23rd international conference on non-contact atomic force microscopy

August 1st to 5th 2022

NCAFM2022
NIJMEGEN

23rd international conference on non-contact atomic force microscopy

Nijmegen (Netherlands), August 1st to 5th 2022

NC-AFM 2022 is the 23rd of a series of conferences devoted to non-contact atomic force microscopy. Previous conferences were held in **Regensburg**, Germany (2019), **Porvoo**, Finland (2018), **Suzhou**, China (2017), **Nottingham**, UK (2016), **Cassis**, France (2015), **Tsukuba**, Japan (2014), **Maryland**, USA (2013), **Ceský Krumlov**, Czech Republic (2012), **Lindau**, Germany (2011), **Kanazawa**, Japan (2010), **New Haven**, USA (2009), **Madrid**, Spain (2008), **Antalya**, Turkey (2007), **Kobe**, Japan (2006), **Bad Essen**, Germany (2005), **Seattle**, USA (2004), **Dingle**, Ireland (2003), **Montreal**, Canada (2002), **Kyoto**, Japan (2001), **Hamburg**, Germany (2000), **Pontresina**, Switzerland (1999), **Osaka**, Japan (1998).

Content

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Zurich Instruments, Zürich (Switzerland)

Welcome reception
Fort Boven-Lent

Conference site
de Lindenberg

Conference dinner
Landgoed Brakkesteyn

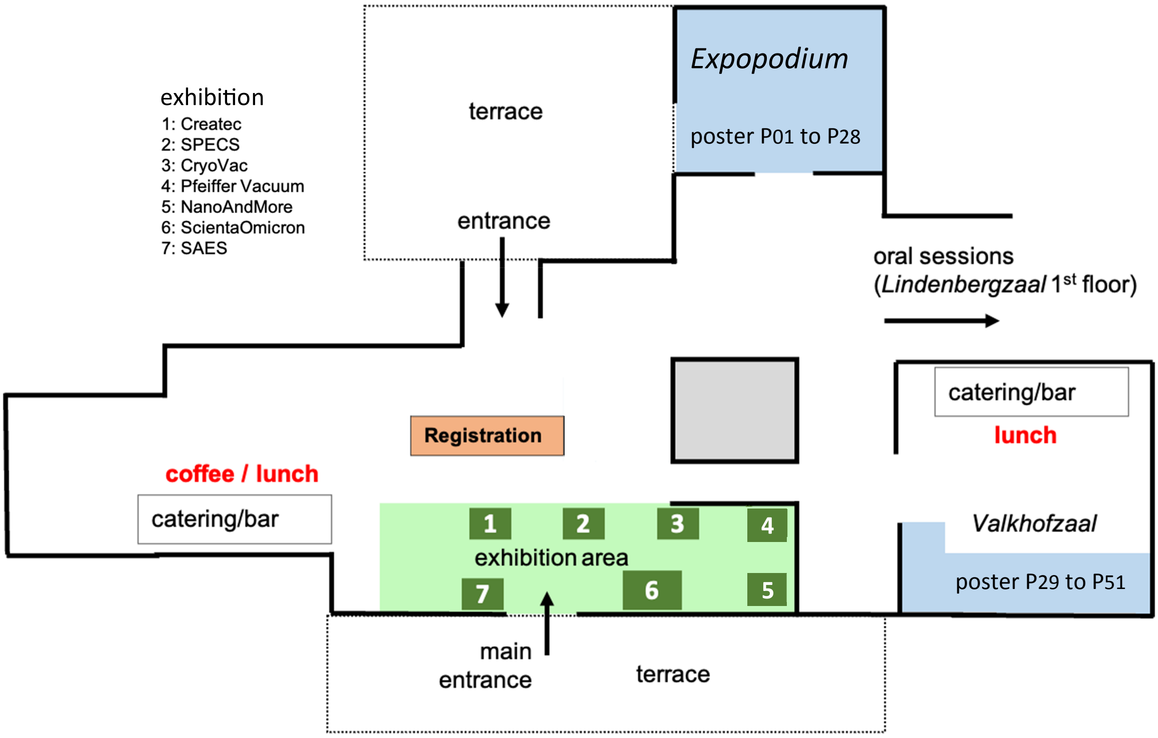
3 Local information

Conference site: de Lindenberg

Lindenberg Cultuurhuis
Ridderstraat 23
6500 AN Nijmegen

The conference is held in the Nijmegen culture house "de Lindenberg" located at Ridderstraat 23 (Nijmegen, Netherlands) close to the Nijmegen waterfront. It is located in walking distance to the historic city centre.

The conference centre can be reached from Nijmegen Centraal Station (main train station) within 8 minutes by bus number 8 (direction Berg en Dal, leave the bus at station Voerweg), bus number 15 (direction Lent Thermion, leave the bus at station Valkhof), or bus number 80 (direction Millingen, leave the bus at station Valkhof). Bus schedules can also be checked via 9292 (https://9292.nl/en). You can furthermore walk for 20 minutes (1.5 km) across the city of Nijmegen.



Welcome reception: Fort Boven-Lent

Fort Boven-Lent
Bemmelsedijk 4
6663 KZ Lent

The welcome reception starts at 4 pm on Sunday and takes place at Fort Boven-Lent (not to be confused with Fort Beneden-Lent located in the west) that is a fortress built in 1862 converted into a meeting place in 2019. Depending on weather conditions, the reception will be open-air on top of the fortress or indoor in the main hall. Fort Boven-Lent can be reached from the conference site by a 35 minute walk (2.8 km) or by a 15 minute bus ride with lines 15 (direction Lent, Thermion, starting at e.g. Nijmegen Centraal station, Waalkade, Valkhof, exit at Lent, Eikenlaan/Laauwikstraat) or 33 (direction Arnehm CS, starting at e.g. Nijmegen Central station, Waalkade, Valkhof, exit at Lent, Duitslandstraat). Bus schedules can also be checked via 9292 (https://9292.nl/en). From the respective stop, take a short walk to Fort Boven-Lent. You can catch buses of the lines 15 and 33 also at the Nijmegen Centraal train station and other places close to the waterfront. There are also direct trains from Nijmegen Centraal to Nijmegen Lent. From Lent station it is a 20 minute walk to Fort Boven-Lent.
After the reception, we have organized a bus ride to Nijmegen central station with two stops on the way (one close to the Trajanusplein and the other at Plein 44). If the weather is nice, you can also enjoy a walk over the historical Waal bridge and enjoy the fantastic view over Nijmegen.

Conference dinner: Landgoed Brakkesteyn

Landgoed Brakkesteyn
Driehuizerweg 285
6525 PL Nijmegen

The conference dinner takes place on Thursday, 6:30pm, at the Landgoed in Park Brakkesteyn (Driehuizerweg 285) that is a traditional farm house located close to the Radboud University campus. The location offers a large terrace with barbecue facilities, a beautiful park, and a dining hall. The Landgoed Brakkesteyn can be reached from the conference site by a 50 minute walk (3.7 km) or by a 30 minute bus ride with the line 15 (from station Valkhof, direction Wijchen, exit at Erasmusgebouw). From other locations take buses 10 (direction Heyendaal, exit at Erasmusgebouw), 12 (direction Druten via Heyendaal, exit at Erasmusgebouw) or 14 (direction NMG Brakkesteyn, exit at Kwekerijweg). Bus schedules can also be checked via 9292 (https://9292.nl/en). From the respective bus station, take a short walk (few minutes) to Park Brakkesteyn.
After the dinner, we have organized a shuttle bus service between the Landgoed Brakkesteyn and Nijmegen central station with two stops on the way (one close to the Trajanusplein and the other at Plein 44). The 50 person bus will depart from the Langoed Brakkesteyn around 21:45, 22:20, and 23:00.

Excursions

Excursion 1: Tour through the oldest city of the Netherlands You will walk through the oldest part of Nijmegen, which is located between the St. Stevenskerk and the Kronenburgerpark. The guides will take you through the oldest shopping street in the Netherlands, past medieval buildings, what's left from the city walls and towers. Also St. Jacob's Chapel and the Jacob's Tower will be visited.

13.40: We meet in front of the de Lindenberg and take a 10 minute walk to the starting point of the tour: Huis van de Nijmeegse Geschiedenis, Mariënburg 26, 6511 PS Nijmegen.
14:00: Start of the tour.
About 16:00: End of the tour (Grote Markt).

Excursion 2: "Rivierpark" To protect Nijmegen against high water, an elongated urban island has been built in 2016 in the river Waal, between the historic city center and the new Nijmegen-Noord district. Together with the secondary river channel "Spiegelwaal", the island forms a unique river park. Do you want to learn more about all the plans and the work involved in making the island and enjoy the nature on it? Join the 1.5 – 2h tour to the island! Please wear suitable footwear as it is a brisk walk. You must be in good physical condition for this walk as there are several stairs and slopes.

13.45: We meet in front of the de Lindenberg and take a 2 minute walk to the Bastei (Lange Baan 4, 6511 XJ Nijmegen).
14:00: Start of the tour from the Bastei.
About 16.00: End of the tour at the Bastei.

Excursion 3: "Stadswaard" The Stadswaard is a beautiful natural area next to the historic city center. Would you like to know more about the plants and animals in the Stadswaard? Or where the river deposits sand and clay after a flood? Join the 1.5 – 2h tour. With a bit of luck, you will suddenly come face to face with grazers such as Konik horses or Galloway cattle. Do you dare?

13.45: We meet in front of the de Lindenberg and take a 2 minute walk to the Bastei (Lange Baan 4, 6511 XJ Nijmegen).
14:00: Start of the tour from the Bastei.
About 16.00: End of the tour at the Bastei.

Excursion 4: Tour through the Bastei De Bastei is the treasure trove of Nijmegen's nature and history, where you can discover everything about life in, around, and on the river. Located in a 16th-century defensive tower, the De Bastei museum offers an exciting wandering garden full of history. Discover the layered history of the oldest city in the Netherlands, on the basis of Roman wall remains, a part of Valkhof castle and of course the Bastei itself.

13.45: We meet in front of the de Lindenberg and take a 2 minute walk to the Bastei (Lange Baan 4, 6511 XJ Nijmegen).
14:00: Start of the tour at the Bastei.
About 15.30: End of the tour at the Bastei.

Excursion 5: Tour and beer tasting in the local brewery de Hemel Come and take a look behind the unique scenes into the oldest craft beer brewery of the Netherlands, located in one of the oldest buildings in Nijmegen and visit the depths of Heaven! In our very own brewery De Hemel (translated to 'Heaven' in Dutch), you will find everything there is to know about the beer, the people, the process, and techniques of brewery. During a guided tour, you get to see the ins and outs of the brewery, and with the help of labels, pictures, short films, machines and equipment, become quickly acquainted with De Hemel. There are also opportunities to take an insight into the production of vinegar, mustard and spirits. Visiting the brewery is naturally accompanied with a tasting session of brewery products to complete the experience.

13.40: We meet in front of the de Lindenberg and take a 10 minute walk to the Hemel (Franseplaats 1, 6511 VS Nijmegen).
14:00: Start of the event.
About 15.30: End of the event.

4 Oral contributions

Session list

Monday, August 1st 2022:

11:00–11:20: Welcome
11:20–12:20: **Atomic scale manipulation**
14:00–15:00: **Novel instrumentation and techniques (A)**
16:00–17:20: **Magnetic properties and artificial structures**

Tuesday, August 2nd 2022:

09:00–10:20: **Force mapping on nanoscale structures and study of water**
11:00–12:20: **Novel instrumentation and techniques (B)**
14:00–15:00: **Nanoscale measurements of charge and work function (A)**
16:00–17:20: **Force mapping in liquid and under ambient conditions**

Wednesday, August 3rd 2022:

09:00–10:20: **Nanoscale measurements of charge and work function (B)**
11:00–12:20: **Study of single molecules**
14:00–15:00: **Lateral forces, friction, and energy dissipation**
16:00–17:20: **Characterisation of molecular systems (A)**

Thursday, August 4th 2022:

09:00–10:20: **Oxide surfaces**
11:00–12:20: **2D materials**

Friday, August 5th 2022:

09:00–10:20: **Characterisation of molecular systems (B)**
11:00–12:00: **Novel instrumentation and techniques (C)**
12:00–12:20: Closing remarks

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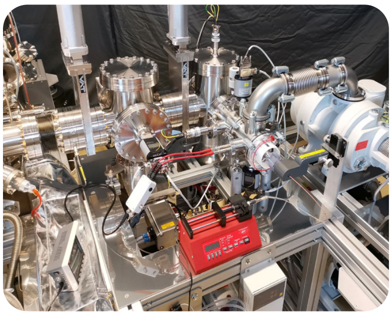
NEW

To deposit complex molecules with a low vapor pressure, CreaTec offers an electrospray ionization system (ESI). The system features several differentially pumped stages, i.e., an ion funnel to focus the molecular beam, a deflector to separate the charged ions from neutral particles, and a mass spectrometer to select the proper molecules to be deposited. The ESI is the perfect tool to deposit large, volatile molecules under clean UHV conditions.



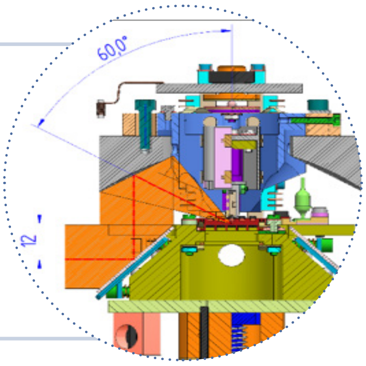
LT-SPM System

Low-temperature scanning probe microscopes are an essential part of CreaTec's product range. The basic 4K-STM can be extended with multiple optional features that make the instrument a versatile platform to conduct experiments on various sample systems. Options are for example nc-AFM, rf-lines, magnetic field and a high NA optical access to the tunneling junction. The low liquid helium consumption (4l lHe / 72h) guarantees stable conditions for prolonged sensitive measurements. Additionally, there is a LT-SPM system with 1K base temperature.

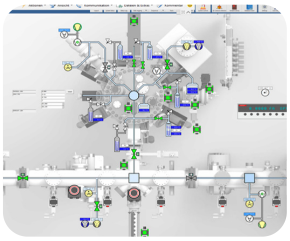
Optical access with parabolic mirrors

NEW

A special version of the SPM features optical access to the tip-sample junction with parabolic mirrors. This allows for the coupling of ultra-fast light pulses as well as long-wavelength radiation (THz) into the tunneling junction. With this pump-probe design, experiments with ultra-fast time resolution and intra-molecular spatial resolution are possible.



System automation



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Monday, August 1st 2022

Welcome

11:00 **The organisers** *Welcome*

Atomic scale manipulation

Chair: Loppacher, C.

11:20 **Ebeling, D.** *Constructing covalent organic nanoarchitectures molecule by molecule via scanning probe manipulation.*

11:40 **Schwarz, U.** *Measuring Energetics of Molecular Motions of Surface Species with Non-contact Atomic Force Microscopy.*

12:00 **Štich, I.** *New ultra-fast method for measuring tunnelling rates between an AFM tip and on-surface species.*

Novel instrumentation and techniques (A)

Chair: Glatzel, T.

14:00 **Zahl, P.** *Automated HR-AFM to facilitate molecular discovery and research for complex molecule mixtures.*

14:20 **Eftekhari, Z.** *Time-resolved mapping of light-induced displacement and photovoltage in on-chip coupled piezo/photodiodes.*

14:40 **Oininen, N.** *Machine learning for nc-AFM image interpretation and tip functionalization.*

Magnetic properties and artificial structures

Chair: Hapala, P.

16:00 **Schwarz, A.** *Probing long and short-range magnetic interactions on the nanoskyrmionic Fe monolayer on Ir(111).*

16:20 **Giessibl, F.** *Very weak bonds to artificial atoms formed by quantum corrals.*

16:40 **Weiss, M.** *Line shape analysis of the resonant eigenstates in a quantum corral by means of tunneling spectroscopy and non contact AFM.*

17:00 **Stilp, F.** *Interaction between an artificial and a natural atom.*

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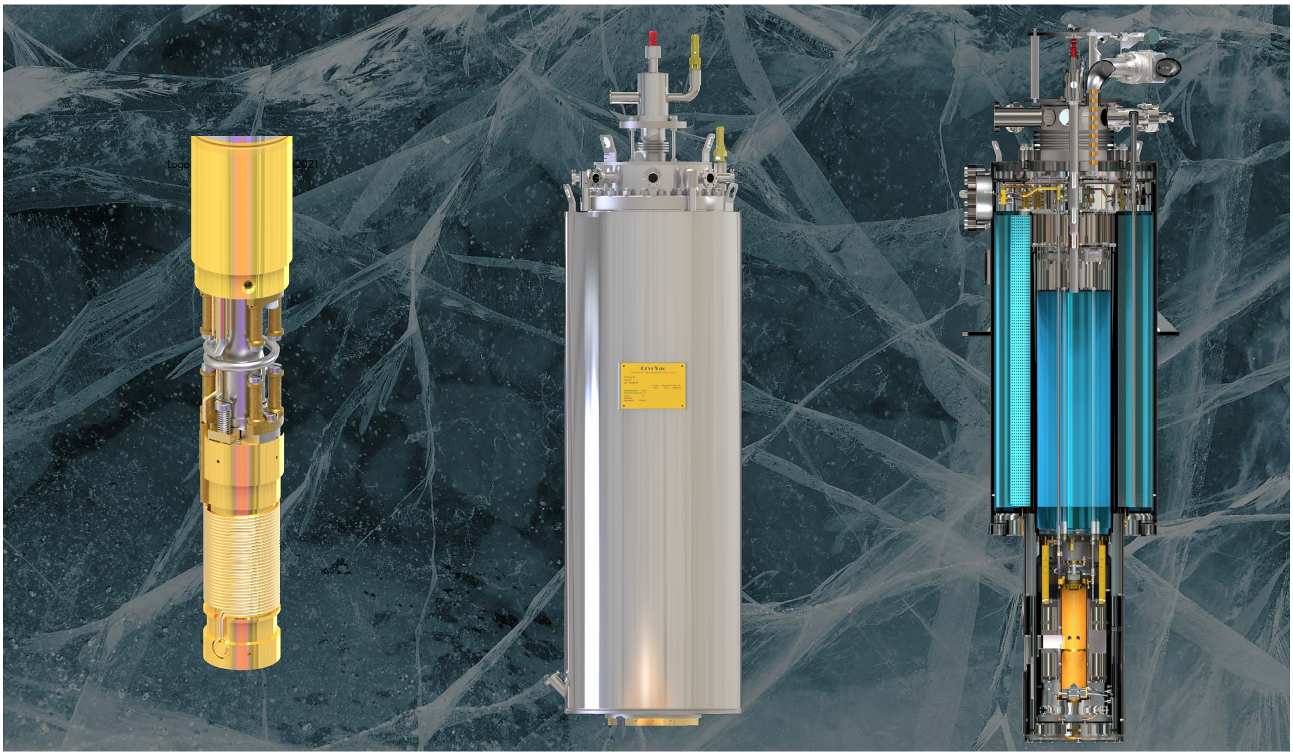

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- hold time up to 300 h
- superconducting 1D/2D/3D coil

low temperature cryostats
- T min: 500 mK - 1.5 K
- compact design / side loading
- upgrade form ^{4}He to ^{3}He operation
- complete UHV compatible / bakeable
- superconducting 1D/2D/3D coil

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Monday 11:20–11:40

Constructing covalent organic nanoarchitectures molecule by molecule via scanning probe manipulation

Qigang Zhong[1], Alexander Ihle[1], Sebastian Ahles[2], Hermann A. Wegner[2], Andre Schirmeisen[1], and **Daniel Ebeling[1,*]**

[1] Institute of Applied Physics, Justus Liebig University Giessen, Giessen (Germany)
[2] Institute of Organic Chemistry, Justus Liebig University Giessen, Giessen (Germany)

*Corresponding author contact: Daniel.Ebeling@ap.physik.uni-giessen.de

Constructing low-dimensional covalent assemblies with tailored size and connectivity is challenging yet often key for applications in molecular electronics where optical and electronic properties of the quantum materials are highly structure dependent. We present a versatile approach for building such structures block by block on bilayer sodium chloride (NaCl) films on Cu(111) with the tip of an atomic force microscope, while tracking the structural changes with single-bond resolution. Covalent homo-dimers in *cis* and *trans* configurations and homo-/hetero-trimers were selectively synthesized by a sequence of dehalogenation, translational manipulation and intermolecular coupling of halogenated precursors. Further demonstrations of structural build-up include complex bonding motifs, like carbon–iodine–carbon bonds and fused carbon pentagons. This work enables synthesizing elusive covalent nanoarchitectures, studying structural modifications and revealing pathways of intermolecular reactions. [1]

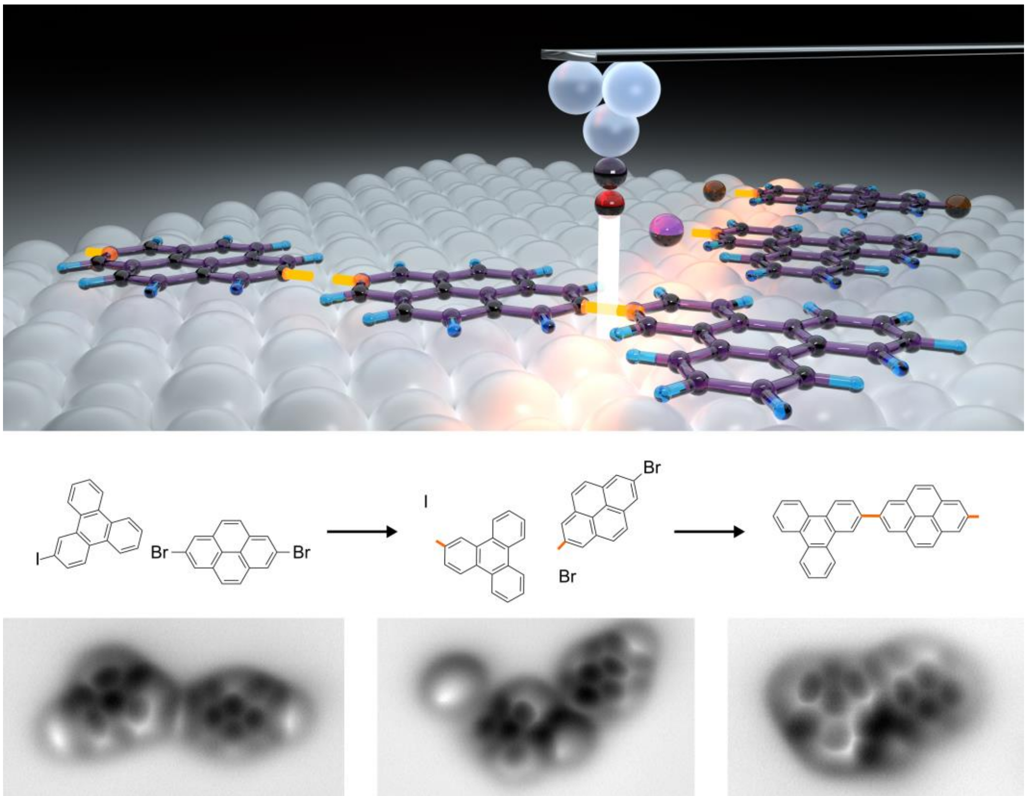

Figure 1: *All reaction steps are induced by voltage pulses with the AFM tip. First, the precursors are activated by dehalogenation. Subsequently, the formed radicals are moved together and finally, a covalent bond is formed (activated and newly formed bonds are shown in orange).*

[1] Zhong et al. *Nature Chemistry* ***13****, 1133 (2021)*

Monday 11:40–12:00

Measuring Energetics of Molecular Motions of Surface Species with Non-contact Atomic Force Microscopy

Omur E. Dagdeviren,[1,2] Chao Zhou,[1] Milica Todorović,[3] Eric I. Altman,[4] and **Udo D. Schwarz**[1,4,*]

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[2] Dept. of Mech. Eng., École de Technologie Supérieure, University of Quebec, Montreal H3C 1K3, Canada
[3] Dept. of Mechanical and Materials Engineering, University of Turku, FI-20014 Turku, Finland
[4] Department of Chem. and Environ. Engineering, Yale University, New Haven, CT 06520, USA

*Corresponding author contact: udo.schwarz@yale.edu

Following adsorption, the next key steps in surface catalytic reactions are diffusion and collision of adsorbed reactants and intermediates. Experimentally measuring the energetics of surface diffusion in isolation is challenging; under reaction conditions, the complexity of the possible molecular interactions makes the problem seemingly intractable. Advances in molecular manipulation using non-contact atomic force microscopy (NC-AFM) methods together with the ability to quantitatively measure the forces imparted by the probe tip using offers promise to measure how surface diffusion barriers are affected by the surrounding environment. This talk will focus on the translation of benzene and phenyl radicals on Cu(100). For benzene, molecules were either pushed, pulled, dragged, jumped to the tip, or did not move with the exact mechanism being reflective mostly of the chemical identity of the tip and its motion relative to the molecule. Comparison with theory suggests that the tip lowers the energy barrier the benzene must overcome to translate on the surface, which evolves with the chemical identity of the tip. In comparison, the missing H of the phenyl radical bonds it tighter to the substrate, thereby lessening the influence of the tip while opening up additional motions including rotation and flipping of the molecule around the C-Cu bond. Different jump distances and barriers were seen that may be associated with these motions (cf. Fig. 1). Together, the results indicate that a reliable methodology where surface reactions can be induced by the tip of a scanning probe microscope and the reaction pathway is chosen at will could be in reach, which would ultimately enable an individualized, site-specific understanding of single-molecule surface chemistry.

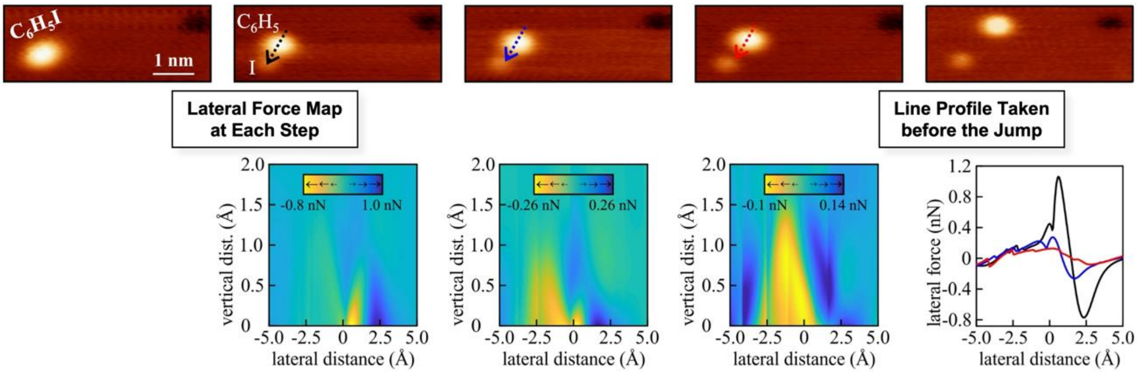

Figure 1: *Manipulation of a phenyl radical. An iodobenzene molecule is deposited on the surface (top row, left image) and then converted to a phenyl radical* C_6H_5 *through a voltage pulse with the iodine atom visible separated (top row, second image). The phenyl is then dragged away from the iodine atom in three successive steps along the pathways highlighted by the black, blue, and red arrows. From the corresponding x-z lateral force maps placed below the topographical images and the line profiles taken before the jump, we can extract that the force needed to move the phenyl changes significantly, indicating different mechanisms of motion.*

Monday 12:00–12:20

New ultra-fast method for measuring tunnelling rates between an AFM tip and on-surface species

L. Kantorovich,[1*] Y. Adachi[2], J. Brndiar[3], H. F. Wen[2], Q. Zhang[2], M. Miyazaki[2], S. Thakur[3], Y. Sugawara[2], H. Sang[4], Y. Li[2*], **I. Štich**[3*]

[1] King's College London, London, WC2R 2LS, United Kingdom
[2] Osaka University, Suita, Osaka, Japan
[3] CCMS, Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia
[4] Jianghan University, Wuhan, China

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A novel method is suggested based on stochastic nature of the tunnelling that enables measuring tunnelling rates between the AFM tip and on-surface species keeping mechanically fixed tip position and hence ensuring a very fast acquisition of data [1]. Due to this, very low temperatures required for existing methods to fight thermal shift are no longer a necessary limitation, and sufficient statistics from which the rates are extracted can be obtained even at elevated temperatures. The method is based on sweeping the bias voltage in both directions at a fixed tip position many times and collecting the voltages at which transitions happen (observed jumps in the frequency shift) into distributions. Then, an exact formula is proposed that allows obtaining the rate from the acquired statistical distributions.

This method is applied to oxygen adatoms adsorbed on TiO_2 surface in the form of reactive oxygen species and single-atom quantum dots, that can exist in two redox states with the charge of minus one or two. The redox state of the oxygen species can be switched by an AFM tip by means of electron tunnelling between the tip and dot. The corresponding tunnelling rates were acquired at 78 K over a wide range of tip-sample distances and applied voltages. This enabled us to study multiple dots and provided unexpected insights into the electronic structure and correlation between the oxygen species; these features remain hidden in the ordinary AFM microscopy. We also show that single-atom quantum dots in the two charge states have drastically different conductance, one conducting while the other non-conducting, which enables one to fabricate a desired binary surface arrangement of such dots (e.g., "anti-" and/or "ferromagnetic" arrangements) that may be considered as a simplest quantum nanodevice.

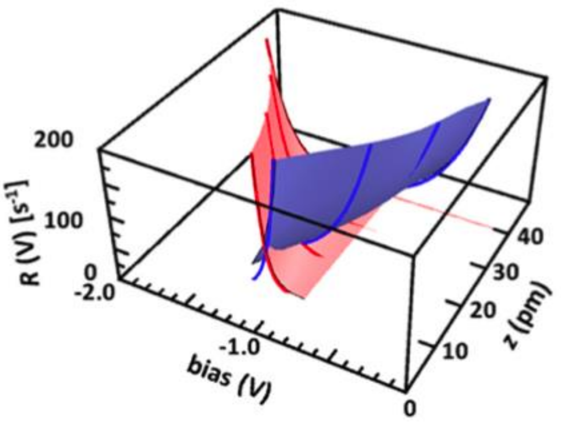

Figure 1: 3D graphs of the recharge (blue) and discharge (red) rates as a function of both the bias, V, and the tip-height, z, for an oxygen adatom quantum dot.

[1] Y. Adachi, J. Brndiar, H. F. Wen, Q. Zhang, M. Miyazaki, S. Thakur, Y. Sugawara, H. Sang, Y. Li, I. Štich and L. Kantorovich, Comm. Mater. **2**, 71 (2021)

Monday 14:00–14:20

Automated HR-AFM to facilitate molecular discovery and research for complex molecule mixtures

Percy Zahl,[1,*] Yunlong Zhang[2], Steven Arias[3]

[1] Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, New York 11973, USA
[2] ExxonMobil Technology and Engineering Company, Annandale, NJ, 08801, USA
[3] University of New Hampshire, Durham, NH, 03824, USA

*Corresponding author contact: pzahl@bnl.gov

Due to its single molecule sensitivity, high-resolution Atomic Force Microscopy (HR-AFM) has proved to be a valuable and uniquely advantageous tool to study complex mixtures, such as petroleum, biofuels/chemicals, and environmental samples. However, significant challenges remain in order to achieve the full potential of the challenging and time-consuming experiments. Automated HR-AFM, in conjunction with machine learning and artificial intelligence, will be the key to overcoming many bottlenecks today, and crucial for research on solutions for the energy transition and environmental sustainability [1]. We showcase first "autonomously acquired" results on petroleum-based mixtures with potential for novel carbon-based composite materials for applications in infrastructures. These are the early steps towards fully autonomous HR-AFM imaging along with a master plan to expand our AI and computer vision based approach further to include all essential steps starting from sample approach, exploration, tip functionalization to molecule selecting and imaging in HR-AFM mode. Our AI steered image "appearance" optimization fine adjusts the sample probe distance. Illustration in figure 1 shows the process we have implemented using a state machine, computer vision and AI (CNN) for decision making using data from QUAM-AFM as references for CNN training [2, 3].

