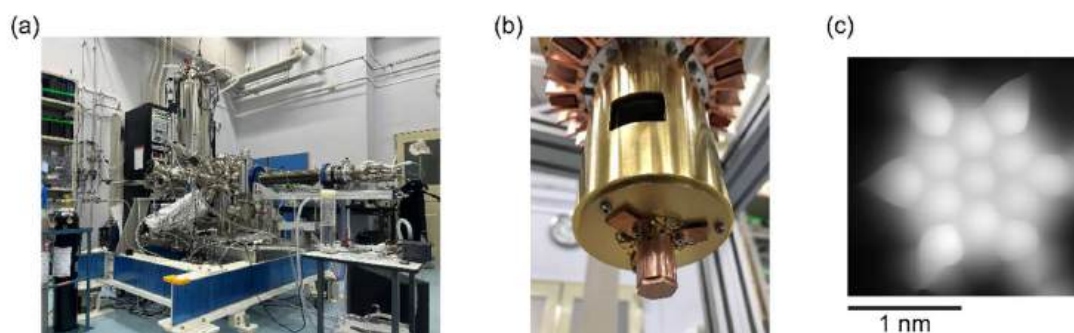


Figure 1: (a) Photograph of LT-AFM/STM system. (b) Low temperature preamplifier for the qPlus sensor. (c) Constant height STM image ($V = 4$ mV)

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Quantifying lateral and normal threshold forces during room-temperature manipulation of C₆₀ on Si(100)-2×1

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Scanning probe microscopy (SPM) enables the controlled manipulation of atoms and molecules with atomic-scale precision. While most molecular manipulation studies are performed at cryogenic temperatures on metallic surfaces [1][2], room-temperature (RT) manipulation remains significantly more challenging due to thermal diffusion and increased adsorbate mobility [3].

Here, we investigate the manipulation of individual C₆₀ molecules on the Si(100)-2×1 surface at RT using non-contact atomic force microscopy (NC-AFM). Two-dimensional force maps were acquired during manipulation events to determine both the normal (F_z) and lateral (F_x) threshold forces required to induce molecular motion both parallel and perpendicular to the Si dimer rows, which occurs via a ‘rolling’ mechanism [4].

We use the reproducibility of these rolling events to obtain direction- and pathway-dependent threshold force distributions from a large number of manipulation events and elucidate the difference in forces required for manipulation in different directions in a highly anisotropic potential landscape, including variations in force response immediately preceding molecular motion.

These results establish NC-AFM as a quantitative probe of molecular manipulation dynamics at RT and provide a framework for the statistical analysis of nanoscale force thresholds during molecular motion.

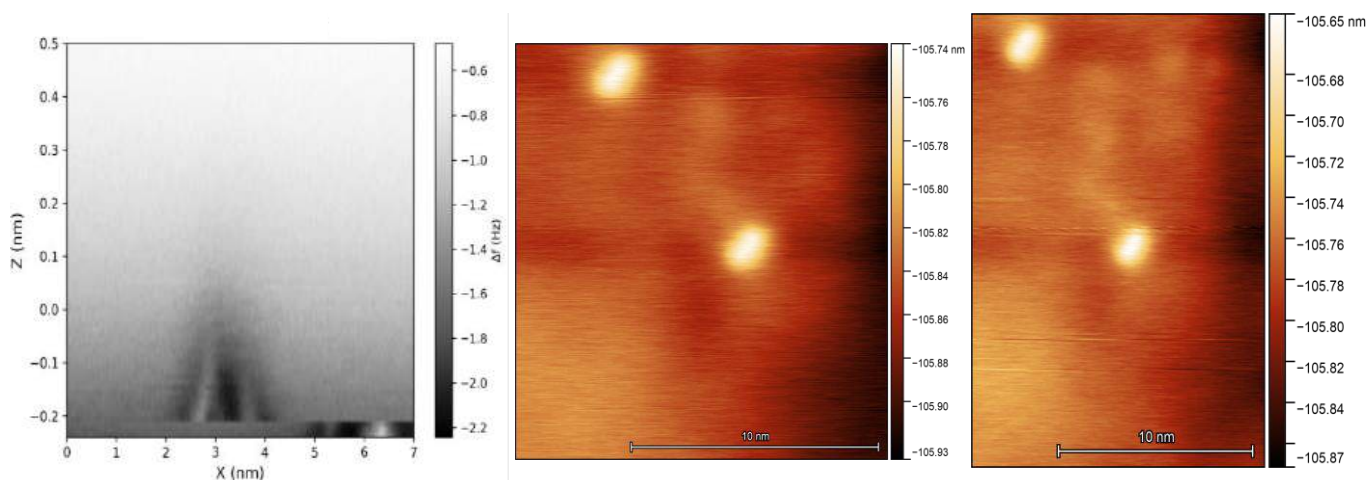


Figure 1: left - xz -frequency shift map of a manipulation event of a C₆₀ (before and after rolling). Right – Constant frequency shift NC-AFM images of C₆₀ on Si(100) at room temperature, before (left) and after (right) manipulation of leftmost C₆₀ along a (vertically oriented) dimer row relative to a static reference molecule.

