Scanning Probe Techniques - Current and Future Trends

844. WE-Heraeus-Seminar

16 Nov - 20 Nov 2025
at the Physikzentrum Bad Honnef/Germany

The WE-Heraeus Foundation supports research and education in science, especially in physics.
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Introduction

The Wilhelm und Else Heraeus-Stiftung is a private foundation that supports research and education in science with an emphasis on physics. It is recognized as Germany's most important private institution funding physics. Some of the activities of the foundation are carried out in close cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft). For detailed information see https://www.we-heraeus-stiftung.de

Aims and scope of the 844. WE-Heraeus-Seminar:

A bit more than 40 years ago, the most powerful tool of surface science was invented at IBM Rüschlikon in Switzerland: the scanning tunneling microscope (STM), soon to be followed by the atomic force microscope (AFM). These scanning probe microscopy techniques are widely considered as the "founding methods of nanotechnology". Ever since their invention, they have evolved into many different directions ranging from surface characterization to contributing to fundamental understanding at the ultimate smallest length-scales, over bottom-up approaches in nanotechnology to exploring interactions between different fundamental properties. We want to honor the continued development in this flourishing field with a WE-Heraeus seminar on "Scanning probe techniques – current and future trends".

Scientific Organizers:

Dr. Shadi Fatayer — KAUST, Saudi Arabia
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Introduction

Administrative Organization:

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Registration:

Mrs. Martina Albert (WE Heraeus Foundation) at the Physikzentrum, reception office Sunday (17:00 h – 20:00 h) and Monday morning

Program

Sunday, November 16, 2025

17:00 – 20:00	Registration	
18:00 – 19:30	*BUFFET SUPPER and informal get-together*	
19:30	Scientific organizers	**Opening and Welcome**
19:45 – 20:45	Ulrike Diebold	**Keynote I** **Non-contact Atomic Force Microscopy: The Ideal Tool for Investigating Insulating Oxides**

Monday, November 17, 2025

08:00	*BREAKFAST*	
Session I: Superconductors		
09:00 – 09:45	Deungjang Choi	**From spins to superconductors: Unlocking Majorana edge states**
09:45 – 10:30	Laétitia Farinacci	**Tuning the properties of Yu-Shiba-Rusinov states induced by magnetic molecules**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Jörg Kröger	**A tour d'horizon: forces, vibrations, spin excitations at the atomic scale**
11:45 – 12:30	**Poster flash**	
12:30 – 12:35	**Conference Photo**	
12:35	*LUNCH*	

Program

Monday, November 17, 2025

14:00 – 15:00	**Poster session I**	
15:00 – 15:45	*COFFEE BREAK*	

Session II: Spins on surfaces

15:45 – 16:30	Stepan Kovarik	**Probing electron spin resonance of molecular spins with scanning tunneling microscopy**
16:30 – 17:15	Taner Esat	**Atomic-Scale Quantum Sensing and Magnetism with Molecular Nanostructures**
17:15 – 18:00	Philip Willke	**Electron Spin Resonance of Individual Atomic and Molecular Spins on Surfaces**
18:00 – 18:15	Stefan Jorda	**About the Wilhelm and Else Heraeus Foundation**
18:15 – 19:30	*DINNER*	
19:30 – 20:30	Nan Jiang	**<u>Keynote II</u>** **Probing Chemistry at the Ångström-Scale via Scanning Tunneling Microscopy Combined Tip-Enhanced Raman Spectroscopy**

Program

Tuesday, November 18, 2025

08:00	*BREAKFAST*	
Session III: Designer quantum matter		
09:00 – 09:45	Daniel Wegner	**Quantum simulator to study electronic structure – from molecules to lattices to the Hofstadter butterfly**
09:45 – 10:30	Peter Wahl	**Atomic scale imaging of emergent quantum states**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Jiani Hong	**Atomic-scale insights into ice and water via high-resolution SPM**
11:45 – 12:30	Fabian Schulz	**Tuning pi-magnetism in atomically precise graphene nanostructures**
12:30	*LUNCH*	
14:00 – 18:00	**Excursion**	
18:00 – 19:30	*HERAEUS DINNER at the Physikzentrum* *(cold and warm buffet, with complimentary drinks)*	
19:30 – 20:30	**Jascha Repp**	**<u>Keynote III</u>** **Non-equilibrium at atomic scales: shaken or stirred… and scanned**

Program

Wednesday, November 19, 2025

08:00	*BREAKFAST*	
Session IV: On-surface chemistry		
09:00 – 09:45	Michael Gottfried	**New Carbon Allotropes and Nanographenes via On-Surface Synthesis and Single-Molecule Manipulation**
09:45 – 10:30	Christian Wäckerlin	**Magnetic functionality of metal-organic low-D materials unraveled by XMCD and SPM**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Pascal Ruffieux	**Nanographene Spin Chains**
11:45 – 12:30	Christian Kuttner	**Inside Nature portfolio: editorial process and innovations**
12:30	*LUNCH*	
14:00 – 15:00	**Poster session II**	
15:00 – 15:45	*COFFEE BREAK*	
Session V: Advanced AFM		
15:45 – 16:30	Florian Albrecht	**Intermediates, Reactions and Products of Cyclocarbons**
16:30– 17:15	Jay Weymouth	**Force microscopy on its side: A unique look at atoms and molecules with Lateral Force Microscopy**
17:15– 18:00	Laerte Patera	**Molecular Assembly and Coupling on Surfaces: From Electrostatics to Heterocyclic Systems**
18:00– 19:30	*DINNER*	
19:30 – 20:30	Katharina Franke	**Keynote IV** **Single-atom Josephson junctions: Shapiro steps and diode-like behavior**

Program

Thursday, November 20, 2025

08:00	*BREAKFAST*	
Session VI: Light-coupled STM		
09:00 – 09:45	Tomáš Neumann	**Theory of Imaging Molecules Using Light in a Scanning Tunneling Microscope**
09:45 – 10:30	Katharina Kaiser	**Tuning the luminescence of single molecules**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Shaoxiang Sheng	**Atomic-scale investigation of electron and phonon dynamics using ultrafast scanning tunneling microscopy**
11:45 – 12:30	Karina Morgenstern	**Laser-induced on-surface processes imaged by STM**
12:30 – 12:45	Scientific organizers	**Poster Awards** **Concluding remarks**
12:45	*LUNCH*	

End of seminar and departure

Posters

Posters

Benjamin Achatz	**Steering interfacial molecular self-assembly by substrate-molecule charge transfer**
Stefanie Adams	**Terahertz field control of surface topology probed with subatomic resolution**
Büşra Gamze Arslan	**Yu-Shiba-Rusinov States at the Edge of a Magnetic Monolayer**
Emma Berger	**Imaging the Quantum Melting of Generalized Wigner Crystals**
Nicolaj Betz	**Energy conversion in single atomic spins exhibiting magnetic exchange forces**
Dasom Choi	**Multi-photon resonant transition in an Er-Ti atomic spin pair**
Jiri Dolezahl	**Raman-detected quantum dot microscopy for nanoscale electrostatic potential imaging**
Alina Drechsler	**STM/STS Studies of Single-Atom Fe Inclusions in MBE-grown Monolayer MoS_2/Gr/Ir(111)**
Florian Faaber	**Influence of atomic-scale defects on coherent phonon excitations by THz near fields in an STM**
Filippo Giovanni Fabozzi	**On-Surface Photopolymerization of Stilbenes via Templating [2+2] Cycloaddition**
Ying Gao	**Orientational switching as an extra degree of freedom in molecular self-assembly on Au(111)**
Patrick Haertl	**Structural, electronic, and magnetic properties of Europium films epitaxially grown on W(110)**
Longfeng Huang	**Molecular Interaction-Directed Self-Assembly and Reorientation of [6]Cycloparaphenylenes on Au(111)**

Posters

Margarete Huisinga	**Revealing Spatial Inhomogeneities in Superconducting 2H-NbS_2 using Magnetic Sensor Atoms**
Tzu-Chao Hung	**Phthalocyanine-based bipartite lattices: Towards a molecular Lieb lattice**
Maneesha Ismail	**Tuning spin transitions in a coupled two-level system using spin-electric control.**
Hao Jiang	**Local activation of on-surface synthesis via laser-illuminated STM tips: toward atomically precise reaction control**
Wouter Jolie	**Magnetic adatom manipulation on monolayer transition metal dichalcogenides**
Kira Junghans	**Realization of separation of time scales for a heterogeneous atomic Boltzmann machine**
Antti Karjasilta	**Evidence of multiferroicity in monolayer $NiBr_2$**
Jinkyung Kim	**Magnetic Quantum Corrals on a Proximity-Superconducting Rasbha Surface Alloy**
Anna Krieg	**Tuning the magnetism of a single atom by local charge gating**
Hitesh Kumar	**Cross-sectional scanning tunneling microscopy study of nearly lattice-matched III–V semiconductor heterostructures**
Paul Laubrock	**PTCDA on calcite(104) - high resolution imaging and charge state control of organic molecules on a bulk insulator**
Henrik Lichtl	**Landau-Zener Dynamics and the Quantum-Classical Crossover in Antiferromagnetic Nanomagnets**

Posters

Ye Liu	**Steering Magnetic Coupling in Diradical Nonbenzenoid Nanographenes**
Janine Lorenz	**Quantitative imaging of the surface potential of a single PTCDA molecule on Pb(111)**
Felix Lüpke	**Momentum-selective tunneling from the edge of a van der Waals scanning probe tip**
Bharti Mahendru	**Josephson diode in a Pb-Pb junction with chiral Fe clusters**
Philipp Maier	**Stochastic resonance realized with a superconducting magnetic impurity state**
Benjamin Mallada	**Atomic-Scale Sequencing of Biomolecules with nc-AFM**
Paola Mantegazza	**Scanning tunnelling microscopy reveals homocoupling-free and exceptionally long pgBTTT as high-performance materials in OECTs**
Alexandra Meerovici Goryn	**Coherent dynamics of magnons by atomic assembly of spin chains with ESR-STM**
Uladzislau Mikhailau	**STM imaging of stripe dynamics in superconducting nickelate**
Matyas Nachtigall	**Effects of Alternating Bias on Spin Resonance in Quantum Devices.**
Jeongmin Oh	**Determination of the coupling regime and Kondo temperature of a spin ½ system at millikelvin temperatures**
Soumyajit Rajak	**Ångström-Resolved Spectro-microscopic Visualization of Surface Catalyzed Metalation Mediated Ring Fusion in Benzoporphyrins**
Luise Renz	**Setup of an ESR-STM at mK Temperatures in a Closed-Cycle Dilution Refrigerator**

Posters

Ángel Rodríguez Alcaraz	**Engineering Spin-1/2 Chains with ESR-STM and NISQ Devices for Time Crystal Realization**
Ricardo Ruvalcaba	**On-Surface Reactions of Electronically Active Self-Assembled Monolayers for Electrode Work Function Tuning**
Sascha Sadewasser	**Conductive atomic force microscopy tomography on Cu(In,Ga)Se2 solar cell absorbers**
Affan Safeer	**Polarons in epitaxial single-layer $MnBr_2$**
Guillaume Schull	**Atomically-controlled fluorescence with STM: from electron to photon excitations**
Lisanne Sellies	**Photoexcitation Atomic Force Microscopy**
Julian Skolaut	**An electrical molecular motor driven by angular momentum transfer**
Sreehari Sreekumar	**Charge Manipulation in Hematite Fe_2O_3 as a Route to Polaron Physics**
Jan ter Glane	**Probing the Electrostatic Potential by AFM with an O-terminated Copper tip: Direct Elemental Discrimination on hBN**
Tfyeche Y. Tounsi	**Inelastic tunneling into multipolaronic bound states in single-layer molybdenum disulfide**
Antonella Treglia	**Dopant-vacancy complexes in transition metal dichalcogenides**
Alkisti Vaitsi	**THz-driven plasmonic STM luminescence**
Lucien Van Assche	**Synthesis and characterization of a spin lattice on superconductors using chlorinated tetraazapyrene radicals**

Posters

Hester Vennema	**Nuclear magnetic resonance on a single atom with a local probe**
Chrisitian von Bredow	**Scanning tunnelling spectroscopy study of proximity superconductivity in Rash-ba-split surface states**
Julian Zeitler	**Manipulating the Crystal Field of Individual Atoms on Surfaces**

Abstracts of Lectures

(in alphabetical order)

Intermediates, Reactions and Products of Cyclocarbons

Florian Albrecht[1], Fabian Paschke[1],Yueze Gao[2], Igor Rončević[2], Hary Anderson[2], Leo Gross[1]

[1] IBM Research Europe — Zurich, Rüschlikon, Switzerland
[2] Department of Chemistry, Oxford University, UK

Cyclocarbons, molecular allotropes of carbon in which all carbon atoms are two-fold coordinated, have been synthesized on surface using tip-induced chemistry [1-4], and the formation of larger cyclocarbons by dimerization of precursors was shown [4]. This presentation will focus on products, reactions and intermediates of cyclocarbons, generated by tip-induced chemistry on ultrathin NaCl layers and characterized by STM and AFM with CO-functionalized tips.

[1] K. Kaiser et al., Science, 365, 1299-1301 (2019)
[2] L. Sun et al., Nature, 623, 972-976 (2023)
[3] Y. Gao et al. Nature, 623, 977-981 (2023)
[4] F. Albrecht et al. Science, 384, 677-682 (2024)

From spins to superconductors: Unlocking Majorana edge states

Deung-Jang Choi[1,2,3]

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Recent advances in quantum science are enabling technologies that manipulate matter at the level of individual atoms and molecules. Here, we demonstrate atomically precise assembly and coherent control of electron-spin qubits using a scanning tunneling microscope (STM), which uniquely combines fabrication and measurement at the single-atomic scale [1,2,3]. By arranging coupled spins on superconducting surfaces, we uncover emergent quantum phenomena, including possible signatures of Majorana bound states [4,5,6]. These engineered spin arrays offer a powerful platform for probing non-Abelian exchange statistics, a key ingredient for topological quantum computing. Our results highlight the potential of atom-by-atom quantum engineering to realize versatile, tunable architectures for future quantum information processing.

References

[1] Colloquium: Atomic spin chains on surfaces. Review of Modern Physics **91**, 041001 (2019)

[2] An atomic-scale multi-qubit platform, Science **382**, (6666), 87-92 (2023)

[3] Electron spin resonance with scanning tunneling microscopy: a tool for an on-surface quantum platform of identical qubits, Nanoscale Adv., **7**, 4551-4558 (2025)

[4] Atomic Manipulation of In-gap States on the β-Bi_2Pd Superconductors, Physical Review B **104**, (4), 045406 (2021).

[5] Calculations of in-gap states of ferromagnetic spin chains on *s*-wave wide-band superconductors, Physical Review B **104**, (24), 245415 (2021).

[6] In-gap states induced by magnetic impurities on wide-band -wave superconductors: Self-consistent calculations, Physical Review B **110**, (20), 205404 (2024)

Non-contact Atomic Force Microscopy: The Ideal Tool for Investigating Insulating Oxides

Ulrike Diebold

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The surface science of metal oxides has evolved into a well-established research field, which provides detailed insights into the atomic-scale properties of these versatile materials. Many technologically interesting oxides are electrical insulators, though, and obtaining the atomically-resolved images that are routine for metallic or semiconducting oxides has remained a real challenge.

A prototypical example is alumina: With a band-gap of 8 eV, Al_2O_3 is unforgivingly insulating. Widely used as a support material for catalysis, as a substrate for epitaxial thin film growth, or as platform for quantum computing, its surfaces have remained a mystery. It has been known for a while that the lowest-energy (0001) surface reconstructs [1], and SXRD [2] measurements have provided a first model for the complex (√31x√31) R9° structure. Solving this reconstruction has also become a test case for ncAFM, with the first atomically-resolved images published more than 20 years ago [3].

Application of the qPlus sensor [4] with O-terminated tips (prepared and judged using a partially O-covered Cu(110) reference sample, as introduced by the Mönig group [5]) has provided superior resolution and helped solve this long-standing puzzle [6]. This approach has also been applied to mica [7] and other silicates [8] and thus opens up the exciting opportunity of investigating oxides that have been inaccessible with established surface science methods.