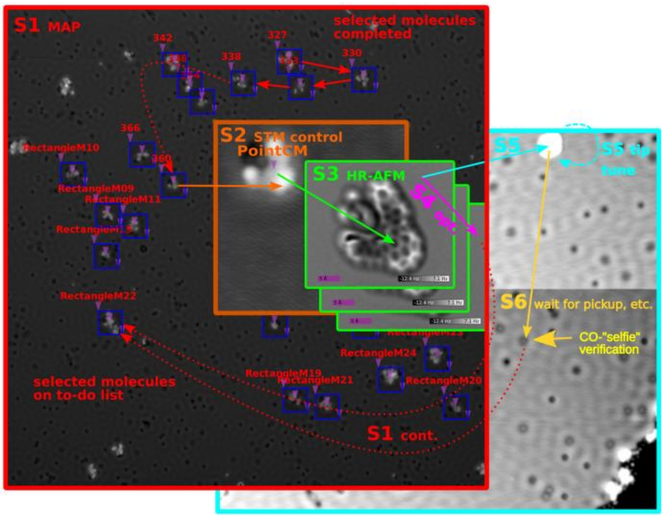

Figure 1: *Automation "Level 00": Computer vision and AI steered Finite-State-Machine. State S1: A STM map of the work area with molecules is used as a starting setup. Auto or manual manual molecule selection. S2: Zoom on the selected next molecule. Precise auto centering and initiation automated HR-AFM transition. S3: HR-AFM imaging with adaptive scan speed at the initial Z setpoint. An autonomous operation at a higher "Level" includes decision making on an image's quality (S4) vs. manual Z choosing. Multiple imaging passes at corrected Z setpoints are evaluated by a CNN with decision making on how to proceed – optimize, continue with the next or bail to S5, S6 for tip/probe cleaning and re-preparation as required. S5: repeated tip cleanup/pulse or tip-form for resharpening. With following CO finding/pickup (S6), verification of CO ``selfie" shapes and task continuation at S1.*

[1] Yunlong Zhang, Energy & Fuels **35** (18), 14422 (2021)
[2] Jaime Carracedo-Cosme, Carlos Romero-Muñiz, Pablo Pou, and Rubén Pérez, J. Chem. Inf. Model. **62** (5), 1214 (2022)
[3] Microscope Control via Gxsm-3 (http://gxsm.sf.net) with included Python interface for all automatisations and real time data access/controls. Utilizing Keras as a deep learning API.

Monday 14:20–14:40

Time-resolved mapping of light-induced displacement and photovoltage in on-chip coupled piezo/photodiodes

Zeinab Eftekhari[1*], Nasim Rezaei[1], Jian-Yao Zheng[1], Andrea Cerreta[2], Ilka Hermes[2], Minh Nguyen[1], Guus Rijnders[1], and Rebecca Saive[1]

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We study hybrid materials systems comprised of a silicon photodiode integrated with a piezoelectric material which show mechanical oscillation upon alternating illumination. Here, we present time-dependent and spatially resolved measurements of the light-induced oscillations.

The hybrid piezo/photodiode system, called piezo-photomotion device enables conversion of light into photovoltage, which can generate mechanical displacement in the piezoelectric membrane [1]. We use atomic force microscopy (AFM) and Kelvin probe force microscopy (KPFM) to investigate the performance of the piezo-photomotion device in a time-resolved fashion to understand the behavior of the device under alternating illumination. Time-dependent and spatially resolved measurement of light-induced displacement and photovoltage were performed with a Park NX 10 scanning probe microscope. The system operated in single-pass sideband KPFM mode which enables high resolution quantitative measurement of topography and surface potential simultaneously. A light source is implemented inside the AFM chamber facilitating the light incoupling and its frequency can be modulated by an internal lock-in amplifier. Therefore, time-dependent deformation and photovoltage which are oscillating with the modulated light frequency can be determined. Time resolved measurements are performed in scan point method for different positions of the membrane and mechanical displacement and corresponding photovoltage are recorded. We only measured one quarter of the active area of the membrane due to symmetry and as expected, the maximum value of displacement (1315 pm) was obtained for position in the center and it decreases to a few picometers at the side edges with the thicker silicon substrate, while the measured photovoltage nearly stayed constant regardless of the scanned position. Therefore, we can attribute the variation of mechanical oscillation only to mechanical reasons and can exclude changes in photovoltage for different positions.

In this report, we have developed a method with which can measure light-induced displacement and photovoltage of a piezo-photomotion device simultaneously. It offers the opportunity to decouple (opto)electric and mechanical response at the nanoscale. I can also be useful for others who would like to know the time-dependence in particular of light-driven systems.

[1] W. M. Luiten, V. M. Van Der Werf, N. Raza, and R. Saive, AIP Adv., vol. 10, no. 10, Oct. 2020.

Monday 14:40–15:00

Machine learning for nc-AFM image interpretation and tip functionalization

Niko Oinonen[1], Lauri Kurki[1], Chen Xu[1], Shuning Cai[1], Markus Aapro[1] , Alexander Ilin[2], Peter Liljeroth[1], Adam S. Foster[1,3,*]

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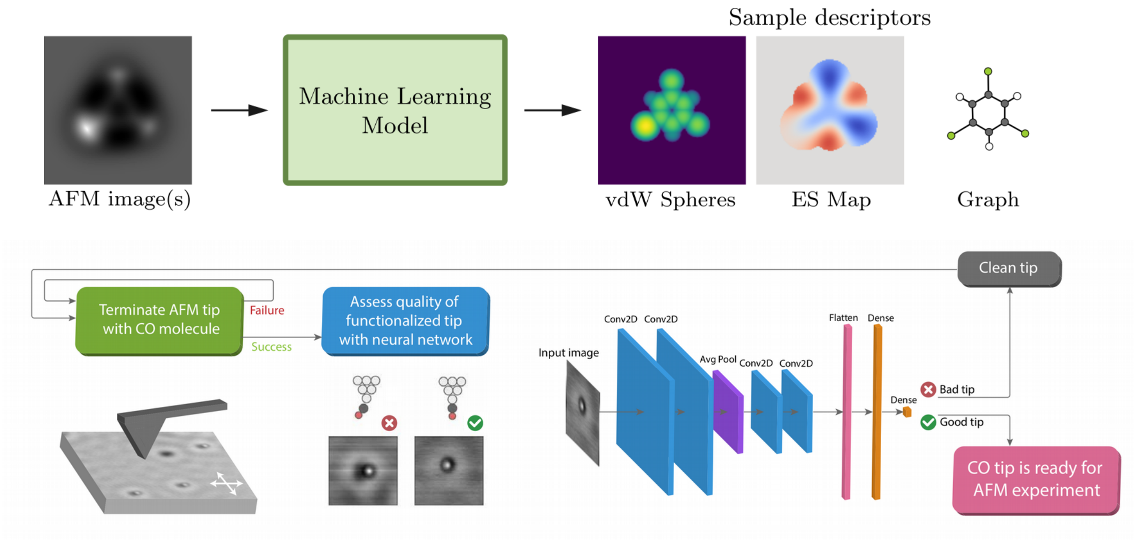
State-of-the-art nc-AFM setups operating in vacuum at low temperatures are able to resolve features on the scale of individual atoms in molecules [1]. However, both the operation of the device and the process of interpreting the resulting AFM images is often a very challenging task even for highly trained experts in the field. We are working towards greater interpretability and greater automation of the processing of AFM images using machine learning methods. We have introduced an approach based on convolutional neural networks for discovering the atomic structure and electrostatic properties of samples directly from AFM images via image descriptors that characterize the sample [2, 3]. Our current work refines the geometry prediction task by predicting the molecule graph of the sample using a model based on graph neural networks [4]. Furthermore, the process of preparing a CO molecule on the apex of the AFM tip can be automated, which greatly reduces the time and effort spent on this trial-and error process [5].

Figure 1: *Machine learning methods can be used both for interpreting AFM images and determining the quality of an functionalized AFM tip.*



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[2] B. Alldritt et al., Sci. Adv. 6(9), eaay6913, 2020.
[3] N. Oinonen et al., ACS Nano, 16, 1, 89–97, 2022.
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Monday 16:00–16:20

Probing long- and short-ranged magnetic interactions on the nanoskyrmionic Fe monolayer on Ir(111)

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Skyrmionic systems are currently investigated, because skyrmions are topologically protected magnetic objects with very interesting and peculiar properties [1]. Particularly, they are discussed as possible candidates for magnetic data storage.

With a lattice constant of just 1 nm the Fe monolayer on Ir(111) exhibits the smallest skyrmion lattice observed so far [2]. Utilizing magnetic exchange force microscopy (MExFM), we are able to simultaneously resolve the atomic and magnetic structure [3]. Unlike antiferromagnetically ordered spin arrangements on surfaces studied previously with MExFM [4,5], the long range dipolar magnetic force does not cancel out completely above the surface.

To investigate the interplay between the short-ranged chemical and magnetic exchange force as well as the long-ranged magnetic dipolar interactions, we recorded site specific force spectroscopy data using the frequency modulation technique (3D Force field spectroscopy: 3D-FFS [6]). As visible in Fig.1, we find that the magnetic lattice can be detected before atomic resolution is actually achieved, indicating that long-range magnetic dipolar forces contribute significantly to the magnetic signal. This finding suggests that magnetic force microscopy (MFM) imaging of such a nanoskyrmion lattice is feasible. Since we observe tip-induced perturbations of the genuine magnetic structure during MExFM data acquisition, this possibility would be very beneficial: MFM experiments are performed at larger tip sample separations than required for MExFM and thus the magnetic structure is less perturbed by the presence of a magnetic tip.

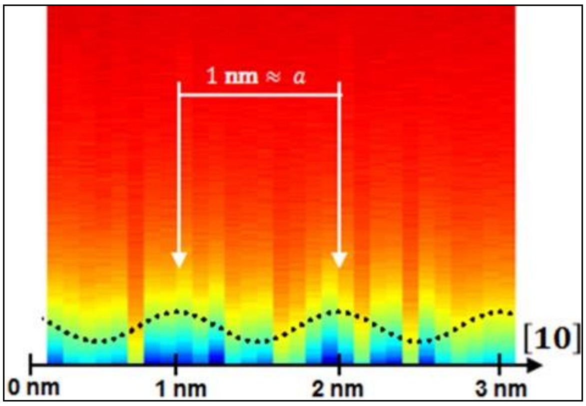

Figure 1: *3D-Force-Field-Spectroscopy on the nanoskyrmion lattice with the 1 nm periodicity of the nanoskyrmion along the [10] direction resolved.*

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[4] U. Kaiser et al., Nature **446**, 522 (2007).
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Monday 16:20–16:40

Very weak bonds to artificial atoms formed by quantum corrals

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We explored the bonding properties of the quantum corral (a circle of 48 iron atoms placed on a copper surface) reported by Crommie, Lutz and Eigler in 1993, along with variants, as an artificial atom using an atomic force micro- scope (AFM). The original corral geometry confines 102 electrons to 28 discrete energy states, and we find that these states can form a bond to the front atom of the AFM with an energy of about 5 millielectron volts. The measured forces are about 1/1000 of typical forces in atomically resolved AFM. The confined electrons showed covalent attraction to metal tips and Pauli repulsion to CO-terminated tips. The repulsion at close distance was evident from the response of corral states created by deliberately placing single iron atoms inside the corral. The forces scaled appropriately with a 24-atom corral.

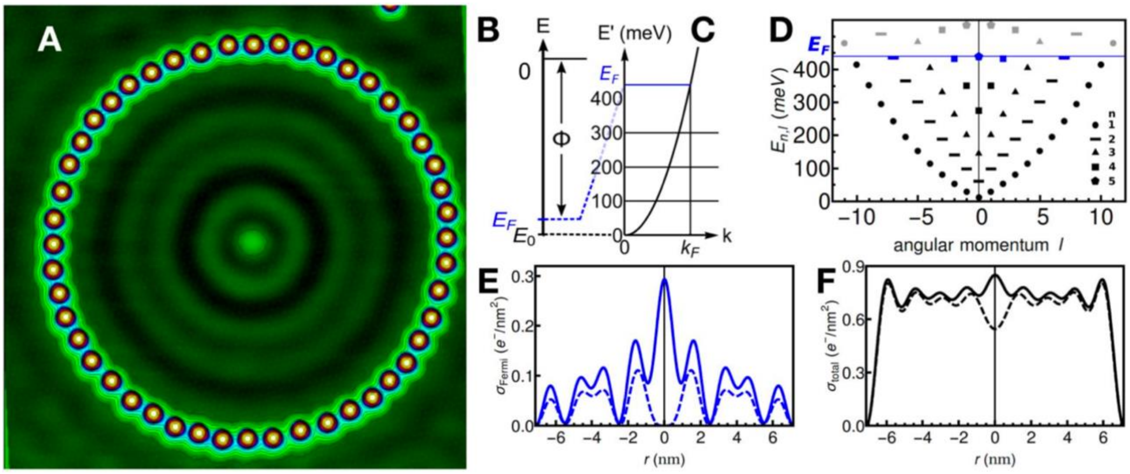

Figure 1: **A** *Topographic STM image at a tip bias of -1 mV and a tunneling current of 20 pA of a quantum corral consisting of 48 Fe atoms on Cu (111) using a CO terminated tip. The ring has a radius of 7.13 nm, the Cu atoms of the Cu(111) substrate appear as small bumps with a height of ≈ 500 fm and a distance of 255 pm.* **B** *Energy diagram of the electrons on the Cu(111)surface with vacuum level at 0, the Fermi energy E_F at -4.94eV, and the lowest energy of the surface state E_0 another -0.44 eV lower.* **C** *Energy spectrum of the occupied surface states on the Cu(111) surface with a shifted energy scale $E' = E - E_0$ with their characteristic dispersion relation $E' = h^2k^2/(2m^*)$.* **D** *Energy spectrum of the occupied corral states, characterized by the number of zeroes n and the angular momentum l. Five of the occupied states, namely $\psi_{n,l} = \psi_{5,0}$, $\psi_{4,\pm2}$ and $\psi_{2,\pm7}$ are imaged by STM at low bias as their energy is close to the Fermi level.* **E** *Calculated surface charge density σ_{Fermi} of the states at the Fermi level, dashed line without contribution of $\psi_{5,0}$.* **F** *Calculated surface charge density of all occupied states σ_{total}, dashed line without contribution of $\psi_{5,0}$.*

[1] F. Stilp et al., *Science* **372**, 1196 (2021).

Monday 16:40–17:00

Line shape analysis of the resonant eigenstates in a quantum corral by means of tunneling spectroscopy and non contact AFM

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Back in 1993 Crommie et al. [1] arranged 48 Fe adatoms on a Cu(111) surface in a circle with a diameter of 14.26 nm. This quantum corral confines surface electrons in a circular potential well. Past investigations with scanning tunneling microscopy and tunneling spectroscopy revealed energetically discrete eigenstates that spatially appear as Bessel functions of the enclosed electrons. But these studies on the Fe quantum corral showed unwanted movement of the corral walls during spectroscopic measurements. [1]

Instead of Fe, we used CO molecules to provide the corral with more stable walls (see Figure 1A). This permitted us to access a larger voltage window and allowed for a detailed line shape analysis of the corrals eigenenergy levels. Surprisingly, we discovered a large Gaussian broadening of the eigenstates.

We also acquired nc-AFM data of the corral. As we have previously done, we determined the occupation of electronic states that cross the Fermi level [2]. Similar to our previous work, we observed that the presence of the probe tip shifts the energy of the electronic states under study. In this work, we show that we can also use the AFM data to estimate the lifetime (i.e. the spectral width) of these states.

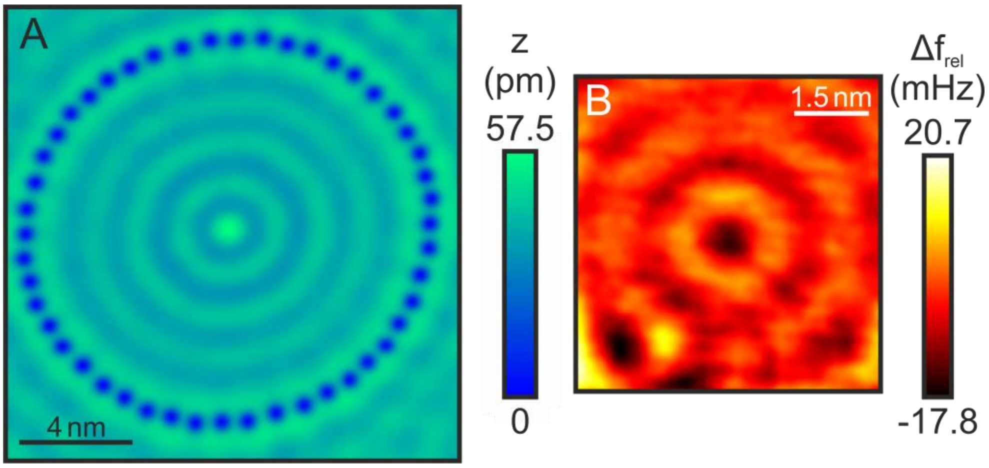

***Figure 1: A** STM image of 48 CO molecules (dark blue spots) forming a circular quantum corral. **B** Constant height AFM image of the corral center.*

[1] M. F. Crommie, C. P. Lutz, D. M. Eigler, Science **262**, 218-220 (1993).
[2] F. Stilp, A. Bereczuk, J. Berwanger, N. Mundigl, K. Richter, F. J. Giessibl, Science **372**, 1196-1200 (2021).

Monday 17:00–17:20

Interaction between an artificial and a natural atom

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The surface state of Cu (111), a quasi-2-dimensional electron gas, is trapped to a small surface area of about 15 x 15 nm^2 by placing 48 CO-molecules in a circular shape on the surface via atomic manipulation. By doing so, one creates a quantum corral with discrete electronic states forming an artificial atom. This structure can be described reasonably well by an infinitely high circular potential well leading to corral states with Bessel-type radial functions and an angular momentum normal to the surface. To investigate the interaction between this artificial atom and a natural atom we bring Fe atoms inside the corral and measure the response of the corral states. Figure 1A shows a STM overview image of this setup.

Thanks to the large size, one can study the structure of the wave functions within that artificial atom by nc-AFM (see Figure 1B) showing an angular dependence of the corral states after placing the atoms inside the corral. This change of the wave functions leads to an energy shift of a few meV confirmed by tunneling spectroscopy measurements. By investigating the change of the wave functions and the energies of the corral states when placing the adatom inside, one can draw conclusion about the interaction between this artificial atom and a natural atom. Here we expand the interpretation of the adatom acting repulsively on the corral states as stated by Stilp et al. [1].

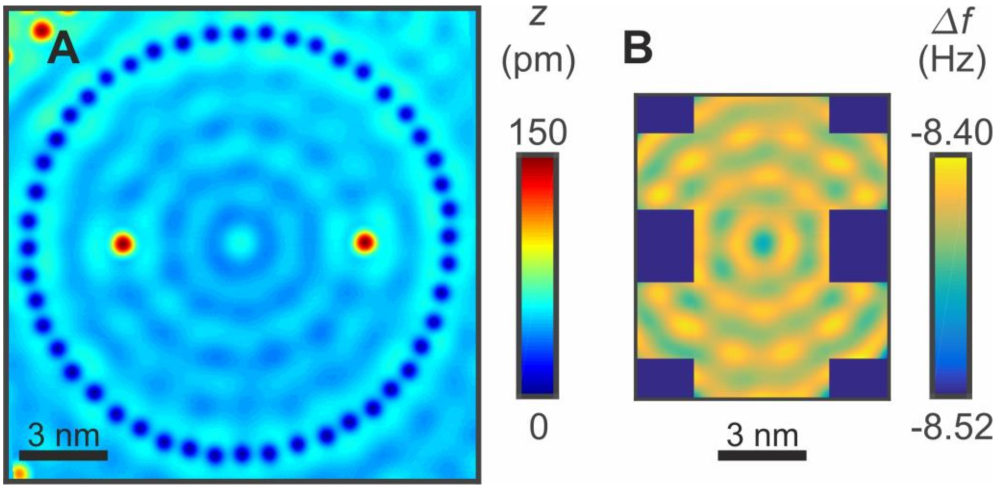

Figure 1: ***A*** *STM image of circular quantum corral formed by 48 CO-molecules (dark spots) as artificial atom and two Fe atoms (bright spots) inside as natural atoms.* ***B*** *Constant height AFM image inside the quantum corral. The subatomic contrast of the artificial atom reveals an angular dependence of the corral states.*

[1] F. Stilp, A. Bereczuk, J. Berwanger, N. Mundigl, K. Richter, F.J. Giessibl, Science **372**, 1196-1200 (2021).

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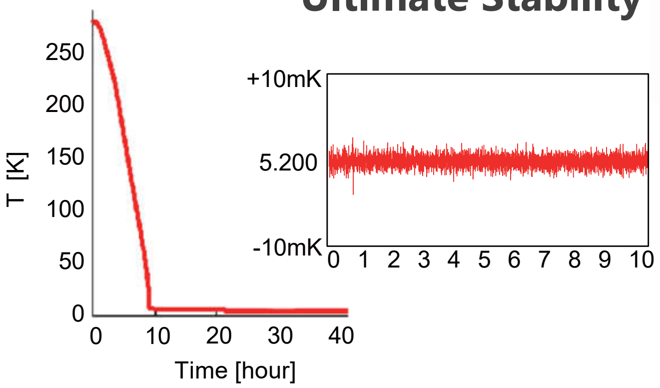
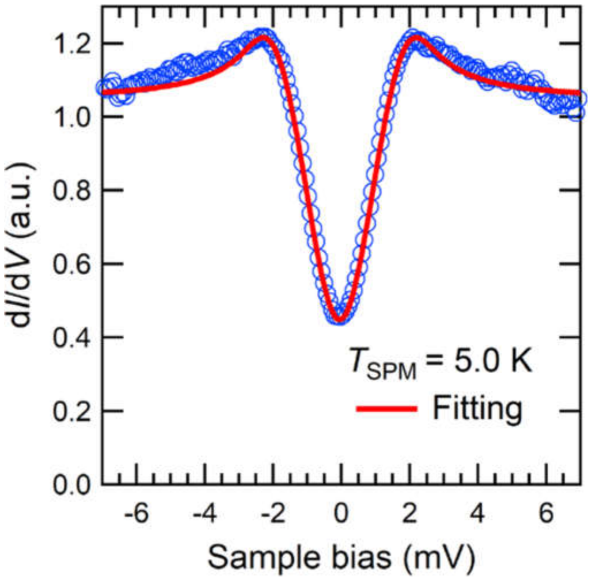
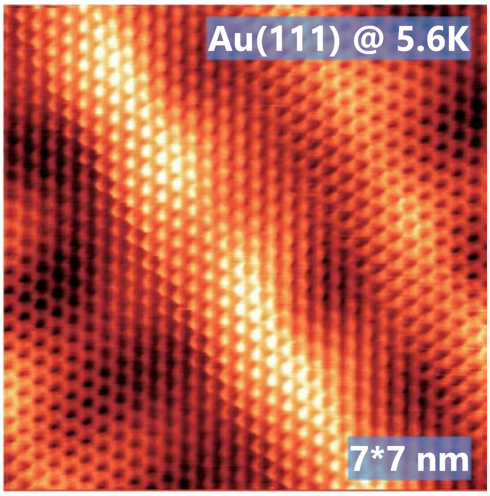


Proven 5K Performance SC gap of Pb



Ultimate STM Resolution



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Tuesday, August 2nd 2022

Force mapping on nanoscale structures and study of water

Chair: Lotze, C.

09:00 **Priante, F.** *Structure discovery in AFM imaging of ice.*

09:20 **Brown, T.** *Room temperature intramolecular force mapping.*

09:40 **Yamamoto, T.** *Atomic-scale measurement of photoinduced force between a tip and the electron orbital of* C_{60} *single-molecule.*

10:00 **Jugade, S.** *Nanomechanical Insights into Graphene-Liquid Interface.*

Novel instrumentation and techniques (B)

Chair: Schwarz, A.

11:00 **Sellies, L.** *Isotope detection inside single molecules in scanning-probe based electron spin resonance.*

11:20 **Martin Jimenez, D.** *Chemical bond imaging using torsional and flexural higher eigenmodes of qPlus sensors.*

11:40 **Sugawara, Y.** *Atomic-scale Optical Properties of Pentacene Molecules Measured by Photoinduced Force Microscopy (PiFM).*

12:00 **Heile, D.** *Alignment method for the accurate and precise quantification of tip-surface forces.*

Nanoscale measurements of charge and work function (A)

Chair: Štich, I.

14:00 **da Lisca, M.** *Cross-sectional Kelvin Probe Force Microscopy on III-V epitaxial multilayer stack: challenges and perspectives.*

14:20 **Hoffmann-Vogel, R.** *Electrostatic Forces above Pb on Si(111).*

14:40 **Navarro Rodriguez, M.** *Characterization of Graphene Oxide charge dynamics with Kelvin Probe Force Microscopy.*

Force mapping in liquid and under ambient conditions

Chair: Balajka, J.

16:00 **Su, S.** *Facet-dependent surface charge and hydration of colloidal* $SrTiO_3$ *nanoparticles at variable pH.*

16:20 **Gisbert, V. G.** *High-Speed Bimodal AFM nanomechanical mapping of collagen self-assembly.*

16:40 **Siretanu, I.** *Correlation between electrostatic and hydration forces on silica and gibbsite surfaces: An Atomic Force Microscopy Study.*

17:00 **Ikarashi, T.** *Visualizing Bias-Dependent Changes in Ionic Liquid/Au Interface Structures by 3D Scanning Force Microscopy.*

Tuesday 09:00–09:20

Structure discovery in AFM imaging of ice

F. Priante,[1] Y. Tian,[2] D. Guan,[2] C. Xu,[1] S. Cai,[1] N. Oinonen,[1] P. Liljeroth,[1] Y. Jiang,[2, 3, 4, 5] and A. S. Foster [1, 6, *]

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[2] International Center for Quantum Materials, Peking University, Beijing, 100871, China
[3] Collaborative Innovation Center of Quantum Matter, Beijing, 100871, China
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The interaction of water with surfaces is crucially important in a wide range of natural and technological settings. In particular, at low temperatures, unveiling the atomistic structure of adsorbed water clusters would provide valuable data for understanding the ice nucleation process. Using high-resolution Atomic Force Microscopy (AFM) and Scanning Tunneling Microscopy, several studies have demonstrated the presence of water pentamers, hexamers, heptamers (and of their combinations) on a variety of metallic surfaces [1 – 4], as well the initial stages of 2D ice growth on an insulating surface [5]. However, in all these cases, the observed structures were completely flat, providing a relatively straightforward path to interpretation. Here, we present high-resolution AFM measurements of several new water clusters on Cu(111), whose understanding presents significant challenges, due to both their highly 3D configuration and to their large size. For each of them, we use a combination of machine learning, atomistic modelling and statistical sampling to propose an underlying atomic structure, comparing the experimental images with simulated AFM from Density Functional Theory. These results provide new insights into the early phases of ice formation, which is a ubiquitous phenomenon ranging from biology to astrophysics.

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[4] A. Dong et al., ACS Nano **12**, 6452–6457 (2018).
[5] R. Ma et al., Nature **577**, 60–63 (2020).

Tuesday 09:20–09:40

Room temperature intramolecular force mapping

Brown T , Blowey P , Henry J , Sweetman A

Non-contact atomic force microscopy (NC-AFM) has yielded enormous progress in our ability to characterise materials at the atomic scale, including the acquisition of dense 3D molecular force fields with intramolecular resolution [1, 2]. To date, intramolecular imaging has almost exclusively been performed at cryogenic temperatures, as the standard CO functionalisation of the metallic tip is only stable at low temperature. In this paper we present the first demonstration of high-resolution three-dimensional force mapping of a single organic molecule at room temperature. The challenges of operating in a room temperature experimental environment are overcome using semiconducting materials to inhibit molecular diffusion and create more robust tip apexes, whilst challenges due to thermal drift are overcome with atom tracking based feedforward correction [3, 4]. Three-dimensional force maps comparable in resolution to those acquired at low temperature are demonstrated, permitting a quantitative interpretation of the adsorption induced changes in the geometry of the molecule.

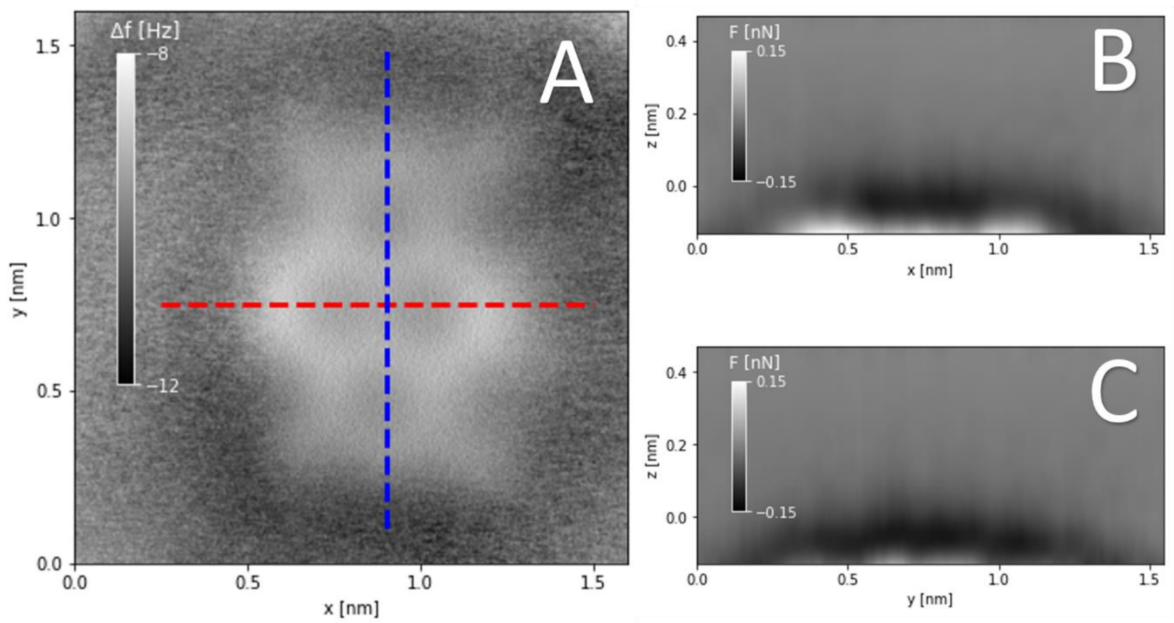

Figure: *(A) Constant height mode image of single NTCDI molecule on Si(111)-(7x7) surface. Image is an average of 10 scans, made possible by continual corrections to the drift compensation. (B), (C) molecular cross sections of the force, measured via grid spectroscopy along the short and long axes respectively. The positions of the cross sections are represented by the dotted lines in (A).*

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1. Leo Gross et al. Science. 28; 325, 5944 (2009)
2. Adam Sweetman et al. Nat Commun 5, 3931 (2014).
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4. Philipp Rahe et al. Rev Sci Instrum 82, 063704 (2011)

Tuesday 09:40–10:00

Atomic-scale Measurement of Photoinduced Force between a Tip and the Electron Orbital of C_{60} Single-molecule

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Photo-induced force microscope (PiFM) has been developed based on the AFM technique to image the optical properties of the sample surface with high spatial resolution [1]. In this microscope, light is irradiated onto the metal tip of AFM and the sample surface, and the dipole-dipole interaction between the dipole induced on the metal tip and the dipole induced on the sample surface is detected as a force (Fig. 1). Using PiFM, optical imaging of various materials such as nanoparticles [1] and quantum dots [2] has been performed. However, optical imaging of single molecules has not been performed to date due to insufficient spatial resolution, and the imaging mechanism is still unclear.