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Influence of the surface corrugation to the charge density wave contrast of 2H-NbSe₂ in SPM images

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A charge density wave (CDW) is a collective phenomenon present in many low-dimensional quantum materials, which can be described as an electronic instability that results into a modulation of the charge density along with a periodic lattice deformation. 2H-NbSe₂ is one of the most-studied materials hosting a CDW owing to a long discussion about the driving mechanism as well as interplay of the CDW with its superconducting properties. Today, it is well established that the incommensurate (almost 3 x 3) CDW originates from momentum and orbital dependent electron phonon coupling [1]. Recent works suggest a multi-band character of the CDW [2] while the role of the vertical displacement of Se atoms to the formation of the CDW is still discussed [3].

In our work we aim at delineating the influence of the vertical displacement of the Se atoms at the surface of 2H-NbSe₂ from the electronic contribution to the almost 3 x 3 CDW superlattice contrast. We utilize combined STM and non-contact Atomic Force Microscopy (nc-AFM) to independently characterize the geometric as well as the electronic structure of the CDW in 2H-NbSe₂. Distance-dependent current and frequency shift images reveal a different evolution of the relative contrast of the atomic and the almost 3 x 3 CDW periodicities. Based on ab-initio calculations, we show that the contrast at small distances is dominated by the displacement of the surface Se atoms. For large distances, the contrast is dominated by the interaction of the permanent dipole of the tip with the potential above the surface that is predominantly modulated by the under lying Nb atoms [4].

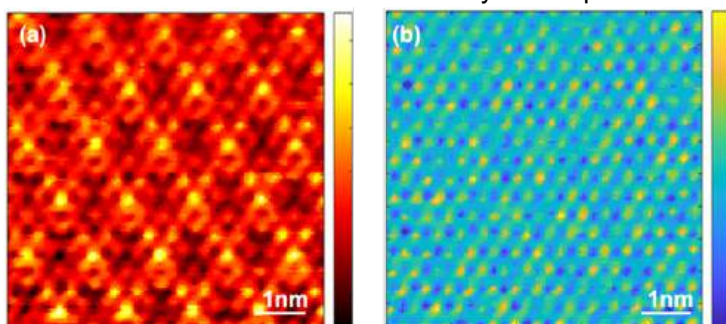


Figure 1: Simultaneously acquired constant-height (a) current and (b) frequency shift.

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Automated, reproducible conditioning of SPM tips

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The quality of scanning probe microscopy data critically depends on the tip: controlled functionalization can both increase image contrast and simplify the interpretation of images. Yet the procedures to prepare well-performing tip terminations rely on operator know-how and vary with individual experience, limiting the reproducibility and throughput of SPM experiments. Efforts to systematize tip preparation range from standardized manual protocols [1] to machine-learning-driven automation [2]. Nevertheless, reproducible, operator-independent tip conditioning remains the exception.

To overcome this bottleneck, we built an open-source software framework [3] that automates tip preparation on scanning probe microscopes, independent of the specific instrument or technique. It connects to the controller through a generalized interface, runs configurable conditioning routines, and logs every step, so that procedures can be reproduced, optimized, shared, and compared between groups.

The current routine applies bias pulses, monitors the frequency-shift response, and evaluates tip quality from the statistics of bias sweeps, repeating the conditioning cycle until a defined criterion is met. We demonstrated unattended multi-hour operation on a Nanonis-controlled microscope [4]. In the future, the framework will be extended to incorporate decision-making based on external image-recognition and numerical analysis, enabling controlled and reliable tip functionalization and termination [5, 6] for AFM measurements. By transforming these operator-dependent recipes into shareable workflows, the framework makes reproducible tip preparation accessible to any laboratory.

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Laser Annealing for Reliable Preparation of Noble Metal–Covered W(111) Single-Atom Tips in UHV