References

[1] T. M. French & G. A. Somorjai, *J. Phys. Chem*. 74, 12 (1970).
[2] G. Renaud, et al., Phys. Rev. Lett. **73**, 1825 (1994)
[3] K. Barth & M. Reichling, *Nature* 414, 27 (2001).
[4] F. J. Giessibl. *Rev. Sci. Instr.* **2019,** *90* (1), 011101
[5] B. S. Schulze Lammers, et al., *Nanoscale* 13, 13617 (2021).
[6] J. Hütner, et al., *Science* 385, 1241 (2024).
[7] G. Franceschi, et al., *Nature Comms*, 14, 208 (2023).
[8] G. Franceschi, et al., *J. Phys.Chem. Lett.*15 (2024) 15 -22

Atomic-Scale Quantum Sensing and Magnetism with Molecular Nanostructures

Taner Esat[1,2]

[1]Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, Jülich, Germany
[2]Jülich Aachen Research Alliance (JARA), Jülich, Germany

Detecting weak magnetic fields from single electrons and nuclear spins at the atomic scale is a long-standing challenge in physics. While current mobile quantum sensors can detect single-electron spins, achieving atomic spatial resolution remains difficult. To approach this scale, we built a quantum sensor with a scanning tunneling microscope (STM) from single atoms and a PTCDA (3,4,9,10-perylenetetracarboxylic acid dianhydride) molecule (Figure 1). The molecule's spin is decoupled from the metal by standing it upright on the STM tip, which mimics its configuration on a pedestal of two transition metal atoms on the surface [1]. This spin-1/2 system acts as a two-level quantum system in a magnetic field [2]. We address the molecular spin by electron spin resonance (ESR) and achieve ~100 neV energy resolution. In a proof-of-principle experiment, we use this sensor to measure the magnetic and electric dipole fields emanating from single atoms with sub-angstrom spatial resolution [3]. Finally, we show that varying the transition metal atoms in the pedestals of standing molecules on a surface controls their spin state. We demonstrate exceptionally long spin lifetimes of up to several minutes on a metal surface using this approach.

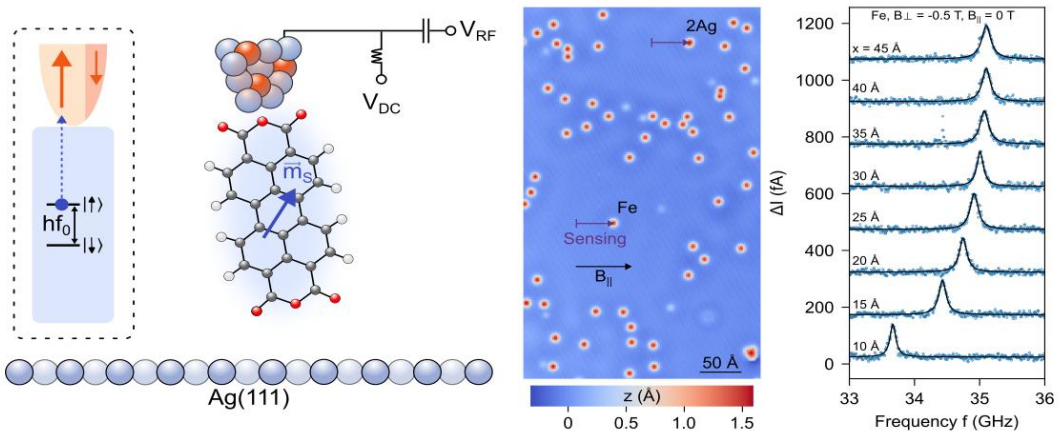

Fig. 1: The spin of the PTCDA molecule on the magnetic tip serves as a two-level quantum system that can be addressed by ESR. When approaching Fe atoms on the surface, the spin resonance frequency shifts due to the electric and magnetic dipole fields from the Fe atom.

[1] Esat et al., Nature 558, 573 (2018)
[2] Esat et al., Phys. Rev. Research 5, 033200 (2023)
[3] Esat et al., Nature Nanotechnology 19, 1466 (2024)

Tuning the properties of Yu-Shiba-Rusinov states induced by magnetic molecules

Laëtitia Farinacci
Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany

Magnetic impurities on a superconductor induce bound states, called Yu-Shiba-Rusinov (YSR) states, within the superconducting gap due to exchange scattering of the Cooper pairs of the substrate onto the magnetic center. The energy of these bound states is dictated by the exchange coupling strength and their electron-hole asymmetry is linked to the potential scattering at the impurity. Importantly, the extent of these states allows for hybridization and under the right conditions, a topological state may emerge in such platforms.

In this talk I will present how the use of magnetic molecules helps tune the properties of YSR states and affects their lineshape in scanning tunneling spectroscopy (STS). First, I will present how the flexibility of the molecular ligand allows to explore various coupling and transport regimes. By approaching the STM tip above a Fe-porphine molecule, we are able to tune the YSR state energy and identify the hallmark of the quantum phase transition in STS. In particular, we are able to identify the ground state of the system and can resolve Andreev processes mediated by the YSR state [1]. Next, I will show that the presence of the magnetic ligand has a direct influence on the lineshape of the YSR state, as well as on that of its counterpart in the normal state: the Kondo resonance. Interferences between tunneling channels lead to an inversion of the electron-hole asymmetry of these resonances across the molecule [2]. Finally, I will demonstrate how molecular self-assembly can be used to tailor YSR hybridization in 2D islands, combining atomic/molecular-precision with long-range order. By tuning the ratio between Fe-porphines and Cl adatoms on Pb(111) we are able to resolve the formation of YSR bands in a kagome lattice and propose that this approach can latter be used to characterize the formation of Kondo lattices on surfaces [3].

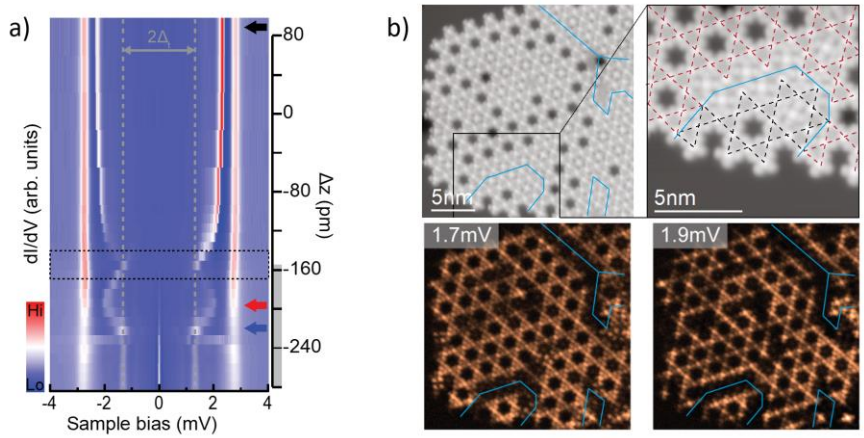

Figure 1. a) Approach of the STM tip toward the Fe center of a Fe-porphine molecule allows to tune the YSR state energy and identify the hallmark of the quantum phase transition in STS. b) Molecular self-assembly leads to the formation of 2D molecular islands in which the formation of YSR bands in kagome domains occurs.

[1] Farinacci et al., *Phys. Rev. Lett.* **121** (19), 196803 (2018)
[2] Farinacci et al., *Phys. Rev. Lett.* **125** (25), 256805 (2020)
[3] Farinacci et al., *Nat. Comm.* **15** (1), 6474 (2024)

Single-atom Josephson junctions: Shapiro steps and diode-like behavior

Martina Trahms[1], Bharti Mahendru[1], Werner van Weerdenburg[1], Jacob F. Steiner[2], Larissa Melischek[2], Clemens B. Winkelmann[3], Felix von Oppen[2], **Katharina J. Franke[1]**

[1]Fachbereich Physik, Freie Universität Berlin, Germany
[2]Fachbereich Physik and Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Germany
[3]Université Grenoble Alpes, CNRS, Institut Néel, Grenoble, France

The scanning tunneling microscope (STM) is a powerful tool for atomic-scale spectroscopy of normal and superconducting materials. By using superconducting tips, Josephson junctions can be formed when approaching a superconducting substrate. A fingerprint of the Josephson junction is a zero-bias peak in voltage-biased differential-conductance spectroscopy. However, an applied bias immediately destroys the phase coherence of the junction.
Replacing the conventional voltage bias with an effective current bias, phase coherence can be preserved in the superconducting state. Here, we investigate the coherence in the phase dynamics in Pb-Pb junctions. We identify switching and retrapping currents that mark the transitions between superconducting and normal states. When then expose the junctions to high-frequency radiation where we find Shapiro steps, signifying the coherent absorption of photons, although phase diffusion is enhanced at the same time.
Adding magnetic adatoms to the surface of a superconductor leads to Yu-Shiba-Rusinov states inside the superconducting gap. Using Josephson spectroscopy, we find that the switching currents are significantly reduced compared to the pristine junction, indicating a local reduction of the superconducting order parameter. Even more interestingly, the retrapping current shows an asymmetric behavior with respect to the biasing direction [1]. This implies that a supercurrent can flow without dissipation in one direction while experiencing resistance in the opposite direction. We attribute this diode-like effect to the electron-hole asymmetry of Yu-Shiba-Rusinov states [1,2].

[1] M. Trahms, L. Melischek, J. F. Steiner, B. Mahendru, I. Tamir, N. Bogdanoff, O. Peters, G. Reecht, C. B. Winkelmann, F. von Oppen, K. J. Franke, Diode effect in Josephson junctions with a single magnetic atom, Nature 615, 628 (2023).
[2] J. F. Steiner, L. Melischek, M. Trahms, K. J. Franke, F. von Oppen, Diode effects in current-biased Josephson junctions, Phys. Rev. Lett. 130, 177002 (2023).

New Carbon Allotropes and Nanographenes via On-Surface Synthesis and Single-Molecule Manipulation

J.M. Gottfried[1]

[1]*Department of Chemistry, University of Marburg, Germany*

Recent advancements in on-surface synthesis techniques enable the fabrication and precise characterization of carbon-based nanomaterials with atomic-scale precision. These materials often exhibit novel (opto)electronic and magnetic properties, arising from both the intrinsic features of the molecular precursors and the unique structures formed during synthesis. On-surface synthesis thus offers a versatile alternative to solution-phase chemistry, granting access to otherwise inaccessible products.

We illustrate this potential with the synthesis of nonbenzenoid carbon allotropes such as the biphenylene network, featuring 4-, 6-, and 8-membered rings and exhibiting metallic behavior [1]. Furthermore, single-molecule manipulation enabled the preparation of tridecacene and pentadecacene—the longest acenes to date—revealing open-shell configurations and low-energy spin excitations [2,3]. Finally, heteroatom doping was used to tune the properties of carbon nanostructures, including acenes, graphene nanoribbons, cycloarenes, and cycloparaphenylenes [4,5].

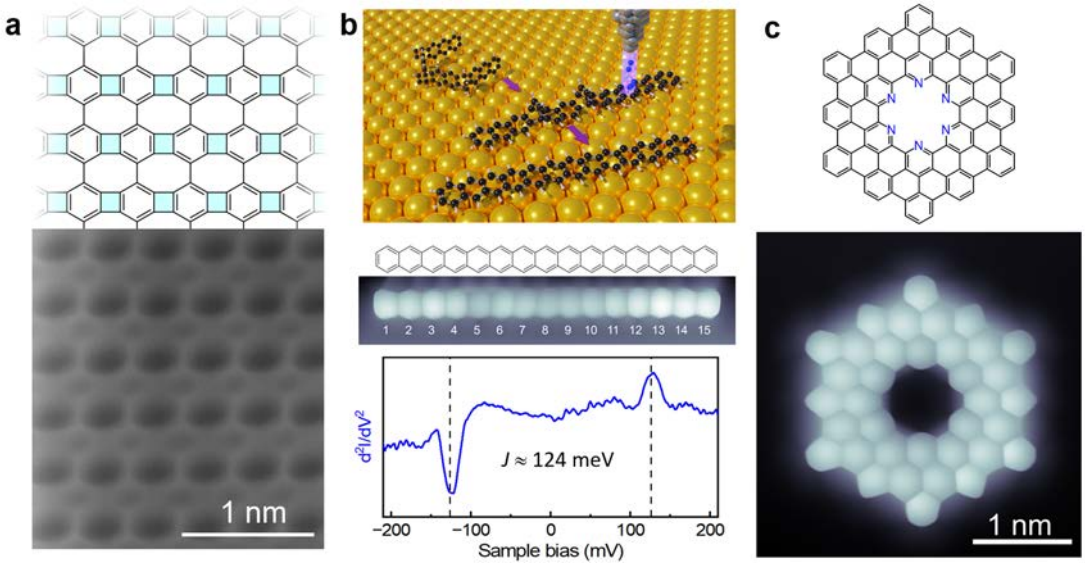

Figure 1. (a) Biphenylene network, (b) long acenes by single-molecule manipulation, (c) N-doped cycloarene.

References

[1] Q.T. Fan et al., J.M. Gottfried, Science **372**, 852-856 (2021).

[2] Z. Ruan et al., J.M. Gottfried, J. Am. Chem. Soc. **146**, 3700-3709 (2024).

[3] Z. Ruan et al., J.M. Gottfried, J. Am. Chem. Soc. **147**, 4862–4870 (2025).

[4] Z. Ruan et al., J.M. Gottfried, Angew. Chem. Int. Ed. e202504707 (2025).

[5] D. Han et al., J.M. Gottfried, J. Am. Chem. Soc. **147**, accepted (2025).

Atomic-scale insights into ice and water via high-resolution SPM

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Water is fundamental to life, and ice, as its solid phase, is ubiquitous in nature, playing a key role in various physical, chemical, biological, and energetic processes. Recently, we developed hydrogen-sensitive scanning probe microscopy (SPM) based on higher-order electrostatic forces[1], successfully applying it to interfacial water/ice systems. Using this technique, we identified two-dimensional (2D) bilayer hexagonal ice grown on a Au(111) surface[2] and demonstrated the symmetrical hydrogen bond through proton doping[3]. This breakthrough provides a foundation for exploring novel properties associated with symmetric hydrogen bonds under ambient conditions and their potential applications. Additionally, we developed a universal high-resolution imaging method for insulating surfaces, allowing direct imaging of bulk hexagonal ice (ice Ih) surfaces[4]. Our observations revealed unique superstructures and premelting phenomena on ice surfaces. By introducing proton doping, recently we successfully engineered a proton-ordered ferroelectric ice phase (ice XI). These findings offer new insights into phase behavior and physicochemical properties of ice, providing a deeper understanding of its fundamental nature and potential applications in materials science.

References:

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Probing Chemistry at the Ångström-Scale via Scanning Tunneling Microscopy Combined Tip-Enhanced Raman Spectroscopy

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Our research investigates how local chemical environments influence single-molecule and nanostructure properties on surfaces with Ångström-scale resolution. Tip-Enhanced Raman Spectroscopy (TERS) combines the spatial resolution of Scanning Tunneling Microscopy (STM) with the chemical sensitivity of Raman spectroscopy. By utilizing a plasmonically active scanning probe, the Raman signal at the tip-sample junction is greatly enhanced, enabling single-molecule probing. This method, further aided by the benefits of ultrahigh vacuum, is uniquely capable of controlling localized plasmons via an atomistic approach. We are able to obtain (1) single-molecule chemical identification;[1] (2) quantum characterization of adsorbate-substrate interactions at the single chemical bond level;[2-4,] (3) atomic-scale insights into the oxygen reactivity on surfaces;[5, 6] (4) local strain effects in an organic/2D materials heterostructure.[7] By investigating single molecules, superstructures, 2D materials lattices, and the adsorption orientations obtained from the vibrational modes, we extract novel surface information at an unprecedented spatial (< 1 nm) and energy (< 10 wavenumber) resolution. Another application of localized surface plasmons is to achieve site-selective chemical reactions at sub-molecular scale. We recently selectively and precisely activated multiple chemically equivalent reactive sites one by one within the structure of a single molecule by scanning probe microscopy tip-controlled plasmonic resonance.[8] Our method can interrogate the mechanisms of forming and breaking chemical bonds at the Ångström scale in various local environments, which is critical in designing new atom- and energy-efficient materials and molecular assemblies with tailored physical and chemical properties.