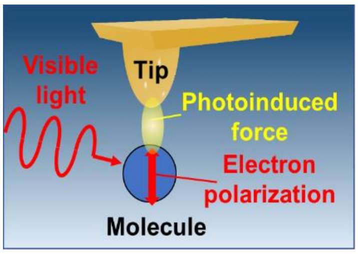

Figure 1: *Photoinduced force between tip and molecule*

In this report, we describe the results of the measurement of photoinduced forces on a single C_{60} molecule at sub-molecular resolution using PiFM. C_{60} molecules were deposited on pentacene bilayer film on Ag (100) substrate. We used a gold-coated cantilever as a force sensor. The wavelength of incident light was 440nm. Figures 2(a) and 2(b) show AFM and photoinduced force images simultaneously measured on a C_{60} at 78K, respectively. While the AFM image of C_{60} had an ordinary round shape because the image is measured in the attractive region, the photoinduced force image of the C_{60} consists of four rings. The minimum diameter of these rings is about 0.45 nm, suggesting that the photoinduced force was successfully measured on an atomic scale. We also measured the photoinduced force curves on the C_{60}, the behavior of which qualitatively agreed with the theoretical calculation. Comparison with the structural model and the distribution of molecular orbitals of C_{60} shows that the bright regions of the photoinduced force image in Fig. 2(b) correspond to the distributions of the highest occupied molecular orbital (HOMO) of the C_{60} (Fig. 2(c)).

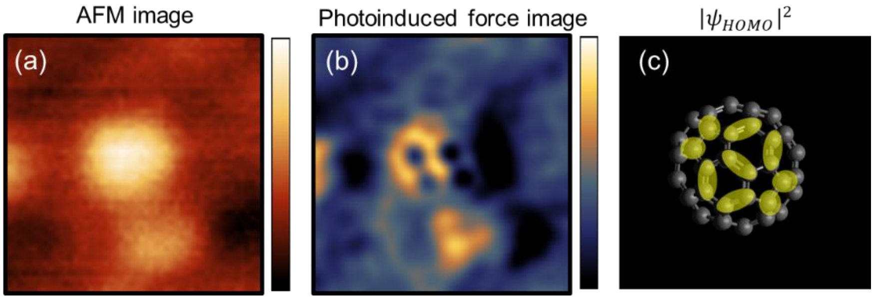

Figure 2: *(a) AFM and (b) photoinduced force image of C_{60} measured at 78K. Scan area is 4nm × 4nm. (c) HOMO distribution of C_{60}.*

[1] J. Jahng et al., Acc. Chem. Res. **48**, 2671–2679 (2015)
[2] J. Yamanishi, Y. Sugawara et al., Nature communications, **12,** 3865 (2021).

Tuesday 10:00–10:20

Nanomechanical Insights into Graphene-Liquid Interface

Sanket Jugade, Prabhat Vashishth, Prosenjit Sen, Akshay Naik*

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Nanoscale insights into Graphene-Liquid interaction allow manipulation of interfacial properties by tuning chemical reactivity, electronic mobilities, adhesion, and friction[1]. Techniques like Atomic Force Microscopy (AFM) that can probe graphene-liquid interface at nanoscale resolution present an opportunity to study the fundamental nature of forces at such unique interfaces[2]. Here, we fabricated suspended graphene on Polydimethylsiloxane (PDMS) microfluidic channels and flowed a liquid mixture of IPA+DI water underneath graphene. We observed a striking phase-contrast of 20^0 between liquid and graphene on liquid (GoL). We demonstrated phase mapping as a simple tool for high-contrast imaging, not achievable on suspended graphene in air, distinguishing topological graphene features like wrinkles, holes, cracks, tears, and pristine regions. Phase measurements coupled with force spectroscopy indicate graphene screens[3] long-range tip-liquid conservative interactions. Nanoscale energy dissipation obtained from these phase measurements shows much lower and uniform dissipation after graphene-liquid contact, mainly due to the absence of tip-adhesion-induced mechanical oscillations otherwise present in air. The dissipation on GoL possibly comes from the short-range hysteresis due to contact with liquid, as indicated by the force spectroscopy data. Therefore, nanoscale dissipation could be utilized to study how contact with different liquids influences the mechanical properties of free-standing 2D materials. Using amplitude-distance spectroscopy in dynamic AFM, we also studied the deformation of graphene membrane during drying of liquid in the channel. Based on these results, we report some interesting observations on capillary forces, trapping of liquid in defects, confinement of liquid in micro-nano holes, and presence of thin layer of liquid below graphene.

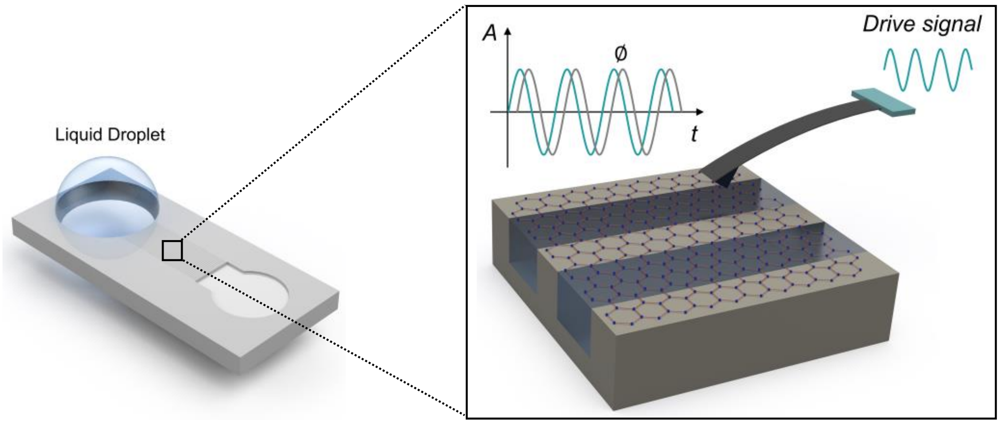

Figure 1: *Schematic of the experimental setup for dynamic AFM measurements on Graphene on liquid*

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[2] M.R. Uhlig, D. Martin-Jimenez, R. Garcia, Nat. Commun. **10**, 2606 (2019).
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Tuesday 11:00–11:20

Isotope detection inside single molecules in scanning-probe based electron spin resonance

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Electron spin resonance (ESR), a versatile technique to study materials with unpaired electrons, was recently combined with scanning tunneling microscopy (STM) [1]. This ESR-STM technique brings an atomic-scale spatial resolution to ESR, allowing for instance to distinguish isotopes of single atoms via the hyperfine interaction between the electron spin under study with the nuclear spin [2]. Furthermore, it enables the coherent manipulation of spins [3, 4] having a great potential for applications in quantum computing.

One of the advantages of ESR-STM is that it has a largely improved energy resolution compared to conventional STM, reaching the nano-electron-volt regime. This energy resolution can even be improved further if the tunneling current as a read-out could be avoided, since this current is the dominating decoherence source for the probed electron spin.

We propose, therefore, a new ESR scanning probe method based on atomic force microscopy (AFM). AFM is a natural choice, well-known for its capability to resolve molecules with sub-molecular resolution [5]. Since our technique does not rely on the tunneling current to read-out the ESR signal, we are able to increase the coherence times of the electron spins and, consequentially, the energy resolution. Therefore, we can resolve the hyperfine interaction inside organic molecules, giving us a tool to distinguish molecules only differing in the isotopic composition. Thus, our technique allows the chemical fingerprinting of molecules and their surroundings.

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Tuesday 11:20–11:40

Chemical bond imaging using torsional and flexural higher eigenmodes of qPlus sensors

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[2] University of Newcastle, Callaghan, NSW, 2308 (Australia).
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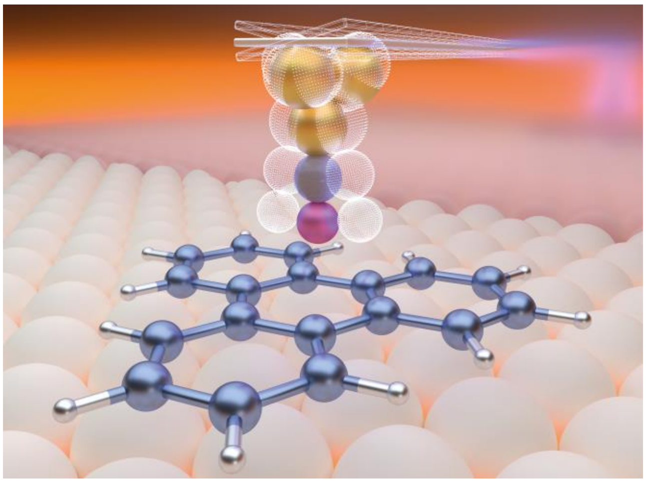
Non-contact atomic force microscopy (AFM) with CO-functionalized tips allows to visualize the chemical structure of adsorbed molecules and identify individual inter- and intramolecular bonds. This technique enables in-depth studies of on-surface reactions and self-assembly processes. Herein, we analyze the suitability of qPlus sensors, which are commonly used for such studies, for the application of modern multifrequency AFM techniques. Two different qPlus sensors were tested for submolecular resolution imaging via actuating torsional and flexural higher eigenmodes and via bimodal AFM. The torsional eigenmode of one of our sensors is perfectly suited for performing lateral force microscopy (LFM) with single bond resolution. The obtained LFM images agree well with images from the literature, which were scanned with customized qPlus sensors that were specifically designed for LFM [1]. The advantage of using a torsional eigenmode is that the same molecule can be imaged either with a vertically or laterally oscillating tip without replacing the sensor simply by actuating a different eigenmode. Submolecular resolution is also achieved by actuating the 2nd flexural eigenmode of our second sensor. In this case, we observe particular contrast features that only appear in the AFM images of the 2nd flexural eigenmode but not for the fundamental eigenmode. With complementary laser Doppler vibrometry measurements and AFM simulations we can rationalize that these contrast features are caused by a diagonal (i.e. in-phase vertical and lateral) oscillation of the AFM tip [2].



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Tuesday 11:40–12:00

Atomic-scale Optical Properties of Pentacene Molecules Measured by Photoinduced Force Microscopy (PiFM)

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The polarization induced in matter by the electric field of light contains information on the excited states of electrons and is a physical quantity that plays a central role in the interaction between light and matter. However, this has never been directly observed on an atomic scale. We have been studying a new concept of optical microscopy (photo-induced force microscopy: PiFM) [1,2]. In photoinduced force microscopy, light is irradiated onto the metal tip of AFM and the sample surface, and the dipole-dipole interaction between the dipole induced on the metal tip and the dipole induced on the sample surface is detected as a force (Fig. 1(a)). This microscope has no light propagation loss, which has been a major problem in conventional near-field optical microscopy, and it is easy to achieve high sensitivity and resolution.

Here we report the results of a high-sensitivity, high-resolution measurement of photoinduced forces acting on pentacene molecules using photoinduced force microscopy. In order to remove the photothermal effect, we used the heterodyne frequency modulation (FM) method, which allows light irradiation at high modulation frequencies [1]. Figure 1(b) shows the photoinduced force image of bilayer pentacene molecules on an Ag(001) surface measured at 78K. The wavelength of the incident light was 690 nm. In the photoinduced force image in Figure 1(b), it can be clearly seen that bright spots are periodically arranged in a row. The minimum spacing of these bright spots is about 0.6 nm, suggesting that the photoinduced force was successfully measured on an atomic scale. Comparison with the structural model shows that the bright spots in the photoinduced force image correspond to the long-axis edge region of the pentacene molecule. The two-dimensional map of the photoinduced force on the pentacene molecule shows that the magnitude of the photoinduced force ranges from 100 fN to 1 pN, and that the interaction region is 1.5 nm (Fig. 1(c)).

This success is a promising development in the search for physical and chemical interactions between light and atoms and molecules at the atomic scale, providing deep insight into various optical processes and functions at surfaces.

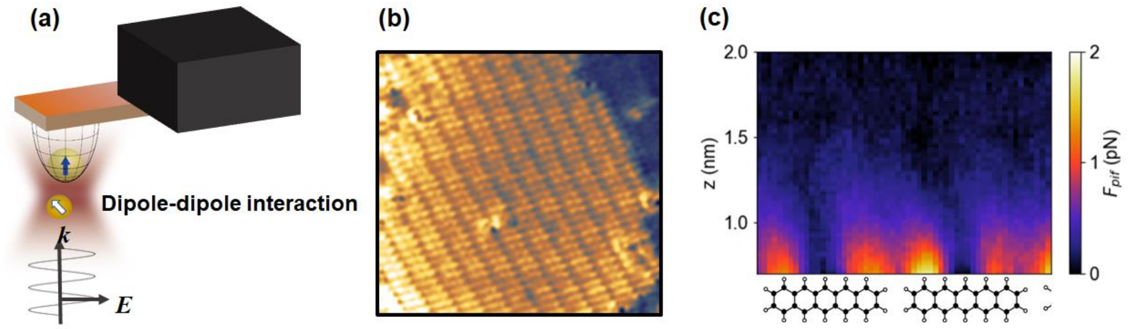

Figure 1: *(a) Concept of PiFM. (b) PiFM image and (c) 2D map of photoinduced force of pentacene molecules on Ag(001) measured at 78K. Wavelength of incident light was 690 nm.*

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Tuesday 12:00–12:20

Alignment method for the accurate and precise quantification of tip-surface forces

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The quantitative interpretation of nanoscale forces requires utmost precision in measuring and analysing force-distance curves. However, the conceptual difficulties in describing tip-surface forces have to be seen alongside experimental challenges that severely limit accurate force measurements with dynamic force microscopy.

Here, we introduce the force curve alignment (FCA) method to determine accurate and precise force-distance curves in force measurements with NC-AFM [1]. While a single force curve can be prone to systematic, often unnoticed errors, we demonstrate the self-consistent retrieval of interaction forces by an alignment procedure using repetitive measurements with the force probe oscillating at varied amplitudes. First, we give evidence for the correctness of this procedure from model data as shown in Figure 1(a). The force curve, the actual oscillation amplitude, and thermal drift parameters are correctly determined as depicted in Figure 1(b). Second, the precision in force measurements by FCA is demonstrated by processing experimental data as depicted in Figure 1(c) and (d). While the acquisition of single curves reveals inconsistent results (Figure 1(c)), precise force data are delivered by FCA (Figure 1(d)).

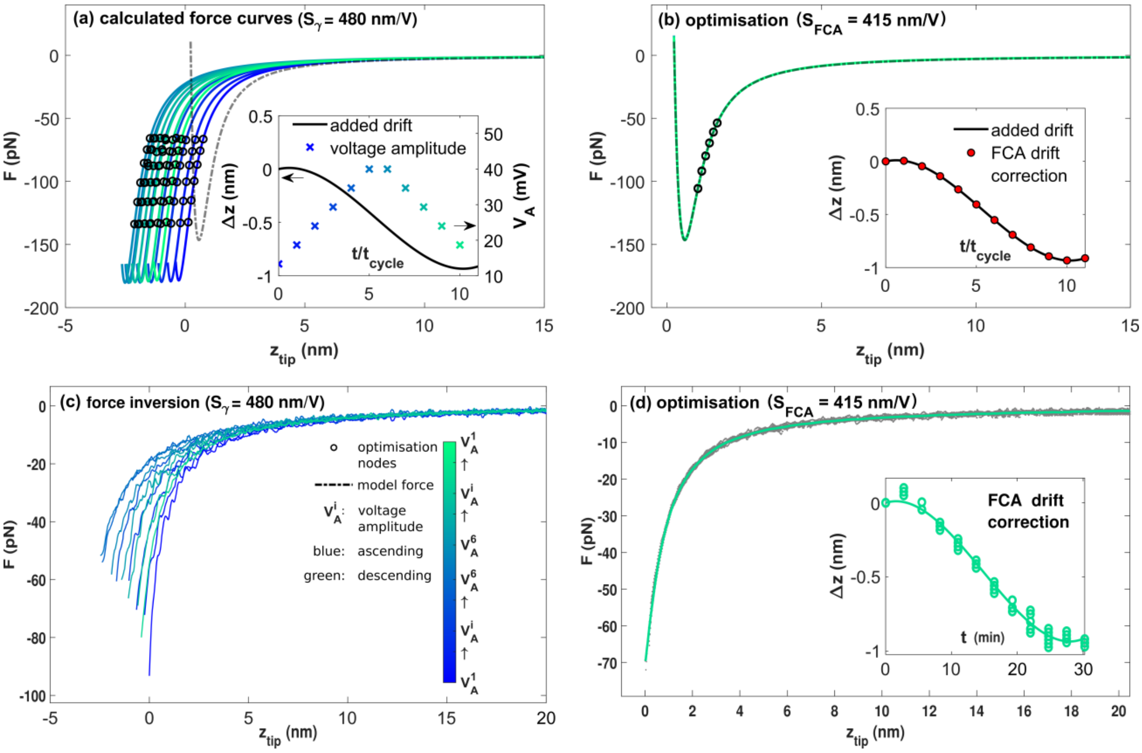

Figure 1: *Simulated (a, b) and measured (c, d) force curves before (a, c) and after (b, d) optimization by FCA.*

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Tuesday 14:00–14:20

Cross-sectional Kelvin Probe Force Microscopy on III-V epitaxial multilayer stack: challenges and perspectives

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The functionality and the electronic performance of semiconductor-based devices greatly depend on the doping profile. Among the wide variety of SPM techniques available [1], Kelvin probe force microscopy (KPFM) is a valuable investigative approach for the study of work functions (WFs) and surface potential. KPFM is a non-contact method which allows the detection of dopant concentrations in a range from 10^{14} to 10^{19} cm^{-3} [2]. In this study, we investigate the capability of FM-KPFM in ambient conditions for the analysis of the doping profile of a p-type zinc doped indium phosphide (InP:Zn) structured sample. For a quantitative interpretation of the KPFM data, the doping profile was extracted directly from the experimental V_{CPD} values acquired in dark and under white light illumination and compared with the doping profile previously determined by electrochemical capacitance-voltage (ECV). The analysis of the KPFM data was assisted by means of theoretical modelling simulating the KPFM measurements, qualitatively reproducing the experimental data by adjusting InP surface defect densities in the simulation.

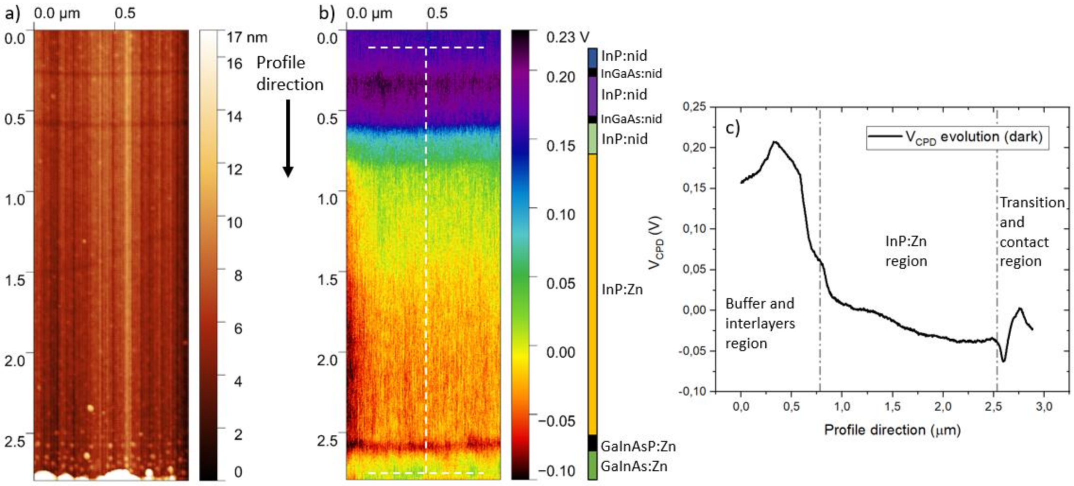

Figure 1: KPFM measurement in ambient conditions on the surface cross-section of the InP:Zn sample in dark. The topography (a) does not show any particular features which may be imprinted in the V_{CPD} image. The V_{CPD} image (b) shows the detection of the different layers which comprise the sample. Note that, the resolution of the images is set to 1024x1024 pixels per point. The profile in (c) shows an average value of the data along the V_{CPD} image and corresponds to the region identified by the dotted white segment.

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Tuesday 14:20–14:40

Electrostatic Forces above Pb on Si(111)

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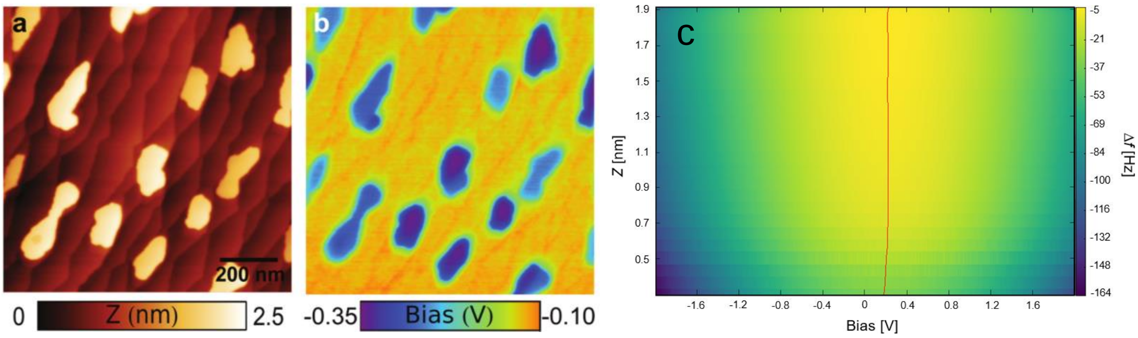
Pb grows on Si(111) in the form of islands combined with a wetting layer. We study both, the wetting layer and the islands: the islands show the quantum size effect due to electrons confined within the islands that form quantized states [1]. The work function, studied by Kelvin probe force microscopy, shows oscillations as a function of film thickness due to this quantum size effect. The wetting layer shows electron-rich areas that we interpret as Si-rich [2]. We discuss that these areas arise when islands disappear in the course of coarsening. During coarsening, some of the islands grow and others disappear. It can also occur that an island first grows and later disappears. We have observed coarsening in scanning force microscopy and Kelvin probe force microscopy over several hours. The results have implications for explosive island growth and collective motion observed on this surface [3,4].

We study in detail electrostatic forces measured both above Pb islands and above the wetting layer as a function of voltage. We measure the frequency shift versus distance and convert our results into force as a function of distance. The data shows a set of parabolae as a function of voltage. The local work function difference is given by the maxima of the parabolae (i.e. by the point used in the Kelvin method). We study the local work function difference as a function of tip-sample distance. The local work function difference is mostly independent of tip-sample distance, only when tunneling distances are reached, there are deviations. This allows to assess the degree to which the the tip shape and sample structure influence the local work function measurement. It also gives information on the onset of chemical bonding between the tip and the surface and how it influences the local work function measurement.

Figure 1: *a) Topography, b) local work function difference (taken from Ref. 1) and c) frequency shift as a function of tip-sample distance. The red line shows the local work function difference*



as a function of tip-sample distance.

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Tuesday 14:40–15:00

Characterization of Graphene Oxide charge dynamics with Kelvin Probe Force Microscopy

Navarro Mario,[1] Jaime Colchero,[1] Miguel Ortuño,[1] Eduardo Colom,[2] Ana M. Benito,[2] Wolfgang K. Maser,[2] Andrés Somoza,[1] Elisa Palacios-Lidón[1,*]

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Graphene Oxide (GO) is a graphite sheet with a wide arrange of oxygen functional groups that decorate its basal plane and edges. Due to its highly disordered and nonstoichiometric nature, complex electronic dynamics take place. These dynamics manifest themselves in the form of localized charge domains which can be characterized with Kelvin Probe Force Microscopy (KPFM) (fig. 1a).

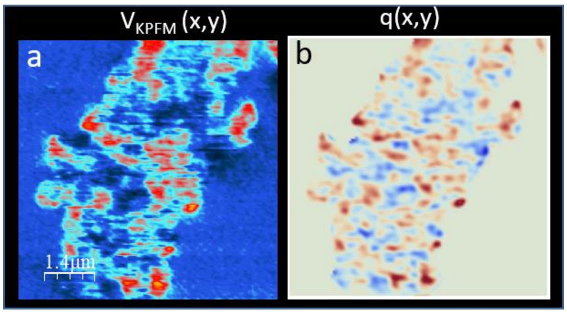

Figure 1: *Single GO a) surface potential distribution, b) real charge distribution*

The real charge distribution is directly obtained from the surface potential distribution [1]. This process allows us to resolve individual charge domains with a charge of around ± 1e and with a radius of about 25 nm (fig. 1b), which is of the order of the correlation length of electrons in the material (~15 nm). The observed correlation length is larger than the localization length of electrons in the material and as such, Efros-Shklovskii conduction is expected to take place [2].

In these works, GO charge distribution as well as its dynamics are measured and compared with "electron glasses" theoretical simulations. This allows us to verify the existence of slow relaxation times as well as fast fluctuations, confirming the presence of different timescales within the material [2]: Furthermore, we performed out of equilibrium charge injection experiments. Monitoring the charge spread evolution (fig. 2A, 2B) together with theoretical modeling, we explore GO's conducting properties.

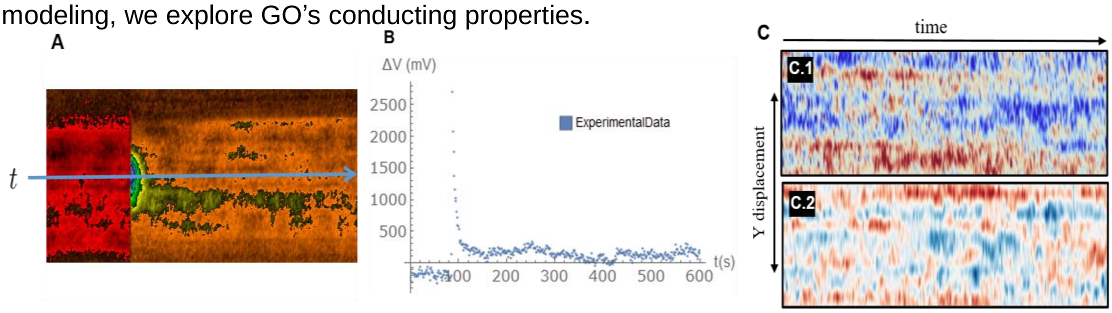

Figure 2: *A) Time evolution of the surface potential at a given line, B) Potential profile at the peak of the distribution as a function of time, C) time evolution of different charge profiles, C1) experimental, C2) simulated data*

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Tuesday 16:00–16:20

Facet-dependent surface charge and hydration of colloidal $SrTiO_3$ nanoparticles at variable pH

Shaoqiang Su[1,*], Igor Siretanu[1], Dirk van den Ende[1], Bastian Mei[2], Guido Mul[2] and Frieder Mugele[1]

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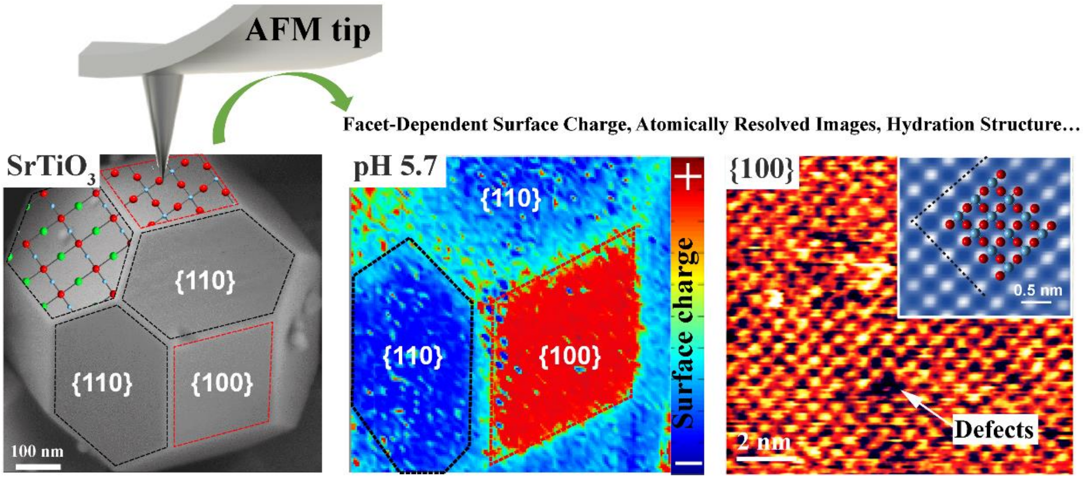
Anisotropy of shape and surface properties determine the functionality of faceted nanoparticles in various contexts including facet selective colloidal self-assembly, crystal growth, biosensing, improved photo/electrocatalytic activity and enhanced selective cellular and ions uptake. The characteristic anisotropy, surface proprieties and function of solid-liquid interfaces of crystalline faceted nanoparticles are believed to be essential for their performance but remains poorly understood and difficult to characterize and quantify. We use dual scale Atomic Force Microscopy to measure electrostatic and hydration forces of faceted $SrTiO_3$ nanoparticles in aqueous electrolyte at variable pH. We demonstrate (i) the ability to quantify strongly facet-dependent surface charges yielding isoelectric points of the dominant {100} and {110} facets that differ by as much as 2 pH units, ii) fluids composition controlled facet-dependent accumulation of oppositely charged (SiO_2) particles, and iii) that atomic scale defects can be resolved but are in fact rare for the samples investigated [1]. Atomically resolved images and facet-dependent hydration structure suggest a microscopic hydration and charge generation mechanism [1].



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Tuesday 16:20–16:40

High-Speed Bimodal AFM nanomechanical mapping of collagen self-assembly

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Collagen is the most abundant structural protein of the extracellular matrix. The assembly of collagen fibrils play relevant roles in a variety biological processes. The formation fibrils during the self-assembly process of collagen I have been studied by AFM [1,2]. Those studies lacked the time and mechanical properties resolution to clarify the mechanism of the earlier stages of collagen assembly and fibril structure formation.

We have developed a high-speed bimodal AFM [3,4] that combines the *ms* time resolution of high-speed AFM [5] with the nanomechanical force sensitivity of bimodal AFM [6,7]. High-speed bimodal AFM characterizes the earliest stages of the self-assembly of the collagen fibrils by proving time-resolved and high-spatial resolution maps of the evolution of the elasticity of the fibrils during the growth.