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A single-atom tip (SAT) is a sharp metal tip terminating in a single atom, enabling atomic resolution in scanning tunneling microscopy (STM) and atomic force microscopy (AFM). Preparing SATs at cryogenic temperatures is extremely time-consuming and often relies on trial and error. It is therefore highly desirable to establish a reliable method for SAT preparation prior to STM/AFM operation. Reliable preparation of noble metal–covered W(111) SATs has been demonstrated through thermal annealing of noble-metal plated W(111) tips to ~ 1000 K in ultrahigh vacuum (UHV) [1,2]. These SATs consist of three-sided W(111) nanopylramids covered with a monolayer of noble-metal atoms (Pd, Ir, Pt, Rh, or Au). A key advantage of this type of SATs is their well-defined apex structures, which provide reproducible electronic signatures for scanning tunneling spectroscopy and predictable potential wells for atomic manipulation. Conventionally, tips were heated by passing current through a V- or arc-shaped tungsten or molybdenum heating loop. However, this approach suffers from mechanical vibration, which is detrimental for STM/AFM applications. In addition, certain designs and materials in tip assemblies cannot withstand annealing at ~ 1000 K. To address these limitations, we report reliable preparation and regeneration of noble metal–covered W(111) SATs using laser annealing [3]. A focused laser beam is directed onto the tip apex to achieve localized heating (Fig. 1a). Field-emission (FE) patterns of noble-metal plated W(111) tips transferred into UHV initially revealed irregular structures that varied from tip to tip (Fig. 1b). When the local laser power exceeded a threshold, the FE pattern evolved over time, indicating structural rearrangement at the apex. After sufficient laser heating, three distinct spots frequently appeared in the FE pattern (Fig. 1c), consistent with the formation of a truncated nanopylramid with a triangular (111) flat-top surface (inset in Fig. 1c). Continued laser heating ultimately produced a SAT characterized by a single round FE spot spanning $\sim 3^\circ$ (Fig. 1d), confirming the controlled formation of a well-defined single-atom tip.

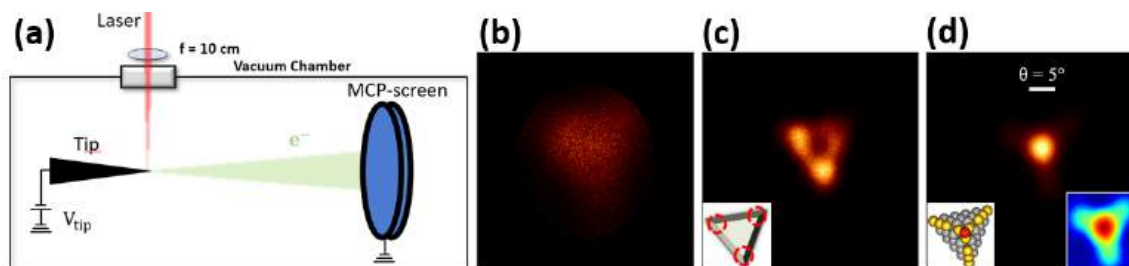


Figure 1: (a) Schematic of laser annealing. (b) FE pattern of an Ir-plated W(111) tip before heating. (c) FE pattern indicating the initial formation of a truncated nanopylramid. (d) FE pattern indicating the formation of an SAT with one narrow emission spot.

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Adsorption of Phthalocyanine on Indium Oxide: Influence of the Metal Ions

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The adsorption and electronic interaction of conjugated organic molecules on oxide surfaces remain insufficiently understood despite their relevance for optoelectronics and model catalytic systems. We investigate the adsorption behavior of metal-free phthalocyanine (H2Pc) on the transparent conductive oxide $\text{In}_2\text{O}_3(111)$ using low-temperature non-contact atomic force microscopy (nc-AFM) and scanning tunneling microscopy (STM).

The comparable size of the molecules and the surface unit cell enables a (1×1) arrangement despite symmetry mismatch (4-fold rotational symmetry of the molecule vs. 3-fold surface symmetry). Across different metalized phthalocyanine (MPc) species (CuPc, CoPc, etc.), we identify a robust adsorption site that enforces molecular overlap in the first layer, as well as a secondary, less frequent site that supports non-overlapping packing [1, 2]. Measurements on H2Pc reveal how the macrocycle interacts with the oxide in the absence of a central metal ion, providing a reference for understanding metal-dependent adsorption.

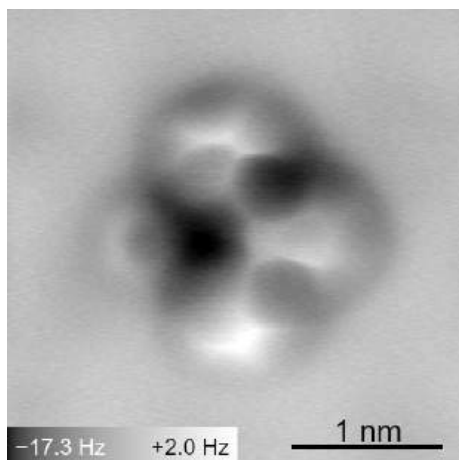


Figure 1: AFM image of a metal-free phthalocyanine, H2Pc, on $\text{In}_2\text{O}_3(111)$; $A = 100 \text{ pm}$, $f_R = 31.2 \text{ kHz}$

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Invasive and non-invasive probes of sub-K molecular diffusion

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Although anisotropic diffusion can define preferred pathways for molecular motion, directed transport requires a perturbation that breaks detailed balance. Tip-driven motion of dibromoterfluorene (DBTF) on Ag(111) is a striking realisation of the latter, where diffusion can be directed over hundreds of nanometres along a preferred crystallographic direction [1]. This novel behaviour arises from an exceptionally shallow corrugation in the potential energy landscape along the preferred direction. The same weak corrugation, however, makes DBTF/Ag(111) an exceptionally challenging system to measure non-invasively: both short-range forces and long-range E-field-mediated interactions strongly perturb the diffusion dynamics.