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Tuning the luminescence of single molecules

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In recent years, tip-enhanced optical microscopy and spectroscopy have demonstrated the ability to overcome the diffraction limit by orders of magnitude, all without the need for fluorescent labels [1]. The key ingredient is the so-called picocavity that is formed between an atomistic plasmonic nanostructure, such as the apex of an STM-tip, and a nearby plasmonic substrate. This arrangement leads to an extreme confinement and enhancement of the electromagnetic field within a picometer-sized volume below the tip [2]. With this, it is now possible to "peak inside" and probe the optical properties of individual emitters, such as molecules, on sub-nanometric length scales [1,3].

When combined with STM, tip-enhanced luminescence experiments such as STM-induced electroluminescence (STML) and tip-enhanced photoluminescence (TEPL) allow not only the characterization of electro-optical properties of single molecules with ultimate spatial resolution, but also the deliberate manipulation of those properties with unprecedented precision. For instance, by controlling the charge state of an emitter it is possible to selectively tune its optical response (Fig. 1) [4] and to explore pathways in between different many-body states of the emitter [5].

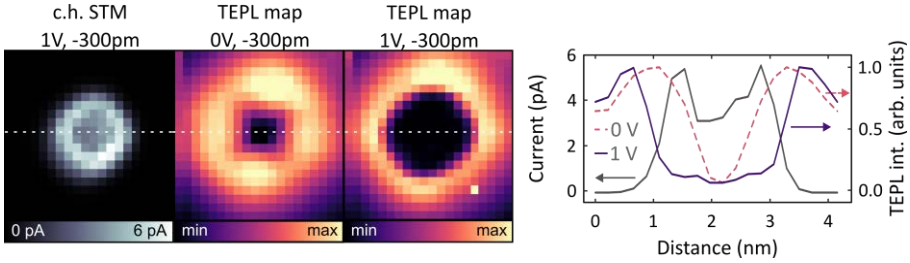

Figure 1: Simultaneously recorded constant-height STM and TEPL images at different bias voltages together with linecuts across the maps.

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Probing electron spin resonance of molecular spins with scanning tunneling microscopy

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Individual spins on surfaces offer a powerful platform for exploring quantum coherence and spin-environment interactions at the atomic scale, an essential step towards the practical implementation of surface-bound quantum systems. By combining scanning tunnelling microscopy (STM) with electron spin resonance (ESR) [1], we can directly image and manipulate atomic-scale environments while probing spin dynamics with high energy and temporal resolution. This unique experimental setting has matured over the last decade, enabling detailed investigations of quantum systems composed mostly of electron spins hosted in atomic and molecular orbitals. While early work centered on single-atom spin manipulation, recent advances have expanded into molecular spin systems, offering new opportunities for tunable spin control and coupling. In this talk, I will present recent developments in detecting and driving spin dynamics in molecules, highlighting their potential for future quantum technologies [2].

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A tour d'horizon: forces, vibrations, spin excitations at the atomic scale

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This talk is about simple model systems showing quantum physics at work. The presented findings rely on the prominent capabilities of scanning tunnelling and atomic force microscopes to manipulate matter atom by atom, to explore quantum excitations with high energy resolution, and to image with atomic resolution. The force involved in a single-molecule metalation reaction, the spectroscopy of graphene phonons, and the occurrence of avoided crossing in coupled molecular spin excitations are at the heart of the presentation. Funding by the DFG through KR 2912 / 17-1, 18-1, 21-1 is gratefully acknowledged.

Inside Nature portfolio: editorial process and innovations

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This talk aims to demystify the editorial journey within Nature-branded journals, revealing the hidden steps that a submitted manuscript goes through on its way to publication. I will explain the editorial criteria our experienced in-house editors use to evaluate submissions and how we decide which manuscripts are sent for peer review.

I will also walk you through the peer review process at Nature Communications [1], highlighting how editors select referees, make decisions based on feedback, and handle interdisciplinary work. We'll touch on recent developments in transparent peer review, the inclusion of early-career researchers in the review process, and initiatives around open data and reproducibility.

We will explore best practices in science communication. Many authors labor under the misapprehension that selective journals look for hyped claims. In contrast, we actively promote honest, transparent, and responsible communication. [2] Along the way, I'll share anecdotes from the life of a scientific editor, and, time permitting, we will reflect on emerging risks in the age of AI, particularly the growing issue of AI-generated images in scientific publications.

Dr. Kuttner is a Senior Editor at Nature Communications and since 2021 responsible for the physical chemistry content with a focus on nanomaterials. [3] Before becoming a full-time editor, he conducted research as a Marie Skłodowska-Curie fellow at the CIC biomaGUNE in Donostia-San Sebastian, Spain, and as a postdoctoral researcher at the Leibniz Institute of Polymer Research (IPF) in Dresden, Germany. [4]
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Laser-induced on-surface processes imaged by STM

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Though largely influencing the efficiency of a reaction, the molecular-scale details of the local environment of the reactants are experimentally inaccessible, hindering an in-depth understanding of a catalyst's reactivity, a prerequisite to maximising its efficiency. We introduced a method to follow individual molecules and their variable environment during a reaction in real space, utilising a combination of a scanning tunnelling microscope (STM) with a femtosecond laser [1] to initiate reactions and extended this approach, more recently, to tunable laser excitation [2]. In this talk, I will introduce the method and present its successful application for direct and indirect excitation of surface-adsorbed molecules through laser excitations. The examples include photo-induced Ullmann coupling of dibromobiphenyl [3], the influence of self-assembly on laser-induced dissociation [4], and how the solvent water steers a photothermal on-surface C-C coupling reaction [5].

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Theory of Imaging Molecules Using Light in a Scanning Tunneling Microscope

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With the advent of light-scanning tunneling microscopy (STML), optically imaging the interior of molecules with light has become an accessible reality. However, acquiring the optical images of molecules by scanning across them by the STML tip is just the first step towards extracting useful information about the molecular transport, excited-state and vibrational properties, among others. The interpretation heavily relies on theoretical models [1,2,3] that can capture the dynamics of electron tunneling, absorption of light and emission of photons or photoelectrons [4]. I will provide an overview of the physical mechanisms shaping the optical images in STML, including a deeper dive into the field of atomic-scale Stark-shift microscopy, discuss the role of vibrations on the optical images [3], and focus on some latest results regarding imaging of photocurrents in STML [4]. I will demonstrate the power of photocurrent detection using an example of the perylenetetracarboxylic dianhydride and discuss how, using this technique, one can disentangle the composition of a molecule's excited eigenstate in terms of its constituent electronic configurations.

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Molecular Assembly and Coupling on Surfaces: From Electrostatics to Heterocyclic Systems

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Understanding the intricate mechanisms governing molecular assembly and coupling on surfaces is essential for advancing surface chemistry and nanotechnology. Here, I will present an exploration of phenomena ranging from electrostatic interactions to the formation of heterocyclic systems, exploiting high-resolution scanning probe microscopy.

The first part will focus on dihydrogen bonding (DHB), a distinctive intermolecular interaction where hydrogen atoms simultaneously act as proton donors and acceptors. Low-temperature scanning tunneling microscopy (LT-STM) reveals single and double DHB motifs within borazine assemblies on Au(111) surfaces. Complementary density functional theory (DFT) calculations provide critical insights into the interplay between substrate adsorption and intermolecular forces, elucidating the stabilization mechanisms driving the formation of borazine clusters.

The second part will examine the self-assembly of fullerene C_{60} and Zn(II)-5,10,15,20-tetrakis(4-aminophenyl)porphyrin (ZnTAPP) on a Ag(111) surface. Kelvin Probe Force Microscopy (KPFM) and Scanning Tunneling Spectroscopy (STS) unveil the intricate role of charge transfer and Coulomb interactions in shaping intermixed molecular phases. Notably, the alleviation of repulsive inter-fullerene Coulomb forces promotes the formation of row-like structures, which, in turn, enhance charge transfer to C_{60} molecules. These findings highlight the delicate balance between substrate-mediated electron transfer and intermolecular forces in directing molecular self-assembly.

The final part will demonstrate the on-surface synthesis of nitrogen-containing heterocycles, which are fundamental building blocks in biomolecules and pharmaceuticals. Thermal activation of a tailored precursor leads to the formation of an N-heterocyclic compound, as visualized by high-resolution non-contact atomic force microscopy (nc-AFM). DFT calculations reveal the reaction mechanism, emphasizing the critical role of hydrogen release as the driving force behind the transformation.

Non-equilibrium at atomic scales: shaken or stirred… and scanned.

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Two complementary approaches that allow accessing non-equilibrium phenomena at atomic scales will be addressed. One of them is ultrafast lightwave-driven scanning tunneling microscopy (LW-STM) [1], which enables observing and even manipulating quantum systems at combined femtosecond and sub-angstrom resolution [2]. We discuss how LW-STM can be expanded to its ultrafast spectroscopy variant [3].

The other approach is enabled by a scanning-probe variant [4] that combines principles of STM with charge detection [5] by means of atomic force microscopy (AFM). Complemented by electronic pump-probe spectroscopy [6], this can be used to address different out-of-equilibrium aspects of individual molecules.

An overview of our recent activities related to the aforementioned two approaches—metaphorically 'shaken' and 'stirred'—will be presented [7-10]. For example, we will highlight the challenges and solutions involved in bringing LW-STM towards laser transients with carrier waves in the near-infrared spectral range to boost the temporal resolution. This way, tunneling-time windows below one femtosecond can be achieved, while maintaining the atomic-scale spatial resolution of STM.

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Nanographene Spin Chains

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Recent advances in on-surface synthesis have enabled the fabrication of prototypical open-shell nanographenes that can be covalently assembled into well-defined quantum spin systems. This presentation focusses on the realization of antiferromagnetically coupled nanographene spin chains, where the choice of the building block and the covalent coupling motif allows for the design of three emblematic quantum spin models: ***i)*** a spin-1/2 Heisenberg chain based on olympicenes [1], ***ii)*** a spin-1 Haldane chain based on triangulenes [2], and ***iii)*** an spin-1/2 alternating exchange Heisenberg chain based on Clar's goblets [3].

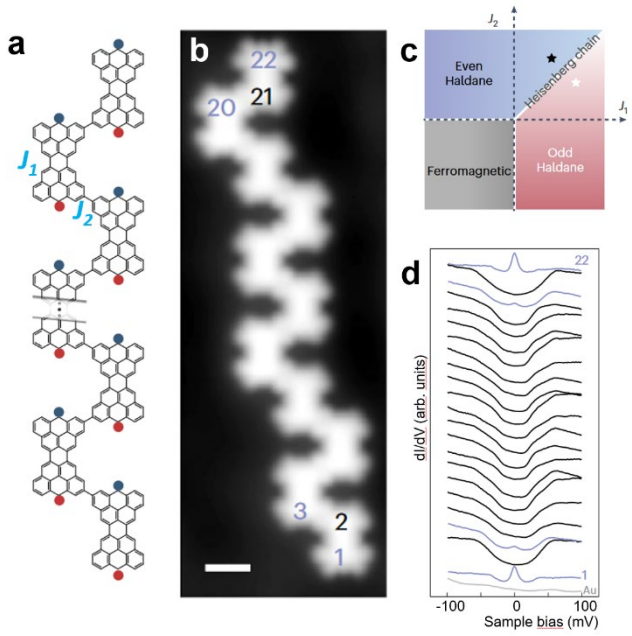

Figure 1: On-surface synthesized spin-1/2 alternating exchange Heisenberg chain based on Clar's goblet revealing gapped bulk excitations and topology-derived end states.

On-surface synthesis and *in situ* scanning probe-based characterization allows testing theoretical predictions for the different quantum systems. This includes length-dependent decay of the magnetic excitation gap in the spin-1/2 Heisenberg chain proving the quantum nature of the realized Heisenberg chain, gapped bulk excitations and fractional edge excitations for the spin-1 triangulene chains and gapped magnetic excitations in the spin-1/2 alternating exchange Heisenberg that depend on the ratio of J_1 to J_2 ($\alpha = J_1/J_2$).

We employ atomic hydrogen to passivate the spin sites via CH_2 group formation, followed by tip-induced reactivation to precisely define chain lengths and control terminal coupling motifs in the alternating exchange Heisenberg chains. This approach enables manipulation of the chain's topological phase and the corresponding selective induction or suppression of topology-dependent end states. Bulk excitations in alternating exchange chains are identified as triplons, and Fourier analysis of inelastic standing wave patterns reveals their energy-momentum dispersion of these spin-1 bosonic quasiparticles. These results establish on-surface synthesis as a powerful route to engineer and explore fundamental quantum spin models with strong exchange interactions at the molecular scale.

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Tuning pi-magnetism in atomically precise graphene nanostructures

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pi-magnetism in carbon-based nanostructures offers a potential route towards molecular spintronics and for integration into quantum information technology. However, realizing this potential relies on the precise control over the charge and spin state of the molecular building blocks. One promising candidate to achieve such level of control are atomically precise nanographenes. These structures allow for realizing pi-magnetism by various means, among them sublattice imbalance and topological frustration.

Here, we show how a combination of solution and on-surface synthesis enables, with atomic precision, the fabrication of different spin-full nanographenes. We characterize their structure as well as electronic and magnetic properties by a combination of low-temperature scanning tunneling microscopy/spectroscopy and noncontact atomic force microscopy and rationalize our findings by extensive electronic structure calculations. Importantly, we demonstrate how spin and charge state, as well as excitation energies of these nanographenes can be tuned by precise control over their atomic structure and through their interaction with the substrate.

*The presented work was carried out in collaboration with the groups of Thomas Frederiksen at Donostia International Physics Center, Diego Peña at Universidade de Santiago de Compostela, and Pavel Jelinek of the Institute of the Czech Academy of Sciences.

Atomic-scale investigation of electron and phonon dynamics using ultrafast scanning tunneling microscopy

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Electrons, phonons, and their interactions play a crucial role in the complex physical phenomena observed in correlated materials. Investigating the dynamics of electrons and phonons at the atomic scale is essential for unveiling the underlying microscopic mechanisms of these phenomena. By integrating terahertz (THz) and femtosecond pulses with scanning tunneling microscopy (STM), we have achieved spatiotemporally resolved measurements of electron and phonon dynamics at the atomic scale [1–4]. The tip-enhanced THz electric field can generate ultrafast Coulomb forces between the STM tip and the sample, thereby exciting coherent acoustic phonons within the sample. In addition, the ultrafast electric field can drive motion of surface charges, modulating the local charge distribution on the sample surface [3]. By analyzing the tunneling current response induced by the THz probe pulse, we are able to resolve the ultrafast evolution of lattice and charge-order parameters with atomic precision [2,3]. Furthermore, by employing femtosecond laser excitation, we have realized atomic-scale characterization of exciton dynamics and nonlinear optical responses in single molecules [4,5]. Our results demonstrate the feasibility of measuring and coherently manipulating electron, phonon, and phase transitions at the atomic scale, thus opening new experimental pathways for understanding and controlling nonequilibrium states in strongly correlated systems.

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Magnetic functionality of metal-organic low-D materials unraveled by XMCD and SPM

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The combination of scanning probe microscopy (SPM) with X-ray magnetic circular dichroism (XMCD) allows to investigate the synthesis, structure, and *magnetic functionality* of low-dimensional metal-organic materials at surfaces. The material under study can be 0D (molecules), 1D (chains) and 2D (sheets), and it can exhibit magnetic functionality such as i) induced magnetization,[1] ii) single-molecule magnetism[2] or iii) collective magnetism[3] such ferromagnetism (Figure 1), antiferromagnetism or ferrimagnetism.
The talk introduces the method XMCD and discusses the important aspect how the quality of samples in synchrotron studies can be guaranteed. Our solution to that problem is to measure the same sample using SPM and XMCD. Transfer is performed without breaking the vacuum by means of a portable vacuum chamber.