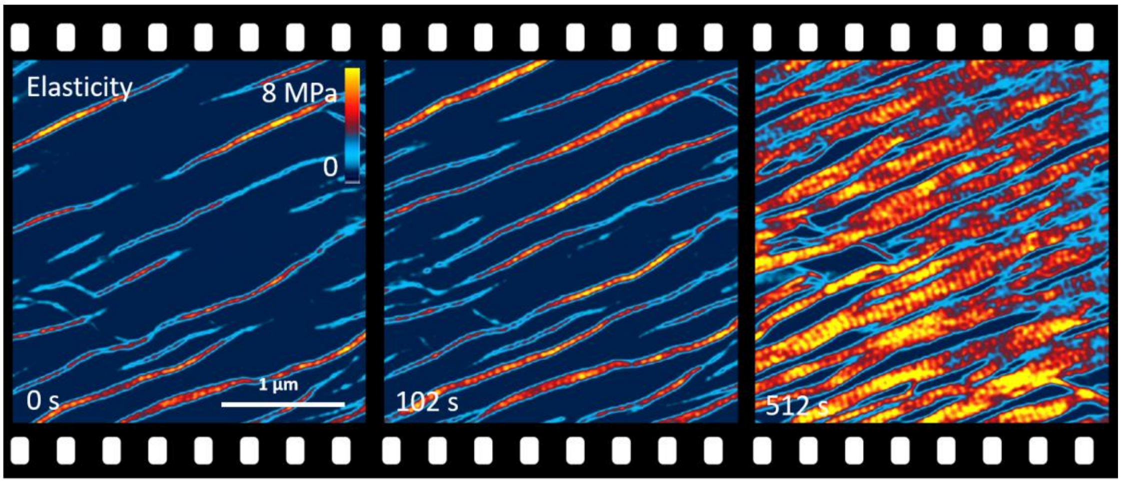

Figure 1: *High-speed bimodal AFM map of elastic modulus. The sequence captures the merging of and the alignment of the D-bands of several microribbons.*

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Tuesday 16:40–17:00

Correlation between electrostatic and hydration forces on silica and gibbsite surfaces: An Atomic Force Microscopy Study

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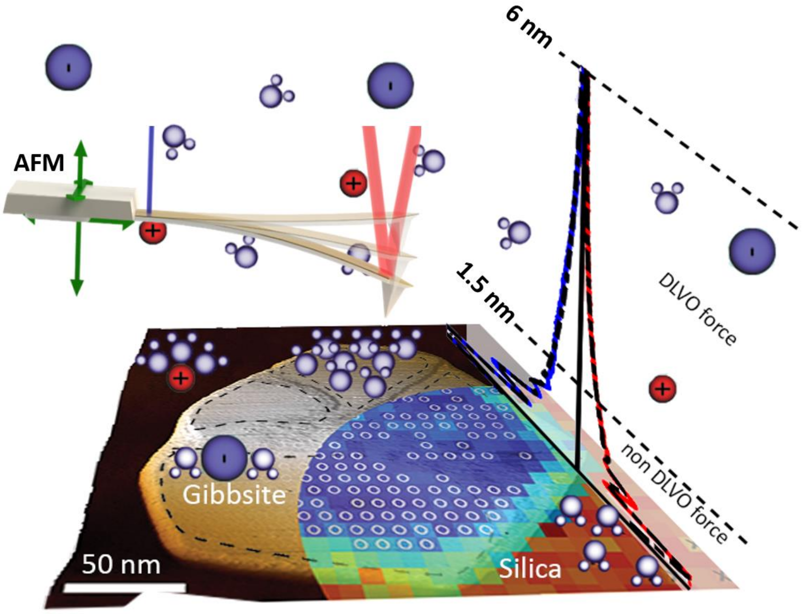
The balance between hydration and Derjaguin–Landau–Verwey–Overbeek (DLVO) forces at solid-liquid interfaces controls many processes, such as colloidal stability, wetting, electrochemistry, biomolecular self-assembly and ion adsorption. Yet, the origin of molecular scale hydration forces and their relation to the surface charge density that controls the continuum scale electrostatic forces are poorly understood. We argue that these two types of forces are largely independent of each other. To support his hypothesis, we performed atomic force microscopy experiments using intermediate-sized tips that enable the simultaneous detection of DLVO and molecular scale oscillatory hydration forces at the interface between composite gibbsite:silica -aqueous electrolyte interfaces. We extract surface charge densities from forces measured at tip-sample separations of 1.5 nm and beyond using DLVO theory in combination with a charge regulation boundary conditions for variable pH and salt concentration. We simultaneously observe both colloidal scale DLVO forces and oscillatory hydration forces for an individual crystalline gibbsite particle and the underlying amorphous silica substrate for all fluid compositions investigated. While the diffuse layer charge varies with pH as expected, the oscillatory hydration forces are found to be largely independent of pH and salt concentration, supporting our hypothesis that both forces indeed have a very different origin. Oscillatory hydration forces are found to be distinctly more pronounced on gibbsite than on silica. We rationalize this observation based on the distribution of hydroxyl groups available for H-bonding on the two distinct surfaces [1].



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Tuesday 17:00–17:20

Visualizing Bias-Dependent Changes in Ionic Liquid/Au Interface Structures by 3D Scanning Force Microscopy

Takahiko Ikarashi[1], Ryo Sakakibara[1], Takumi Yoshino[1], Keisuke Miyazawa[1], Takashi Sumikama[1], Kazuki Miyata[1], Sunao Shimizu[2], Yoshihiro Iwasa[3,4] and Takeshi Fukuma[1,*]

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[2] CRIEPI, Nagasaka 2-6-1, Yokosuka, Kanagawa 240-0196, Japan.
[3] Faculty of Engineering, The University of Tokyo, Hongo 7-3-1, Bunkyo 113-8656, Japan.
[4] RIKEN CEMS, Hirosawa 2-1, Wako, Saitama 351-0198, Japan.
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In recent years, electric double layer transistors (EDLTs) using ionic liquid (IL) as a gate insulator have received great attention [1]. EDLTs allows to accumulate charges with a much higher density than conventional field-effect transistors. Due to their unique characteristics, applications of ILs to a wide range of devices have been explored. Elucidation of the nanostructures of IL/solid interfaces is required to achieve better charge storage and carrier mobility. However, such interfacial structures are poorly understood because conventional techniques do not allow direct observation of the interfaces.

In this study, we used three-dimensional scanning force microscopy (3D-SFM) [2] that can visualize solid-liquid interfaces with a subnanometer-scale resolution to solve these problems. We performed 3D-SFM imaging of interfaces between IL (DEME-TFSI) and an atomically flat Au (111) surface with a variable bias voltage as shown in Figure 1(a) and investigated the bias voltage dependence of the interfacial structures. Figures 1b(i) and 1c(i) show the *z* cross-sections of the obtained 3D-SFM images. With a negative bias voltage, 3-4 layer-like contrasts were observed. Each layer has a thickness corresponding to the size of an ion pair. Meanwhile, with a positive bias, the layer-like contrasts becomes obscured, and the vertical positions of individual layers were changed. To understand this difference, we compared them with the results of molecular dynamics (MD) simulation as indicated in Figures 1b(ii) and 1c(ii). This suggests that 3D-SFM mainly visualizes the distribution of TFSI^- with a larger mass than DEME^+. The results demonstrate that 3D-SFM can visualize the 3D structures of IL/electrode interfaces. Such unique capability should help understanding the correlation between the interfacial structures and EDLT device functions.

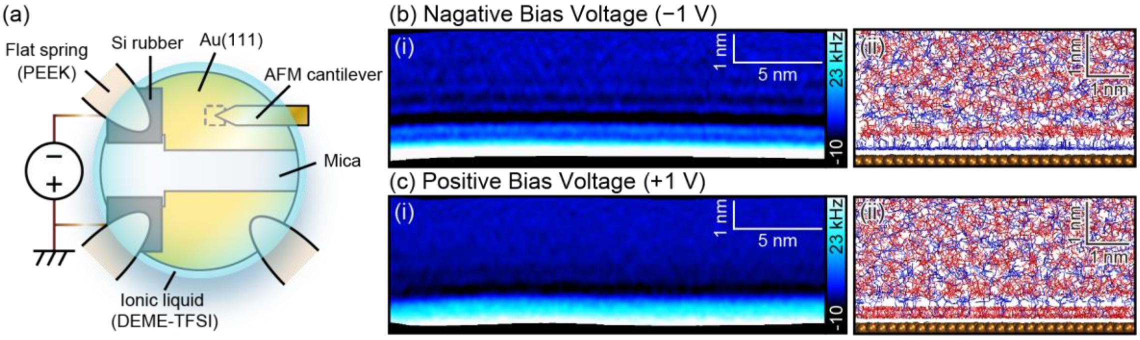

***Figure 1**: (a) Schematic of the measurement setup. (b,c) (i) 3D-SFM images and (ii) MD simulation snapshots of DEME-TFSI/Au(111) interface with (b) negative bias and (c) positive bias voltages.*

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Wednesday, August 3rd 2022

Nanoscale measurements of charge and work function (B)

Chair: Farinacci, L.

09:00 **Setvín, M.** *Real-space view on polaron kinetics in oxides.*

09:20 **Glatzel, T.** *Work Function and Friction Measurements of 2D KBr/Graphene Heterostructures.*

09:40 **Miyazaki, M.** *Measurement of spatially resolved surface photovoltage on* TiO_2*(110) by ac bias KPFM.*

10:00 **Cowie, M.** *Single-dopant band bending fluctuations in* $MoSe_2$ *measured with electrostatic force microscopy.*

Study of single molecules

Chair: Telychko, M.

11:00 **Pérez, R.** *Molecular identification with AFM images and deep learning.*

11:20 **Vilhena, G.** *Nanomanipulation and Dynamics of Single-Molecules at Surfaces.*

11:40 **Gallardo, A.** *Real-space imaging of* σ*-hole by means of Kelvin probe force microscopy.*

12:00 **Henry, J.** *Measuring the change in reactivity of a single molecule: Does The Bottom Effect The Top?*

Lateral forces, friction, and energy dissipation

Chair: Schwarz, U.

14:00 **Nam, S.** *The importance of the dipole at the metal tip apex when approaching closer with a CO tip.*

14:20 **Ollier, A.** *Energy dissipation on twisted bilayer graphene at magic angle twist.*

14:40 **Song, Y.** *Superlubric sliding in atomic friction in the case of molybdenum disulfide on gold.*

Characterisation of molecular systems (A)

Chair: Pawlak, R.

16:00 **Ihle, A.** *Tuning Halogen Bond Directed Self-Assembly: Substrate Snapping vs Intermolecular Interactions.*

16:20 **Ventura-Macias, E.** *Identifying* CO_2 *adsorption defects on Au surfaces with HR-AFM and STM.*

16:40 **Loppacher, C.** *[4+4] Photodymerization of Tripticene Derivatives with Anthracene Blades on Ionic Crystal Substrates.*

17:00 **Li, C.** *JT-SPM study of electron acceptor molecules on Ag(111).*

Wednesday 09:00–09:20

Real-space view on polaron kinetics in oxides

J. Redondo,[1,2] V. Gabriel,[1] G. Franchesci,[2] D. Wrana,[1] E. Rheinfrank,[2] I. Sokolovic,[2] G. S. Parkinson,[2] M. Riva,[2] M. Schmid,[2] U. Diebold,[2] P. Kocan,[1] **M. Setvin[1,2]**

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The behaviour of excess electrons and holes in a semiconductor determines the material's physical and chemical properties. In ionic lattices, charge carriers typically adopt certain degree of localization due to strong electron-phonon coupling. The resulting quasiparticle consisting of the charge carrier and the accompanying phonons is called a polaron [1]. Polarons influence many intriguing materials properties such as charge transport, superconductivity, colossal magnetoresistance, magnetism, or thermoelectricity.

Understanding of polaron physics is limited, and novel experimental approaches are needed to address this problem. Here we show that combined AFM/STM holds potential for understanding polaron dynamics. We report results on the hematite Fe_2O_3 (1-102) surface (see Fig. 1a), where electrons and holes form small polarons with high activation energies for hopping to adjacent sites. The STM functionality allows injection of electrons into the surface; the electrons remain localized near the injection site for days. The electrostatic potential induced by such electrons is shown in the LCPD map in Fig. 1b. The polarons become mobile under the influence of electric fields, illumination by visible light, or upon thermal activation.

The thermal exciations of polarons has been investigated in detail, see Fig. 1c. Annealing to gradually increasing temperatures results in a gradual spreading of the polaronic cloud due to the thermal activation combined with electrostatic repulsions among the polarons. Experiments were performed on stoichiometric and Ti-doped hematite samples; the doped samples show a significantly higher polaron mobility.

The work was supported by GACR project 20-21727X, GAUK Primus/20/SCI/009 and FWF project SUPER (P32148-N36.

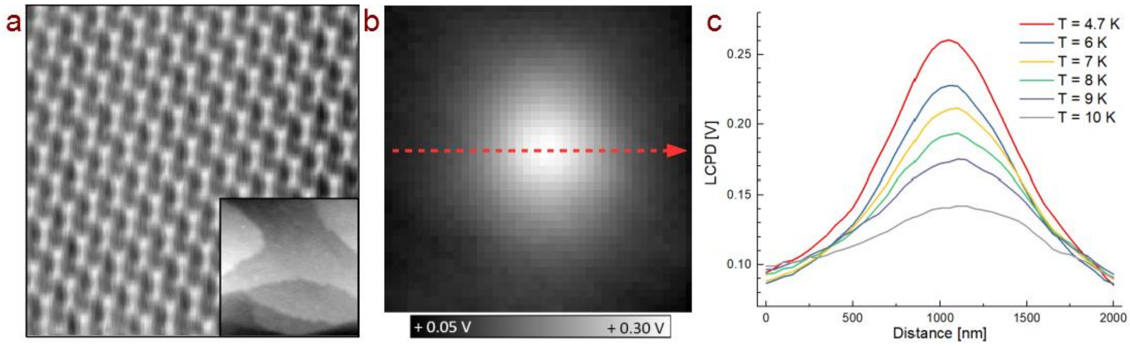

***Figure 1:** a) Atomically-resolved AFM image of the hematite (1-102) surface. The inset shows a 100 × 100 nm2 topographic image. b) 2×2 µm2 map of the electrostatic potential, measured by KPFM, induced by local injection of electrons into the surface. c) Evolution of the electrostatic potential after annealing the sample to various temperatures, measured along the line marked in b). Data obtained for hematite doped with 3% Ti.*

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Wednesday 09:20–09:40

Work Function and Friction Measurements of 2D KBr/Graphene Heterostructures

Zhao Liu[1], Antoine Hinaut[1] , Stefan Peeters[2] , Sebastian Scherb[1] , Ernst Meyer[1] , Maria Clelia Righi[2] and **Thilo Glatzel[1,*]**

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The intercalation of graphene is an effective approach to modify the electronic properties of two-dimensional heterostructures for attractive phenomena and applications. In this presentation, we show the characterization of the growth and the surface properties of ionic KBr layers altered by graphene using ultra-high vacuum atomic force microscopy at room temperature (Fig. 1). We observed a strong rippling of the KBr islands on Ir(111), which is induced by a specific layer reconstruction but disappears when graphene is introduced in between. The latter causes a consistent change in both the work function and the frictional forces measured by Kelvin probe force microscopy and frictional force microscopy, respectively [1]. Systematic density functional theory calculations of the different systems show that the change in work function is induced by the formation of a surface dipole moment while the friction force is dominated by adhesion forces.

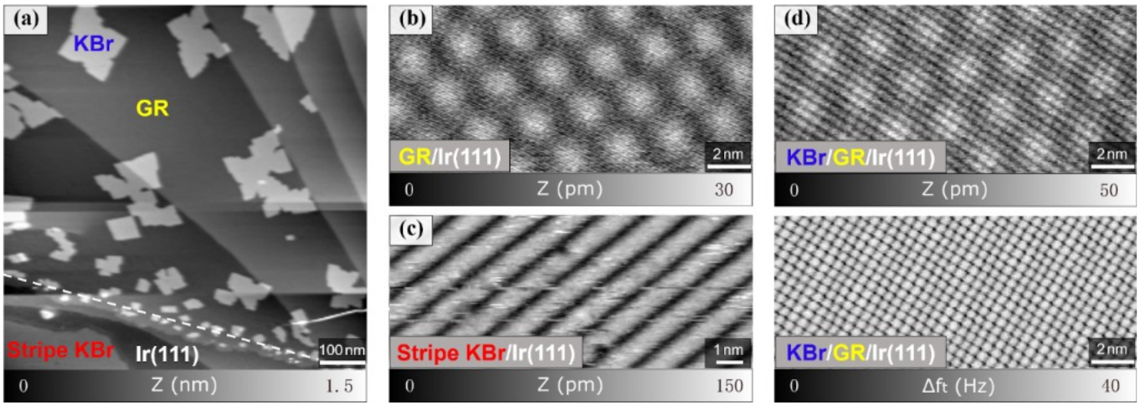

Figure 1: *Cubic KBr on the GR/Ir(111) surface. (a) Two different KBr structures have been discovered on GR/Ir(111) and bare Ir(111). (b) Single moiré pattern of GR/Ir(111) ($A_1 = 2nm$, $\Delta f_1 = -85Hz$, $\gamma = -70pN.nm^{1/2}$). (c) Corrugated KBr on bare Ir(111) with the stripe structure ($A_1 = 2nm$, $\Delta f_1 = -50Hz$, $\gamma = -41\ pN.nm^{1/2}$). (d) Multiple moiré pattern of GR/Ir(111) ($A_1 = 2nm$, $\Delta f_1 = -300Hz$, $\gamma = -247pN.nm^{1/2}$), with the torsional frequency shift Δf_t image below ($A_t = 30pm$) [2].*

[1] Z. Liu et al., Beilstein J. Nanotechnol. **12**, 432 (2021).
[2] Z. Liu et al., Nanomaterials **12**, 968 (2022).

Wednesday 09:40–10:00

Measurement of spatially resolved surface photovoltage on TiO_2(110) by ac bias KPFM

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Surface photovoltage (SPV) measurement [1,2] is a crucial way of investigating optoelectronic and photocatalytic semiconductors. The local SPV is generally measured by Kelvin probe force microscopy (KPFM) under dark and illumination consecutively, in which the thermal drift degrades the spatial and energy resolution. In this study, we present the ac bias Kelvin probe force microscopy (AC-KPFM) which operates an ac bias feedback to directly measure the local SPV except the influence of thermal drift, allowing the higher resolution (Figure 1a,b) [3].

We used a rutile TiO_2(110) sample to demonstrate the AC-KPFM for SPV measurement. AC-KPFM successfully resolved the inhomogeneous SPV distribution fluctuating in a few tens of nanometer and in a few millivolts scale (Figure 1c,d), while the classical KPFM has observed the homogeneous SPV distribution over the TiO_2 surface due to limited resolution [4].

AC-KPFM breaks the time barrier and can measure the faster SPV response by about 1-8 orders of magnitude rather than in classical KPFM which operates dc bias feedback. AC-KPFM is applicable to both amplitude modulation (AM) mode and frequency modulation (FM) mode, so it would contribute to the advancing SPV measurements in various environments such as in vacuum, air, and liquid.

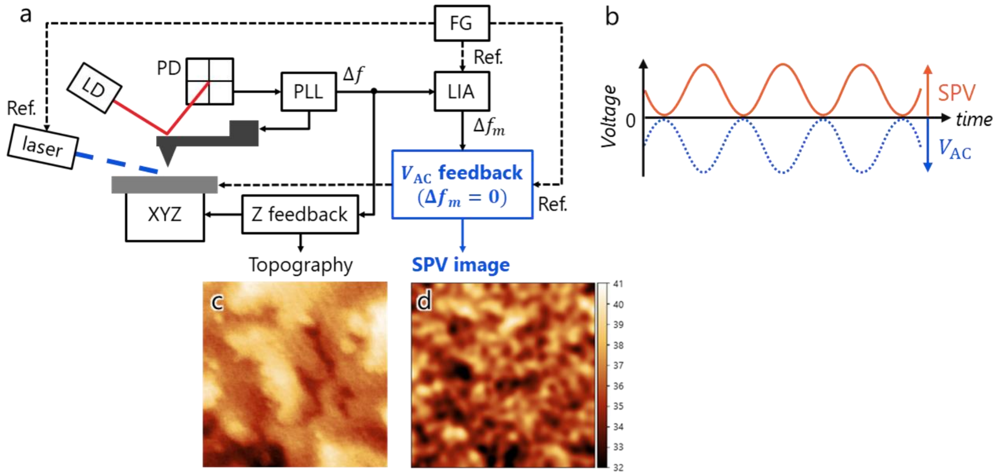

Figure 1: *Schematics of AC-KPFM for direct SPV measurement. (a) Block diagram of AC-KPFM. (b) Compensation scheme with ac bias feedback that nullifies the SPV. (c) Topographic and (d) SPV images of TiO_2(110) surface (200×200 nm^2).*

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[4] K. Emiko and T. Tatsuma, *Adv. Mater. Interfaces* **1**, 1400066 (2014)

Wednesday 10:00–10:20

Single-dopant band bending fluctuations in $MoSe_2$ measured with electrostatic force microscopy

Megan Cowie,[1,*] Rikke Plougmann,[2] Zeno Schumacher,[3] and Peter Grütter[1]

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For systems involving metallic samples and probes, the origin of the frequency shift in electrostatic force microscopy (including Kelvin probe force microscopy) is well-understood. However, in systems with semiconducting samples or probes, band bending effects must be considered. A complete understanding of the frequency shift origin must account for both the delocalized nature of the electrons contributing to band bending (i.e. the bias-dependent surface potential), as well as the spatially localized nature of the AFM probe.

In this work, we measured the bias-dependent surface potential of exfoliated multilayer $MoSe_2$ on SiO_2 with a metal-coated cantilevered probe using frequency-modulated atomic force microscopy in ultra-high vacuum. We also modelled this system as a 1D metal-insulator-semiconductor (MIS) capacitor. The modelled surface potential, force, and frequency shift are shown for two acceptor concentrations in Figure 1 in blue and green. Bias-dependent two-state fluctuations in the frequency shift, shown in Figure 1c in black, were measured. This two-state effect arises due to a change in global band bending as an electron moves into and out of an acceptor state. It is not due to a varying Coulomb potential of an electrically isolated state being occupied and unoccupied. Importantly, the amplitude of this random telegraph noise can be fully explained as being due to the bias-dependent surface potential, and does not depend specifically on the energy levels of the acceptor states themselves

Finally, we demonstrate that the bias-dependent fm-AFM excitation channel may be used to provide an order-of-magnitude estimate of band bending (i.e. charge reorganization) timescales for a conservative system. These timescales, which in this work are on the order of 30 ns, exhibit strong bias and spatial dependence.

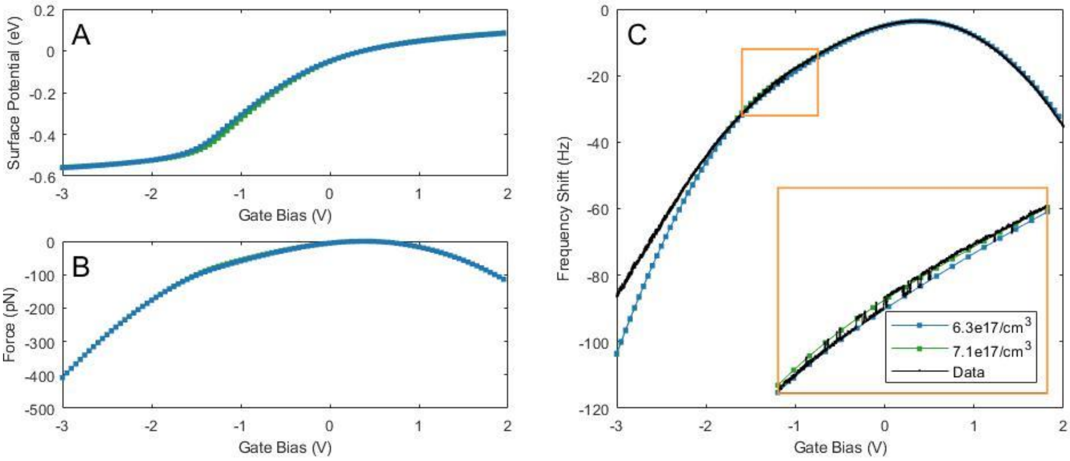

Figure 1: *a) Modelled bias dependence of the surface potential, b) force, and c) frequency shifts of an MIS capacitor for two ionized acceptor concentrations: 6.3e17/cm*^{3} *(blue) and 7.1e17/cm*^{3} *(green). Experimental fm-AFM results also shown in (c) (black). Inset: A zoom-in of the frequency shift (yellow rectangle) for which fluctuations in the data were observed.*

Wednesday 11:00–11:20

Molecular identification with AFM images and deep learning

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Recent advances in the interpretation of the contrast provided by AFM with CO-functionalized on porphycenes [1] and on self-assembled molecular layers driven by either halogen [2] or hydrogen bonds [3], shows that there are clear connections between fundamental chemical properties of the molecules and key features imprinted in AFM images. Inspired by these results, we address the problem of the complete identification (structure and composition) of molecular systems solely based on AFM images, without any prior information, exploiting deep learning (DL) techniques.

In a first step, we restrict ourselves to a small set of 60 flat molecules and demonstrate the automatic classification of AFM experimental images by a DL model trained essentially with a theoretically generated data set [4]. We analyze the limitations of two standard models for pattern recognition when applied to AFM image classification and develop a model with the optimal depth to provide accurate results and to retain the ability to generalize. We show that a variational autoencoder (VAE) provides a very efficient way to incorporate into the training set, from very few experimental images, characteristic features that assure a high accuracy in the classification of both theoretical and experimental images.

Learning from the successes and the limitations of this proof-of-concept, we have developed QUAM-AFM, the largest data set of simulated AFM images generated from a selection of 685,513 molecules that span the most relevant bonding structures and chemical species in organic chemistry [5]. QUAM-AFM contains, for each molecule, 24 3D image stacks, each consisting of constant-height images simulated for 10 tip–sample distances with a different combination of AFM operational parameters, resulting in a total of 165 million images. The data for each molecule includes, besides AFM images, ball-and-stick depictions, IUPAC names, chemical formulas, atomic coordinates, and map of atom heights. A graphical user interface allows the search for structures by CID number, IUPAC name, or chemical formula.

Using QUAM-AFM to train different deep learning models, we explore different alternatives to go beyond the classification of limited groups of molecules and achieve the complete identification of an arbitrarily complex, unknown molecule. Firstly, we frame the molecular identification as an image captioning problem and design an architecture, composed of two multimodal recurrent neural networks, capable of providing the IUPAC name of an unknown molecule using a 3D image stack as input [6]. Secondly, we use a Conditional Generative Adversarial Network (CGAN) to convert the 3D stack of AFM images into a ball--and--stick depiction, where balls of different color and size represent the chemical species and sticks represent the bonds, providing complete information on the structure and chemical composition [7]. Tests with a large set of theoretical images and few experimental examples demonstrate the accuracy and potential of the two approaches for molecular identification from AFM images.

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[2] J. Tschakert, et al., Nat. Commun. 11, 5630 (2020)
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Wednesday 11:20–11:40

Nanomanipulation & Dynamics of Single-Molecules at Surfaces

J.G. Vilhena[1,2], Remy Pawlak[2], Philipp D'Astolfo[2], Shi-Xia Liu[2], Silvio Decurtins[3], Thilo Glatzel[2], Alexis Baratoff [2], Ernst Meyer[2]

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Understanding the motion/dynamics of a single molecule over a surface is a problem of a paramount importance in designing advanced molecular nanostructures/assemblies capable of meeting specific needs[1,2,3]. The interest is better realized by the broad spectrum of promising applications including molecular electronic devices, tribology/corrosion inhibition, and 3D nanopatterning[4]. One possible route to achieve a higher control on molecular diffusion along predetermined pathways would be to access the single-molecule mechanics during their on-surface displacements[5]. This in turn would provide a mean to rationally design molecules with improved assembly/diffusion properties. Nevertheless, to date, understanding the interplay between molecule mechanics, surface displacements and dynamics at a atomic level is highly challenging as it requires knowing not only the forces needed to manipulate them but also to relate them with particular molecular/atomic motion.

Almost 20 years passed after the first scanning probe microscopy[6] atomic-manipulation until it became possible to record the time variations of mechanical forces during manipulation[7]. As this technique[7,8,11,12] – *cryo-force-spectroscopy* – relies on a dynamic AFM operated at 4.8K in Ultra-High-Vacuum it allow us to perform successive manipulations a in a clean and controlled environment but also enable us to characterize both the surface and the molecule with atomic resolution prior and after the manipulation. This breakthrough opened new and exciting possibilities to explore mechanical properties at a single molecule level with an unrepresented resolution and control over the system. In this talk I shall discuss some of the major achievement and the versatility of this technique including: the discovery of a state of almost vanishing friction of graphene nanoribbons when sliding over a gold surface[8,9,10]; measuring the stiffness of a single DNA nucleotide and the detection[11] of a C-C bond twist at a single bond level[12]. Altogether this provides a comprehensive understanding of complex on-surface dynamics of the molecules over surfaces and how dynamic balancing of intra-molecular mechanics and surface comensurability play out in a broad range of conditions.

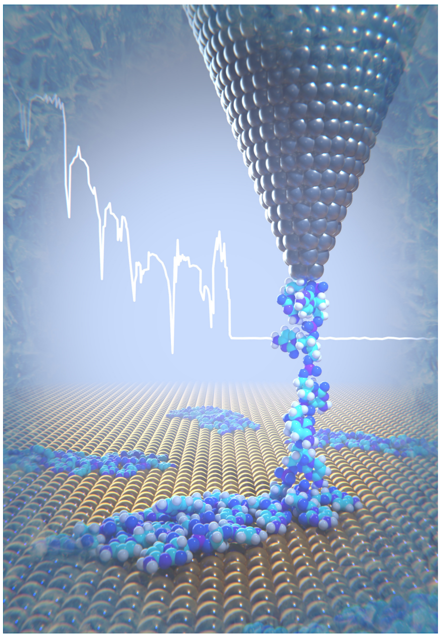

Figure 1*: Single molecule cryo-force spectroscopy: Lifting a single-stranded DNA molecule deposited over Au(111).*

References:
[1] Vanossi, A. et al. Rev. Mod. Phys. 85, 529 (2013).
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[12] J.G. Vilhena, R. Pawlak, et al. Accepted in PRL (2022)

Wednesday 11:40–12:00

Real-space imaging of σ-hole by means of Kelvin probe force microscopy.

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Anisotropic charge distributions on individual atoms, such as σ-holes, are crucial for the structural properties of certain systems. Nevertheless, the existence of σ-holes has only been demonstrated indirectly, either observing the interaction between halogenated molecules or by theoretical calculations.

We show that Kelvin probe force microscopy (KPFM) with a properly functionalized tip can provide a direct visualization of the anisotropic charge of the σ-hole (see Fig. 1), as well as the quadrupolar character of the carbon monoxide molecule. [1]

To assist the designing of the experiment and the posterior interpretation of the experimental data, we propose and implement a computational method to simulate the KPFM contrast at close tip-sample distances.

The KPFM contrast at macroscopic tip-sample distances is well understood as the difference between the work functions of tip and sample. On the other hand, at close tip sample distances we found the local contact potential difference (LCPD) to be given by an interplay of different interactions between intrinsic charges and polarizations on the tip-sample junction.

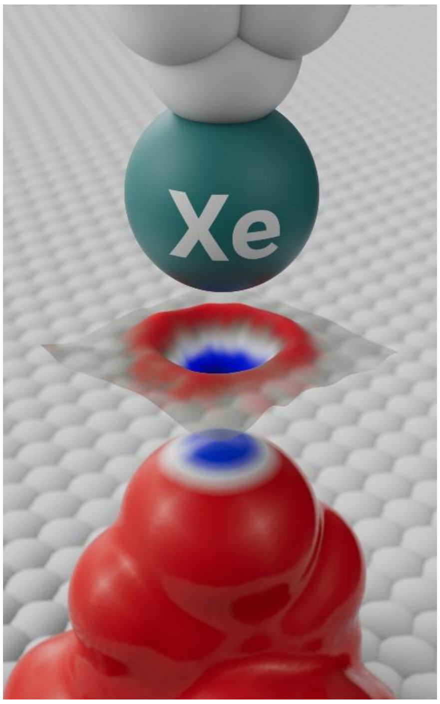

Figure 1: *Schematic description of the acquisition method of the σ-hole KPFM image.*

[1] B. Mallada, A. Gallardo, M. Lamanec, B. de la Torre, V.Špirko, P. Hobza and P. Jelinek, Real-space imaging of anisotropic charge of σ-hole by means of Kelvin probe force microscopy, Science **374**, 863–867 (2021).