To separate tip-induced behaviour from the “native” diffusion of DBTF on Ag(111), we combine non-invasive measurements with perturbative $df(z)$ spectroscopy. For the former, DBTF is positioned under the tip, the tip is retracted (~ 10 nm) for a fixed time and then restored. Repeated trials provide temperature-dependent (350 mK - 4.2 K) occupation probabilities. Comparison with the predictions of canonical 1-D random walk theory and the output of kinetic Monte Carlo simulations yields a “tip-free” barrier in the 1 – 5 meV range. We then use the approach of Ternes *et al.* [2], to determine the vertical and lateral forces required to move the same DBTF molecule. At nominally zero sample bias (Fig. 1C), 2-4 pN of lateral force is required for molecular translation. With a bias of -500 mV, the corresponding forces required for manipulation remarkably fall below the noise floor of our measurement (cf Fig 1C, 1D).

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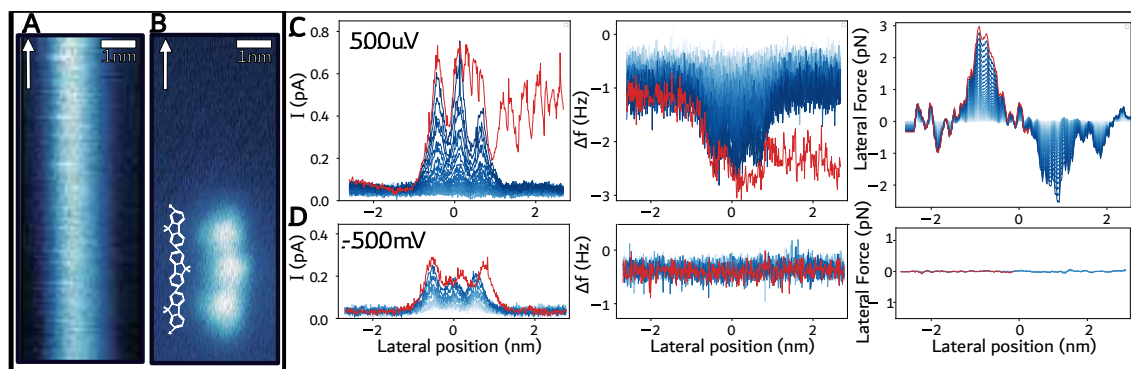


Fig. 1. Left panel: STM images of (A) DBTF “stripe”, and (B) static DBTF molecule at 350 mK. Arrow to the left indicates scan direction. **Right panel:** tunnel current, frequency shift, and extracted lateral forces for two different sample biases, nominally 0V (~ 500 μ V residual DAC offset) and -500 mV. Molecular motion is indicated in red, with the lateral force after the movement omitted.

Adsorption geometry determination of three-dimensional molecular architectures

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Noncontact atomic force microscopy (nc-AFM) with a CO-functionalized tip [1] is widely used to determine the chemical structure of nearly planar molecules. However, resolving the detailed bond structure and adsorption geometry of three-dimensional molecular architectures remains challenging [2-6] because conventional scanning trajectories are typically set parallel to the surface plane. In this work, a macrocyclic 1,8-anthrylene-ethynylene tetramer, which exhibits a chiral diamond-prism three-dimensional structure with switchable chirality in the gas phase [7], is deposited onto a thin NaCl film on Au(111). Upon adsorption, the upper two anthrylene moieties protrude into the vacuum, whereas the lower two face the substrate. Because of the flexible and rotatable C-C bonds in the bridging ethynylene units, the diamond-prism structure may not be preserved on the surface. To determine the actual adsorption geometry, we reveal the chemical structure of the upper anthrylene moieties by employing scanning trajectories tilted by approximately $\pm 25^\circ$ with respect to the surface plane. The lower anthrylene moiety exhibits a nearly planar adsorption geometry due to van der Waals interactions with the surface. Based on these observations, the molecule is determined to adopt a tent-shaped adsorption geometry. Our work demonstrates that tilted scanning trajectories provide a route toward bond-resolved nc-AFM imaging of complex three-dimensional molecular architectures.

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Metallic Longitudinal Electrostatic Screening in a Type-I Superconductor

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In an alternative electrodynamic theory of superconductivity, J.E Hirsch proposed a modification to the London electrodynamic equation for superconductors to allow electric fields to penetrate further into the superconductor without generating infinite supercurrent. One of the outcomes of this change is that the electrostatic screening of a superconducting condensate should scale with the London penetration depth (typically $\lambda_L \sim 100$ nm) rather than the traditional Thomas-Fermi length ($\lambda_{TF} \sim 100$ pm) [1].