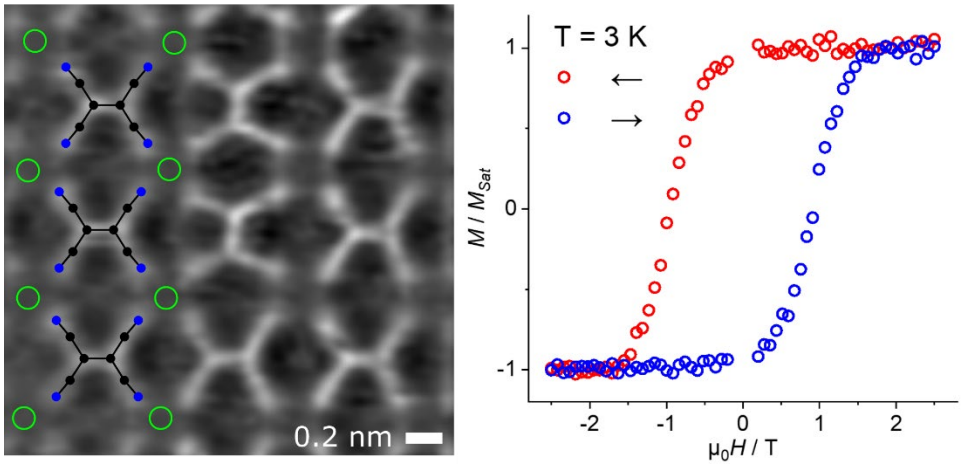

Figure 1: **Structure and magnetic properties of the metal-organic 2D ferromagnet NiTCNE on Au(111).** (left) Laplace filtered, constant height nc-AFM image, recorded with CO modified tip. (right) Field dependent magnetization, obtained using XMCD along the surface normal.

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Atomic scale imaging of emergent quantum states

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A characteristic property of quantum materials is that their ground state is highly sensitive to external stimuli, making it possible to control their ground states. This property makes them in principle highly desirable for applications, however in many cases we do not understand the ground state sufficiently will to be able to control it at will. Studying their low energy electronic structure by low temperature scanning tunnelling microscopy and spectroscopy had proven a very successful route to connect microscopic and macroscopic properties in these materials. It relies on real space maps of the differential conductance, from which, via quasiparticle interference, information about the electronic structure can be extracted

In my talk, I will show a few examples of strongly correlated electron materials, where we have achieved linking the microscopic and macroscopic properties[1-3]. The successful interpretation of quasiparticle interference relies on realistic simulation of the experimental data starting from microscopic models. I will discuss how this is done in practice[4].

This work was done in close collaboration with C.A. Marques, L.C. Rhodes, W. Osmolska, H. Lane, I. Benedičič, and M. Naritsuka.

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Quantum simulator to study electronic structure – from molecules to lattices to the Hofstadter butterfly

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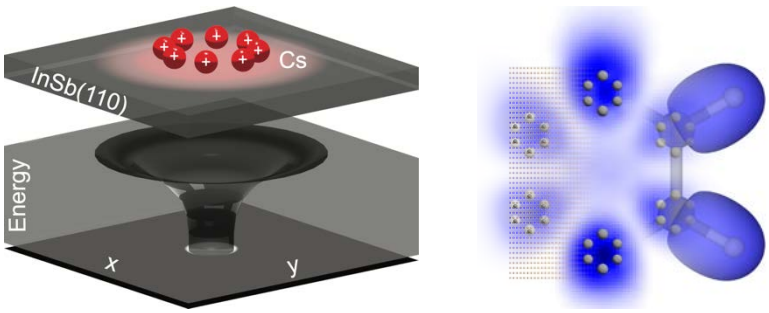
Quantum simulators are a pathway to study novel physical phenomena which are difficult to predict or observe in synthesized materials. To this end, the physical behavior of materials ranging from gasses to superconducting qubits has been used to emulate Hamiltonians. A promising route is to create bottom-up platforms based on assembling adsorbates on surfaces via the atomic manipulation capabilities in scanning tunneling microscopy (STM). This way, tunable artificial atoms, molecules and lattices can be created, and their electronic properties can be studied by means of scanning tunneling spectroscopy (STS).

In my talk, I will introduce a novel solid state quantum simulator based solely on patterned Cs atoms on the surface of semiconducting InSb(110). We use this platform to locally bind electrons in traps that emulate artificial atoms, by precisely positioning Cs atoms with the STM tip [1]. The bound localized states are probed and mapped via STS. These artificial atoms serve as building blocks to realize artificial molecular structures with different orbital symmetries. We realize textbook examples of molecular physics such as bonding/anti-bonding splitting in dimers, higher orbital symmetries (p_x, p_y, sp^2 hybrids) and the emulation of entire organic molecular electronic structure (e.g. benzene, *cis*-, *trans*, and cyclobutadienes, triangulene). I will discuss the transition from the molecular limit to band formation in extended artificial structures, and I will give an outlook of our most recent studies in strong magnetic fields, where we can observe Fock-Darwin states and Hofstadter bands.



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Force microscopy on its side: A unique look at atoms and molecules with Lateral Force Microscopy

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Atomic force microscopy can be used to image surfaces and flat molecules from "above" with remarkable clarity. These images combine advances in dynamic modes with techniques that allow the tip to be controlled at the atomic level. We make use of these achievements and turn atomic force microscopy on its side, oscillating the tip laterally to perform lateral force microscopy (LFM). By using the qPlus sensor, which doesn't require optics but instead makes use of the piezoelectric effect, we can easily use an LFM sensor in a commercial low-temperature atomic force microscope operating in ultra-high vacuum. In this talk, I will review how we've used the unique data LFM provides to investigate surfaces and adsorbates at the atomic scale [2], from laterally flexible adsorbates [1] and the sides of molecules [4], to measurements of energy loss over single chemical bonds [3, 5].

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Electron Spin Resonance of Individual Atomic and Molecular Spins on Surfaces

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In this talk, I will present recent advances for molecular spins on surfaces probed by electron spin resonance scanning tunneling microscopy (ESR-STM). First, by employing tip-assisted on-surface assembly, we construct a molecular ferrimagnet composed of an iron-phthalocyanine (FePc) molecule coupled to an additional Fe atom anchored beneath a benzene ligand on 2 monolayers of MgO/Ag(001) [1]. A strong Heisenberg exchange coupling between the spin-½ FePc and a spin-1 Fe atom yields a correlated ground-state doublet that is energetically well separated from excited states. The spin lifetime exceeds 1.5 µs (in the limit of large tip-distance) and Rabi drive shows π-times of ≈ 5 ns - roughly a factor of two improvement compared to simpler spin-½ counterparts on this substrate. This demonstrates that on-surface *spin engineering* via intra-molecular design and controlled coupling can yield molecular spin units with enhanced coherence and tunable spin–spin interactions when assembled into dimers.

Second, we demonstrate *spin-electric coupling* (SEC) for individual molecules on surfaces [2]. Using ESR-STM, we show how the resonance frequency of FePc and Fe–FePc complexes can be tuned via the applied bias voltage of the STM tip. The nonlinear dependence of the ESR frequency on bias is attributed to a transport-mediated exchange field from the magnetised tip, which shifts the spin energy levels when additional molecular orbitals come into resonance. This SEC enables all-electrical coherent spin control: Rabi oscillations of the individual and coupled molecular spins can be tuned electrically, opening a pathway to quantum operation driven purely by voltage rather than local magnetic fields.

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Abstracts of Posters

(in alphabetical order)

Steering interfacial molecular self-assembly by substrate-molecule charge transfer

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Scanning probe microscopy studies of organic molecules on metal substrates have furthered our understanding of substrate-molecule charge transfer processes [1]. On surface self-assembly of the electron acceptor C_{60} is driven by an interplay of short-range attractive Van der Waals forces and long-range repulsive electrostatic interactions [2,3]. Here we report the formation of an intermixed phase composed of C_{60} and Zn(II)-5,10,15,20-tetrakis(4-aminophenyl)porphyrin (Zn-TAPP) molecules on Ag(111). An approach combining scanning tunneling microscopy/spectroscopy (STM/STS) and Kelvin probe force microscopy (KPFM) was used to investigate the degree of substrate-molecule charge transfer for C_{60} in close-packed islands and a row-like intermixed structure. Analysis of our tunneling and force spectroscopy measurements revealed that mitigation of the coulomb repulsion drives the formation of the intermixed phase and promotes additional charge transfer to the C_{60} molecules [4]. These results demonstrate that controlling long-range Coulomb interactions can steer the formation of distinct self-assembled structures on metal substrates, offering insights for the design of new charge-optimized molecular nanostructures.

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Terahertz field control of surface topology probed with subatomic resolution

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Light-induced phase transitions offer a method to dynamically modulate topological states in bulk complex materials. Yet, next-generation devices demand nanoscale architectures with contact resistances near the quantum limit and precise control over local electronic properties. The layered material WTe_2 has gained attention as a likely Weyl semimetal, with topologically protected linear electronic band crossings hosting massless chiral fermions. Here, we demonstrate a topological phase transition facilitated by light-induced shear motion of a single atomic layer at the surface of bulk WTe_2 [1], thereby opening the door to nanoscale device concepts. Ultrafast terahertz fields enhanced at the apex of an atomically sharp tip of a terahertz scanning tunnelling microscope (THz-STM) [2] couple to the key interlayer shear mode of WTe_2 via a ferroelectric dipole at the interface, inducing a structural phase transitions at the surface from T_d-WTe_2 to a metastable state resembling 1T'-WTe_2 (Fig. 1a). Subatomically resolved differential imaging (Fig. 1b), combined with hybrid-level density functional theory, reveals a shift of 7 ± 3 picometres in the top atomic plane. Tunnelling spectroscopy links electronic changes across the phase transition with the electron and hole pockets in the band structure (Fig. 1c), suggesting a reversible, light-induced annihilation of the topologically-protected Fermi arc surface states in the top atomic layer.

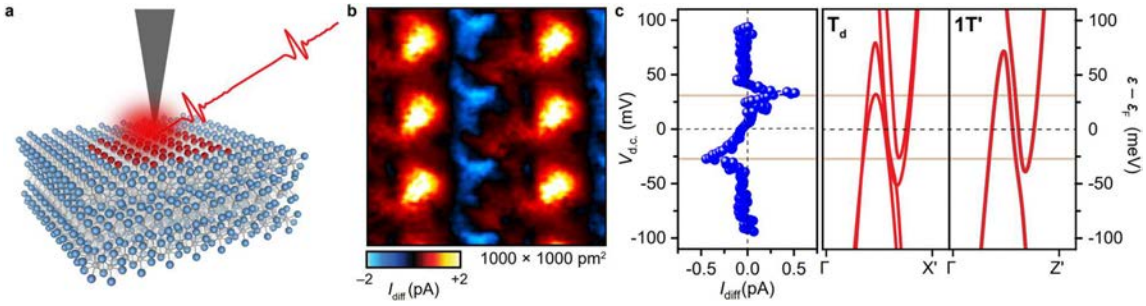

Figure 1: **a,** Schematic of a THz-STM junction and local light-driven phase transition. **b,** The differential tunnelling current signal I_{diff} reveals differences in the surface charge density between the phases. **c,** The bias voltages $V_{d.c.}$ at which the differential signal appears corresponds to the energy regimes that show a difference between T_d-WTe_2 and 1T'-WTe_2 in the calculated bandstructure.

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Yu-Shiba-Rusinov States at the Edge of a Magnetic Monolayer

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The ability to control interactions between magnetic and superconducting materials can lead to intriguing phenomena, such as topological superconductivity. At atomic scale, a single magnetic impurity interacting with a superconductor can induce in-gap bound states, so-called Yu-Shiba-Rusinov (YSR) states. Individual YSR states can couple in chains or lattices of magnetic impurities to create YSR bands. Together with spin-orbit coupling, these bands can be topological, leading to the emergence of topological superconductivity. There are only a few examples of topological superconductors to date, and the need to explore material platforms to engineer topological superconductors with desirable properties remains. Toward this aim, stacked van der Waals materials are a highly promising platform to engineer topological phases in superconductors. Recently, multiferroicity of nickel diiodide (NiI_2) was shown down to monolayer limit [1,2,3]. With its helical magnetic order and intrinsic spin-orbit coupling [4], NiI_2 is an excellent candidate for heterostructures realizing topological superconductivity.

Here, we present our study on monolayer NiI_2 grown on superconducting bulk $NbSe_2$. This system is characterized using scanning tunnelling microscopy and spectroscopy. The effect of doping due to the growth of NiI_2 on different substrates is investigated. Our observations revealed that NiI_2 does not show ferroelectricity, likely due to the charge transfer from the $NbSe_2$ substrate. In addition, we have investigated the edges of the NiI_2 islands, where we found clear signatures of YSR states and zero bias peaks in the $NiI_2/NbSe_2$ system. Our results show that the combination of 2D materials is a promising way to create designer materials with scientifically and technologically relevant properties.

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Imaging the Quantum Melting of Generalized Wigner Crystals

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Abstract

The emergence of unconventional phases from electron correlations exemplifies one of the most formidable challenges in condensed matter physics.[1,2] Moiré superlattices of two-dimensional materials offer a highly versatile platform to explore such phenomena through gate-tunable interaction strength and carrier density.[3,4] Using scanning tunneling microscopy (STM), we directly image the density-tuned melting of generalized Wigner crystals (GWCs) and Mott insulators (MI) in an electron-doped twisted AB-stacked $MoSe_2$ moiré bilayer. Our local imaging reveals how melting is influenced by strain inhomogeneities inherent to realistic samples. We find a striking electron-hole asymmetry in the density-tuned GWC melting at slight departures from commensurate filling. Removing electrons from a GWC yields glassy, disordered states with local charge fluctuations, providing the first experimental evidence for amorphous phases that have long been hypothesized to exist at incommensurate fillings. Adding electrons instead forms uniform, liquid-like phases, consistent with delocalization in a Fermi liquid. We find this electron-hole asymmetry to reflect the broken particle-hole symmetry of the triangular lattice, which produces distinct Fermi pockets for electrons and holes in momentum space. Meanwhile, this asymmetry is absent for the doped MI. Our study provides a platform to investigate how interactions, frustration, and the underlying lattice affect correlation-driven phase transitions.

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Energy conversion in single atomic spins exhibiting magnetic exchange forces

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Single atomic spin dynamics provide direct access to quantum mechanical effects and to the atoms fundamental interactions at the smallest length-scales. In that, spin-polarized scanning tunnelling microscopy (STM) can detect individual spin switches in quantum jump trajectories and the interaction between coupled spins. Atomic force microscopy (AFM) on the other hand, gives access to atomic-scale magnetic forces, such as chemical, electrostatic or magnetic exchange forces. The magnetic exchange force has for example been investigated on fully stable spins in magnetically ordered lattices [1,2].

Here instead, we show magnetic exchange force detection on a dynamically switching single Fe atom on MgO/Ag(100) and show how the interplay between tunnelling induced spin transitions and magnetic exchange force can drive the mechanical motion of the AFM cantilever. The atom is thereby converting electrical to mechanical energy. Further, we investigate the underlying dynamics by resolving real-time information on the state of the spins in the tunnel current and by simultaneously tracking its effect on the magnetic forces between the spin and the cantilever. We find that the switching spin synchronizes its dynamics with the AFM cantilever while exhibiting significant magnetic forces. This interplay between magnetic exchange interactions and spin dynamics not only reveals deep insights into the behavior of strongly driven spins, it also provides access to quantum thermodynamics, a novel field with largely unexplored prospects.

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Multi-photon resonant transition in an Er-Ti atomic spin pair

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The interaction between radiation and matter involving the absorption or emission of multiple photons underpins various modern technologies, including Raman scattering and harmonic generation. The coherent control of quantucm states through two-photon processes facilitates the creation of quantum entanglement [1, 2, 3], a cornerstone of quantum information processing. Despite the significance, the coherent control of such a process in atomic spin qubits remains largely unexplored [4-7]. In this presentation, we show our recent experimental results demonstrating the observation of a two-photon process in a pair of erbium (Er) and titanium (Ti) spins on a MgO surface. Using pulsed electron spin resonance in a scanning tunneling microscope, we achieve coherent control of the Er-Ti spin pair using two-photon interaction, further identifying a novel way for implementation of quantum gates to atomic spin qubits on a surface.