Wednesday 12:00–12:20

Measuring the change in reactivity of a single molecule: Does The Bottom Effect The Top?

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Decades of surface science studies on adsorbed molecules have shown the surface a molecule is adsorbed on can affect the molecule's electronic and geometric structure [1]. However, the change in reactivity of a single molecule induced by the presence of a surface has not been rigorously investigated. The influence of molecule-substrate bonding on the interactions experienced by a scanning probe microscope (SPM) tip was investigated by studying C_{60} molecules adsorbed on the Cu(111) surface, using simultaneous non-contact atomic force microscopy (NC-AFM) and scanning tunnelling microscopy (STM). C_{60} can form distinctly different structures when adsorbed on the Cu(111) surface [2][3], two of which were utilized in this work. In the first structure, the Cu(111) surface remains relatively unperturbed. In the second, the presence of the C_{60} induces a reconstruction of the underlying Cu(111) surface, with the C_{60} molecules occupying a 7 atom vacancy. Despite this, both configurations adopt a (4x4) periodicity. This provides an ideal system to probe the effect the molecule-substrate bonding has on the physico-chemical properties of the molecule. As the molecules adsorb in the same orientation in both structures, any difference in the interaction between the SPM tip and the C_{60} molecules can be attributed to differences in the molecule-substrate bonding [2][4][5][6].

In this work, the physico-chemical properties of C_{60} molecules (in different adsorption structures) were investigated using NC-AFM force spectroscopy, through comparing the minima in collected force spectra. Complementary ab initio simulations of the spectra were also performed in DFT to gain a deeper understanding of the experimental results.

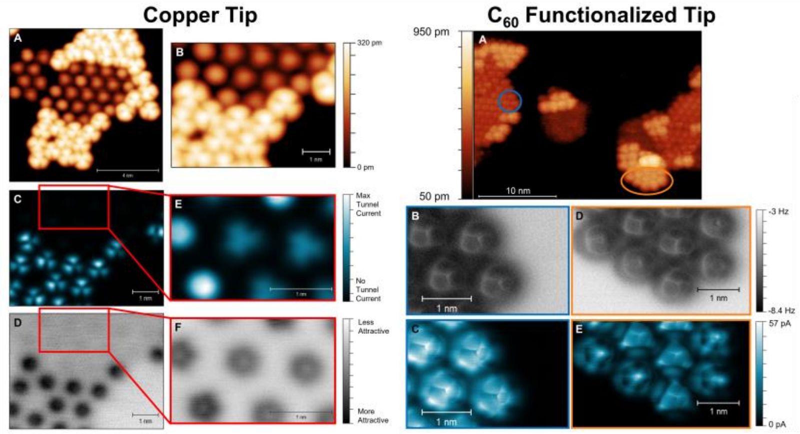

Figure 1: *Constant current STM images (black and orange), and simultaneous constant height AFM (greyscale) and tunnel current images (black and blue) taken over of islands of C_{60} on the Cu(111) surface with Cu and C_{60} tips.*

[1] L. Gross, F. Mohn, N. Moll, P. Liljeroth, and G. Meyer, Science 325, 1110 (2009).
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Wednesday 14:00–14:20

The importance of the dipole at the metal tip apex when approaching closer with a CO tip

Shinjae Nam, Oliver Gretz, Thomas Holzmann, Franz J. Giessibl and Alfred J. Weymouth

By functionalizing the tip with a single CO molecule, the spatial resolution of atomic force microscopy (AFM) can be drastically increased. Much of the contrast in AFM images has been explained by a flexible CO at the tip apex and an empirical description (e.g. Morse, Lennard-Jones) of the interaction between the CO and the surface atoms. Although Pauli repulsion plays a dominant role at very close distance, reports have indicated that additional phenomena (e.g. the electrostatic field [1], total charge density [2]) are also relevant to understand the AFM signal.

Here, we use Lateral Force Microscopy employing qPlus sensors that are tilted by 90° such that the tip oscillates parallel to the surface to quantify the short-range interaction between a CO tip and a CO on the Cu (111) surface [3]. Previously we studied this system by scanning an area centered over the CO on the sample down to tip heights at which the surface CO laterally moved. In this study, we offset the scan area laterally with respect to the CO molecule, allowing to come closer to the surface.

Interestingly, an additional dip appears for these very close distances which cannot be explained with CO relaxation and a Morse potential. Following the results of other investigations, we include the electrostatic force in our simulations. We modeled our tip as a quadrupole, including a dipole at both the metal tip and on the CO molecules [4]. Our model matches the experimental result when assuming a negative charge at the apex of the CO on the surface. The dipole of the metal apex of the tip (i.e. with the positive charge pointing towards the surface) is the reason we see this additional dip and becomes a much greater influence as we approach closer to the surface.

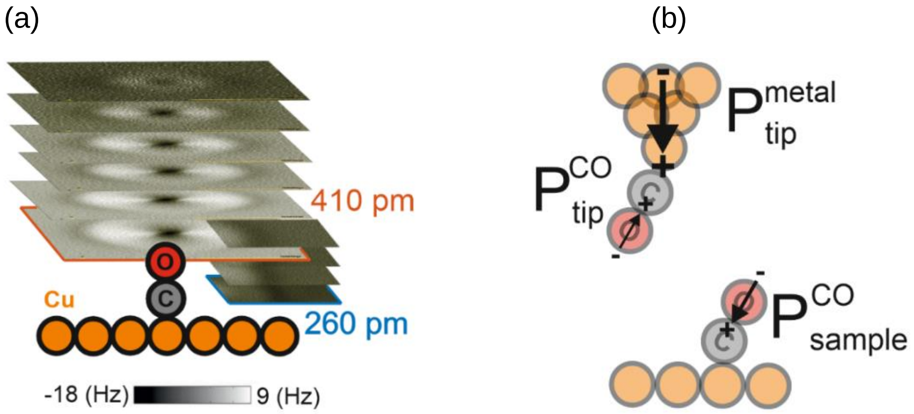

Figure 1. *(a) Full slices above the CO molecule can be acquired down to a position marked by orange. Then, to avoid the CO moving, we acquire data at one side down to a lower point, indicated by the blue outline. (b) The schematic figure of the calculated model. The tip is modeled as a quadrupole, including the metal tip apex and the CO on it. The best agreement with the data came from a CO on the surface with a negative charge at the apex.*

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Wednesday 14:20–14:40

Energy dissipation on twisted bilayer graphene at magic angle twist

A. Ollier[1], M. Kisiel[1], U. Gysin[1], E. Tosatti[2] and E. Meyer[1]

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Understanding nanoscale energy dissipation is nowadays among few priorities particularly in quantum systems. Whilst traditional Joule dissipation omnipresent in today's electronic devices is well understood, the energy loss of the strongly interacting electron systems remains largely unexplored. Twisted bilayer graphene (tBLG) is a host of interaction-driven correlated insulating phases, when the relative rotation is close to the magic angle (1.08^{o}).

Here, we report on low temperature (5 K) nanomechanical energy dissipation of tBLG measured by sharp tip of the pendulum atomic force microscope (pAFM). Ultrasensitive cantilever tip acting as oscillating plunger gate over the quantum device showed giant dissipation peaks attributed to different fractional filling of the flat energy bands. Dissipation spectroscopy allows to determine the twist angle distribution of tBLG. Thus, nanomechanical energy dissipation provides a rich source of information on the dissipative nature of the correlated electronic system of tBLG, with implications for coupling a mechanical oscillator to the quantum devices. Application of magnetic fields provoked strong oscillations of the force and dissipation signal which is strongly enhanced for fractional 3/4 band filling.

Wednesday 14:40–15:00

Superlubric sliding in atomic friction in the case of molybdenum disulfide on gold

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[2] International School for Advanced Studies (SISSA), 34136 Trieste, Italy
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Molybdenum disulfide (MoS2), a single layer of Mo atoms sandwiched in between two layers of S atoms, shows a wide range of potential applications in the fields of electronics, optoelectronics and micro and nanomechanical systems requiring ultralow friction[1,2]. The structural and superlubric properties of single layer MoS_2 on Au(111) forming moiré structures have been investigated by means of ultrahigh vacuum atomic force microscopy with bimodal and contact modes. Monolayer MoS_2 flakes was grown on an Au(111) surface under ultrahigh vacuum having a hexagonal superstructure of patches with ~45 pm corrugation and about ~3.3 nm periodicity. Friction force microscopy measurements at the atomic scale indicate a superlubric regime between the tip apex and the MoS_2 surface in which the friction force remains at an ultralow value and is independent from normal load. Superlubricity conditions are observed for different loads which indicates the absence of out-of-plane deformations. We do find that the MoS_2 layer including the moiré superlattice modulation originating from the natural misfit between MoS_2 and the Au(111) substrate is relatively rigid. We also demonstrate a nonmonotonic frictional speed dependence of the MoS_2 surface induced by multi-slip effect. Our results open up a new avenue for minimizing friction in nanoscale electronic devices and other dry rigid contacts used in aerospace lubrication.

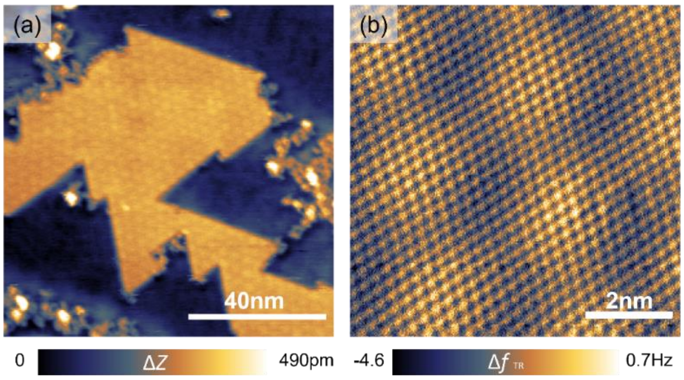

Figure 1: Use (a) 100 nm × 100 nm topographic nc-AFM image of a single layer MoS_2 flake. (b) High-resolution image showing the moiré and the atomic structure of the MoS_2 islands in the torsional frequency shift Δf_{TR} recorded in bimodal AFM. Parameters: (a) Δf_{1st} = -10 Hz, A_{1st} = 2.5nm, (b) Δf_{2nd} = -100 Hz, A_{2nd} = 800 pm, A_{TR} = 80 pm.

[1] A. K. Geim, et al., Nature 499, 419–425 (2013)
[2] O. Hod, et al., Nature 563, 485–492 (2018)

Wednesday 16:00–16:20

Tuning Halogen Bond Directed Self-Assembly: Substrate Snapping vs Intermolecular Interactions

Alexander Ihle[1,4,*], Daniel Martin Jimenez[1,4], Sebastian Ahles[2], Doreen Mollenhauer[2,4], Hermann A. Wegner[3,4], Andre Schirmeisen[1,4] and Daniel Ebeling[1,4]

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[2] Institute of Physical Chemistry, Justus Liebig University Giessen, Germany
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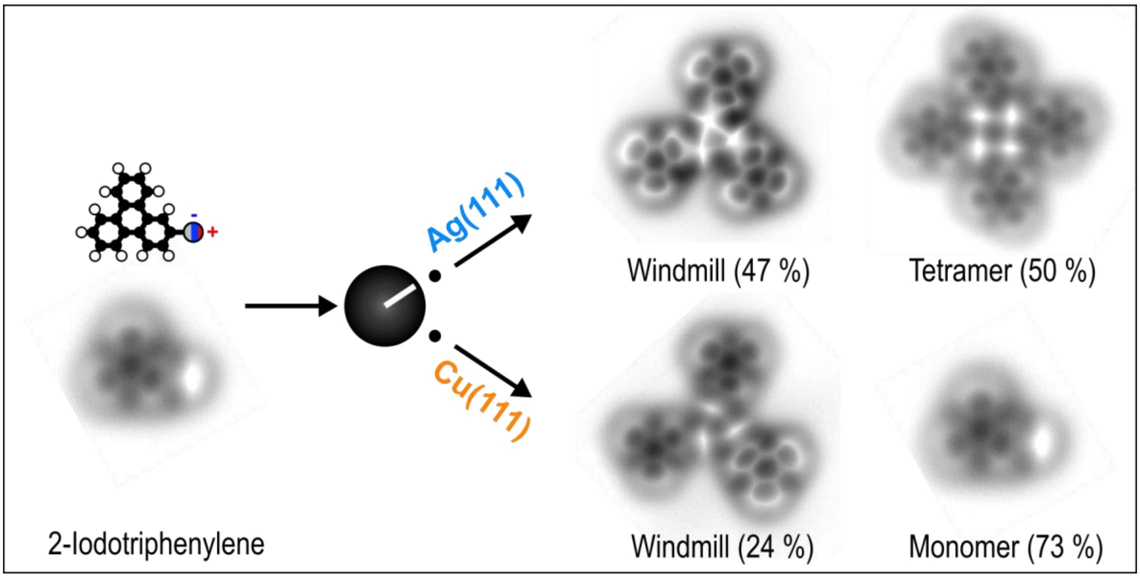
Intermolecular halogen bonds are interesting for applications in supramolecular chemistry, crystal engineering, drug design, or catalysis because of their strong directionality and tunability. The self-assembly processes of halogenated molecules on surfaces are still not well understood since the bond lengths, bond angles and adsorption positions cannot be determined precisely enough with conventional scanning tunneling microscopy. Here, we use the bond imaging technique, namely low temperature atomic force microscopy with CO functionalized tips, to study the self-assembly process of 2-iodotriphenylene on Cu(111) and Ag(111). We recently observed that the surface material strongly influences the selectivity of intermolecular halogen bonds. [1] Here, we found that also the bonding configuration is tunable via the substrate material (see Scheme 1). On Cu(111) we mostly find molecular monomers and clusters with threefold symmetry (windmill type). On Ag(111), however, we find clusters with threefold and fourfold symmetry. The bond imaging technique allows to precisely determine the orientations and adsorption positions of the individual molecules on the different substrates, which gives useful insight into the mechanisms of the assembly process and the nature of intermolecular halogen bonds.



Scheme 1: Tuning the bonding configuration of halogen bond directed assemblies via the surface material.

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

Wednesday 16:20–16:40

Identifying CO_2 adsorption defects on Au surfaces with HR-AFM and STM

Emiliano Ventura-Macias,[1] Oscar Custance,[2] Oleksandr Stetsovych,[2,3] Tomoko K. Shimizu,[2] Pablo Pou,[1,4] Shigeki Kawai,[2] Ruben Perez* [1,4]

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CO_2 adsorption is a key mechanism for current and future carbon capture technologies. Metal-organic frameworks are relevant for them as their presence on metal surfaces can significantly enhance CO_2adsorption and packing. In particular, 1,4-phenylene diisocyanid (PDI) chains on Au(111) allow CO_2 to assemble between these chains in a herringbone pattern that is often broken by lines of defects surrounded by a hexagonal arrangement of CO_2 molecules [1]. These hexagonal defects also appeared in free-standing CO_2 islands, where different structural patterns are observed, an precise characterization may give clues about the formation of these structures.

Using measurements from an AFM/STM system with a CO-functionalized tip, combined with theoretical simulations of AFM [2,3] and STM images –where the effect of the CO relaxation is included [4]– , we determined the nature of these defects. The basic hexagonal arrangement was found to be a windmill structure. It is formed by at least three subunits of three molecules arranged in a triangle (Fig. 1). Moreover, we identified a rich variety of windmill structures that enclosed different chemical species, giving rise to very complex STM and AFM contrast: (1) a gold adatom that appears as a void in AFM, but it clearly shows in STM. (2) a vertical CO molecule that appears as a very defined spot in AFM and as a blur in STM. (3) and a vertical CO2 molecule that shows when the tip is far but disappears when it approaches.

The disappearance of the vertical CO_2 while approaching the tip posed a significant problem for understanding both AFM and STM contrast. DFT calculations showed that the molecule protrudes from the CO_2 layer by around 1 Å and that the CO on the tip is very flexible compared to the vertical molecule. The difference in flexibility deflects the apex of the tip further away from the surface and results in a smaller measurement than expected from the topography of the defect.

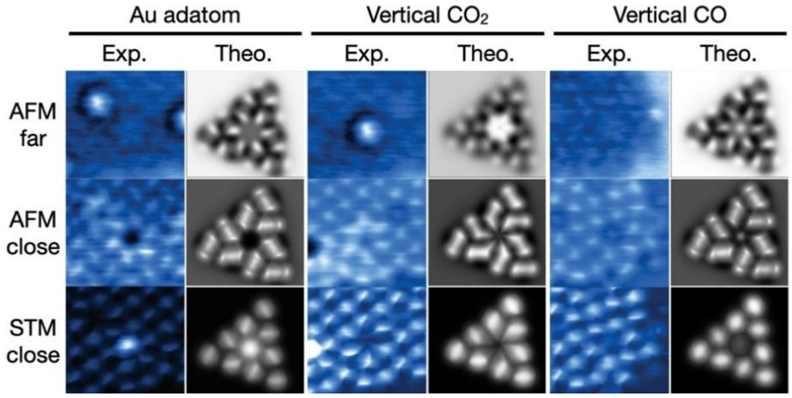

Figure 1: *Comparison of experimental and theoretical images of windmill-type defects.*

[1] M. Feng, et al. ACS Nano **9 12**, 12124–12136 (2015)
[2] M. Ellner, P. Pou, R. Perez, ACS Nano **13 1**, 786–795 (2019).
[3] P. Zahl, et al., Nanoscale 13, 18473 (2021).
[4] E. Ventura-Macias, et al., (2022) submitted.

Wednesday 16:40–17:00

[4+4] Photodimerization of Triptycene Derivatives with Anthracene Blades on Ionic Crystals

Elie Geagea,[1] Franck Para,[1] Laurent Nony, [1] Sylvain Clair,[1] and **Christian Loppacher**; [1*]
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Iptycenes are highly stable compounds with three-dimensional aromatic structures. Derivatives with extended anthracene blades have successfully been self-assembled and subsequently photodimerized both at the air/water interface [1] as well as on various substrates.[2] On metal substrates it has been shown that reducing the molecule-substrate interaction by iodine-passivation of the Au(111) surface is promoting the formation of large and highly-organized layers with a photopolymerizable arrangement.[3]

In this work, we present the self-assembly of three-fold anthracene-triptycene derivatives without (antrip) and with peripheral fluorine substitution (fantrip) on ionic crystal surfaces. The extended anthracene blades enhance the stability of the supramolecular structures and favor a self-assembly in which all anthracene blades of each monomer are stacked face-to-face. This organization is essential to facilitate the subsequent lateral polymerization by intermolecular [4+4] photocycloadditions. Our results show, that on ionic crystals, both the molecule-substrate and molecule-molecule interaction must be enhanced. This is attained by peripheral fluorine substitution, which increases attractive electrostatic interactions. Figure 1 shows the photopolymerized monolayers on a KBr substrate after light-induced dimerization and subsequent annealing. We discuss, how the deposition and illumination parameters as well as the used ionic substrate can be adapted to optimize the structure quality of the on-surface photo-polymerized 2D polymer.

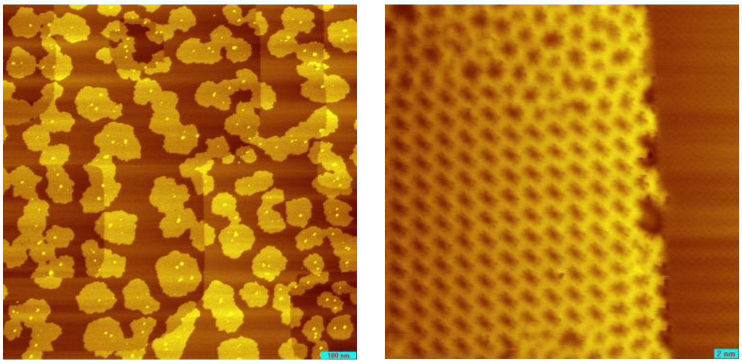

Figure 1: *Left: 1µm size nc-AFM topography image of 0.5 monolayers of fantrip deposited onto KBr with simultaneous illumination; polymerized domains with 0.7 nm apparent height are formed. Right: 20 nm size nc-AFM image showing the polymerized network with different local organization as well as the KBr substrate (right margin, upper terrace).*

[1] D.J. Murray *et al.*, J. Am. Chem. Soc. **137**, 3450 (2015), https://doi.org/10.1021/ja512018j
[2] Grossmann *et al.*, Nat. Chem. 13, 730–736 (2021), https://doi.org/10.1038/s41557-021-00709-y
[3] L. Grossmann *et al.*, Angew. Chem. Int. Ed. e202201044 (2022), https://doi.org/10.1002/anie.202201044

Wednesday 17:00–17:20

JT-SPM study of electron acceptor molecules on Ag(111)

Chao Li,[1] Rémy Pawlak,[1] Jung-Ching Liu,[1] Outhmane Chahib,[1] Thilo Glatzel,[1] Ping Zhou,[2] Silvio Decurtins,[2] Shi-Xia Liu,[2] Ernst Meyer[1,*]

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We investigated the Tetra-bromopyrimido perimidine (TBTP) molecules on Ag(111) using our latest JT-SPM installation. Close-packed arrays with orientational disorder of TBTP molecules were determined by high-resolution nc-AFM imaging with CO-tips. Tunnelling conductance spectra show TBTP molecules were negatively charged at equilibrium conditions (without bias) and can be discharged with positive bias voltages.[1] dI/dV mapping images of the discharging peaks at positive bias voltage show the Coulomb blockade rings in real space.[2] In addition, the ion resonance peaks are split into several satellite peaks due to electron-vibration coupling.[3] According to our measurements, JT-SPM is capable of working at submolecular resolution and generating high-quality tunnelling conduction spectra.

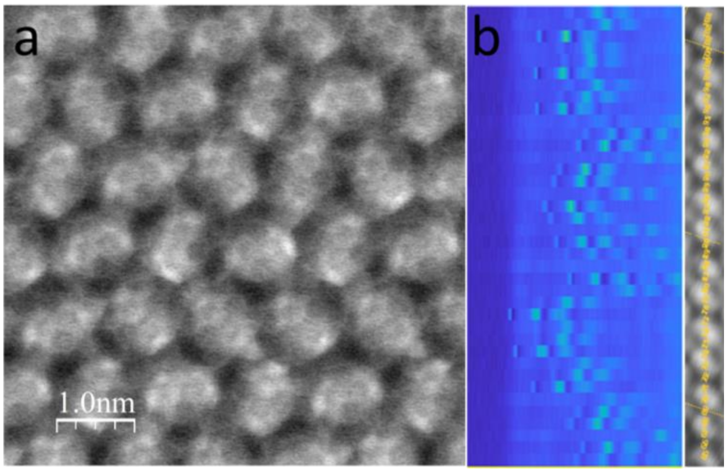

Figure 1: (a) nc-AFM image of TBTP molecules on Ag(111). (b) Spectra maps of dI/dV between 0 to 1.5 V along the molecular chains show the ion resonance peaks distributed in molecules.

[1] Gonzalez-Lakunza, N., Fernández-Torrente, I., Franke, K., Lorente, N., Arnau, A., Pascual, J. I. *Phys. Rev. Lett.* **100**, 156805 (2008).
[2] Fernández-Torrente, I.; Kreikemeyer-Lorenzo, D.; Stróżecka, A.; Franke, K. J.; Pascual, J. I. *Phys. Rev. Lett* **108**, 036801 (2012).
[3] Repp, J.; Liljeroth, P.; Meyer, G. *Nat. Phys.* **6**, 975–979 (2010).

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Thursday, August 4th 2022

Oxide surfaces

Chair: Setvín, M.

09:00 **Wrana, D.** *Ferroelectricity on oxide perovskite surfaces.*

09:20 **Sokolović, I.** *Charge trapping on a truly bulk-terminated* $SrTiO_3$*(001).*

09:40 **Heggemann, J.** *The (2×1) reconstruction of calcite(104).*

10:00 **Li, Y.-J.** *CO oxidation on Au adatom on oxidized rutile* TiO_2 *surface.*

2D materials

Chair: Temirov, R.

11:00 **Telychko, M.** *Sub-angstrom noninvasive imaging of atomic arrangement in 2D hybrid perovskites.*

11:20 **Gou, J.** *Observation of monoelemental ferroelectrics by scanning probe microscopy.*

11:40 **Behn, W.** *Tuning and measuring the potential landscape in 2D materials.*

12:00 **Spiegelberg, J.** *Spatially Resolved Nonlinear Optical Response in 2D* WS_2*.*

Thursday 09:00–09:20

Ferroelectricity on oxide perovskite surfaces

Dominik Wrana[1,*], Igor Sokolović[2], Jesus Redondo[1], Pavel Kocán[1], Aji Alexander[1],
Llorenç Albons[1], Martin Setvin[1,2]

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In many bulk materials transition to the ferroelectric phase can be triggered by the ion displacement from its equilibrium position in the matrix. For example, in barium titanate, $BaTiO_3$, the Ti^{4+} ion rests in a double-well potential landscape, resulting in a switchable polarization [1]. If this potential barrier in a well is low, which is in the case of potassium tantalate, $KTaO_3$, ferroelectric state can be reached by the application of a small stimuli, e.g. stress, doping or external fields, causing the material to be incipient-ferroelectric (quantum paraelectric).

In this talk, I will present the similarities and differences between two representative perovskite oxide surfaces – $KTaO_3$(100) and $BaTiO_3$(100), showcasing the manifestation of the (incipient-) ferroelectricity on the atomic and electronic structure. Both surfaces were prepared by cleaving single crystals *in situ* and characterized by means of qPlus nc-AFM at temperatures ranging from 4K to 100K.

$BaTiO_3$(100), a model ferroelectric perovskite, cooled down to 4K adopts a rhombohedral crystal structure, where titanium atoms can easily break a symmetry causing a spontaneous polarization. I will present that a biased tip placed a few nanometers above the surface allows for reversible manipulation of individual atoms on the surface, writing and erasing polarized ferroelectric domains (as demonstrated in Fig. 1a,b).

For a similar experimental conditions, incipient-ferroelectric $KTaO_3$ remain paraelectric, hence tip-induced electric fields influence it via different mechanisms. Excess charges injected from the AFM tip form quasiparticles called polarons (charges coupled with lattice distortions) which can be further shaped into 1D or 2D structures by intrinsic surface electric fields, emerging from two alternating domains of KO and TaO_2, developed to compensate the surface polarity [2]. Careful analysis of the frequency shift signal enables tracing single injections (Fig. 1c inset), whereas Kelvin Probe Force Microscopy mapping reveals the 1D or 2D shape of charged domains (Fig. 1c).

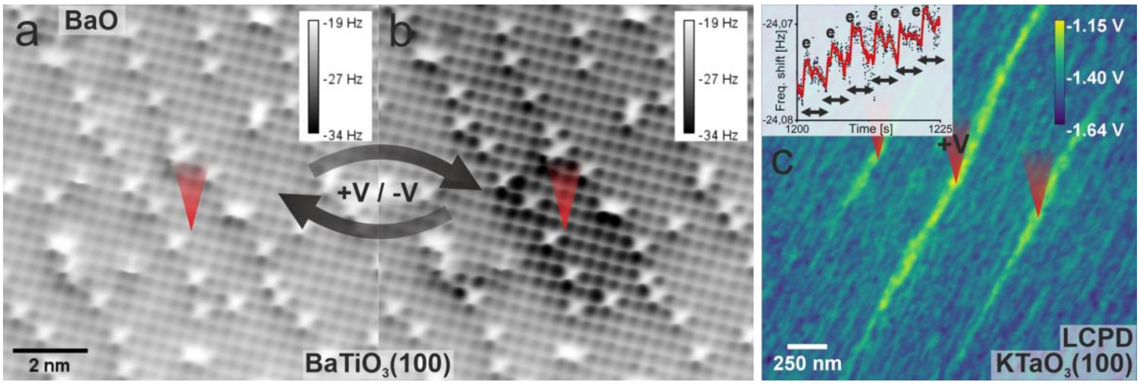

Figure 1: *Nanoscale characterization of (incipient-)ferroelectricity. a,b) Reversible manipulation of atomic displacements on $BaTiO_3$(100), c) Injecting single electrons (inset) to form 1D polaronic domains on $KTaO_3$(100).*

[1] H. Kwei, A. C. Lawson, S. Cheong and S. Billinge, J. Phys. Chem. **97**, 2368-2377 (1993).
[2] M. Setvin, M. Reticcioli, …, and U. Diebold, Science, **359(6375)**, 572-575 (2018).

Thursday 09:20–09:40

Charge trapping on a truly bulk-terminated $SrTiO_3(001)$

Igor Sokolović[1]**,** Dominik Wrana[2] ,Florian Ellinger[3] , Michele Reticcioli[3], Michael Schmid[1],
Cesare Franchini[3], Ulrike Diebold[1], Martin Setvín[1,2]*

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[2] Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic
[3] Faculty of Physics and Center for Computational Materials Science, University of Vienna, Vienna, Austria

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$SrTiO_3$ attracts significant attention in the last two decades as a model cubic pervoskite oxide, particularly since the discovery of the two-dimensional electron gas appearing on the (001) surface of this otherwise wide-band gap semiconducting solid. We derived a method for obtaining truly-bulk terminated $SrTiO_3(001)$ surfaces *in situ* [1], by exploiting the incipient ferroelectric character of the bulk [2]. Besides coming the closest to the pristine surface [3], the cleaved $SrTiO_3(001)$ surfaces exhibit a series of interesting phenomena due to the symmetry breaking during cleaving.

In this talk, I will demonstrate that the cleaved $SrTiO_3(001)$ surface can accommodate electron-hole separation, a process forbidden by its inversion symmetry [4]. Following UV irradiation, both, the Nb-doped and the nominally undoped $SrTiO_3$ accumulate positive charges on the cleaved (001) surfaces, indicated by Kelvin probe force microscopy. The charging proceeds through the formation of hole polarons on the O 2p orbitals, as corroborated by DFT. The lifetime of the trapped charges is exceptionally long, measuring in days, at both LHe and LN_2 temperatures. The trapped holes can be easily annihilated by injecting electrons from the tip. On Nb-doped $SrTiO_3$ (Fig. 1a) the injected electrons annihilate holes highly locally, while on the undoped $SrTiO_3$ (Fig. 1b) the injected electrons discharge the surface even several micrometers away in a highly anisotropic manner from the point of injection. Single hole discharging events were observed (positions marked with “1” and “2” in Fig. 1a), while STS recorded the changes to the electronic structure. Atomically-resolved imaging with an O-terminated tip confirms no structural changes following the charge accumulation and dissipation.