These dramatic changes to electrostatic screening should correspond to significant, measurable differences in a local scanning probe microscope, as discussed by A. Peronio and F.J. Giessibl [2]. Here, we use a series of complementary scanning tunnelling microscopy (STM) and non-contact atomic force microscopy (nc-AFM) experiments at 300 mK on the surface of Pb(111) both in the superconducting and normal state to probe the changes in electrostatic screening across this phase transition.

Using nc-AFM, we probe the distance-dependent electrostatic force between a tip and the sample to quantify the induced image dipole on the Pb(111) surface (Figure 1). We then cross-correlate this information with STM-based measurements of field-emission resonances between the tip and sample; these resonances are also incredibly sensitive to the screening of image dipoles in the substrate and are used to quantify changes through the superconducting phase transition. The data converges on the conclusion that the screening length is nearly unchanged through the superconducting transition.

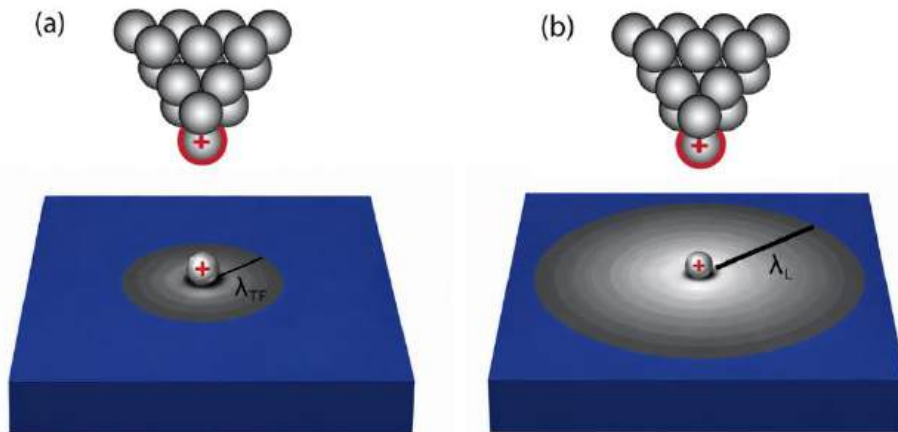


Figure 1: Schematic illustration of the screening of the tip-induced electric field (mirror-charge response) by a superconductor as described by (a) Conventional London equation where screening occurs over the Thomas–Fermi screening length. (b) Alternative theory of superconductivity proposed by Hirsch, predicting a substantially longer-range electrostatic screening response.

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Molecular Resolution Imaging of Trisodium Citrate Cluster on NaCl (001) in Air Using Frequency Modulation Atomic Force Microscope

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Trisodium citrate (TSC) has been reported to alter the growth morphology of NaCl crystals from the cubic {100} habit to octahedral {111} faces presumably through selective adsorption on crystal surfaces. To observe TSC adsorption behavior while suppressing NaCl dissolution, we have previously examined TSC adsorption on NaCl (001) through a thin adsorbed water layer. Low relative humidity (RH) favored the formation of TSC clusters at step edges, whereas increasing RH enhanced TSC mobility and promoted the development of water-containing islands.

In this study, we focus on high-resolution imaging of the molecular structure of TSC clusters adsorbed on NaCl (001). Such imaging enables evaluation of the adsorption orientation of TSC molecules and provides insight into the adsorption mechanism. To suppress molecular mobility, which hinders high-resolution imaging, FM-AFM imaging was performed under low RH, where the adsorbed water layer was minimized. A freshly cleaved NaCl surface was dripped with 2 microliters of TSC solution (1 mM in pure water) under RH < 40%. Subsequently, the surface was dried overnight using silica gel until a low RH was achieved in the thermostatic chamber. Imaging was performed using a frequency modulation atomic force microscope (SPM-8000FM prototype, Shimadzu). We used a commercial Si cantilever (ppp-NCHR, Nanosensors) with an Al coating on its backside with a resonance frequency (f_0) of 257 kHz. Under low RH (~14%), molecular-resolution imaging of TSC adsorbed on NaCl (001) was successfully achieved (Fig.1). The result suggests that TSC molecules are not randomly distributed, but instead form an ordered adsorbed layer on the NaCl surface. Based on the molecular patterns, we will discuss the adsorption orientation of TSC molecules on NaCl (001) and its implications for the adsorption mechanism.

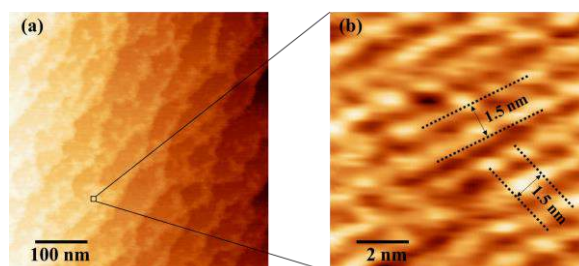


Figure 1: FM-AFM images of a NaCl (001) surface on which a TSC water solution was dripped under RH 14%. (a) Wide-view image, showing TSC clusters preferentially adsorbed along step edges of the NaCl surface. (b) Zoomed image of the rectangular region in (a). The dashed lines highlight the molecular ordering of TSC molecules.