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Raman-detected quantum dot microscopy for nanoscale electrostatic potential imaging

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Mapping the electrostatic potential of nanoscale objects on surfaces is crucial for understanding their fundamental properties, including self-assembly or chemical reactivity. While atomically resolved methods like Kelvin probe force microscopy (KPFM) and scanning quantum dot microscopy [1] (SQDM) provide quantitative access via electrostatic force detection, a comparable technique for scanning tunneling microscopy (STM) has remained elusive.

Here, we introduce a novel photon-based approach, tip-enhanced Raman scattering scanning quantum dot microscopy (TERS-SQDM), which detects the charge state of a PTCDA molecular quantum dot on the tip from its Raman scattering signal using a 1.96 eV HeNe laser. Voltage-dependent Raman spectra reveal distinct intensity changes that coincide with single-electron charging thresholds, in direct correspondence with the frequency-shift charging dips in conventional SQDM.

We validate TERS-SQDM performance by mapping the local electrostatic potential of several nanoscale objects, including a subsurface defect and an Ag adatom on Ag(111). Our results establish TERS-SQDM as an alternative to AFM-based electrostatic imaging, combining the standard low-temperature STM setup with an easily implemented optical readout scheme. Furthermore, we envision the use of tip-enhanced Raman scattering and photoluminescence from the molecular quantum dot to experimentally probe excited molecular states and their transition dipoles.

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STM/STS Studies of Single-Atom Fe Inclusions in MBE-grown Monolayer MoS_2/Gr/Ir(111)

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Transition metal dichalcogenides (TMDs) have drawn significant attention due to their scalability and the thickness-dependence of their electronic density of states (DOS). Moreover, dimensionally confined TMDs, mainly 2D monolayers (MLs), are highly sensitive to structural defects, such as vacancies, interstitial and substituent atoms. Even in very low-density regimes, these impurities significantly affect various properties by introducing stress and/or modifying the DOS [1-4]. Consequently, there are ongoing efforts to engineer defects in TMDs to tune their electronic, magnetic, optical, and catalytic properties. While most of the current research focuses on naturally occurring defects in chemical vapor deposited TMDs, to improve control over defect engineering, we focus on intentional single-atom inclusions in TMDs grown by molecular beam epitaxy (MBE).

Here, I present our scanning tunneling microscopy (STM) and spectroscopy (STS) studies of Fe inclusions in ML MoS_2 on Gr/Ir(111), which we realize by co-evaporating Fe during MoS_2 MBE growth. We identify the Fe inclusions upon comparison with naturally occurring defects found on the undoped MoS_2 grown previously in the same UHV chamber. STS experiments reveal the presence of in-gap states arising from the incorporation of Fe atoms, whose spatial distributions are imaged by means of bias-dependent differential conductance mapping. Furthermore, resonant tunneling spectroscopy shows that the image potential states (IPS) are modified by the Fe inclusions, influencing the IPS' energetic positions due to a variation in the local work function.

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Influence of atomic-scale defects on coherent phonon excitations by THz near fields in an STM

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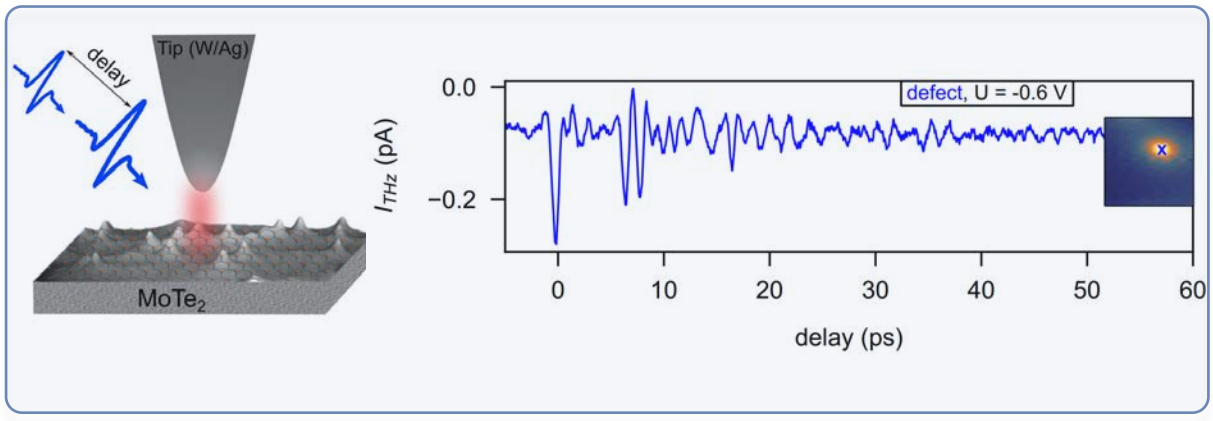
Coherent phonons are collective, ultrafast vibrations of atoms and central to understanding and controlling light-driven structural changes in solids [1,2]. Using terahertz scanning tunneling microscopy (THz-STM), we excite and detect coherent phonons in semiconducting bulk 2H-$MoTe_2$ with atomic-scale spatial resolution. In a THz pump–probe scheme, we detect long-lived oscillations corresponding to out-of-plane breathing and in-plane shear modes—vibrations that in the bulk crystal are inactive and difficult to detect, respectively [3,4].
We conclude, that local band bending must induce a dipole to which THz near fields can couple efficiently. In line with this conclusion, we find that the relative excitation strengths of the two modes change with bias voltage and in the vicinity of defects. We propose that atomic defects modulate the coupling between phonons and the THz field through local band bending. This defect-dependent coupling mechanism enables selective excitation of specific vibrational modes at the nanoscale, offering a pathway for tuning material properties via engineered defect landscapes.



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On-Surface Photopolymerization of Stilbenes via Templating [2+2] Cycloaddition

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On-surface synthesis has emerged as a powerful strategy for constructing covalent nanostructures, exploiting the templating and catalyzing roles of solid surfaces. Light-induced activation offers a fast, reliable means of triggering chemical reactions potentially accessing new mechanistic pathways via excited-state chemistry. Photochemical processes such as UV-induced polymerization of diacetylenes and photodimerization of stilbene derivatives exemplify this potential. Among light-driven reactions, [2+2] photocycloaddition is particularly valuable for generating cyclobutane-containing compounds, hardly accessible by thermal synthetic methods. However, achieving high regio- and stereoselectivity—especially in forming extended oligomers or polymers—remains a significant challenge.

In this work, we explore the use of supramolecular templating to drive the formation of 1D polymers via [2+2] photocycloaddition, employing scanning probe microscopy techniques to manipulate and characterize the resulting macromolecules with nanometer precision. The monomer design is based on a stilbene dimer, devised to engage in specific π-π stacking contacts thereby leading to the formation of densely packed and precisely preorganized supramolecular networks on 2D materials' surfaces. Both the supramolecular monomer assembly as well as the resulting photoproduct are characterized by scanning probe microscopies as well as photoelectron spectroscopy to confirm the light-induced covalent bond formation and to characterize the electronic properties of the final polymeric material.

Our work combines molecular design involving non-covalent assembly on surfaces with advanced surface characterization techniques and demonstrates a novel and selective route to direct light-induced on-surface polymerization.

Orientational Switching as an Extra Degree of Freedom in Molecular Self-Assembly on Au(111)

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Abstract: We investigated the co-assembly of oval-shaped C_{70} and rod-like octanethiol on the Au(111) substrate. We find that C_{70} can switch between two orientations: i) long axis perpendicular to the substrate; ii) long axis parallel to the substrate. This switching capability offers an extra degree of freedom in optimising space-filling, and it leads to structure diversity. By switching between two orientations, the C_{70} molecule effectively plays a dual role in creation of self-assembled structures. The orientation of the octanethiol rod can also change in response to local environment. Such a dual role of a single element is expected to exist in many other physical systems covering multiple scales.

Structural, electronic, and magnetic properties of Europium films epitaxially grown on W(110)

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Rare earth metal (REM) films are renowned for their complex magnetic properties, primarily governed by the element-specific sign and wavelength of the RKKY interaction. Due to the complexity of their cleaning procedures, the magnetic domain structure of REM surfaces has remained largely unknown until today and is an ongoing topic of debate. In this study, we investigate the structural, electronic, as well as the complex magnetic structure of Europium (Eu) films on W(110) using spin-polarized scanning tunneling microscopy (SP-STM). In the bulk, Eu has a half-filled 4*f*- and an empty 5*d*-shell and adopts a body-centered crystal structure. In thin epitaxial films, however, a metastable hexagonal close-packed structure is expected, accompanied by helical spin ordering below $T_{\text{Néel}}$ = 91 K. With optimal preparation conditions, we successfully grew clean, smooth films. In the tunneling spectra of these Eu films, we observed two intense peaks at positive bias voltages which we interpret as the unoccupied and exchange-split $5d_{z^2}$-like surface state. Beyond a critical film thickness, striped regions with a periodicity of ≈ 3 nm were identified. Experiments with differently magnetized STM tips and the application of an external magnetic field up to ±2.5 T revealed the magnetic nature of the stripes, which turned out to be bulk-terminated spin spirals in hcp Eu propagating along $\langle\bar{1}\bar{1}23\rangle$-directions in the surface-near region.

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Molecular Interaction-Directed Self-Assembly and Reorientation of [6]Cycloparaphenylenes on Au(111)

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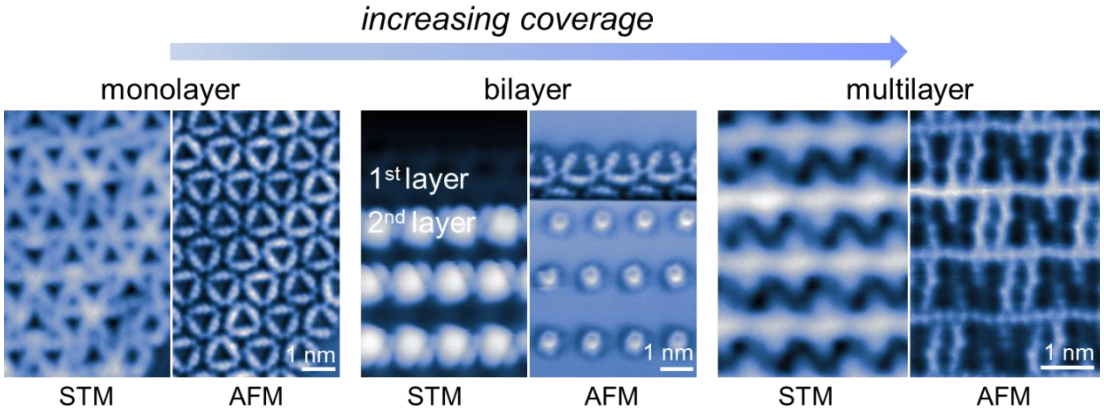
Cycloparaphenylenes (CPPs) represent a fascinating class of polycyclic aromatic hydrocarbons (PAHs) distinguished by their unique optical and electronic properties. Moreover, CPPs are useful for developing supramolecular complexes[1] and thin-film technologies[2]. In this work, we investigate the self-assembly behavior controlled by supramolecular interactions of [6]CPPs on Au(111) using low-temperature scanning tunneling microscopy/spectroscopy (STM/STS) and non-contact atomic force microscopy (NC-AFM). In the sub-monolayer regime, flat-lying species with the CPP-ring oriented parallel to the substrate and distinct phenyl-tilting are clearly resolved by AFM characterization, whereby reorientation of tilted phenyl rings occurs as the tip-sample distance changes. With increasing coverage, Volmer-Weber growth of [6]CPPs is identified. Surprisingly, at medium coverage, the second-layer CPPs form one-dimensional standing chains accommodated at the gaps generated within the first layer, which configuration is stabilized by C-H···π interactions[3]. This flat-standing complex architecture exhibits a HOMO-LUMO gap reduced by approximately 20% compared to single-layer islands. At higher coverage, stacked multilayer islands evolve that could be again characterized by AFM. This insight into complex interaction-directed assembly of CPPs offers valuable guidance for controlling film morphology in future electronic or optoelectronic applications.



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Revealing Spatial Inhomogeneities in Superconducting 2H-NbS_2 using Magnetic Sensor Atoms

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Transition metal dichalcogenides (TMDs) provide a versatile platform to explore the interaction between magnetic atoms and superconductors, which realizes long-range Yu-Shiba-Rusinov (YSR) states [1, 2]. Among the TMDs, 2H-NbS_2 is unique as it lacks a charge density wave (CDW) in the pristine material. However, the presence of local, defect-induced CDW patterns is being debated in literature [3, 4].

Using low-temperature scanning tunneling microscopy and spectroscopy, we investigate the 2H-NbS_2 surface and observe wave-like modulations around defects in differential conductance maps. These features suggest either local CDW nucleation or quasiparticle interference (QPI). To distinguish the origin of the wave patterns, we use YSR states arising from individual Fe adatoms as local probes, as the YSR state energy is expected to scale with the local density of states. By manipulating a single Fe atom across the surface, we detect a strong variation in YSR energies in identical adsorption sites. The spatial correlation analysis between YSR peak energies and the wave patterns reveals that the observed wave patterns are not purely electronic (e.g., QPI). Our results highlight the utility of YSR states as sensitive probes of spatial inhomogeneities in superconducting materials.

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Phthalocyanine-based bipartite lattices: Towards a molecular Lieb lattice

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Designed molecular systems allow us to exploit the engineered energy spectrum originated from the topology [1-5]. A Lieb lattice is an example for how topology can emerge material properties such as the sublattice imbalance induced extended degenerate states, resulting in a flat band [6]. Whereas the physical properties of Lieb lattice have been widely studied in cold-atom systems and photonic lattices, experimental realization in solid-state systems with atomic precision remain scarce [7].

Here, we realize several different Lieb-lattice prototypical structures by means of on-surface synthesis. Owing to the C_4 symmetry and on-surface synthesizability of phthalocyanines (Pcs), Pcs are utilized as the building blocks, having identical molecular subunits, yet different coordination numbers. We present atomically precise, covalently bonded structures with increasing dimensionality, starting with a simple bipartite unit, having only one A site and four B sites, to a linearly extended prototypical structure to the two-dimensional (finite) Lieb lattice, as evidenced by bond-resolving AFM imaging. All the structures are planar and feature π-conjugation over the network. The electronic properties of the structures are analyzed by combining differential conductance mapping, density-functional theory calculations, and tight-binding models. The formed structures exhibit a strong inter-site electronic coupling and are in accordance with Lieb's rules for quantum states of bipartite lattices.

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Tuning spin transitions in a coupled two-level system using spin-electric control

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The milestone of controlling individual spins one-by-one is a prerequisite for numerous applications such as miniaturization of data storage or quantum computing. In the field of Electron Spin Resonance Scanning Tunneling Microscopy (ESR-STM), a spin-polarized tip allows for such atomic scale spin manipulations, which has consolidated the technique of ESR-STM in the recent years. In our case, we have a high Zeeman energy (corresponding to 60 – 90 GHz) and we exploit a local electric field in the tunnel junction to tune the energy of the transitions.

Here we experimentally measure a dimer system as a function of the electric field. We are demonstrating that we can control the coupled spins through an avoided level crossing, thereby introducing an additional tuning parameter. We then use non-equilibrium Green's function techniques and density matrix theory to disentangle the different terms in the tunneling current.

We find excellent quantitative agreement between theory and experiment, allowing us to establish a better understanding of excitation dynamics. Given that lately there has been a considerable interest in more complex arrangements of multiple spins, the versatility of our theory can open the possibility to predict and explain the outcome of a variety of experiments under different conditions.

Local activation of on-surface synthesis via laser-illuminated STM tips: toward atomically precise reaction control

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One of the ultimate goals of nanotechnology is the precise fabrication of functional nanostructures and nanoelectronic devices. On-surface synthesis, through the rational design of molecular precursors, has made significant contributions toward this objective by enabling the bottom-up construction of tailored nanostructures. However, most of the on-surface synthetic approaches employ thermal annealing as a reaction trigger, which hinders atomically precise fabrication. In contrast, tip-induced and light-induced strategies offer tunability and higher precision[1,2]. Notably, laser-illuminated plasmonic tips can generate near-field effects[3], which may further promote reactions with enhanced efficiency and precision.