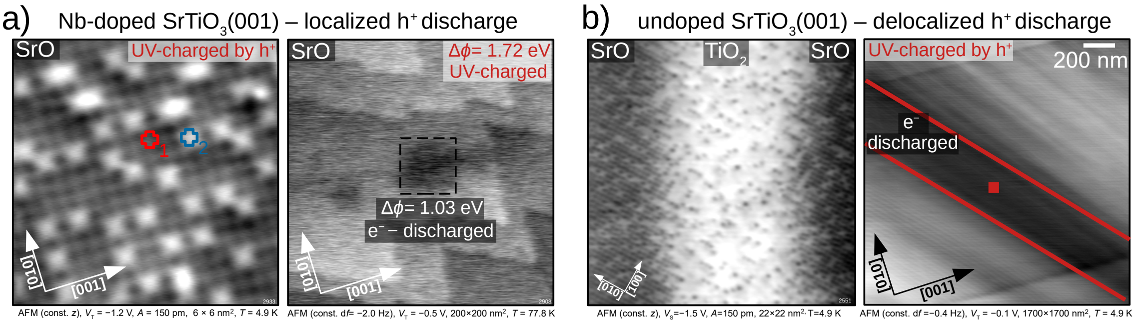

***Figure 1:** Charging via UV light and discharging via electron injection on the bulk-truncated (001) surfaces of a) Nb-doped and b) undoped* $SrTiO_3$*.*

[1] I. Sokolović, M. Schmid, U. Diebold, and M. Setvín, Phys. Rev. Mater. **3**, 034407 (2019).
[2] K. A. Müller and H. Burkard, PRB **19**, 3593 (1979).
[3] I. Sokolović, G. Franceschi, Z. Wang, J. Xu, J. Pavelec, M. Riva, M. Schmid, U. Diebold, and M. Setvín, PRB **103**, L241406 (2021).
[4] M. M. Yang, D. J. Kim, and M. Alexe, Science **360**, 904 (2018).

Thursday 09:40–10:00

The (2×1) reconstruction of calcite(104)

Jonas Heggemann,[1,*] Yashasvi Ranawat,[2] Ondřej Krejčí [2], Adam S. Foster,[2] Philipp Rahe,[1]

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Calcite, the most stable polymorph of calcium carbonate ($CaCO_3$), is an abundant material in the Earth's crust, a central constituent of biominerals in living organisms [1], and currently investigated as a capture material for CO_2 to offset greenhouse emissions [2]. However, and despite intensive studies of the pristine and hydrated calcite(104) surfaces, there is still serious ambiguity regarding the properties of this surface: effects such as a row-pairing [3] or a (2×1) reconstruction [4] have been reported, yet so far with conflictive conclusions and without a structural explanation.

Here, we use a combination of non-contact atomic force microcopy (NC-AFM) with CO-functionalized tips at 5K, density functional theory calculations with state-of-the-art dispersion corrections, and NC-AFM image simulations to clarify the microscopic geometry of the calcite(104) surface. A (2×1) reconstruction is consistently found in the experimental data and DFT calculations (see panel (a)), expressed by an alternating row structure (see panel (b,c)) with a rotation of every second carbonate group. Most importantly, we find that two different adsorption positions are generated for CO molecules within the (2×1) unit cell. Furthermore, we develop an algorithmic symmetry test to assess the symmetry properties of the surface. When using symmetric tips, excellent agreement is found with an assignment of calcite(104) to the planar space group *pg*, thus rendering the row-pairing to be a tip artefact. Last, it is found that the calcite surface bequeaths its glide plane symmetry to CO molecules as a glide plane related counterpart is found for each adsorbed species (see panel (d)).

In conclusion, our study confirms the presence and determines the microscopic geometry of the (2×1) reconstruction of calcite(104) and assigns the surface to the planar space group *pg*. These findings are most critical for future studies where physical, chemical or geological processes on calcite(104)–(2×1) are influenced by the surface geometry.

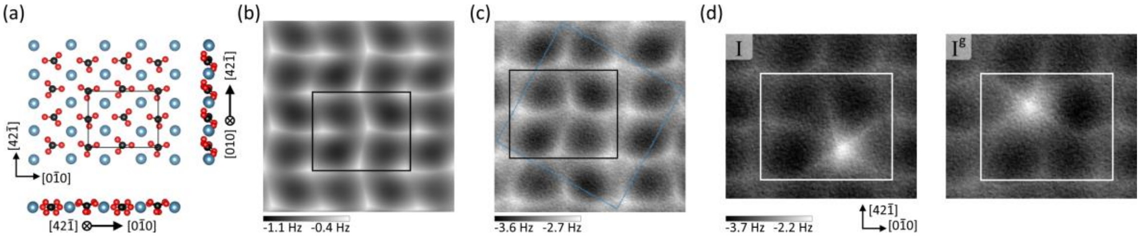

Figure 1: *(a) DFT-derived geometry of the calcite(104)-(2×1) surface (top-layer shown). (b) Simulated and (c) experimental NC-AFM data calculated for or acquired with a CO tip at 5K. (d) Identical CO adsorption positions related by the glide plane symmetry imaged by a CO terminated tip. The black and white rectangles indicate (2×1) unit cells at equivalent positions.*

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Thursday 10:00–10:20

CO oxidation on Au adatom on oxidized rutile TiO_2 surface

Yuuki Adachi,[1] Ján Brndiar,[2] Martin Konôpka,[2] Robert Turanský,[2] Yasuhiro Sugawara,[1] Lev Kantorovich,[3]* Ivan Štich,[2]* and **Yan Jun Li**[1]*

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Single-atom catalysis of CO oxidation on metal-oxide surfaces is of paramount importance for greenhouse recycling, automotive catalysis, and beyond, but the atomic-scale mechanism is still missing. Here, using scanning probe microscopy techniques, Fig. 1, we show that charging single Au atoms (Au_1) on oxidized rutile TiO_2 surface, both positively and negatively, considerably promotes adsorption of CO. Two different CO adsorption geometries (bean/donut image, see Fig.1) on Au atoms are identified. We demonstrate a full control over the redox state of adsorbed Au single atoms, the CO adsorption geometry and CO adsorption/desorption by the AFM tip. On charged Au atoms, we activate Eley–Rideal oxidation reaction between CO and a neighboring oxygen adatom by the tip. Our results suggest that the Au dual activity for CO oxidation after is the key ingredient also in photocatalysis under realistic conditions.

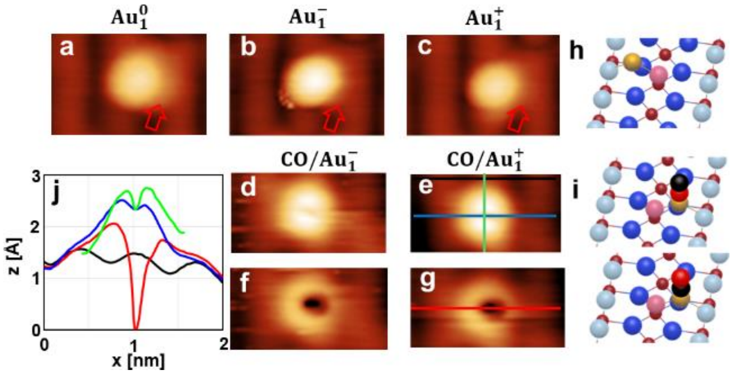

***Figure 1**: Atomic-scale CO adsorption on the Au_1/O-rutile TiO_2 (110) surface. AFM images of Au_1, **a**-**c**, and of CO/Au_1, **d**-**g**. O_{ad} on top of which Au_1 adsorbs asymmetrically is indicated by the red arrows in **a**-**c**. **h, i,** Schematic models of Au_1 and of CO/Au_1, respectively. **j**, Line scans over CO/ Au_1^+ in both bean (green and blue lines) and donut (red line) adsorption geometries as indicated in panels **e** and **g**, respectively. The black line corresponds to the underlying surface.*

[1] Y. Adachi, J. Brndiar, M. Konôpka, R. Turanský, Y. Sugawara, L. Kantorovich, I. Štich, and Y.J. Li, submitted (2022).

Thursday 11:00–11:20

Sub-Ångstrom noninvasive imaging of atomic arrangement in 2D hybrid perovskites

Mykola Telychko,[1] Shayan Edalatmanesh,[2,3] Kai Leng,[4] Ibrahim Abdelwahab,[1,5] Na Guo,[6]
Chun Zhang,[6] Jesús I. Mendieta-Moreno,[2] Matyas Nachtigall,[2] Jing Li,[5] Kian Ping Loh,[1,*]
Pavel Jelínek, [2,3]* Jiong Lu[1,5]*

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[5] Centre for Advanced 2D Materials (CA2DM), National University of Singapore, Singapore.
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Non-invasive imaging of the atomic arrangement in two-dimensional (2D) Ruddlesden-Popper hybrid perovskites (RPPs) is challenging because of the insulating nature and softness of the organic layers. Here, we demonstrate a sub-angstrom resolution imaging of both soft organic layers and inorganic framework in a prototypical 2D lead-halide RPP crystal via combined tip-functionalized scanning tunneling microscopy (STM) and noncontact atomic force microscopy (ncAFM) corroborated by theoretical simulations [1]. STM measurements unveil the atomic reconstruction of the inorganic lead-halide lattice and overall twin-domain composition of the RPP crystal, while ncAFM measurements with a CO-tip enable nonperturbative visualization of the cooperative reordering of surface organic cations driven by their hydrogen bonding interactions with the inorganic lattice. Moreover, such a joint technique also allows for the atomic-scale imaging of the electrostatic potential variation across the twin-domain walls, revealing alternating quasi-1D electron and hole channels at neighbouring twin boundaries, which may influence in-plane exciton transport and dissociation.

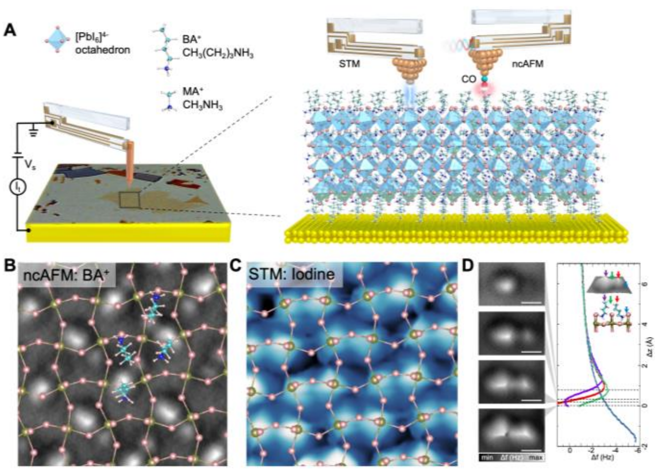

Figure 1: *(A) Schematics showing a combined STM and ncAFM imaging of the RPP surface using a tuning fork–based qPlus sensor. (B) ncAFM image and (C) STM image collected over the same surface area. D) $\Delta f(\Delta z)$ curves acquired over the sites marked by color-coded arrows in the experimental 3D-rendered ncAFM image in the inset (top) and side view of the butylammonium pair structure in the (inset bottom).*

[1] M. Telychko *et al*., *Science Advances.* **8**, eabj0395 (2022)

Thursday 11:20–11:40

Observation of monoelemental ferroelectrics by scanning probe microscopy

Jian Gou[1,*], Chao Yang[2], Lan Chen[3], Ariando Ariando[1], Wei Chen[1], Yunhao Lu[2,*], Andrew Thye Shen Wee[1,*]

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Ferroelectrics are well known for the applications on the non-volatile memories and electric sensors, and recently have been extended to the areas of renewable energy harvesting and neuromorphic computing. Though vast progresses have been made on the two-dimensional limits regarding the development of perovskite thin film and van der Waals monolayer ferroelectrics, the microscopic behaviors of the ferroelectric polarization and dipole switches have barely been characterized directly in the experiment. On the other hand, the ferroelectric instability demands the charge ordering that forms the cations/anions center and the spatial inversion symmetry breaking that creates the ferroelectric polarization, which hardly happen simultaneously in one system. The coupling of these two degrees of freedom in the ferroelectric phase transition therefore is rare to be investigated.

Alternatively, monoelemental ferroelectrics is an ideal platform to realize both charge ordering and spatial inversion symmetry breaking in one system when there is a transition between the parent phase and the polarized phase [1]. In this work, we report the experimental observation of the in-plane polarized monoelemental ferroelectrics in the black phosphorous-like bismuth [2]. By the combination of scanning tunneling microscopy (STM) and non-contact atomic/Kelvin probe force microscopy (AFM/KPFM), we directly measured the electric dipole and visualized the ferroelectric dipole reversion at the atomic scale. The further lattice distortion and band bending measurement at the 180° charged domain walls exhibited the screened Coulomb interaction and the modulated electronic structure at the tail-to-tail domain wall, which was verified to be the results of the interplay between the charge ordering and ferroelectric lattice distortion. Our work explicitly observed the interlock between the charge ordering and the spatial inversion symmetry in one system. This demonstrated a new route of electronic states modulations during the ferroelectric phase transition.

[1] C. Xiao, F. Wang, S. A. Yang, Y. Lu, Y. Feng, and S. Zhang, Elemental Ferroelectricity and Antiferroelectricity in Group-V Monolayer, Adv. Funct. Mater. 1707383, 1 (2018).

[2] J. Gou, L. Kong, L. Kong, X. He, Y. L. Huang, J. Sun, J. Sun, J. Sun, S. Meng, S. Meng, K. Wu, K. Wu, K. Wu, L. Chen, L. Chen, L. Chen, A. T. S. Wee, and A. T. S. Wee, The Effect of Moiré Superstructures on Topological Edge States in Twisted Bismuthene Homojunctions, Sci. Adv. 6, (2020).

Thursday 11:40–12:00

Tuning and measuring the potential landscape in 2D materials

Wyatt A. Behn,[1,*] Zachary J. Krebs,[1] Keenan J. Smith,[1] Kenji Watanabe,[2] Takashi Taniguchi,[3] and Victor W. Brar[1]

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[2] Research Center for Functional Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan
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Accurately mapping the local electrostatic potential of 2D materials is critical to understanding how the electronic structure is modified in the presence of perturbing potentials [1,2]. Potentials from superlattices and defects are of particular importance due to the affects they may have on transport properties and the strength of el-el interactions [3,4]. Invasive probes, such as Scanning Tunneling Microscopy (STM), can alter the potential landscape of materials sensitive to doping effects and reveal misrepresentative results [5]. Kelvin Probe Force Microscopy (KPFM) measurements of local electrostatic potentials also suffer inaccuracies due to long-range forces [6]. We present KPFM measurements with a calibration scheme that accurately reconstructs the potential well profile of user-created, electrostatically defined quantum dots (QDs) in monolayer graphene/hexagonal boron nitride (MLG/hBN) heterostructures (Fig. 1). We show that experimentally extracted energy level spacings measured by scanning tunneling spectroscopy (STS) compare well to reconstructed KPFM data. This technique combining STM and KPFM allows for the response of quasiparticles as a function of carrier concentration to be determined in a self-consistent way. Such methods could be implemented to further investigate nanometer-scale optically active atomic defects in 2D transition metal dichalcogenides [7,8].

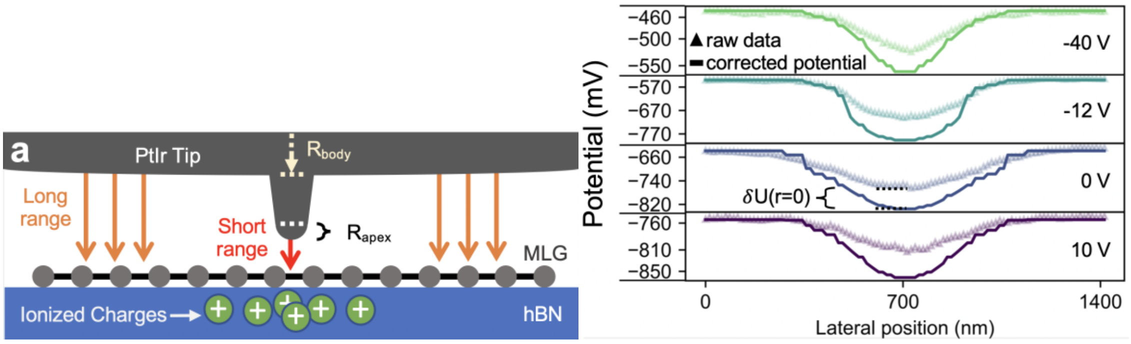

Figure 1: *Left: Diagram illustrating short/long-range contributions in a KPFM measurement of a charged QD. Right: Extracted surface potential variations moving laterally across the QD in the graphene surface before and after removing long-range contributions.*

[1] J. Lee, et al., Nat. Phys. **12**, 1032 (2016).
[2] J. Velasco, et al., Nano. Lett. **18**, 5104 (2018).
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[6] H. Jacobs, P. Leuchtmann, O. Homan, A. Stemmer, J. Appl. Phys., **84**, 1168 (1998).
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Thursday 12:00–12:20

Spatially Resolved Nonlinear Optical Response in 2D WS_2

Josephine Spiegelberg,[1,*] Rasa Rejali,[2] Zeno Schumacher,[3] Megan Cowie,[1] Peter Grütter[1]

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Transition metal dichalcogenides (TMDC) represent a new class of quantum materials with many applications in nano- and opto-electronics due to their direct bandgap, high mobility, and layered structure [1,2]. Their lack of inversion symmetry also means that they exhibit particularly strong non-linear optical (NLO) responses. Current experimental measurements of 2D TMDC nonlinear optical susceptibility often do not agree with theoretical values and can vary over several orders of magnitude depending on growth and measurement techniques [3,4]. These discrepancies are likely related to the presence of defects in the monolayers which may be due to atomic scale structural defects, local oxidation, atomic kinds in steps, or extended nanometer size wrinkles from the deposition of monolayer material. The influence of these defects on nonlinear optical properties is not yet well understood. Our work aims to spatially resolve the nonlinear optical response of defects in TMDCs using a novel combination of non-contact AFM and femtosecond optical excitation. In this setup, an optically excited nonlinear response can be mechanically measured via variations in the electrostatic interactions between an AFM tip and the sample [5]. The small size of the AFM tip allows for high spatial resolution in the measurement of the non-linear properties and correlation with atomic scale structure.

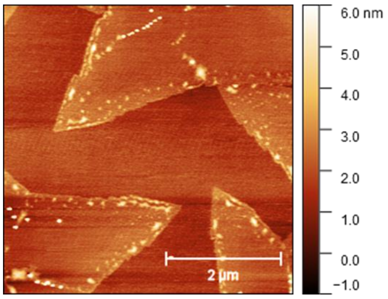

Figure 1: *Tapping mode AFM image of CVD-grown WS_2 flake topography.*

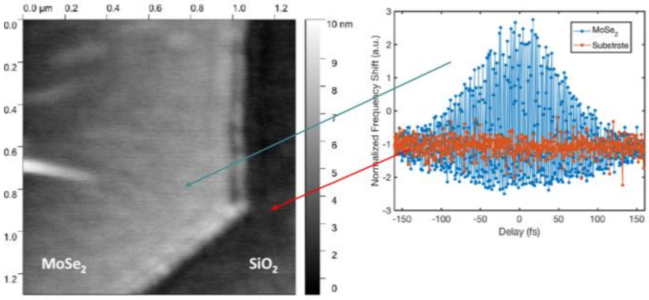

Figure 2: *Illumination of $MoSe_2$ flake by pulsed laser induces a polarization, due to its nonlinear optical response, which varies the electrostatic tip-sample interactions measured by frequency shift of an AFM cantilever. As the delay between two beams is varied, the AFM records an interferometric autocorrelation function. No signal is measured on SiO_2 substrate.*

[1] N. Kumar, S. Najmaei, Q. Cui, F. Ceballos, P. M. Ajayan, J. Lou, and H. Zhao, Phys. Rev. B - Condens. Matter Mater. Phys. **87**, 1 (2013).
[2] X. Zhang, Z. Lai, C. Tan, and H. Zhang, Angew. Chemie - Int. Ed. **55**, 8816 (2016).
[3] K. Bredillet, J. Riporto, G. T. Forcherio, J. R. Dunklin, J. P. Wolf, L. Bonacina, Y. Mugnier, and R. Le Dantec, Phys. Rev. B **102**, 1 (2020).
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[5] Z. Schumacher, R. Rejali, R. Pachlatko, A. Spielhofer, P. Nagler, Y. Miyahara, D. G. Cooke, and P. Grütter, Proc. Natl. Acad. Sci. U. S. A. **117**, 19773 (2020).

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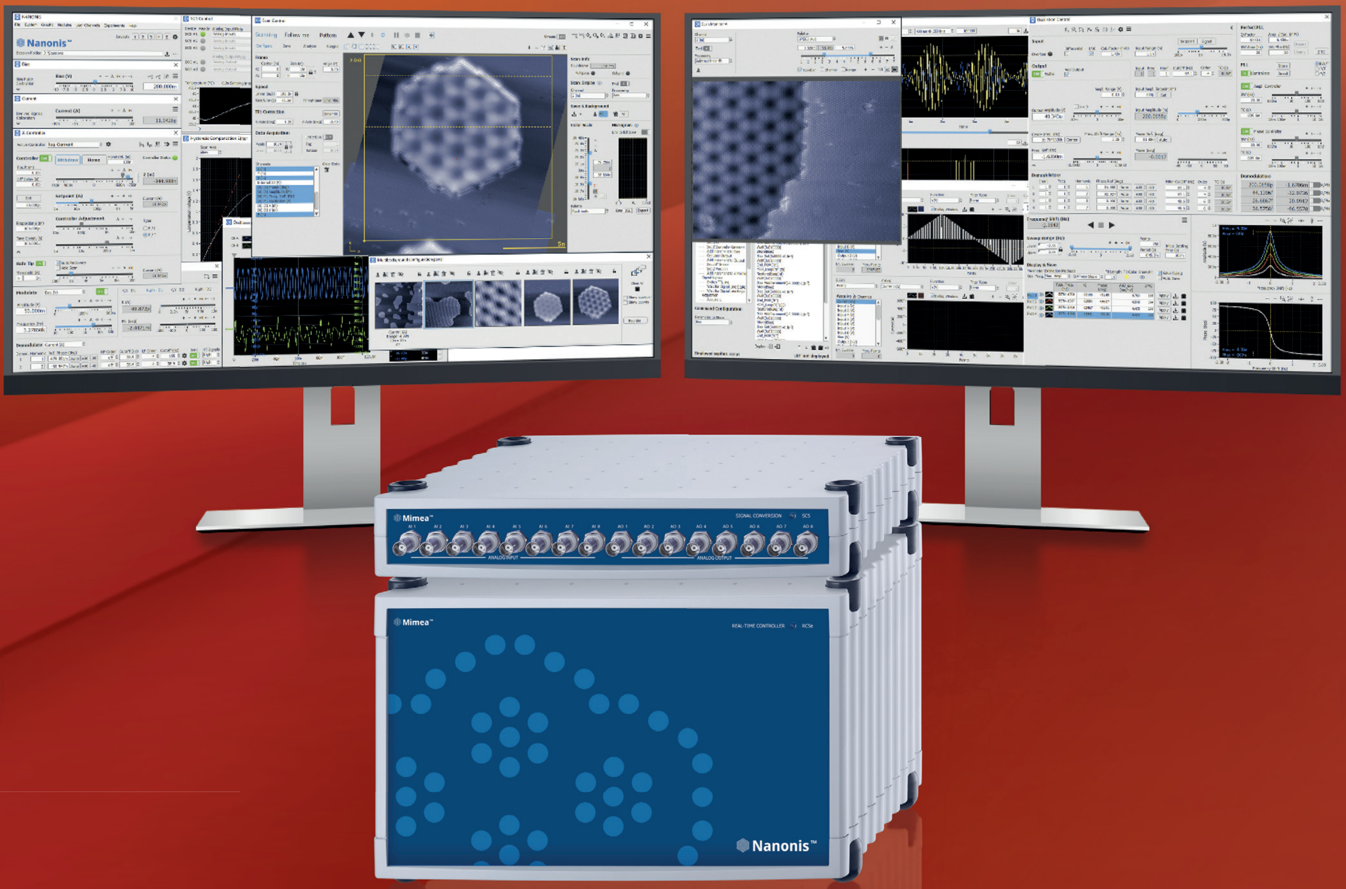

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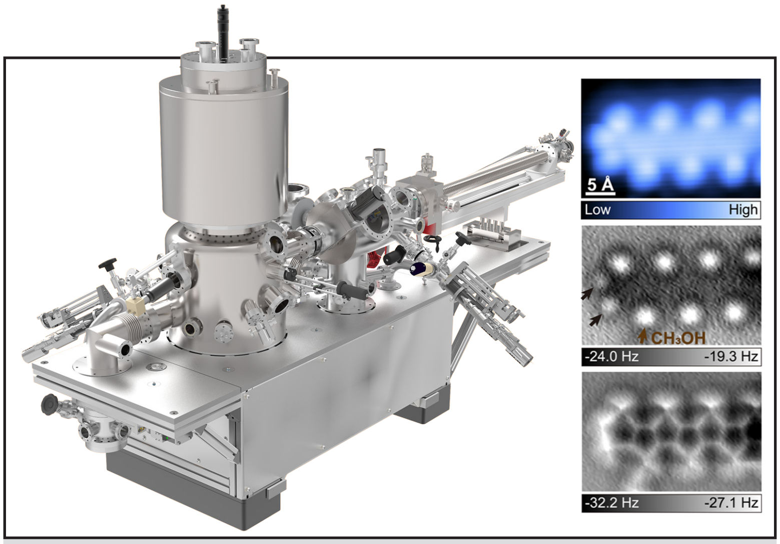

Right column: Atomic Insight into the Interfacial Effect on the Molecular Solvation, Jia Dong, Pu Yang, Chen Zhang, Duanyun Cao, Ying Jiang, and Jing Guo; The Journal of Physical Chemistry C 2022 126 (7), 3756-3763; DOI: 10.1021/acs.jpcc.1c10296.

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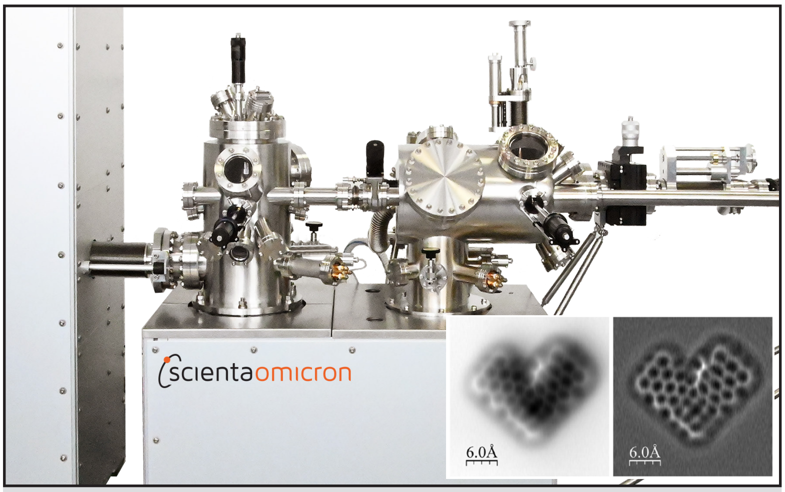
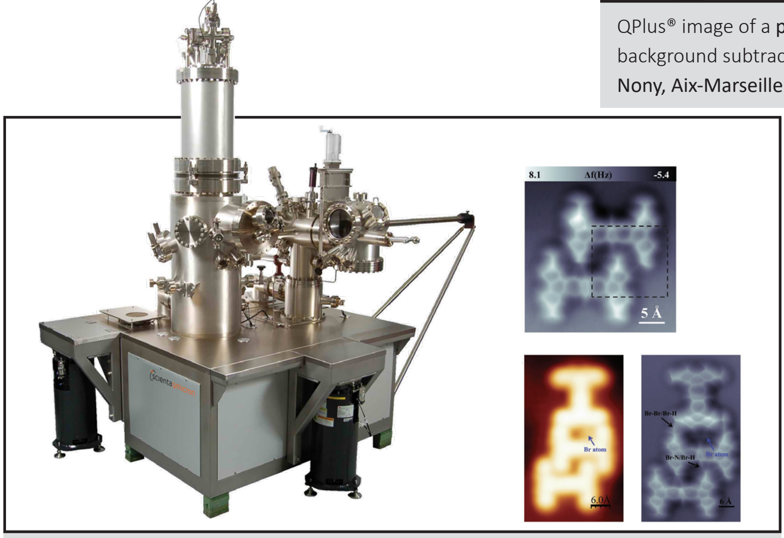


QPlus® image of a **porphyrinoid molecule on Au(111)**. Left: raw image. Right: after background subtraction. **Data courtesy: Sylvain Clair, Christian Loppacher and Laurent Nony, Aix-Marseille Univ, Marseille, France.**



Right column: QPlus® and STM of 2-TBQP dimers (top) and trimers: Real-Space Investigation of the Multiple Halogen Bonds by Ultrahigh-Resolution Scanning Probe Microscopy, Dingguan Wang, Zishen Wang, Wei Liu, Arramel, Siying Zhong, Yuan Ping Feng, Kian Ping Loh, and Andrew Thye Shen Wee; NUS Singapore, DOI: 10.1002/smll.202202368.

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Friday, August 5th 2022

Characterisation of molecular systems (B)

Chair: Pérez, R.

09:00	**Scherb, S.** *Tuning thermal expansion of supramolecular networks by alkyl chain modification.*
09:20	**Laflör, L.** *The search for iron: NC-AFM imaging of the trimesic acid – iron self-assembled networks on Au(111).*
09:40	**Liu, J.-C.** *Proximity-Induced Superconductivity in Atomically Precise Nanographenes.*
10:00	**Pawlak, R.** *On-surface synthesis of nitrogen-doped nanographene characterized by low-temperature atomic force microscopy.*

Novel instrumentation and techniques (C)

Chair: Ebeling, D.

11:00	**de Campos Ferreira, R. C.** *Real Space Visualization of Entangled Excitonic States in Charged Molecular Assemblies.*
11:20	**Sekatskii, S.** *High spatial resolution PhotoThermal Induced Resonance imaging in visible spectral range based on Scanning Near-field Optical Microscope fibre probes and electronics.*
11:40	**Khachatryan, K.** *Understanding signal generation in NC-AFM with interferometric displacement detection.*

Closing remarks

12:00	**The organisers** *Closing remarks*

Friday 09:00–09:20

Tuning thermal expansion of supramolecular networks by alkyl chain modification

Sebastian Scherb,[1]* Antoine Hinaut,[1] Rémy Pawlak[1], J.G. Vilhena[1], Yiming Song[1], Klaus Müllen[2], Thilo Glatzel[1], Akimitsu Narita[2], Ernst Meyer[1]

[1] Department of Physics, University of Basel, Klingelbergstrasse 82, 4056, Basel, Switzerland
[2] Max Plank Institute for Polymer Research, Ackermannweg 10, 55128, Mainz, Germany

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Two-dimensional supramolecular materials present unique possibilities to achieve highly ordered structures while offering exceptionally high response to external stimuli. Combining the functionalities possible in supramolecular assemblies with well controlled response to head, could open the possibility to tune thermal expansion of functional materials. Such tuning is of high interest for mechanical and sensing applications, like sensorics, artificial muscles or aerospace [1].

Here, we present the tuning response of 2D supramolecular assemblies of three hexabenzocoronene based molecules equipped with three length of peripheral alkyl chains - butyl, octyl and dodecyl groups, using nc-AFM and STM at different temperatures. Based on analysis of nano-scale images of the assemblies between 5 and 300 K on Ag(111) and Au(111) surfaces, we find thermal expansion coefficients to be tuned from 69 ± 12 × 10^{-6} K^{-1} to 880 ± 28 × 10^{-6} K^{-1}, as shown in Fig. 1. A shortening of the chains, thereby, corresponds to an increase of the expansion coefficient. Generally, the expansion is increased on Au(111) in comparison to Ag(111) with a limit reached for the longest chains [3].