Force-Based Characterisation of Bond Formation in Coupled Artificial Atoms

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The scanning tunnelling microscope (STM) provides a powerful platform for constructing nano-scale systems atom by atom, enabling the realisation of artificial quantum matter [1]. Charged Cs adatoms on InSb(110) represent a particularly flexible system in this regard, facilitating precision engineering of potential energy landscapes within a dilute two-dimensional electron gas [2]. Because the Cs/InSb(110) system is intrinsically electrostatic in nature, Kelvin probe force microscopy (KPFM) can be used to directly interrogate the underlying confinement potential.

Using simultaneous Kelvin probe force microscopy (KPFM) and scanning tunnelling spectroscopy (STS) with qPlus sensors, we directly measure both the electrostatic confinement potential and the spatially delocalised ground-state charge density of artificial molecules fabricated by STM manipulation (Fig. 1). By combining these measurements with simple quantum mechanical models, we extract quantitative information on the energetics of artificial bonding interactions, enabling direct analogies to real chemical systems while simultaneously probing the limits of the simulator itself. This work establishes force-based scanning probe microscopy as a powerful tool for electrostatic quantum simulation, moving these platforms towards tunable analogue simulators capable of exploring fundamental two-dimensional chemistry in regimes where simple analytical approaches, and even sophisticated computational methods, become intractable.

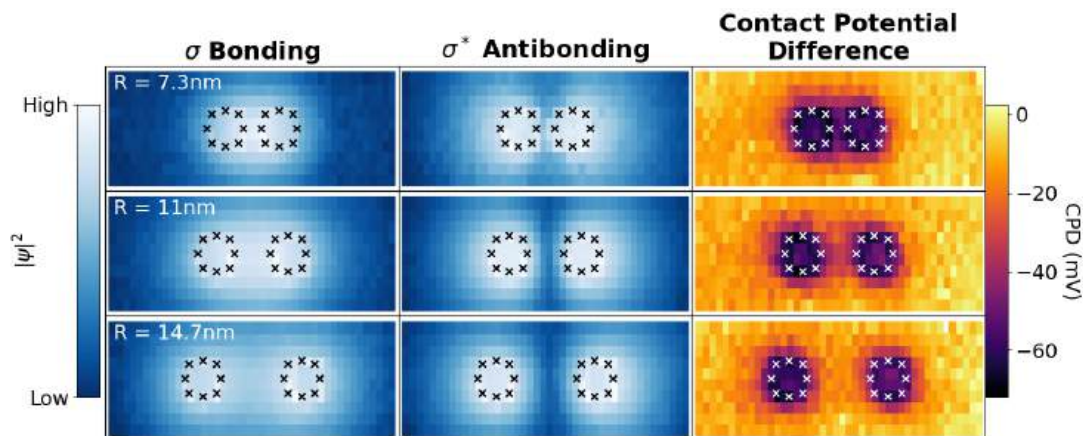


Fig. 1. (Left) Bonding and anti-bonding maps of artificial atom dimers realised via tracking of the bound state amplitude from dI/dV spectroscopy. R represents the interatomic separation. (right) KPFM maps of the contact potential difference for each of the associated dimers. Marked crosses represent positions of Cs atoms

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Force Microscopy at the Electrified Solid-Liquid Interface with Tip Apex Modification

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qPlus sensor AFM operated under electrochemical potential control (EC-AFM) [1,2] now resolve both electrode surfaces and solvent layering at electrified solid-liquid interfaces with (sub)-nanometer precision.[2] Yet the contrast mechanisms governing AFM measurements in liquid environments are not fully understood. Commonly employed Si tips acquire a pH-dependent surface charge in aqueous electrolyte. In pure water, where this charge is absent or negligible, the observed frequency-shift oscillations are well described by treating the tip apex as a single water molecule interacting with the density-modulated interfacial water - the so-called solvent-tip approximation (STA), successfully applied at many neutral and charged solid-liquid interfaces [3]. In electrolyte solution [4], the charged Si apex introduce contrast contributions, such as electric double-layer overlap that the STA does not account for. Systematically isolating these contributions demands precise control over tip apex chemistry under well-defined electrochemical conditions.

To address this, we functionalize Si tips with covalently bound, charge-neutral methyl groups, producing an apex of known composition and minimal permanent charge. Using these probes alongside bare Si tips at Au(111)-electrode interfaces, we investigate how the charge at the tip apex modulates the interfacial solvent contrast and the ability to discriminate between water and ion layering using force spectroscopy. In these experiments we measure the frequency shift induced by the interaction of the tip with the solvent structure. We show that the charged Si tip reveals an alternating cation-anion layering, yielding a characteristic layer spacing of ~ 0.5 nm at the potential of zero charge (PZC) that reflects the periodicity of the ionic charge-density profile, whereas the methyl-terminated tip returns a spacing of ~ 0.3 nm consistent with the molecular density oscillations of interfacial water at the same electrode potential (see Figure 1). Taken together, these experiments shed new light on the molecular-scale contrast mechanisms in liquid-phase AFM and underscore the decisive influence of tip-apex chemistry [4] in resolving interfacial water layers and in discriminating water from ions at electrified solid-liquid interfaces.