In this poster, through the synergistic combination of scanning tunneling microscopy (STM) and laser excitation, we present the local activation of on-surface synthesis processes. Using two representative precursors for thermal on-surface synthesis, 10,10'-dibromo-9,9'-bianthryl (DBBA) and 4,4''-dibromo-p-terphenyl (DBTP), we observed the dehydrogenative cyclization and debromination, respectively, by visible-laser-illuminated STM tips on Au(111) at low temperature. Our systematic controlled experiments reveal that specific combinations of the STM bias voltages and incident-light wavelength can induce the local reactions, thereby providing insights into the underlying reaction mechanisms. Our findings highlight the potential of this combined triggering strategy toward atomically precise fabrication of nanostructures.

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Magnetic adatom manipulation on monolayer transition metal dichalcogenides

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Two-dimensional materials are found to host a large variety of correlated phases. A promising approach towards understanding and controlling these phases is by means of atomic manipulation. Here we compare two systems for atomic manipulation experiments: Fe on 1H-MoS_2 and Fe on 1H-TaS_2. We find that manipulation of Fe on 1H-MoS_2 results in point defects (sulfur vacancies) [1], which we investigate using scanning tunneling microscopy and spectroscopy. In contrast, we find that single Fe adatoms can be laterally moved on 1H-TaS_2, enabling construction of lattices consisting of tens of adatoms. We additionally report on the observation of two inequivalent adsorption sites for Fe, hollow and Ta-top sites, which manifest as differences in the adatom's apparent height.

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Realization of separation of time scales for a heterogeneous atomic Boltzmann machine

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The Boltzmann machine (BM) describes an energy-based neural network formed by coupled, fluctuating Ising spins [1]. A material realization of the Boltzmann machine was constructed using the complex stochastic dynamics of coupled Co atoms on the surface of black phosphorus (BP) [1]. Neurons and synapses were realized by a separation of time scales exploiting the anisotropic electronic structure of BP [1]. Using the anisotropy of the substrate is a limitation in scaling this concept.

Here, we study the coupled dynamics of different types of atoms on BP, which exhibit orbital memory [2,3]. We study the influence of the coupling on stochastic dynamics in heteroatomic dimer and trimer configurations with scanning tunneling microscopy (STM). Further, we discuss how the multi-well energy landscape can be influenced by an applied AC signal.

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Evidence of multiferroicity in monolayer $NiBr_2$

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Multiferroic materials exhibit more than one primary ferroic order, such as ferromagnetism and ferroelectricity. Progress in two-dimensional (2D) materials has proven monolayer NiI_2 to be the first multiferroic material at single-layer limit[2]. Here we present experimental evidence of multiferroicity in monolayer $NiBr_2$, another transition metal dihalide (TMDH), by using scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS). These techniques have demonstrated the capacity to investigate monolayer multiferroicity at atomic scale[2]. Surprisingly, we observe two different stripe periodicities, ~14 Å and ~28 Å. Furthermore, we are able to switch between these by altering our setpoint or applied external magnetic field. These findings are important for further understanding of multiferroicity down to monolayer limit.

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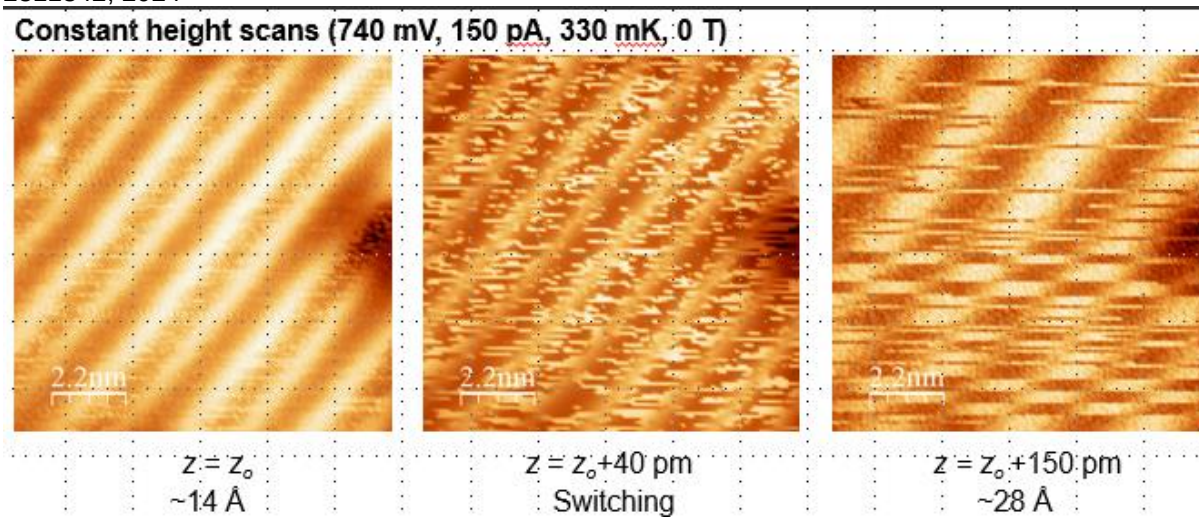

Figure 1: Change of stripe periodicity when the tip-sample distance increases.

Magnetic Quantum Corrals on a Proximity-Superconducting Rasbha Surface Alloy

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Artificial nanostructures made with on-surface atoms offer tunable quantum platforms for exploring emergent phenomena such as Kondo resonance, quasiparticle interference as well as topological bound states [1]. Quantum corrals, as closed atomic structures, can confine and resonate surface-state electrons at discrete eigenmodes. When coupled to superconducting substrates, recent research has demonstrated that quantum corrals can support spin-degenerate Machida-Shibata (MS) as well as Yu-Shiba-Rusinov (YSR) in-gap states due to proximity-induced Cooper pairing [2,3]. However, leveraging this framework, especially including magnetic interactions and strong spin-orbit coupling, to potentially achieve non-trivial topological phases or spinful quantum dots remain a significant challenge.

Here, we investigated quantum corrals crafted from Fe magnetic atoms on the Rashba surface alloy BiAg2/Ag(111) with proximity-induced superconductivity from a Nb(110) substrate. The shape of the quantum corrals was chosen hexagonal, imposing a boundary condition fitting to the lattice symmetry. The magnetic Fe atoms placed on the superconductor, which are used to build the quantum corral walls, induce YSR confined states of a similar spatial distribution as the quantum corral eigenmodes in the gap of the substrate. The spatial oscillations of these confined states show an almost perfect antiphasing between the particle- and hole-like components, similar to long-range YSR states of individual magnetic atoms [4]. In addition, we observe confined states close to the coherence peaks, which resemble MS states. By further studying the change of these two types of states with corral size, our work characterizes the interplay between the YSR and MS states within the quantum corral.

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Tuning the magnetism of a single atom by local charge gating

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The description of single-atom magnetism depends on the interplay of various degrees of freedom and the balance of different interactions. This includes the interplay between the orbital, spin and charge degrees of freedom, as well as the balance between spin-orbit coupling, hybridization, and different exchange interactions, such as Hund's and Kondo exchange. To date, the strategy to change the magnetic behavior of a single atom is to explore different atom/surface combinations. However, in this way, nearly all these various parameters are fixed by the material system and when changing the material system, the entire set of parameters changes. Here, we use variations in the local charge density on semiconductor surfaces as a platform to modify the magnetic properties and tunneling transport of individual Fe atoms. We start with Fe atoms on the surface of InSb [1,2], and characterize its magnetic excitations as a function of magnetic field. We then harness a newly developed quantum simulator platform, based on patterning Cs atoms on the surface of InSb [3]. We show that by varying the local density of Cs on InSb(110), we can change the magnetic properties and excitations of an individual Fe atom. These results serve as a starting point to develop quantum simulation to study magnetic models in which the spin, charge, and orbital degree of freedom can be tuned.

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Cross-sectional scanning tunneling microscopy study of nearly lattice-matched III–V semiconductor heterostructures

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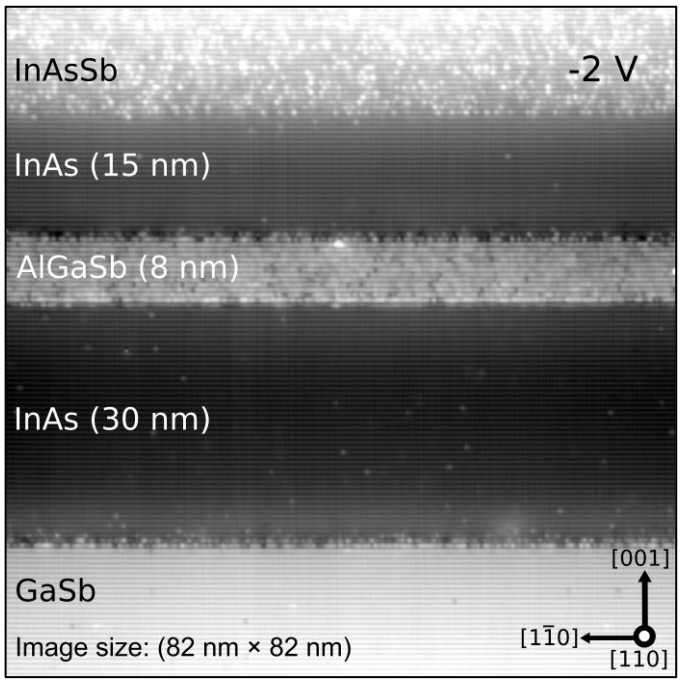
Cross-sectional scanning tunneling microscopy (X-STM) is a powerful technique for investigating the structural and electronic properties of III-V semiconductor heterostructures [1,2]. These heterostructures are grown along the (001) direction by molecular beam epitaxy and accessible in cross-sectional view by cleaving the sample in ultrahigh vacuum to expose the (110) cleavage surface.

We used this approach to study a **GaSb-InAs-AlGaSb-InAs-InAsSb** layered heterostructure (as shown in the figure) grown on a Te-doped GaSb substrate. Voltage-dependent chemical contrast in STM imaging allows differentiation between anions and cations in the III-V semiconductors. We took advantage of this capability to determine the degree of homogeneity in the ternary materials, that is to say, the degree of Al-Ga mixing in the AlGaSb layer, as well as the As-Sb mixing in the InAsSb layer.



With the help of scanning tunneling spectroscopy, we precisely determined the band gaps of the individual layers and locally probed the band lineup across the entire heterostructure. This allowed us to investigate the charge carriers' behavior governed by the band lineup. Specifically, we studied the spatial confinement and quantization of conduction band states in the InAs layer as well as their decay into the gap region of the neighboring layers.

Finally, we show preliminary spectroscopy results on single In atoms transferred from the (In-coated) STM tip to the surface of the InAs and GaSb layer, respectively.

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PTCDA on calcite(104) - high resolution imaging and charge state control of organic molecules on a bulk insulator

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The development of functional single-molecule nanosystems for future information technology and (opto-)electronics relies on innovative approaches for realizing molecular self-assembly on insulating substrates, given the electronic isolation from the supporting material together with a variety of proven concepts for molecular structure formation. Nowadays, it is understood that molecular anchoring [1] is essential for the realization of molecular structures on dielectrics, as it impedes molecular dewetting [2].

Here, we study the adsorption structure and functional aptitude of single perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA) molecules on the calcite(104) surface. Non-contact atomic force microscopy performed with CO-functionalized tips achieves sub-molecular contrast of PTCDA on the bulk dielectric surface, with resolution comparable to molecule-on-metal systems [3]. In combination with density functional theory calculations, the high-resolution data evidences a strong molecular deformation as a consequence of strong molecule-surface interaction. Furthermore, we investigate the charging behavior of isolated and paired PTCDA molecules by tunneling single electrons from the tip contact [4]. The charging of isolated molecules reveals not only minor molecular reorganization, but also shows that the influence of residual charges typical for bulk dielectrics after cleaving in ultrahigh vacuum [5] has negligible effect on the charging process. For the case of paired PTCDA molecules, we find that an intermolecular Coulomb repulsion [6] strongly influences the charging behavior of the individual molecules.

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Landau-Zener Dynamics and the Quantum-Classical Crossover in Antiferromagnetic Nanomagnets

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Avoided level crossings give rise to quantum superposition states that significantly speed-up the spin dynamics by enhancing tunneling of magnetization. As the size of a spin system increases, these superpositions, and accordingly the crossings, become smaller which gradually suppresses tunneling of magnetization leading to a quantum to classical crossover.
To explore this, we measure magnetization reversal in antiferromagnetic Fe spin chains on a Cu_2N surface [1], shown in Fig. 1, using a scanning tunneling microscope (STM). By oscillating the magnetic STM tip, we induce an oscillating field at the spin chain, which allows us to drive the system through the avoided level crossing at ramp speeds up to 40 kT/s and simultaneously track the real-time spin switching with microsecond resolution.
We observe a clear dependence on chain length: Longer chains predominantly exhibit thermally activated switching, consistent with a collapse of the avoided level crossing. In contrast, shorter chains with five atoms or less show increased switching at the avoided level crossing.
We demonstrate that the switching probability follows the Landau-Zener dependence on ramp speed. Our results highlight that magnetic state transitions can be induced via fast modulation of the STM tip, opening new possibilities for rapid control of spins at the nanoscale.

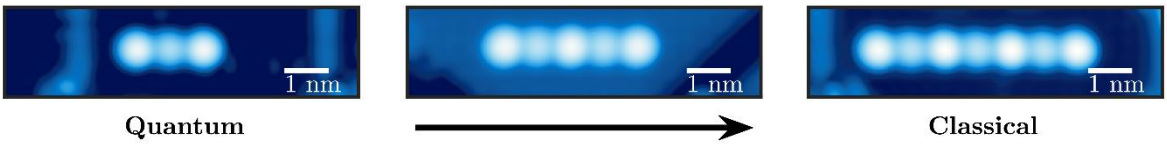

Figure 1: Spin polarized topographies of Fe nanomagnets containing three to seven atoms on a Cu_2N surface representing the transition from a quantum to a classical nanomagnet.

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Steering Magnetic Coupling in Diradical Non-benzenoid Nanographenes

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Magnetic properties arising from controlled spin–spin interactions hold great promise for applications in spintronics and quantum technologies [1,2]. In nanographenes, pentagonal and heptagonal rings introduce geometric frustration and sublattice imbalance, fundamentally altering spin localization and facilitating the emergence of open-shell structures [3-5]. The precise engineering of magnetic order and coupling strength in the resulting nonbenzenoid nanographenes, however, remains a challenging and underexplored area. Here, we demonstrate an on-surface synthesis of nanographenes incorporating five- and seven-membered rings through a sequence of intramolecular C–C bond formations between methyl and aryl units. Two products are generated: the partially cyclized intermediate MAAT and the fully cyclized end product MAZC. Due to the presence of iodo groups, the resulting monomers obtained can be covalently connected via Ullmann-like coupling in variable modes, enabling programmable spin arrangements. While MAZC exists as a nonmagnetic species, MAAT featuring one seven-membered ring holds an unpaired S = 1/2 spin and exhibits Kondo resonance on a metal surface. By change of the connectivity between two MAAT units, tunable magnetic ground states and precise control over the exchange-interaction strength can be achieved. These findings, supported by scanning probe microscopy and density functional theory, establish a novel strategy for designing defined carbon nanostructures with tailored topological defects and offer fine-tuned manipulation of molecular magnetism.

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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 and was first introduced in 2015 by researchers at Peter-Grünberg-Institute (PGI-3) at Forschungszentrum Jülich [1]. From 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.

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Momentum-selective tunneling from the edge of a van der Waals scanning probe tip

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Scanning tunneling microscopy (STM) has become an important tool for studying the properties of van der Waals materials, such as graphene, because it enables the characterization of localized electronic states, such as moiré and edge states. Adapting our previously developed vdW stacking methods [1, 2] we have fabricated scanning tunneling tips made from exfoliated graphite flakes. Such vdW tips were characterized by tunneling on the Ag(111) surface, where differential conductance measurements evidence tunneling through zigzag/armchair edges of the graphene-like tips. Additionally, we find that Friedel oscillations observed on the Ag(111) surface with such tips show an anisotropic tunneling conductance. Theoretical considerations support that this anisotropy stems from momentum-selective tunneling between the quasi-one dimensional tip apex and the Ag surface. To further validate this finding, we resolved the momentum-dependent superconducting gap of FeSe.