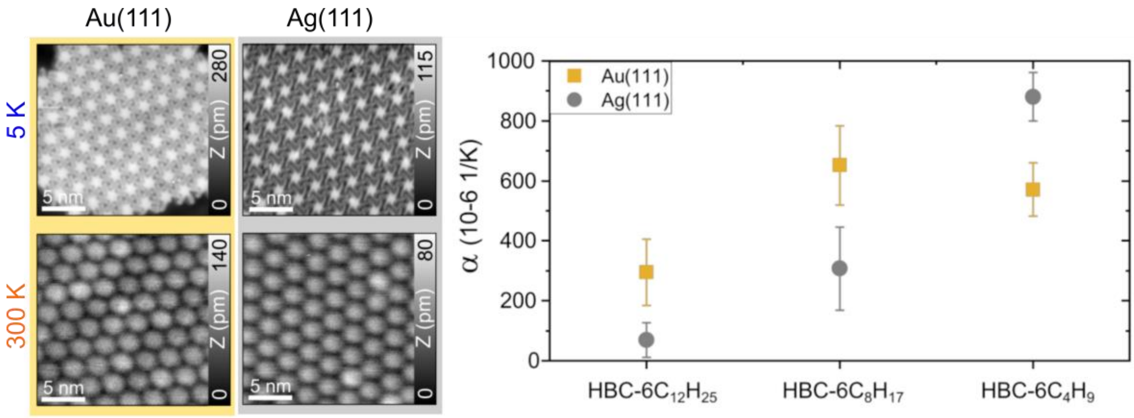

Figure 1: *Thermal response of 2D supramolecular assemblies depending on alkyl chain length.*

[1] Zhu *et al*. Matter 4, 1832 (2021)
[2] Scherb *et al.* Commun. Mater. **1**, 1 (2020).
[3] Scherb *et al. in preparation*.

Friday 09:20–09:40

The search for iron: NC-AFM imaging of the trimesic acid – iron self-assembled networks on Au(111)

L. Laflör, P. Rahe*

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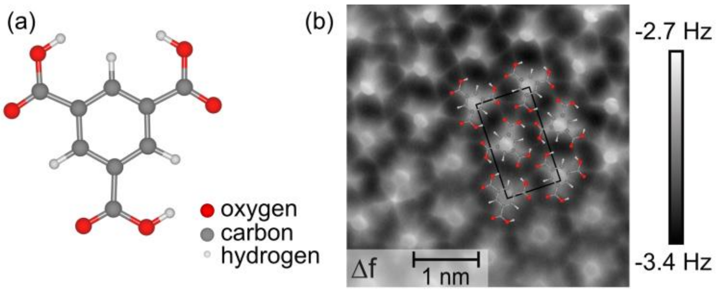
Surface metal-organic networks are tuneable, two dimensional networks with a number of functions including the scaffold for host-guest systems or magnetic elements. These networks are formed by organic linker molecules coordinating to metal centres [1]. However, identifying the metal centres and coordination bonds within the networks using non-contact atomic force microscopy (NC-AFM) can be a challenge. So far, two different types of contrast have been observed at the metal centre's position with high-resolution NC-AFM: First, the metal centre is imaged as a protrusion with sharp features connecting the metal centre to the binding partner [2,3]. Second, the organic linkers are connected via a bond-like feature in NC-AFM images at the position of the metal centre [4]. In the latter contrast mode, no protrusion is observed at the metal centre position, thus, the position of the metal centre cannot be identified directly. Still, the identification of the metal centre's position is crucial for understanding the bonding within the network.

Here, the aim is to determine the presence of iron atoms in a network formed by iron and trimesic acid (TMA, see panel (a)), on Au(111) using NC-AFM with CO functionalised tips. After the deposition of TMA and iron, the formation of an ordered network with a rectangular supercell containing two TMA molecules and having a size of 0.89×1.49 nm is observed (see panel (b)). We find the supercell formation to be robust against a change of different preparation parameters such as the deposition order, sample temperature, and TMA:Fe ratio.

Principally, the intermolecular bonding can be stabilised by both, coordination or hydrogen bonds. Along these lines, the supercell is investigated with constant-height imaging using CO-functionalised tips and the bond-like features connecting the oxygen atoms of the carboxylic acid groups are investigated. Within the images, no intermolecular protrusions are observed, hence, iron cannot be identified directly. Therefore, we statistically analyse the oxygen-oxygen distances between the oxygen atoms via unit cell averaged images to clarify the intermolecular bonding situation. A deductive approach is followed considering the possibilities of different carboxylic acid orientations as well as deprotonation, ultimately shedding light on the bonding situation within the network.



(a) Ball and stick model of trimesic acid. (b) NC-AFM image of TMA and iron on Au(111). Six TMA models are included; the black rectangle highlights the supercell. Imaging parameters: Δf*=-3 Hz,* U_s*=0.65 mV,* f_0*=36461 Hz,* T_s*=4.6 K.*

[1] L. Dong, et al. Prog. Surf. Sci. **91**, 101 (2016).
[2] C. Chiang, et al. Science, **344**, 885 (2014).
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[4] M. Telychko, et al. Angew. Chem. Int. Ed. **58**, 18591 (2019).

Friday 09:40–10:00

Proximity-Induced Superconductivity in Atomically Precise Nanographenes

Jung-Ching Liu[1], Rémy Pawlak[1], Xing Wang[2], Philipp d'Astolfo[1], Carl Drechsel[1], Ping Zhou[2], Silvio Decurtins[2], Ulrich Aschauer[2], Shi-Xia Liu[2], Wulf Wulfhekel[3], Ernst Meyer[1,*]

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Atomically precise nanographenes (NGs) can be efficiently synthesized through on-surface reactions. By proximizing tailored NGs to a s-wave superconductor, topological superconductivity could be fostered. However, on-surface synthesis of NGs is restricted to noble metals [1-2] or metal oxides [3], and is still missing on superconducting surfaces. To fill the gap, we first fabricate a Ag buffer layer on the Nb(110) superconductor [4], and grow atomically precise NGs on the Ag/Nb substrate using DBBA as the precursor. Through the investigation of non-contact atomic force microscopy with a CO-functionalized tip, we demonstrate successful synthesis of polymeric chains and NGs, and reveals their atomic structures on the superconducting Ag/Nb(110) substrate. We believe our method provides a promising platform for studying the role of topology in the interaction between carbon magnetism and superconductivity [5].

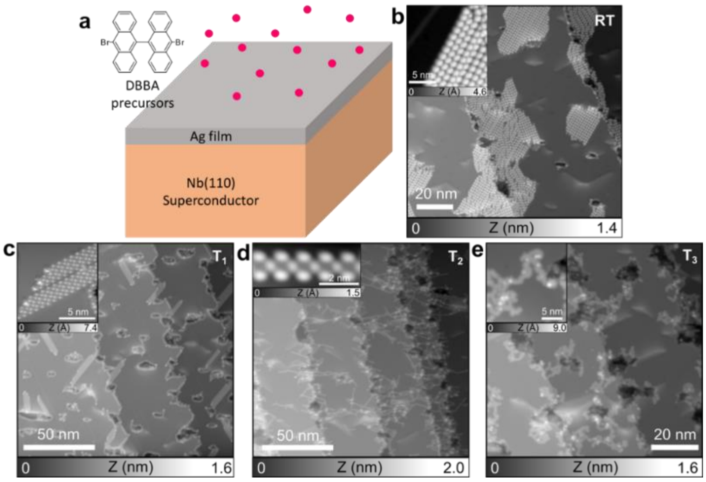

Figure 1: *An overview of the bottom-up synthesis on the superconducting Ag/Nb with DBBA as the precursor.* ***a*** *The drawing of the sample.* ***b*** *DBBA assemblies after deposition.* ***c-e*** *Synthesized polymeric chains and NGs after annealing the sample at different temperatures.*

[1] J. Cai *et al.,* Nature **466**, 470-473 (2010).
[2] K. A. Simonov *et al.,* Sci. Rep. **8**, 3506 (2018).
[3] M. Kolmer *et al.,* Science **369**, 571-575 (2020).
[4] T. Tomanic *et al.*, PRB **94**, 220503 (2016).
[5] J.-C. Liu *et al.,* arXiv:2202.00460

Friday 10:00–10:20

On-surface synthesis of nitrogen-doped nanographene characterized by low-temperature atomic force microscopy

Rémy Pawlak,[1,*] Jung-Ching Liu,[1] Chao Li,[1] Outhmane Chahib,[1] Xunshan Liu,[2] Ulrich Aschauer,[2] Silvio Decurtins,[2] Shi-Xia Liu,[2] Ernst Meyer[1,*]

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Heteroatom doping in nanographene [1] offers unique opportunities to tune electronic band gaps, realize donor-acceptor (D-A) heterostructures [2] or enhance edge magnetism [3]. Among the potential dopants, nitrogen is of particular interest for its electron-accepting character in graphene and the possibility of inducing robust ferromagnetism at high doping concentration [4].

In this presentation, our recent works that explore the assembly and surface-assisted chemical reactions of N-doped precursors at surfaces will be discussed [6]. I will present the on-surface synthesis of porous GNR [4] and Kagome graphene [5], whose structures are systematically characterized by low temperature scanning tunneling microscopy (STM) and atomic force microscopy (AFM) supported by density functional theory (DFT). Besides high-resolution imaging with CO-terminated tips, the charge-state control of these N-doped nanographene will be also demonstrated using force spectroscopy [6].

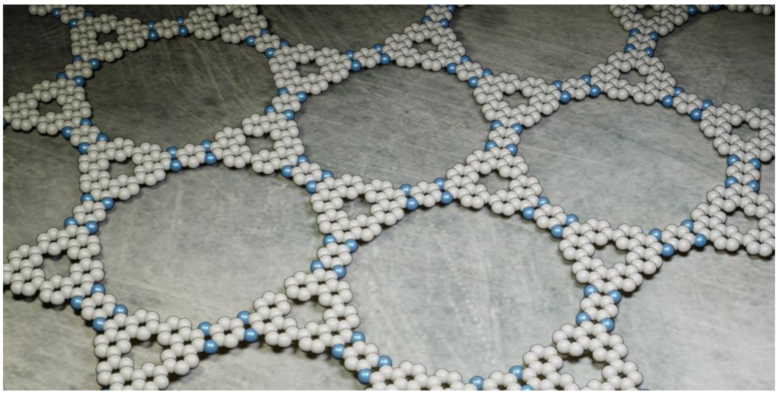

Figure 1: *Artistic view of the N-doped Kagome graphene synthesized on Ag(111) [5].*

[1] J. Cai et al. Nature **466,** 470 (2010).
[2] T. Meier et al. ACS Nano **11,** 8413-8420 (2017).
[3] R. E. Blackwell et al. Nature **600,** 647-652 (2021).
[4] R. Babar et al. Phys. Rev. B **99,** 5442 (2019).
[4] R. Pawlak et al. J. Am. Chem. Soc. **42**, 12568-12573 (2020).
[5] R. Pawlak et al. Angew. Chem. Int. Ed. **60**, 8370-8375 (2021).
[6] C. Drechsel et al. Submitted.

Friday 11:00–11:20

Real Space Visualization of Entangled Excitonic States in Charged Molecular Assemblies

Jiří Doležal,[1,2] Sofia Canola,[1] Prokop Hapala,[1] **Rodrigo Cezar de Campos Ferreira**,[1*] Pablo Merino,[3,4] and Martin Švec,[1,5]

[1] Institute of Physics,Czech Academy of Sciences; Czech Republic
[2] Faculty of Mathematics and Physics, Charles University; Czech Republic
[3] Instituto de Ciencia de Materiales de Madrid; CSIC, Madrid, Spain
[4] Instituto de Física Fundamental, CSIC; Serrano 121, E28006 Madrid, Spain
[5] Regional Centre of Advanced Technologies and Materials; Czech Republic

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The study of the optoelectronic properties of single-molecule emitters and their aggregates paves the way for new quantum computing and cryptography technologies, as well as molecular-based memory devices and sensors. Nanoscale information into the photophysics of these intriguing phenomena could be gained through the so-called STM-induced luminescence (STML) technique, which allows us to get deep insight into the fundamental mechanism behind the molecular electronic and vibronic transitions responsible for the photoluminescence. In contrast to far-field spectroscopies, near-field spectroscopic mapping allows for direct identification of individual eigenmodes, exciton coupling type, and excited states that would otherwise be inaccessible [1]. Here, we used STML in conjunction with atomic force microscopy (AFM) to examine delocalized single-exciton states of charged molecular assemblies built from individual perylenetetracarboxylic dianhydride (PTCDA) molecules. The results, in comparison with calculated many-body optical transitions, reveal a second low-lying excited state of the anion monomers and its role in exciton entanglement within the assemblies. By changing the charge states of the assembly, we demonstrate control over the exciton coupling. This work shows the possibility of tailoring the excitonic properties of exciton aggregates for advanced functionalities and lay the groundwork for addressing them individually at the nanoscale.

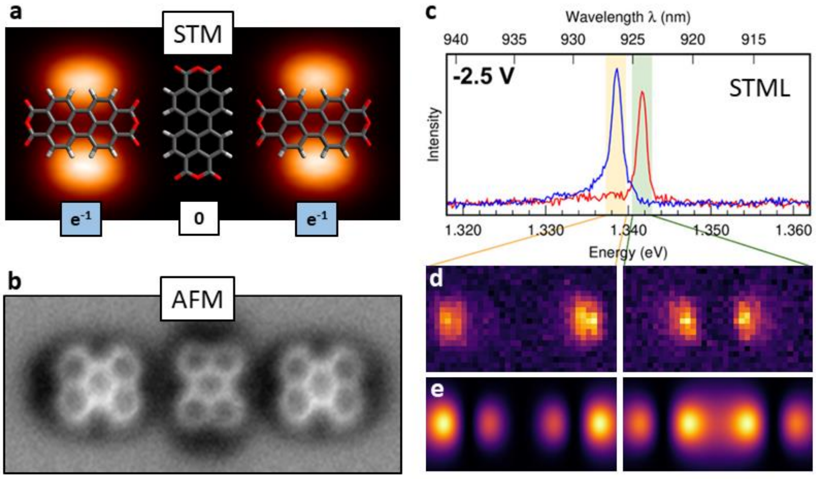

Figure 1: *a) constant-height current images of the trimer at -2.5 V. b) AFM constant-height image of the backbones taken at 5 mV. c) STML spectrum of the trimer taken at -2.5 V. d) Experimental photon maps with ranges marked in the spectrum. e) Simulated photon maps.*

[1] J. Doležal, S. Canola, P. Hapala, R.C.C. Ferreira, P. Merino, and M. Švec, ACS Nano, **16**, 1, 1082–1088 (2022).

Friday 11:20–11:40

High spatial resolution PhotoThermal Induced Resonance imaging in visible spectral range based on Scanning Near-field Optical Microscope fibre probes and electronics

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Recently, we have demonstrated high spatial resolution (up to 5 nm) and monolayer sensitivity PhotoThermal Induced Resonance (PTIR) imaging in visible spectral range based on “classic” cantilever-based Atomic Force Microscopy setup [1]. These results profit also from the coincidence of the laser pulse repetition rate (these pulses induce thermal expansion) with the resonant dithering frequency of an AFM cantilever, and gap plasmon resonance attainable in the visible spectral range for the gold coated AFM tip - sample gap thickness of a few nm.

Here we present the newest modification of this approach: Scanning Near-field Optical Microscope (SNOM) electronics and SNOM fiber probes, mounted onto the quartz tuning fork, were used for PTIR measurements. We exploited also the proprietary “double-resonant” montage of such SNOM probes onto the tuning fork: the working frequency of the latter coincides with the resonant dithering frequency of the free-standing part of the probe (glass beam). Earlier, we have demonstrated that such a montage enables to obtain excellent topographical images, including those of single strand DNA molecules [2]. The value of the working frequency of the tuning fork is around 33 kHz, so that a great variety of commercially available ns pulsed lasers in visible (routinely having the working frequency up to 100 – 200 kHz) can be used as a source of light for PTIR in conditions of a “triple resonance”. This additionally increases the sensitivity of the method. In Fig. 1 below we present the first images obtained with such approach. Further perspectives of the method will be also discussed.

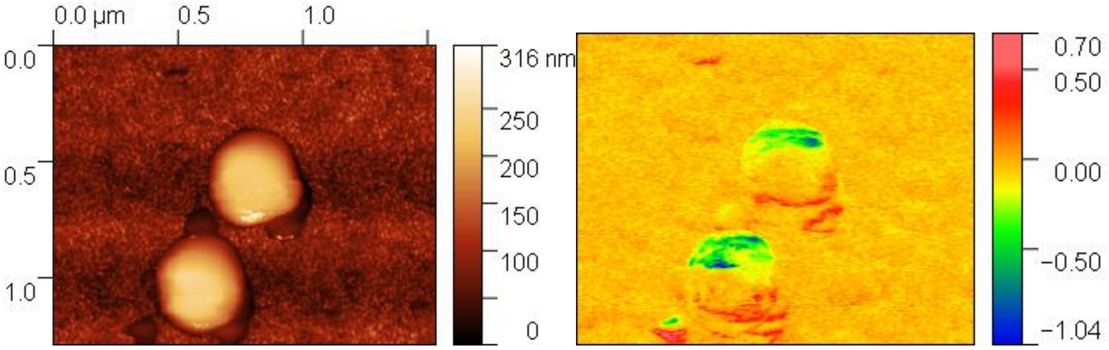

Figure 1: *Topographical (left) and PTIR (right) images of 200 nm-size nanospheres stained with dark red dye (ThermoFischer Scientific) well absorbing the laser radiation used (671 nm) delivered via SNOM probe. Control experiments without laser reveal flat structureless pictures.*

[1] J. Zhou, A. Smirnov, G. Dietler and S. K. Sekatskii, Nano Letters **19**, 8278 (2019).
[2] S. K. Sekatskii, K. Dukenbayev, M. Mensi, *et al.*, Faraday Disc. **184**, 51 (2015).

Friday 11:40–12:00

Understanding signal generation in NC-AFM with interferometric displacement detection

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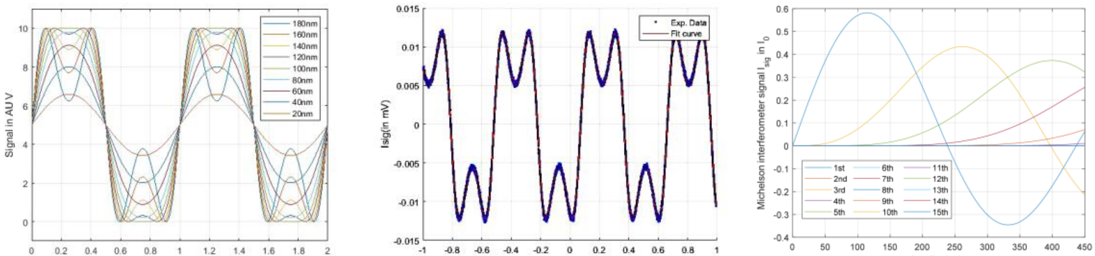
Interferometry is a standard method for detecting the cantilever displacement in NC-AFM where the interferometer is mostly operated in the Michelson mode [1] while operation in the Fabry-Pérot mode allows the study of opto-mechanical coupling phenomena [2]. Assuming a freely, hence, harmonically oscillating cantilever, we investigate the convolution of the cantilever displacement with the interferometer response function of the spatially modulated cavity light field. The interferometer responds with a periodic signal with non-trivial time dependence that we investigate in both, the time and frequency domain. Figure 1(a) shows time traces of a simulation while Fig 1(b) shows representative experimental data together with a fit curve. Fitting the model curve to experimental data yields the cantilever oscillation amplitude A_0, detector sensitivity and reflectivity factor V_0, alignment error of the interferometer d_{err}, fundamental cantilever eigenfrequency f_0 and excitation phase φ_0 with a remarkable precision. Having the laser wavelength as a length standard, interferometric detection specifically allows a most accurate determination of the oscillation amplitude that is a critical parameter for the quantitative interpretation of NC-AFM data.

A harmonic analysis of the Michelson interferometer signal yields a series expansion in Bessel functions of the first kind that is typical for a frequency modulated signal. A perfectly aligned Interferometer with the zero point of the cantilever oscillation exactly placed in the inflection point of the interferometer response function yields a spectrum solely consisting of odd Bessel functions. Representative model data are shown in Fig. 1(c). The presence of a 2nd harmonic signal in experimental data reveals an interferometer misalignment and a fit of the 2nd harmonic model curve to experimental data allows the evaluation of d_{err}. Evaluating the zero crossings of the harmonic contributions allows determining an accurate value for A_0.



(a) (b) (c)

Figure 1 (a) *Model of time domain interferometric signal for different oscillation amplitudes* A_0. (b) *Fitted experimental interferometric signal.* (c) *Harmonic analysis of a model interferometric signal.*

Our study demonstrates the precise and accurate determination of the cantilever oscillation amplitude with a method solely based on inherent interferometer properties rather than involving a tip-surface interaction that is prone to introducing uncertainty.

[1] A. v. Schmidsfeld et al., Beilstein J. Nanotech. **7**, 841 (2016).
[2] A. v. Schmidsfeld and M. Reichling, Appl. Phys. Lett. **107**, 123111 (2015).

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5 Poster contributions

Poster session A, Monday, August 1st 2022

P01 **Cai, Shuning** *Water-induced hydrogen-bond mismatch in a 2D supramolecular DNA bases assembly*

P03 **Temirov, Ruslan** *Design of an NC AFM operating at millikelvin temperatures: A progress report*

P05 **Rothe, Karl** *Atomic forces and relaxations in single-molecule reactions*

P07 **Qu, Zhang** *Atomic structure and electron distribution of ring-like Co cluster on Si(111) surface by NC-AFM/KPFM at 78 K*

P09 **Wang, Ziying** *Engineering Topological Phases in a Two-dimensional Transition Metal Dichalcogenide*

P11 **Xu, Chen** *Electrostatic Discovery Atomic Force Microscopy*

P13 **Jiuyan, Wei** *Study of Co adsorption model on Si(111)-7×7 surface using DFT calculation*

P15 **Balajka, Jan** *CO adsorption on* Fe_3O_4*(111) imaged by scanning probe microscopy*

P17 **Priante, Fabio** *Probing the structural details of cellulose and chitin nanocrystal-water interfaces by 3D-AFM*

P19 **Heile, Daniel** *Modelling nanoscale charge measurements*

P21 **Karimi, Amin** *Adsorption structures of mixed red-PTCDA and PTCDA on Ag(111)*

P23 **Schwarz, Alexander** *A novel method akin to magnetic force microscopy to sense tiny bio-magnetic fields using magnetically sensitive resonators*

P25 **Rothhardt, Daniel** *Local Work Function on Graphene Nanoribbons and on the Au(111) herringbone reconstruction*

P27 **Dierker, Tim** *Systematically mapping the distance-dependent tip-sample interaction for the PTCDA/Ag(111) system*

P29 **Wiesener, Philipp** *Atomic-scale characterization of triazine-based copper nitrides and their catalytic performance in an oxygen reduction reaction*

P31 **Ranawat, Yashasvi** *Workflow for prediction of hydration layers on surfaces*

P33 **Loppacher, Christian** *Investigating UV-Induced Polymerization of Pre-Assembled Supramolecular Layers on Ionic Crystal Substrates*

P35 **Khachatryan, Knarik** *Automated and highly accurate adjustment of a fibre interferometer for NC-AFM displacement detection*

P37 **Sun, Shuo** *Epitaxial Growth of Ultraflat Bismuthene with Large Topological Band Inversion Enabled by Substrate-Orbital-Filtering Effect*

P39 **Chahib, Outhmane** *Characterization of one-dimensional silicene structure on Au (110) by atomic force microscopy*

P41 **Verhage, Michael** *Applications of the tuning fork planar probe: on-tip magnetic SPM sensor in UHV*

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P45 **Tomitori, Masahiko** *Surface resistivity evaluated by frequency modulation atomic force microscopy through Joule heat energy dissipation*

P47 **Huang, Shuyu** *In-situ characterization of atomic friction of pristine and Nitrogen-doped graphene in ultrahigh vacuum*

P49 **Arai, Toyoko** *Oscillatory behavior of dissipation energy in hydration layers at the interface between a nanometer-thin water film and a KBr(100) surface observed by frequency modulation atomic force microscopy*

P51 **Seeja Sivakumar, Nikhil** *Development of a low-temperature scanning probe microscopy setup to study atomic-scale magnetism in 2D materials*

Poster 01

Water-induced hydrogen-bond mismatch in a 2D supramolecular DNA bases assembly

Shuning Cai,[1] Chen Xu,[1] Lauri Kurki,[1] Adam S. Foster,[1] Peter Liljeroth[1,*]

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As ubiquitous as bulk water, nano-confined water plays a key role in biological and chemical processes and determines some unique properties of materials. However, there is limited evidence on the real-space structures of confined waters. Here, we observed that the initial hydration of the ordered hydrogen-bonded adenine assembly increases the distance between the rows of adenines on Ag (111). Intriguingly, the homochiral molecules between the rows are converted into a heterochiral ‘mismatching’ hydrogen bonding pattern, which is driven by the energy gain from the hydration by the water molecules. Our observations provide direct evidence of hydration processes at the single molecule level and suggest that the counter-intuitive mismatch of hydrogen bonding can exist in the water-related processes and materials. This can offer new insights into topics where hydrogen bonding plays a prominent role, such as crystal engineering, DNA nanotechnology and heterogenous catalysis.

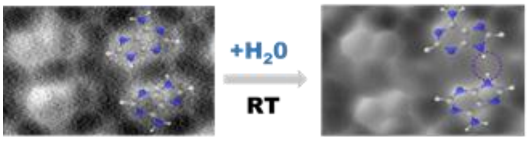

Figure 1: *Schematic illustration of the water-induced adsorption sites change in the 2D supramolecular self-assembly of adenine molecules on Ag(111) with counterintuitive hydrogen-bond ’mismatch’.*

Poster 03

Design of an NC AFM operating at millikelvin temperatures: A progress report

Ruslan Temirov[1,2,*], Taner Esat[1,3], Sven Just[1,3], Denis Krylov[1,3], Peter Coenen[1,4], Vasily Cherepanov[1,4], F. Stefan Tautz[1,3,7]

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We have recently developed and launched into operation a millikelvin scanning tunneling microscope (mK STM) powered by an adiabatic demagnetization refrigerator (ADR) [1]. One of the unique features of our design is its modularity, which facilitates further setup development. This contribution will describe the ongoing effort of extending the microscope's capabilities to the NC AFM mode of operation.

[1] T. Esat, P. Borgens, X. Yang, P. Coenen, V. Cherepanov, A. Raccanelli, F. S. Tautz, and R. Temirov, Rev. Sci. Inst. **92**, 063701 (2021)

Poster 05

Atomic forces and relaxations in single-molecule reactions

K. Rothe,[1] N. Néel,[1] M.-L. Bocquet,[2] J. Kröger[1,*]

[1]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

[2]PASTEUR, Département de chimie, École normale supérieure, PSL University, Sorbonne Université, CNRS, F-75005 Paris, France

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We combine atomic force microscopy (AFM) experiments on single phthalocyanine (Pc) molecules adsorbed on Ag(111) with density functional theory (DFT) simulations to probe structural relaxations upon the atom-by-atom abstraction of pyrrolic H, to gain insight into the subsequent on-surface metalation with a single Ag atom and the bonding behavior of the resulting two conformational Ag-Pc isomers with a CO-terminated AFM tip.

The atomwise abstraction of pyrrolic H leaves its footprints in spatially resolved force spectra with a CO-terminated tip. The magnitude of the point of maximum attraction unveils the macrocycle center as the most attractive region of the molecule; its vertical shift towards the substrate surface upon moving from the molecular periphery to the center matches well DFT predictions of the relaxed adsorption geometry.

On-surface metalation of a single free-base Pc is achieved by adding a single Ag atom from the AFM tip to the macrocycle center. Lower bounds of the force and energy for the metalation process can be inferred from probing the force variation at the verge of the chemical reaction. The spontaneous atom transfer is in agreement with the DFT energy profile determined in a nudged-elastic-band approach.

The metalation leads to two conformational isomers with clearly distinct bonding behavior to an approached CO molecule. The isomer with the central Ag atom pointing to CO (Ag-Pc↑) exhibits a complex evolution of the distance-dependent interaction, while the conformer with Ag bonded to the metal surface (Ag-Pc↓) gives rise to a Lennard-Jones behavior. Simulations within DFT comprising the entire junction highlight the role of structural relaxations, physisorption and chemisorption for Ag-Pc↑, while Ag-Pc↓ exhibits chemical inertness to the bonding with CO.

Poster 07

Atomic structure and electron distribution of ring-like Co cluster on Si(111) surface by NC-AFM/KPFM at 78 K

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The adsorption of metal nanoclusters on semiconductor surfaces has been intensively investigated for the past several decades because of low dimensional and quantum properties. They are promising for many novel applications in ultrahigh density recording, nanoelectronics and nanocatalysis, etc. [1]. Co adsorption on Si(111)-7×7 surface is highly related to the Co coverage, expose temperature and annealing temperature [2]. However, the atomic structure and model of Co atoms adsorbed on Si(111)-7×7 surface are still unknown. In this work, we have performed an NC-AFM/KPFM measurement of Co atoms adsorption on Si(111)-7×7 surface at 78K.

For the first time, the ring-like Co cluster with the atomic resolution was obtained as shown in the topographic image (the inserted image) in Fig. 1(a). As a result, the Co cluster was adsorbed on an off-center site in FHU of Si(111)-7×7 surface, and two center Si adatoms were missing on the surface. From the site-dependent force curve, we found that cluster atom, cluster hole and Si adatom have different maximum attractive forces, which reveals the different bond energy. Fig. 1(b) show the experimental V_{LCPD} image and DFT calculation of ring-like Co cluster which exhibits the same charge distribution of six atoms of Co cluster with more positive charged. Combing AFM and KPFM results, we analyze the atom structure of ring-like Co cluster on Si(111)-7×7 surface, and propose a structure model including three Co atoms and six Si atoms as shown Fig.1 (c).

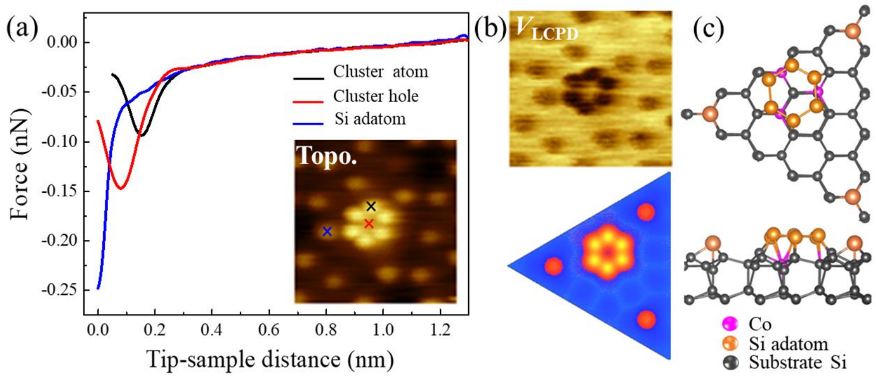

Figure 1: *(a) Force as a function of tip-sample distance at cluster atom, cluster hole and Si adatom, the inserted image is a topographic image of ring-like Co cluster on FHU of Si(111)-7×7. (b) The experimental V_{LCPD} image and DFT Calculation of ring-like Co cluster. (c) Model of ring-like Co cluster. Imaging parameters: 5×5 nm^2, f_0 = 960 kHz, A = 2 nm, Q = 12800, T = 78 K.*

[1] H. Roder, E. Hahn, et al., Nature **366**, 141-143(1993).
[2] A.E. Dolbak, B.Z. Olshanetsky, et al., Surf. Sci. **373**, 43-55 (1997).