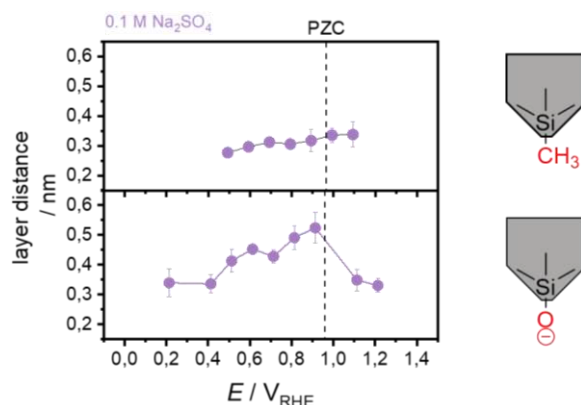


Figure 1: Layer distance vs. potential plots in 0.1 M Na_2SO_4 with methyl modified (top) and unmodified (bottom) tips.

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qAFM: A Python toolbox for quantitative analysis in NC-AFM

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The theory for non-contact atomic force microscopy (NC-AFM) in the harmonic approximation is well developed and widely used [1]. Yet, connecting measured observables such as the frequency shift, oscillation amplitude, and dissipation signals to physically interpretable force curves can be a demanding data-analysis task. Additionally, there is often need for numerically simulating various aspects of NC-AFM, both for didactic and scientific reasons.

To meet these requirements in an efficient and modern way, we here present the Python toolbox **qAFM** designed to support quantitative NC-AFM data workflows from analytical force modelling to the reconstruction of tip-sample forces from experimental data. The toolbox is built on the harmonic approximation of dynamic AFM by solving the equation of motion of the force sensor with tip-surface interaction and describing the tip movement in the force field of the sample. **qAFM** implements core routines for FM-AFM and AM-AFM, including conversions between frequency shift and cap-averaged force gradients, cap and cup averaging procedures, as well as solvers for calculating quantities based on the three fundamental AFM equations [1]. Analytical interaction models are organized according to their physical origin and include short-range chemical interactions, van-der-Waals forces for different tip geometries, and electrostatic force laws.

Beyond forward modeling, **qAFM** provides deconvolution workflows for quantitative force measurements. For example, frequency-shift curves can be converted into conservative force curves and interaction potentials using established force-inversion approaches, including the Sader-Jarvis algorithm [2] and the matrix-based inversion method introduced by Giessibl [3].

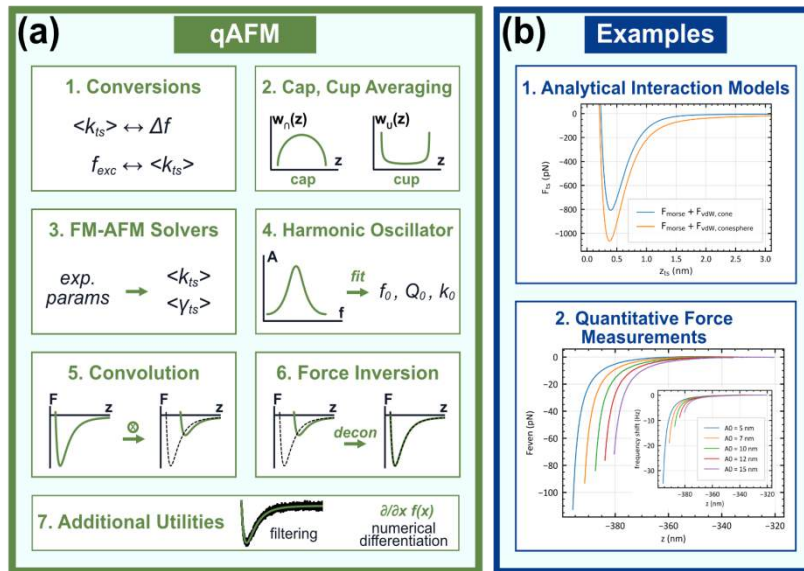
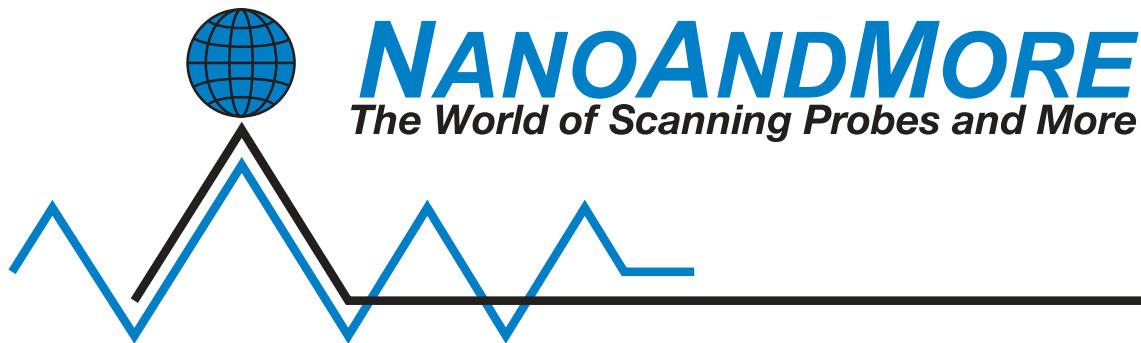