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Josephson diode in a Pb-Pb junction with chiral Fe clusters

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Josephson junctions are junctions where Cooper-pairs can tunnel between two weakly-coupled superconductors with a phase difference. The phase dynamics of Josephson junctions can be accessed via current-biased Josephson spectroscopy revealing the switching and retrapping currents [1]. Switching currents mark the transition from Cooper-pair tunneling to quasi-particle tunneling whereas retrapping currents indicate the opposite. Recently, it has been found that a single magnetic adatom inside a Josephson junction in a scanning tunneling microscope (STM), leads to diode-like behavior in the retrapping currents. This asymmetry in retrapping currents has been attributed to quasi-particle tunneling through the electron-hole asymmetric Yu-Shiba-Rusinov states [1,2].

Here, we investigate self-assembled clusters of Fe on Pb(111). We find different types of clusters, one type of them exhibits spatially chiral YSR wavefunctions in the differential conductance (dI/dV) maps. Current-biased Josephson spectroscopy over these chiral clusters does not only show asymmetry in retrapping currents but also in switching currents. These results point towards the presence of a magnetic moment of the cluster that breaks time-reversal symmetry.

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Stochastic resonance realized with a superconducting magnetic impurity state

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The phenomenon of stochastic resonance was originally studied in the context of climatic changes and has since been observed in a variety of systems, both classical and quantum. Here, we employ this phenomenon to infer the rates of tunneling processes in the course of quantum electronic transport [1,2]. We theoretically investigate the emergence of stochastic resonance in superconducting junctions, focusing on a system where one electrode hosts a Yu-Shiba-Rusinov state – a discrete bound state within the superconducting gap induced by the magnetic exchange interaction between a magnetic impurity and its superconducting host. Applying the framework of full counting statistics, we demonstrate that stochastic resonance manifests as the reduction of the Fano factor and a resonance of the tunneling current. The frequency of the resonance reveals information about the rate of microscopic electronic processes, e.g. the process responsible for quasiparticle-occupation parity breaking.

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Atomic-Scale Sequencing of Biomolecules with nc-AFM

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Glycans, peptides, and cyclodextrins present major challenges for structural analysis due to branching, heterogeneous modifications, and stereochemical diversity. Conventional tools such as MS and NMR often fail to resolve these features at the single-molecule level. Non-contact AFM, combined with STM and KPFM under cryogenic UHV conditions, has recently demonstrated chemical sensitivity sufficient to discriminate functional groups and stereochemical arrangements by probing electrostatic and non-covalent interactions. Applications include the direct visualization of glycans in protein and lipid conjugates [1], submolecular resolution of cyclodextrins [2], and progress toward sequencing of complex carbohydrates and peptides. These results underline the potential of nc-AFM to expand the scope of SPM from imaging and identification toward true atomic-scale sequencing of biomolecules.

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Scanning tunnelling microscopy reveals homocoupling-free and exceptionally long pgBTTT as high-performance materials in OECTs

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Conjugated polymers, among organic semiconductors, have attracted significant attention due to their remarkable conductivity, mechanical flexibility and cost-effective processability. These attributes make these materials highly promising candidates for a wide range of applications, including optoelectronics, thermoelectrics, sensors, and bioelectronic devices.

The innovative combination of electrospray deposition (ESD) with scanning tunnelling microscopy (STM) in an ultrahigh vacuum environment, developed by the Costantini Group, provides an unprecedented opportunity to achieve detailed, molecular-scale insights into the structure, conformation and assembly of surface-adsorbed conjugated polymers. This level of analysis remains unattainable with any other existing analytical technique. The electrospray ionisation process enables the controlled and intact soft-landing of sub-monolayer coverages of macromolecules onto atomically clean and flat single-crystal surfaces while preserving their original sequence and structure. High-resolution STM analysis then reveals preferential assembly configurations, stacking distances, polymer mass distributions, exact backbone sequences and side chain conformations.

In this study, we specifically quantify homocoupling defects in the benchmark *p*-type material pgBTTT synthesised via two different pathways: conventional Stille polymerisation and an alternative symmetric Stille approach. Our findings indicate that polymers synthesised via the alternative approach are exceptionally long and exhibit no homocoupling defects, in contrast to those obtained through conventional Stille polymerisation. This structural advantage translates into significantly improved performance in organic electrochemical transistors (OECTs). STM measurements enable a crucial statistical investigation of the relationship between homocoupling defects and molecular weight, interestingly revealing no significant correlation between the two, and challenging the common assumption that homocoupling defects hinder polymer growth.

Coherent dynamics of magnons by atomic assembly of spin chains with ESR-STM

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The coherent free evolution of coupled spins [1] and an electron and nucleus within a single atom [2] has previously been demonstrated using ESR-STM. Here, we extend this approach to atomically assembled spin chains, which provide a tunable platform for investigating magnon transport and interactions with nanosecond-resolution pump-probe spectroscopy. These chains offer a powerful testbed for quantum simulation, enabling the realization of exotic magnetic states at the atomic scale [3]. By exploiting the spectral resolution of ESR-STM, we achieve controlled excitation, and tuning of coherent spin-wave modes, while pump-probe techniques allows us to directly map their dynamics on a nanosecond scale. In particular, by engineering stronger exchange coupling within the change itself and the readout atom, we observe many more oscillations within the coherence times, demonstrating dynamical timescales significantly faster than those reported by Veldman *et al.* [1]. This work addresses the coherent magnon dynamics within precisely engineered atomic spin chains and paves the way for probing more complex collective excitations in larger spin systems.

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STM imaging of stripe dynamics in superconducting nickelate

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The Hubbard model on the square lattice predicts stabilization of a unique correlated stripe order for small dopings, a finding that has been discussed a lot in the context lightly doped cuprates. This charge-spin stripe modulation has been experimentally observed originally in non-superconducting nickelate La_2NiO_4, and then also in some high-temperature superconducting cuprates. Recently, high-temperature superconductivity has been discovered in the higher order members Ruddlesen-Popper nickelates $La_{n+1}Ni_nO_{3n+1}$ n=2,3,4. We show that similar stripe order is observed in STM imaging on the surface of La4Ni3O10 in the metallic state. Additionaly, it turns out that low frequency local stripe fluctuations can be induced by electrons tunnelling from the tip, hinting on a weak pinning of the electronic order to the lattice. Such observations point out further similarities between high-temperature cuprates and nickelates suggesting similar correlated physics in these systems.

Effects of Alternating Bias on Spin Resonance in Quantum Devices.

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Electron spin resonance with the scanning tunneling microscope (ESR-STM) is a successful technique that detects single-atom spin resonances by measuring the tunneling DC current as a function of driving frequency. Although ESR–STM experiments continue to proliferate, their exact mechanism remains debated, with multiple theoretical models proposing how time-dependent electric fields modulate spin-polarized transport electrons [1]. Furthermore, ESR-STM has been proposed as a potential setup for a single-molecule quantum computer [2–4].

Here, we expand upon the master equation approach developed by Reina-Gálvez et al. [5], to examine a many-body problem for different atomic level parameters. In particular, we replace an effective time-dependent transition by explicitly including the effects of the RF bias.

We employ our model to examine the effects of DC and RF bias applied to the junction. Our findings could be used in the development of single-molecule quantum devices in the ESR-STM setup. We will further compare our predictions with the experimental results to better understand the effects of time-dependent electric fields.

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Determination of the coupling regime and Kondo temperature of a spin ½ system at millikelvin temperatures

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Scanning tunneling microscopy (STM) is a powerful tool for fabricating and studying artificial nanostructures on surfaces. Recent studies have shown that the electronic coupling between a planar aromatic molecule and a metallic substrate can be strongly reduced by lifting the molecule into an upright configuration using STM manipulation [1,2]. Here, we extend this approach by investigating an upright-standing NTCDA (1,4,5,8-naphthalenetetracarboxylic dianhydride) molecule on an Ag(111) surface. The molecule-substrate interaction is characterized via the Kondo effect arising from an unpaired electron in a molecular orbital of NTCDA. We show that, in the weak-coupling regime, the temperature dependence of the Kondo resonance alone is insufficient to determine the Kondo temperature. Instead, a combined magnetic-field- and temperature-dependent analysis is required. By measuring differential conductance (dI/dV) spectra between 30 mK and 1 K under various magnetic fields and comparing them with numerical renormalization group (NRG) calculations, we find that the Kondo temperature lies between 1 fK and 100 fK, and is thus far below the experimental temperature in the millikelvin range.

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Ångström-Resolved Spectro-microscopic Visualization of Surface Catalyzed Metalation Mediated Ring Fusion in Benzoporphyrins

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Understanding and controlling surface-supported physicochemical transformations at the molecular level is crucial for advancing functional materials in catalysis and optoelectronics. However, precise control over reaction outcomes requires sub-molecular-scale characterization of the local structure of chemical intermediates and products. Scanning tunneling microscopy (STM) plays a central role in this effort, offering sub-molecular resolution of adsorption geometries, conformational dynamics, and electronic states. The incorporation of single transition metal atoms into molecular systems has opened new directions in optoelectronics and single-site catalysis. Yet, the role of surface chemistry in stabilizing specific molecular configurations under the influence of metal substrates remains largely unexplored. Porphyrins are ideal candidates for such studies due to their electronic and catalytic versatility, as well as their ability to coordinate metal atoms. While STM reveals intramolecular topographic and electronic features, integrated tip-enhanced Raman spectroscopy (TERS) complements the structural insight from the viewpoint of chemical identification. A combined ultra-high vacuum (UHV) STM and TERS approach has been employed to probe vibrational and structural changes at the molecular level in the investigation of the thermal transformation of tetraphenyl tetrabenzoporphyrin on a Cu(100) surface. Notably, STM visualizes the in-situ formation of a Cu-porphyrin complex at room temperature, demonstrating a potential single catalytic site. TERS revealed the chemical identity and the origin of altered symmetry in the nonplanar intermediate. Upon further annealing, STM-TERS confirms increased planarity and stronger molecule–substrate interaction in the final product. TERS also identifies the bonding scheme in the products, offering a comprehensive view of the reaction landscape.

Setup of an ESR-STM at mK Temperatures in a Closed-Cycle Dilution Refrigerator

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By combining Electron Spin Resonance (ESR) with Scanning Tunneling Microscopy (STM), electronic and magnetic properties of single atoms and molecules can be studied. However, for these measurements a setup that both enables a low electronic temperature and a good RF transmission to the STM junction is required.

Here, we describe the setup of an ESR-STM mounted in ultra-high vacuum (UHV) in a compact closed-cycle Dilution Refrigerator (DR) providing both a low vibrational level and a fast cooldown. The electronic temperature of our setup measured on Al(111) is 150 mK while maintaining a reasonable RF transmission up to 20 GHz. To realize this, RF voltages up to 1 GHz are applied to the tip, while higher RF frequencies are applied to an RF antenna.

Engineering Spin-1/2 Chains with ESR-STM and NISQ Devices for Time Crystal Realization

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Recent advances in quantum technologies have opened new avenues for probing and controlling quantum systems at the atomic scale. In particular, the combination of electron spin resonance scanning tunneling microscopy (ESR-STM) with noisy intermediate-scale quantum (NISQ) devices provides a powerful platform for investigating spin dynamics and implementing quantum operations with unprecedented spatial and temporal resolution. By performing NISQ simulations to benchmark and guide ESR-STM experiments, we gain experimental access to regimes beyond the reach of classical computation. Here, we propose a scheme for realizing discrete time crystals in engineered spin-1/2 chains assembled atom-by-atom by positioning Ti atoms on MgO/Ag(100). The interplay between periodic driving and Heisenberg-like interactions in these atomically precise chains enables the exploration of non-equilibrium quantum phases with direct relevance to quantum information processing and nanoscale magnetism. Our approach builds on recent demonstrations of atomic spin chains fabricated with STM manipulation [1,2] and establishes a pathway to experimentally access Floquet-engineered phases of matter with single-site control.

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On-surface reactions of electronically active self-assembled monolayers for electrode work function tuning

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Self-assembled monolayers (SAMs) help improve the performance of organic electronic devices through interface passivation and enhanced carrier transport. Yet, there is limited information as to the chemical structure of the SAMs upon functionalisation and subsequent thermal treatment. Here, we studied the on-surface reaction of carbazole derived SAMs on model gold electrodes, focusing on the chemical structure changes induced by thermal treatments. Furthermore, we correlate the microscopic changes with their impact on the electrode's work function. The carbazole-based SAMs first transform into organometallic complexes. At higher annealing temperatures, SAMs convert into oligomeric complexes. The observed chemical reactions significantly reduce the electrode work function and facilitate electron injection in n-type organic thin film transistors. Our results highlight on-surface synthesis of electronically active SAMs as an alternative approach for modifying the work function of electrodes for organic electronics.

Conductive atomic force microscopy tomography on Cu(In,Ga)Se_2 solar cell absorbers

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Alkali-fluoride (AlkF) post-deposition treatments (PDT) have led to significant increases in the power conversion efficiency of polycrystalline Cu(In,Ga)Se_2 (CIGSe) thin-film solar cells. Kelvin probe force microscopy has revealed that the AlkF-PDT passivates grain boundaries [1]. However, these results rely on surface potential information collected at the surface of the AlkF-PDT CIGSe, and the electronic structure of grain boundaries in the bulk remains unknown [2]. Here, we explore the nano-scale electronic properties of CIGSe absorbers into the bulk of the layer, by using an emerging conductive atomic force microscopy (C-AFM) tomography method. Highly-doped diamond-coated AFM tips are scanned repeatedly across the same area using high tip-load forces of several µN, leading to a tip-induced material removal [3]. Simultaneously, the local tip-sample current is recorded. The layer-by-layer C-AFM images lead to a three-dimensional current image, reaching deep into the bulk of the CIGSe layer.

We present a methodology for the quantitative analysis of the C-AFM current signals, in consistency with a mechanical model describing the materials removal [4]. The analysis enables to determine the charge-carrier concentration of individual grains in the polycrystalline CIGSe absorber. For CIGSe with various AlkF-PDT treatments, we find that a lower efficiency solar cell with a KF-PDT shows a stronger inhomogeneity of charge-carrier concentration, while RbF- and CsF-PDT lead to narrow distributions at higher charge-carrier concentrations. The charge-carrier concentration and its homogeneity relate directly to the open-circuit voltage of solar cell devices, thereby impacting the device performance. Thus, the success of the AlkF-PDT can be hampered by spatial inhomogeneities on the sub-micrometer scale in the charge-carrier concentration. Furthermore, analysis of grain boundary currents reveals that they behave similar in the bulk to what is observed near the surface.

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Polarons in epitaxial single-layer $MnBr_2$

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Beyond their intriguing magnetic properties, epitaxially grown single-layer transition metal dihalides exhibit spontaneous self-trapping of charge carriers, forming quasiparticles with exceptional long lifetimes, identified as polarons [1-2]. Here, we study polaron formation in epitaxially grown single-layer $MnBr_2$, which has a larger band gap than other previously studied transition metal dihalides [3]. We observe strong similarities in the polaronic behavior of $MnBr_2$ compared to $CoCl_2$, yet also uncover new features unique to $MnBr_2$. Our results show that the polarons are thermally stable up to room temperature, though their density drops as temperature increases. Notably, polarons in $MnBr_2$ on Gr/Ir(110) exhibit significant interaction with the underlying moiré superstructure. Additionally, we discover that polaron characteristics depend heavily on the substrate: while $MnBr_2$ on Gr/Ir(110) hosts four different polarons, only two intrinsic types remain on Gr/Ir(111). On Au(111), polarons become more confined, and their densities rise significantly compared to the Gr/Ir substrates.

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Atomically-controlled fluorescence with STM: from electron to photon excitations

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STM-induced luminescence [1,2] and tip-enhanced photoluminescence [2] enable fluorescence imaging of molecules with sub-nanometer spatial resolution. While the former approach relies on tunneling electrons as an excitation source, the latter involves exciting the molecule with light. This poster will highlight recent results from our team and compare the respective benefits of each method.

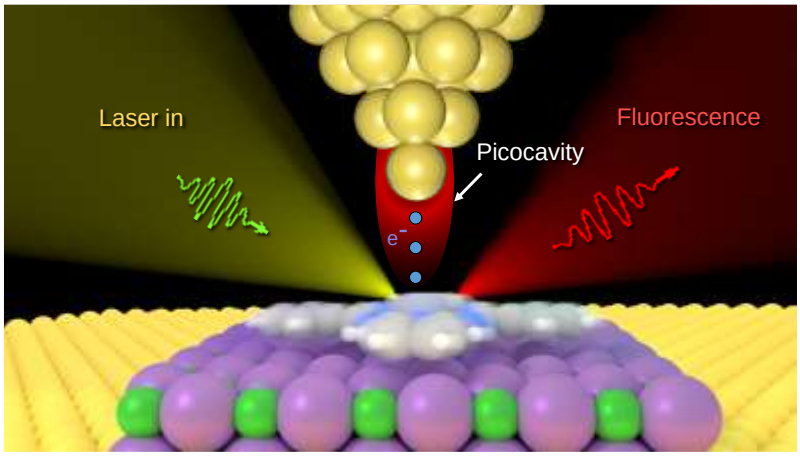

Figure 1: Tip-enhanced photoluminescence of a free-based phthalocyanine molecule decoupled from Ag(111) by few layers of NaCl in a scanning tunneling microscope.

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Photoexcitation Atomic Force Microscopy

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The combination of scanning tunnelling microscopy (STM) with luminescence provides atomic-scale insights into light-matter interaction. More recently, photoexcited charge carriers have been detected by means of STM, opening the door to study photo-physical processes with atomic-scale spatial resolution [1] – from exciton generation to charge transport.

We propose a novel approach to detect photoexcitation in single molecules adsorbed on thick insulating films (> 20 monolayers NaCl). Suppressing substrate tunnelling enables single-charge sensitivity and allows separating the subsequent steps involved. We detect single-electron tunnelling events that follow photoexcitation using atomic force microscopy (AFM), in a similar way as in alternate-charging STM [2]. Key to this approach is the synchronization of the laser pulses to the oscillation of the AFM sensor.

We demonstrate this technique for individual copper phthalocyanine molecules, where the observed smeared-out contrast in the photoexcitation AFM images indicates the involvement of a long-lived quadruplet excited state. The nature of these states is further elucidated using the recently developed excited-state spectroscopy method [3]. This combination of methods enables the detection of long-lived excited states, including a quadruplet state, and underscores the potential of photoexcitation AFM to advance the study of light-matter interactions at the single-molecule level.

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An electrical molecular motor driven by angular momentum transfer

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The generation of unidirectional motion on a molecular level has been a long-standing challenge in the engineering of molecular machines. Often, it is generated by excitation and directional relaxation caused by steric hindrance.
We present results concerning a molecular motor driven by an angular momentum transfer from the current in an STM to the molecule. The molecular complex is comprised of a helical moiety (rotor) mounted on a tripodal platform (stator) via a C-C triple bond (axle). The molecules are anchored to a Au(111) surface and studied at 4.2 K. Employing a codeposition technique we ensure that the rotors are well separated.
Fixing the tip position on a molecule and recording time traces of the current, we find three distinguishable current levels, which we interpret as meta-stable rotational states. As directional rotation processes potentially compete with random motion, we scrutinize the directionality via a binomial test. Unlike ratchet type motors which typically rely on excitation of vibrational states, voltages of about 1.8 V are required to observe directed rotation. Most notably, the direction of rotation does not change when the bias voltage polarity is reversed. These counter-intuitive results exclude any momentum transfer via a chiral tip, the chiral geländer type head group or the chiral foot structure.
Instead, our DFT calculations show that the rotation sense is linked to transport across specific helical orbitals in the axle. The current flowing across these orbitals leads to a backaction torque on the molecular rotor. Crucially, the relevant orbitals at positive and negative voltages have opposite helicity. In combination, reversal of both the direction and the helicity of the current leads to backaction and rotation in the same direction, in full agreement with the experiment.
We believe that our combined experimental and theoretical results are proof of an entirely new driving mechanism for directed rotation on the molecular scale.

Charge Manipulation in Hematite Fe_2O_3 as a Route to Polaron Physics

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The non-contact Atomic Force Microscopy (nc-AFM) technique has enabled breakthroughs in single-electron charge manipulation [1]. Here we use this capability to study polaron dynamics. Polarons are self-localized electrons or holes in ionic lattices that are crucial to material properties like conductivity, catalysis, and exotic phenomena such as high-temperature superconductivity and colossal magnetoresistance [2]. This research explores the behavior of polarons in hematite Fe_2O_3 at the single quasiparticle level, with a particular emphasis on the fundamental mechanisms governing their injection, formation, migration, and interactions with defects. [3]. The latest findings that will be presented highlights advances in localized charge injection technique, assessments of polaron stability, and the ability to track individual polarons in real space.

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Probing the Electrostatic Potential by AFM with an O-terminated Copper tip: Direct Elemental Discrimination on hBN

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Monolayer hexagonal boron nitride (hBN) is an insulator of great interest owing to its point defects, some of which are suspected to act as room-temperature single-photon emitters [1]. Understanding the microscopic structure of these defects is crucial for quantum optics. Although conventional scanning probe techniques such as STM and AFM provide insights on the atomic scale, they cannot reliably distinguish boron from nitrogen atoms [2]. This exemplifies a broader challenge in scanning probe microscopy: the lack of elemental and chemical selectivity on heterogeneous surfaces, where complex contrast mechanisms require interpretations to rely on indirect assumptions about tip and surface structure. Non-contact AFM with oxygen-terminated copper tips (CuOx-tips) has recently been shown to provide elemental selectivity in atomic-scale imaging, allowing for defect identification on complex metal oxide surfaces by directly accessing the metal and oxygen sublattices [3, 4]. The oxygen termination leads to electron accumulation at the tip apex, dominating electrostatic interactions with the surface and enabling site-specific probing of the local atomic potential defined by the underlying elemental composition. Recently, we successfully applied this approach also to NaCl thin films and inherent defect structures, which indicated its universal applicability.

On the basis of these results, we utilize CuOx-tip AFM imaging for investigations of hBN. We present electrostatic potential calculations of DFT-optimized monolayer hBN, demonstrating its feasibility. Also, since the controlled growth of hBN is challenging, these experiments further demand the development of advanced experimental methods for the in-situ growth of hBN on single-crystalline surfaces. We then discuss the advantages of CuOx-tip AFM for structural characterization of hBN and its defects, and present first results toward correlative studies of optoelectronic properties with STM and STS. This work aims to open the path to chemically resolved, atom-specific studies of quantum defects in two-dimensional materials.

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Inelastic tunneling into multipolaronic bound states in single-layer molybdenum disulfide

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A polaron is a quasiparticle that forms when an excess of electrons or holes interacts with the vibrations of the surrounding atomic lattice. This interaction causes the nearby ions to displace from their equilibrium positions, creating a localized trap for charges. When the Coulomb interaction is suppressed, strong electron-phonon coupling takes place. As a result, the individual polarons couple to each other giving rise to multipolarons.

In this work, we investigate the role of electron-phonon coupling and its link to multipolarons in single layer (SL) MoS_2 on graphene (Gr) on Ir (111) substrate. We use scanning tunneling microscopy and spectroscopy to measure the inelastic excitations of polaronic bound states emerging from the coupling of non-polar zone-boundary phonons to Bloch electrons in n-doped metallic SL MoS_2. Tunneling into the vibrationally coupled polaronic states leads to a series of evenly spaced peaks in the dI/dV spectra on either side of the Fermi level as shown in figure (1.c). Combining density functional (perturbation) theory with a recently developed *ab initio* electron-lattice downfolding technique, we show that the energy spacing stems from the longitudinal-acoustic phonon mode that flattens at the Brillouin zone edge and is responsible for the formation of stable multipolarons in metallic MoS_2 [1].

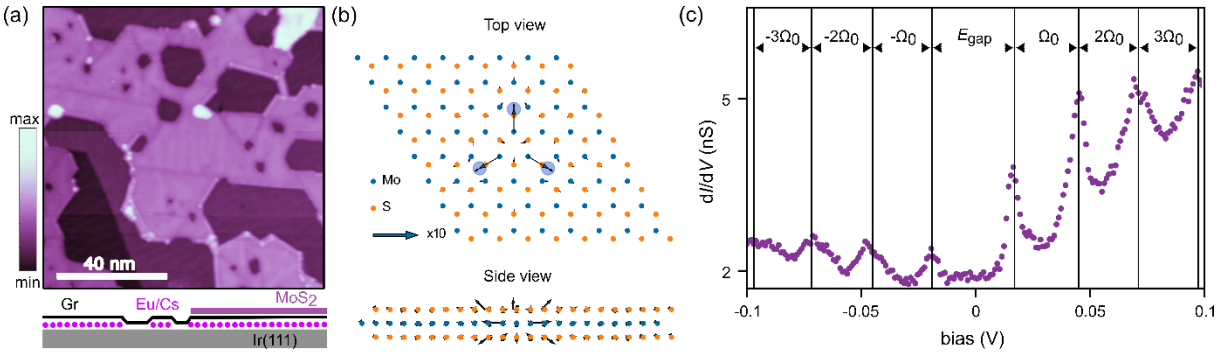

Figure 1: (a) STM image of MoS_2 on Eu intercalated Gr on Ir(111). Below STM topograph is a cross-sectional schematic view of the system. (b) Relaxed crystal structure based on *ab initio* model calculations on an 18 × 18 supercell. (c) Low-bias STM dI/dV spectrum of metallic SL MoS_2, revealing peak-dip features and a gap at the Fermi level.

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Dopant-vacancy complexes in transition metal dichalcogenides

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Solid-state quantum emitters are central to the development of quantum sensing and communication technologies.[1] Atom-like centers in crystals such as diamond[2] and SiC[3] provide spin-selective optical transitions, exceptional coherence times, stability at room temperature, and compatibility with wafer-scale integration.[4] However, their 3D bulk nature makes it difficult to control defect structures, achieve spatially precise integration, and fully exploit their optical properties. Embedding emitters in atomically thin 2D materials offers a promising alternative, where electronic behavior is highly sensitive to defects and their interaction with the surrounding lattice.

Here, we explore a pathway to emulate diamond NV^- centers in a 2D platform by introducing donor- and acceptor-type substitutional dopants with non-isovalent transition metals.[5–8] Using atomically resolved scanning tunneling microscopy (STM) spectroscopy (STS) and non-contact atomic force microscopy (nc-AFM) we directly visualize the atomic and electronic structure of dopant-vacancy complexes in MoS_2. We show that (Re_{Mo} + Vac_S) structures can be generated with high chemical specificity and give rise to both filled and empty in-gap states. Furthermore, we demonstrate controlled p-type doping via vanadium incorporation, uncovering how the V charge state evolves in both single- and few-layer MoS_2 and how it interacts with vacancies induced by thermal annealing.

Our results establish a versatile strategy for defect engineering in 2D semiconductors, opening opportunities for scalable quantum emitter platforms that combine atomic precision with tunable electronic environments.

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THz-driven plasmonic STM luminescence

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We demonstrate THz-induced STM-luminescence (THz-STML) from a plasmonic tunnel junction driven by broadband single-cycle THz pulses generated from a high-power rotating spintronic THz emitter. [1] A detailed analysis of the THz-STML spectra under a range of different tunneling conditions shows the absence of a quantum cutoff in THz-STML, indicating that overbias emission strongly contributes to the observed plasmonic luminescence. We aim to estimate the THz peak bias and gain insight into the processes that lead to light emission, via reconstruction of the THz-STML spectra from the static reference STML spectra and by measuring the dependence of the THz-STML yield on the static STM bias. Our work contributes to the enduring discussion on the nature of overbias photon emission and hot-electron processes in tunnel junctions. [2,3]

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Synthesis and characterization of a spin lattice on superconductors using chlorinated tetraazapyrene radicals.

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Designing spin lattice using radical molecules is crucial for engineering molecular electronics. Here, we study, 5,9,10-tetrachloro-1,3,6,8-tetraazapyrene (TClTAP) [1] molecules on Pb(111) using Scanning Tunneling Microscopy (STM) and spectroscopy. TClTAP molecule is a strong acceptor allowing to transfer one electron from the substrate into the lowest unocuppied molecular orbital (LUMO). This result in molecule becoming negatively charged with an additional electron and behaving like a magnetic impurity. To quantify the resulting magnetic impurities, we probed the local density of states (LDOS) near the Femi level to observed the appearance of in-gap Yu-Shiba-Rusinov (YSR) bound states within the superconducting gap [2]. The pair of YSR states confirms that the electron is in an anionic state with spin states = ½. At larger bias voltages, the chemical potential of the surface can be tuned to induced the controlled discharge of the molecule [3].

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Nuclear magnetic resonance on a single atom with a local probe

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The nuclear spin is a prime candidate for quantum information applications due to its weak coupling to the environment and inherently long coherence times. However, this weak coupling also challenges the addressability of the nuclear spin. Here we demonstrate nuclear magnetic resonance (NMR) on a single on-surface atom using a local scanning probe. We employ an electron-nuclear double resonance measurement scheme and resolve nuclear spin transitions of a single ^{47}Ti isotope with a nuclear spin of $I = 5/2$. Thanks to the quadrupole interaction, it proves possible to resolve multiple NMR transitions, which energies we can support with calculations. Our results indicate that the nuclear spin can be driven efficiently irrespective of its coupling to the electron spin, which is required for direct control of the nuclear spin in the long-lifetime regime. Moreover, investigation of fundamental interactions of a nuclear spin with its environment studied in a platform with atomic-scale control provides valuable knowledge for other platforms deploying nuclear spins for characterization techniques or quantum information technology.

Scanning tunnelling spectroscopy study of proximity superconductivity in Rashba-split surface states

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Adding superconductivity to gapless materials via the proximity effect [1,2,3] can lead to a variety of interesting physical phenomena including topologically non-trivial states [4]. Rashba-split surface states, proximitized by a superconducting substrate, are of particular interest, as they combine strong spin-orbit coupling with a sizable superconducting gap, making them a promising system in the search for topological superconductivity. More recently, proximitized surface states have also been shown to enable coherent quantum projections of Yu-Shiba-Rusinov states, highlighting their potential as a platform to explore fundamental interactions between superconductors and magnetic impurities [5].

We investigate the mechanism of proximity-induced superconductivity in the Shockley-type surface states of thin Cu and Ag films grown on Nb(110) [6], the elemental superconductor with the highest critical temperature. Using scanning tunneling spectroscopy, we observe a multitude of sharp low-energy peaks in the spectra. These features can be attributed to two distinct types of Andreev bound states—one associated with the thin film bulk states, and one with the surface state. Through statistical analysis, we show that the surface-state–related bound state energy depends on the Cu/Ag-island-surface area, indicating that the proximity effect into the surface state is driven by bulk–surface electron scattering, which is enhanced on smaller islands due to their higher step-edge density. The bulk-state related energy follows the island-thickness dependence of de Gennes-Saint-James states [2].

To increase the Rashba-type spin-orbit coupling of the surface, a third monolayer of Bi was deposited onto the noble metal islands leading to the formation of the surface alloys BiCu2 and BiAg2 [7] which exhibit surface states with very large Rashba spin-splitting. These surface states couple strongly to the bulk electrons leading to large proximity induced gaps.

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Manipulating the Crystal Field of Individual Atoms on Surfaces

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The magnetic behavior of ions in solid-state materials is predominantly driven by their immediate atomic-scale environment. The specific arrangement of charges in the immediate vicinity shapes the electrostatic energy landscape, altering and mixing electronic states. This interaction is described as the crystal field (CF) and is, for magnetic impurities on insulating thin-films, strongly influenced by the adsorption site on the underlying lattice. We use combined scanning tunneling microscopy (STM) and atomic force microscopy (AFM) to resolve the influence of the CF on individual titanium and iron atoms on a double layer of magnesium oxide (MgO).

The forces between the STM/AFM tip and the adsorbed atoms enable precise repositioning of atoms within their binding site. This grants direct access to the modification of the local CF, and thereby allows us to tune the atom's magnetic anisotropy. The combined STM/AFM can further be used for Kelvin probe force microscopy (KPFM) measurements to investigate the local contact potential difference (LCPD) and resolve induced changes.

Our measurements pave the way for harnessing magneto-elastic effects in individual atoms either by manipulating their magnetic properties via electric fields or local forces, such as mechanical strain.