Figure 1: (a) Overview of the **qAFM** Python toolbox for quantitative non-contact AFM analysis. The package combines numerical and analytical routines for conversion of physical quantities, cap/cup averaging, FM-AFM solvers, harmonic-oscillator fitting, convolution, force inversion, and numerical utilities. (b) Examples for force evaluation and simulating an NC-AFM experiment.

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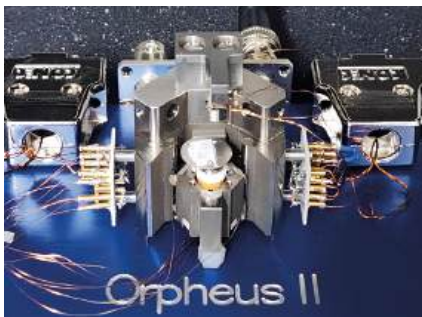
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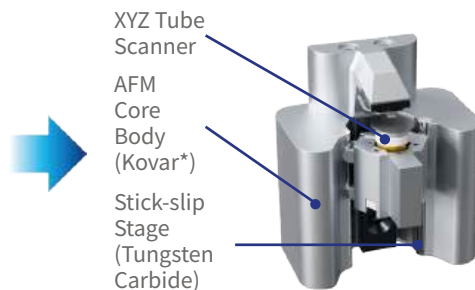
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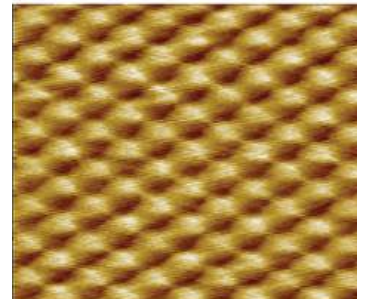
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08:00 – 09:00	REGISTRATION				
09:00 – 09:20	TECHNICAL SYMPOSIUM	Amogh Kinikar	Alexander Schwarz	Akash Gupta	Mong-Wen Gu
09:20 – 09:40		Ye Liu	Aris Lafranca	Shuyu Huang	Orlando Jose Silveira Junior
09:40 – 10:00		Lisanne Sellies	Yuuki Adachi	Jay Weymouth	Ondřej Krejčí
10:00 – 10:20		Yuejian Zhang	Susanne Baumann	Sophia Schweiss	Martin Ondráček
10:20 – 10:40		COFFEE BREAK			J. G. Vilhena
10:40 – 11:00				Mengxi Liu	
11:00 – 11:20	TECHNICAL SYMPOSIUM	Mithun Manikadan	Jascha Repp	EXCURSIONS	Ruben Perez
11:20 – 11:40		Manuel González Lastre	Christian Loppacher		Tobias Dickbreder
11:40 – 12:00		Prokop Hapala	Indranil Mal		Sarah Tobisch
12:00 – 12:20		Farzin Irandoost	Antoine Hinaut		Ulrike Diebold
12:20 – 14:00	LUNCH				CLOSING REMARKS
14:00 – 14:20	OPENING REMARKS	Rémy Pawlak	Peter Grutter		
14:20 – 14:40	Yoichi Miyahara	Jie Huang	Yuto Nishiwaki		
14:40 – 15:00	Brian Kiraly	Daniel Rothhardt	Yasuhiro Sugawara		
15:00 – 15:20	Ryota Fukuzawa	Jonas Heggemann	Vijayalaxmi Sankeshwar		
15:20 – 16:00	COFFEE BREAK				
16:00 – 16:20	Leo Gross	Jing Guo	Daniel Martin-Jimenez		
16:20 – 16:40	Xinnan Peng	Paul Laubrock	Omur Dagdeviren		
16:40 – 17:00	Shijing Tan	Davoud Pourzadeh	Udo Schwarz		
17:00 – 17:20	Percy Zahl	Jara Trujillo-Mulero	Daniel Ebeling		
17:20 – 17:40	WELCOME RECEPTION (from 17:20)	Barbara Hissa			
17:40 – 18:00		POSTER SESSION (17:40–20:00)	POSTER SESSION (17:40–20:00)	CONFERENCE DINNER (from 18:00)	
18:00 – later					