Poster 09

Engineering Topological Phases in a Two-dimensional Transition Metal Dichalcogenide

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Topological states of quantum matter hold promise as platforms for the next generation of electronics. Notable examples include topological insulators[1, 2], which exhibit insulating bulk and gapless surface or edge modes that are protected by time-reversal symmetry, and Weyl semimetals[3, 4], which are characterized by the gapless bulk states with Fermi arcs on the surface. The 2D topological insulator was originally theorized to exist in graphene, followed by hunting for the type-II Weyl semimetals in WTe_2, $MoTe_2$, and related compounds. In this work, by first-principle calculations, we predict that bilayer 2H-TaS_2 possesses a Z2 topological metal phase at a specific self-intercalation concentration of 50% ($Ta_{10}S_{16}$). Ultrathin $Ta_{10}S_{16}$ film is synthesized with molecular beam epitaxy and its edges state is studied by scanning tunnelling microscopy. $Ta_{10}S_{16}$ consists of mosaic intercalation domains where the intensity of electronic states at Fermi energy is greatly enhanced on the domain edges. The intensities of electronic states form a linear oscillation with an external magnetic field, which is a manifestation of Aharonov–Bohm oscillations. Wafer-scale $Ta_{10}S_{16}$ film of high quality allows potential applications to electronic and spintronic devices based on the quantum spin Hall effect and its possible candidates for the realization of Majorana fermions.

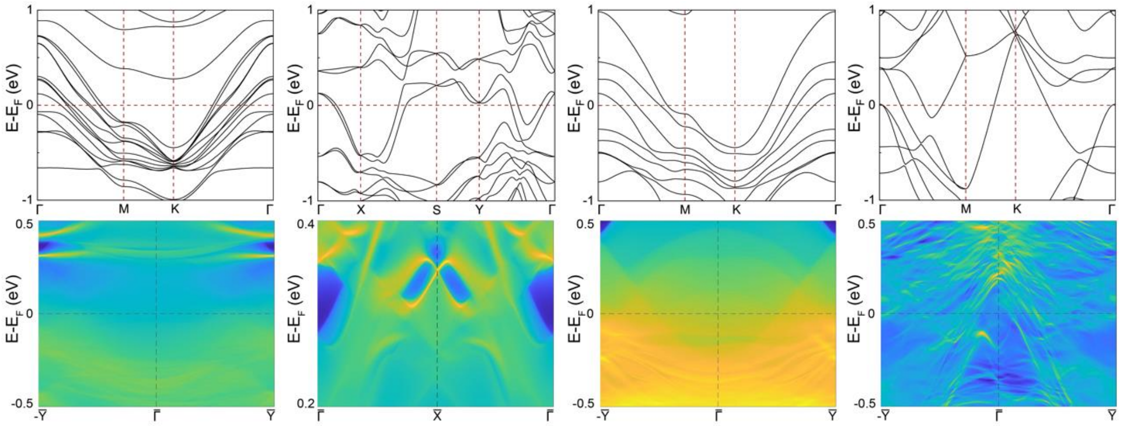

Figure 1: Simulated band structures and edge states of different intercalation concentrations. From left to right: intercalation concentration of 33.3%, 50%, 66.7% and 100%.

Reference

[1] Kane, C. L., Mele, E. J., Physical review letters, 95(22), p.226801 (2005).
[2] Fu, L., Physical Review Letters, 106(10), p.106802 (2011).
[3] Xu, S., et al., Science, 349(6248), pp.613-617 (2015).
[4] Wan, X., et al., Physical Review B, 83(20), p.205101 (2011).

Poster 11

Electrostatic Discovery Atomic Force Microscopy

Niko Oinonen[1], **Chen Xu**[1], Benjamin Alldritt,[2]
Filippo Federici Canova[1,2], Fedor Urtev[1,3], Shuning Cai[1], Ondřej Krejčí[1]
Juho Kannala[3], Peter Liljeroth[1], *, and Adam S. Foster[1,4], *

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[2] Nanolayers Research Computing Ltd, London N12 0HL (United Kingdom)
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While offering high resolution atomic and electronic structure, scanning probe microscopy techniques have found greater challenges in providing reliable electrostatic characterization on the same scale. In this work, we offer electrostatic discovery atomic force microscopy, a machine learning based method which provides immediate maps of the electrostatic potential directly from atomic force microscopy images with functionalized tips. We apply this to characterize the electrostatic properties of a variety of molecular systems and compare directly to reference simulations, demonstrating good agreement. This approach offers reliable atomic scale electrostatic maps on any system with minimal computational overhead.

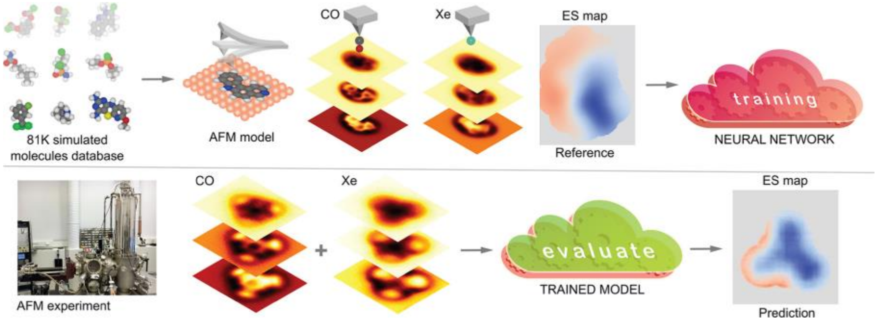

Figure 1: Schematic of the ED-AFM method. We train a neural network that takes two sets of AFM images as input and translates them to the ES Map descriptor, which is the vertical component of the electrostatic field over the sample molecule. The model is trained on simulated sets of input–output pairs calculated from a database of several tens of thousands of molecule geometries. The trained model can then be applied to experimental AFM images to produce a prediction of the sample electric field.

[1] N. Oinonen, et al. ACS Nano **16**, 89-97 (2021).

Poster 13

Study of Co adsorption model on Si(111)-7×7 surface using DFT calculation

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The adsorption of metal nanoclusters on Si surfaces has been widely investigated for several decades. However the model of Co adsorbed on Si(111)-7×7 surface and the process of Co diffusion on Si surface are still uncertain [1]. Density functional theory (DFT) method is one of the most successful theoretical method to investigate the electronic structure and properties of solids in various fields of material research [2,3]. Recently, we have observed the ring-like Co clusters adsorbed on Si(111)-7×7 by AFM/KPFM at 78K as shown in Fig.1. Here, The Co cluster was adsorbed on an off-center site in HUC (half unit cell), two center Si adatoms were missing. According to AFM/KPFM images, to reveal the proper Co adsorption model on Si(111)-7×7 surface, we have calculated two models, which are one or three Co atoms adsorbed on Si(111)-7×7 surface with DFT calculation. We found that two structure models are more stable than that of the initial state as the adsorption energy of one or three Co atoms (-27.46 eV or -136.54 eV). Fig1. (c) and (d) show the result of electron localiazation functional (ELF) of three Co atoms adsorbed model by DFT calculation. The details will be presented in NC-AFM conference.

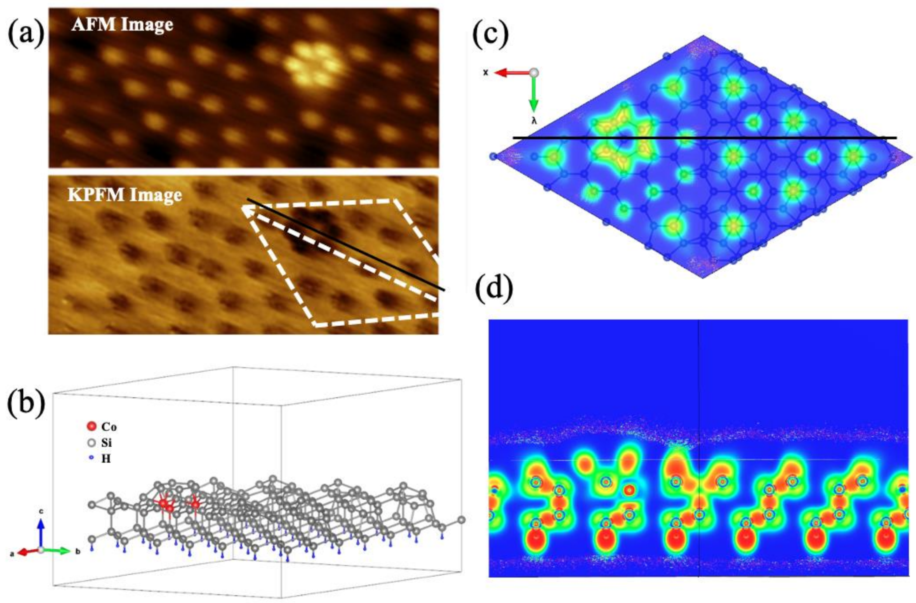

Figure 1： *Co cluster adsorbed on Si(111)-7×7. (a) AFM and KPFM images. The white dotted line marks the calculated basic cell and the black line is the section line. (b) The model of three Co atoms adsorbed on Si(111)-7×7. (c) Corresponding electron localiazation functional (ELF) by DFT calculation. (d) Cross-section of the black line in (c).*

[1] AE Dolbak, BZ Olshanetsky, et al., Surf. Sci. **373**, 43-55 (1997).
[2] ED Farias, MEZ Michoff, et al. Appl. Surf. Sci. **565**, 150552 (2021).
[3] RA Zhachuk, DI Rogilo, et al. Phys. Rev. B **104**.12, 125437 (2021).

Poster 15

CO adsorption on $Fe_3O_4(111)$ imaged by scanning probe microscopy

Johanna Hütner,[1] Florian Kraushofer,[1] Matthias Meier,[1,2] Zdeněk Jakub,[3] Michael Schmid,[1] Ulrike Diebold,[1] Gareth S. Parkinson,[1] **Jan Balajka**[1]

[1] Institute of Applied Physics, Vienna University of Technology, Vienna, Austria
[2] Computational Material Physics, University of Vienna, Vienna, Austria
[3] CEITEC, Brno University of Technology, Brno, Czech Republic

*Corresponding author contact: balajka@iap.tuwien.ac.at

Magnetite $Fe_3O_4(111)$ surface has been investigated thoroughly with surface science techniques. Across a wide range of O_2 chemical potentials, the surface is terminated by tetrahedrally coordinated Fe atoms (Fe_{tet}), forming a hexagonal lattice [1]. Models of CO adsorption on $Fe_3O_4(111)$ have been proposed based on TPD and IRAS measurements combined with DFT calculations [2]. At sub-monolayer coverages, all TPD features have been assigned to the CO molecules adsorbed on defects [2]. Using scanning probe microscopy, we identified the CO adsorption sites on $Fe_3O_4(111)$ and relate them to published spectra.

Specifically, we dosed CO onto a UHV-prepared $Fe_3O_4(111)$ surface at 105 K and imaged the surface at 77 K with STM and noncontact AFM using a qPlus sensor. With a CO-functionalized AFM tip, the adsorbed CO on the $Fe_3O_4(111)$ surface yields a bright contrast (Fig. 1a) due to the repulsive interaction between the two CO molecules [3]. The tunneling current image (Fig. 1b) was simultaneously recorded during the constant-height AFM imaging.

We observed that CO molecules dosed at 105 K never occupy neighboring Fe_{tet} sites. Instead, their spacing locally corresponds to a $(\sqrt{3}\times\sqrt{3})R30°$ pattern or longer-distance (2×2) ordering. The CO molecules adsorb directly atop the surface Fe_{tet} atoms occupying ~20% of the available sites at the chosen experimental conditions.

I will discuss CO adsorption patterns at different dosages and temperatures imaged by scanning probe microscopy and relate them to the previously published TPD and IRAS analyses. The direct identification of adsorption sites precludes surface defects from solely responsible for CO adsorption at low coverages. The results will refine the existing models for CO adsorption on $Fe_3O_4(111)$ and contribute to the ongoing debate on the structure and reactivity of this surface.

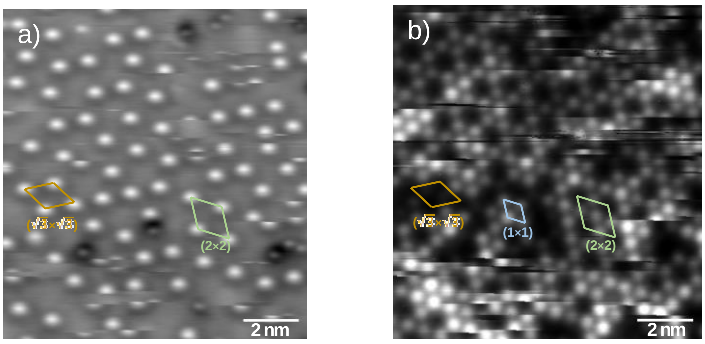

***Figure 1.** Noncontact AFM images of CO adsorbed on $Fe_3O_4(111)$ a) Frequency shift signal, CO molecules yield a bright, repulsive contrast. b) Simultaneously recorded tunneling current image.*

[1] G. S. Parkinson, Surf. Sci. Rep. **71,** 272-365 (2016).
[2] X. Li, et al., J. Phys. Chem. B **122**, 527-533 (2018).
[3] M. Ellner, et al., Nano Lett **16**, 3 (2016).

Poster 17

Probing the structural details of cellulose and chitin nanocrystal-water interfaces by 3D-AFM

A. Yurtsever,[1] P. Wang,[2] **F. Priante**,[3] Y. M. Jaques,[3] K. Miyazawa,[1] K. Miyata,[1] M. J. MacLachlan,[2] A. S. Foster [3,] * and T. Fukuma [1]

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Cellulose and chitin are among the most abundant biopolymers in nature, constituting the building block of numerous materials deriving from plants, tunicates, fungi, and crustaceans [1 - 3]. However, an accurate picture of the crystalline surfaces of cellulose and chitin at the molecular level is still missing. Here, using atomic force microscopy (AFM) and molecular dynamics (MD) simulations, we revealed the molecular details of the chain arrangements at the surfaces of cellulose and chitin nanocrystals in water. We further visualized the three-dimensional (3D) local arrangement of water molecules near these surfaces by 3D-AFM (see Fig. 1 for e.g. chitin). In both materials, the AFM experiments and MD simulations showed an anisotropic water layer structuring, determined by the different surface topologies and exposed chemical moieties. These findings provide important insights to our understanding of interfacial interactions on cellulose and chitin nanocrystals in water at the molecular level.

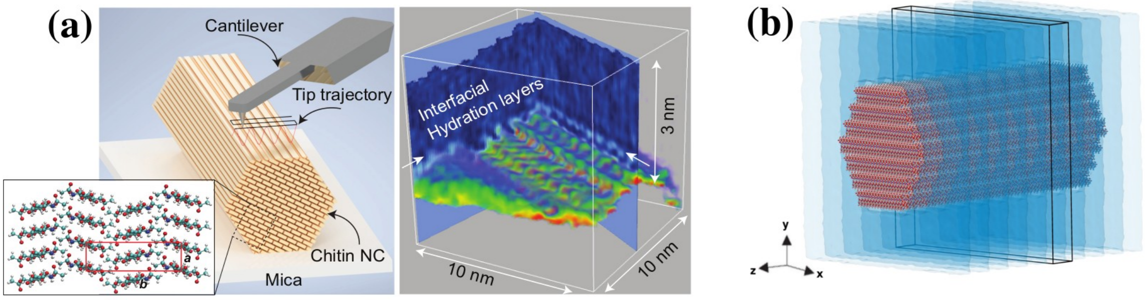

Figure 1: *(a) Experimental setup scheme (left) and 3D-AFM image of the chitin-water interface (right). The 3D map indicates the variations of the frequency shift of the oscillating cantilever as function of the xyz coordinates. (b) Model structure for chitin nanocrystal employed by the MD simulation, exposing different crystallographic planes.*

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Poster 19

Modelling nanoscale charge measurements

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Charge state measurements at the nanoscale are of utmost importance for the characterization of application-relevant elements, for example in catalysts as well as semiconductors or energy harvesting devices. From a fundamental research point, charge measurements will deliver critical insights into the involved physical, chemical, or biological processes. However, quantitative charge measurements with atomic force microscopy (AFM) and Kelvin probe force microscopy (KPFM)-based methods are still a challenge. In particular, a large number of parameters contribute to the voltage $V_{\text{Bias}}^{\text{COMP}}$ determined to compensate the contact potential difference (CPD) and to minimize the forces due to charges [1, 2].

Here, we present a detailed investigation of numerous factors that contribute to the measurement observable $V_{\text{Bias}}^{\text{COMP}}$ and which, consequently, need to be considered when aiming for quantitative charge measurements. In particular, we unravel a dependence on the oscillation amplitude and analyze the influence of the tip geometry and system parameters such as the dielectric constant (Figure 1a). Furthermore, we discuss the influence of charges depending on their lateral (Figure 1b and 1c) and vertical position. As KPFM is a non-local technique, we find that charges far away from the tip position still give a contribution. In conclusion, we argue that charge quantification from regular imaging bears many ambiguities, while mapping the progress of $V_{\text{Bias}}^{\text{COMP}}$ with respect to the vertical tip position z_{ts}^{min} allows to untangle many of these contributions on the path to charge quantification.

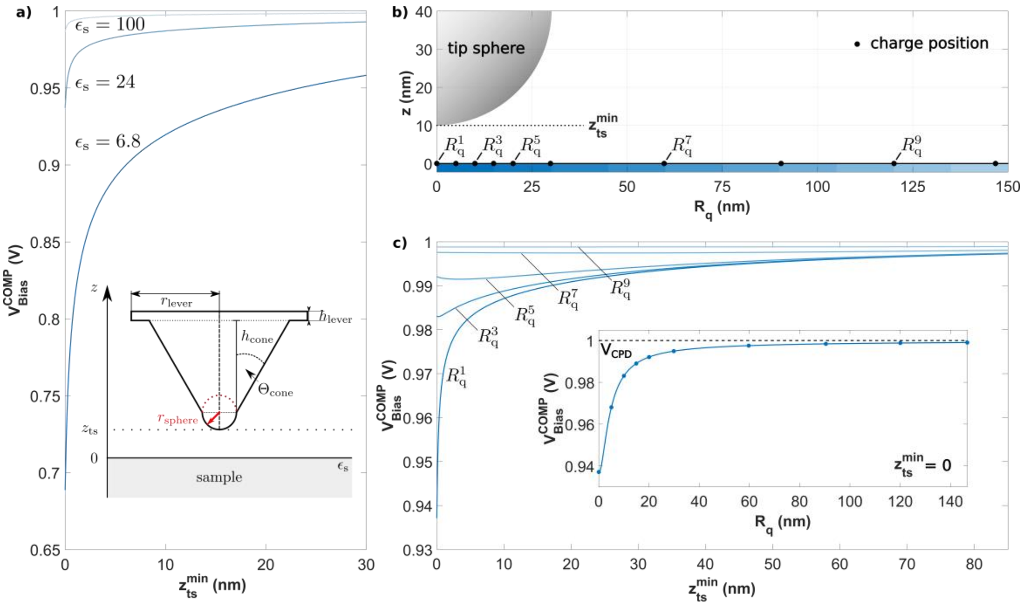

Figure 1: *Dependence of* $V_{\text{Bias}}^{\text{COMP}}(z_{ts}^{min})$ *on (a) the dielectric constant* ϵ_s *and on (b, c) the lateral position* R_q *of a single elementary charge. Model parameters:* $V_{CPD} = 1V$, $\epsilon_s = 24$, $r_{sphere} = 30nm$, $\Theta_{cone} = 23.3°$, $h_{cone} = 12.5\mu m$, $r_{lever} = 34.55\mu m$ *and* $h_{lever} = 4\mu m$ *(inset in a).*

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Poster 21

Adsorption structures of mixed red-PTCDA and PTCDA on Ag(111)

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For molecular manipulation and SPM tip functionalization, the mode of anchoring molecules to the tip is decisive [1,2]. We recently found that PTCDA ($C_{24}H_8O_6$) binds to a Ag tip with *two* oxygen-metal bonds when it is retracted from the surface [3]. While this is crucial for its stabilization in a vertical state, the two bonds reduce the degrees of freedom during manipulation in the tip-molecule-surface junction.

To overcome this problem, we synthesized a PTCDA derivative ("red-PTCDA", $C_{24}H_{10}O_5$), in which one carboxylic oxygen is replaced by two H atoms (inset of Fig. 1a). For molecular manipulation, this allows choosing between one or two tip-oxygen bonds. Here, we present a study on the absorption structures formed by a mixture of PTCDA and red-PTCDA on the Ag(111) surface with the help of low-temperature NC-AFM/STM. In constant height Δf images with a decorated tip, red-PTCDA can be identified by a pronounced feature caused by one of the out-of-plane H atoms (Fig.1).

We observed that despite the minimal modification of red-PTCDA compare to PTCDA, the mixture of both molecules exhibits a strongly different behaviour compared to the regular island growth of pure PTCDA. Particularly striking is the coexistence of zero-, one-, and two-dimensional structures (Figure 1). A likely explanation for such diverse structures is the influence of long-range electrostatic interactions related to the in-plane dipole moment of red-PTCDA.

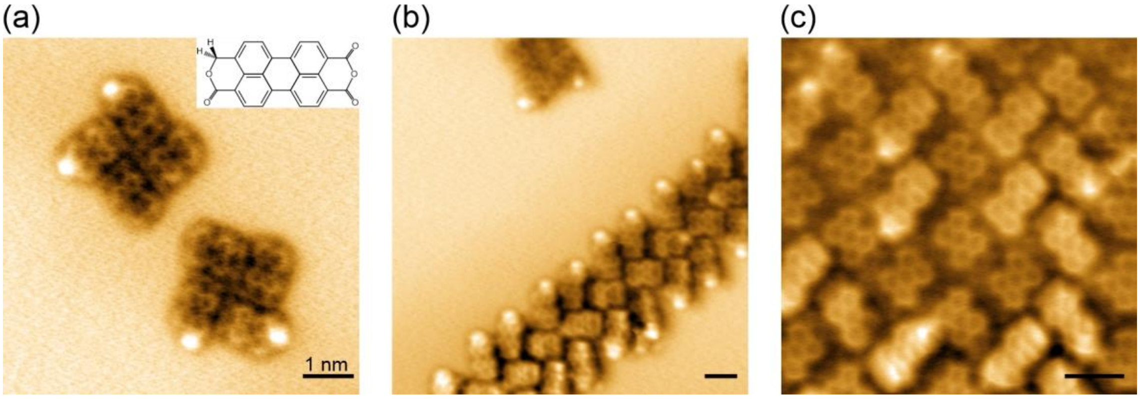

Figure 1: (a) Zero-, (b) one-, and (c) two-dimensional structures of a mixture of red-PTCDA and PTCDA adsorbed on Ag(111). The tetramer in panel (a) is the most common growth motif.

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Poster 23

A novel method akin to magnetic force microscopy to sense tiny bio-magnetic fields using magnetically sensitive resonators

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Magnetoencephalography is used to map brain activity by detecting magnetic fields in the fT regime that are generated by current pulses in the neurons. Currently, SQUID-based detector arrays (SQUID: superconducting quantum interference device) that operate at liquid helium temperatures are employed for this task. Here we present a patented idea [1] envisaged in the OXiNEMS project [2] to replace these delicate and susceptible sensors by more robust magnetically sensitive mechanical resonators in conjunction with a superconducting field-to-gradient converter.

As visible in Fig.1, a superconducting loop picks up a weak magnetic field and thereby generates a current. This current in turn produces an Oersted field. By introducing a constriction, the field is strongly magnified. A magnetically sensitive resonator, e.g., a cantilever, bridge or membrane, located above the constriction can sense the magnetic field by tracking the induced frequency shift using the same detection schemes as in force microscopy set-ups. The design is similar to the concept of magnetic force microscopy (MFM) and the same equations to determine the sensitivity of the device apply.

This project has received funding from the European Union’s Horizon 2020 research and innovation program under grant agreement No 828784.

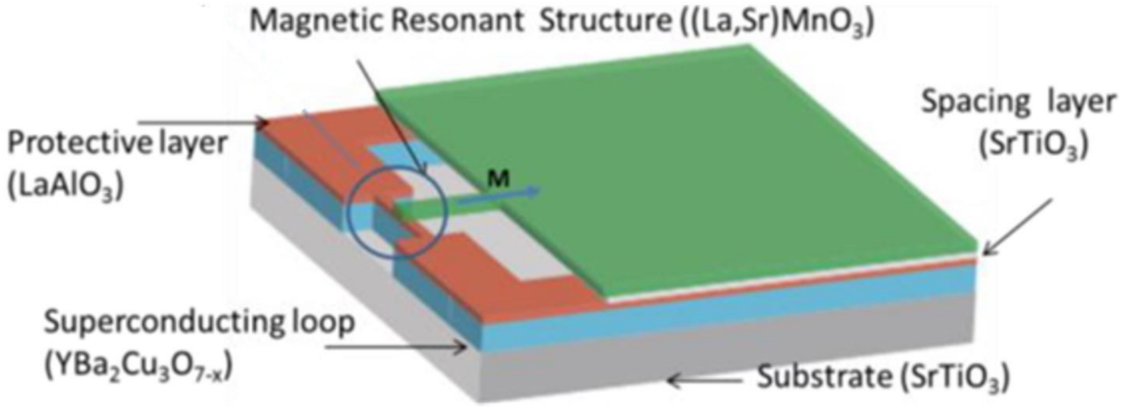

Figure 1: *Concept of the detection scheme to sense weak bio-magnetic fields in the fT-regime using a design similar to an MFM set-up as envisaged in the OXiNEMS project.*

[1] European application No.: EP20169544.2
[2] OXiNEMS: Oxide Nanoelectromechanical Systems for Ultrasensitive and Robust Sensing of Biomagnetic Fields (www.oxinems.eu)

Poster 25

Local Work Function on Graphene Nanoribbons and on the Au(111) herringbone reconstruction

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Graphene nanoribbons (GNRs) exhibit remarkable electronic properties due to the nature of the charge carriers and local confinements [1]. We prepared the GNRs via on-surface synthesis on an Au(111) substrate [3]. The precursor molecule 10,10′-dibromo-9,9′-bianthracene (DBBA) was vapour-deposited onto the Au(111) surface at 470 K and then kept at 470 K for 10 min for dehalogenation. The dehydrogenation takes place during a second annealing step. We investigated the variation of the local work function (LCPD) of the GNRs on the Au(111) surface using frequency modulation scanning force microscopy in ultra-high vacuum. The LCPD images were acquired by parallel recording of topography and Kelvin probe force microscopy. The LCPD images reveal a charge transfer between the GNRs and the underlying substrate and confirm the p-type doping of the GNRs on Au(111) [2]. We observed a modification of the work function at the edges of the GNRs, which is due to the screening of electrostatic fields from the GNR by the Au(111). Changes in the work function between 15-30 mV due to the herringbone reconstruction were observed in addition. This indicates a change in surface reactivity [4]. Density functional theory (DFT) calculation supports the experimental findings.

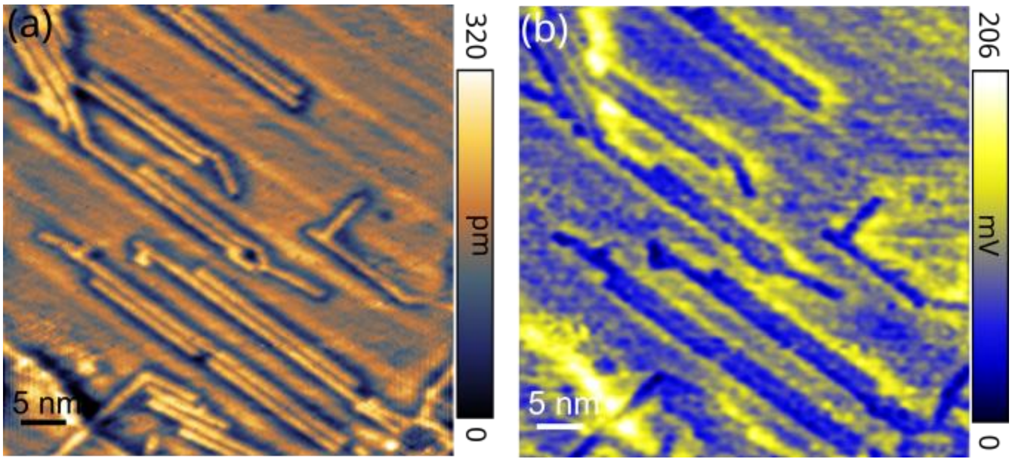

Figure 1: *(a) Topography, (b) local work function difference of GNRs on Au(111).*

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Poster 27

Systematically mapping the distance-dependent tip-sample interaction for the PTCDA/Ag(111) system

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Over the last years, significant progress with scanning probe microscopy (SPM) has been made after successfully establishing controlled tip functionalization [1]. One example of these accomplishments is the development of scanning quantum dot microscopy (SQDM) [2]. By attaching the π-conjugated molecule 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) to the apex of a metallic SPM tip, the electrostatic potential near the sample surface can be quantitatively mapped [3]. In order to reliably apply this technique, the expedient pick-up of a single molecule is required [4].

Here, we investigate the tip-molecule interaction between a metallic tip and surface-adsorbed PTCDA molecules by means of systematic measurements. Scanning tunneling microscopy (STM) and atomic force microscopy (AFM) measurements of PTCDA molecules on a Ag(111) surface are carried out to especially investigate the vertical dependencies of the STM tunnelling current and the AFM frequency shift. Data are acquired by systematically mapping these quantities along different axes of single PTCDA molecules embedded in the molecular film. Fingerprints for the dynamic behaviour of the molecules are clearly revealed and guide the vertical manipulation for molecular pick-up.

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Poster 29

Atomic-scale characterization of triazine-based copper nitrides and their catalytic performance in an oxygen reduction reaction

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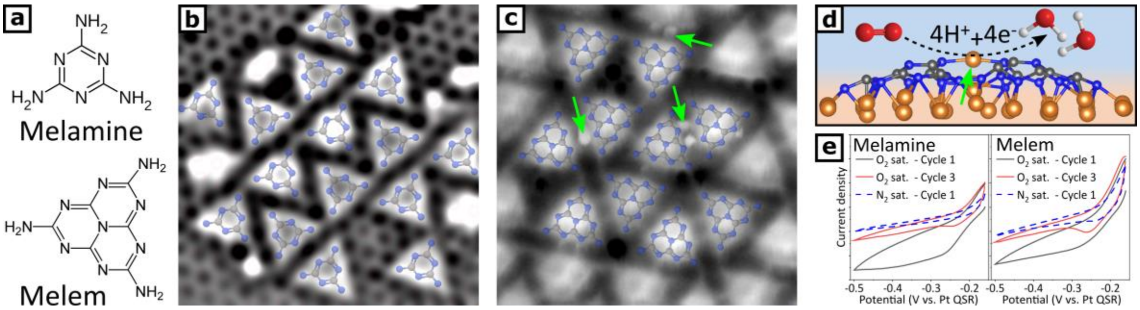
In heterogenous catalysis via surface supported metal nanostructures the performance strongly depends on the size and coordination of the specific catalytically active sites. Reducing the size to the lower limit results in isolated metal atoms constituting a promising approach for the design of single atom catalysts (SACs) [1]. The desired low coordination leads to technical issues like the chemical stability as well as the prevention of agglomeration. One possibility is the use of supramolecular nanostructures allowing to immobilize catalytically active single metal atoms.

Here we investigate triazine- and heptazine based molecules (Fig. **a**) and their strong interaction with a Cu(111) substrate to build a catalytically active surface according to the principle of SACs. The supramolecular nanostructures (Fig. **b**,**c**) are resolved by an O-terminated copper tip [2] in constant-height nc-AFM mode. Cu atoms at intermolecular sites show a pronounced interaction with the O-terminated tip (green arrows in Fig. **c**) [3]. Supporting DFT simulations (Fig. **d**) confirm a drastic lifting of the intermolecular Cu atoms and a strong interaction of gaseous oxygen species with the N-Cu-N sites.

A potential catalytic activity of the elevated copper atoms with their reduced coordination is investigated by ex-situ cyclic voltammetry experiments (Fig. **d,e**). In particular, we studied the actual electrochemical performance towards the oxygen reduction reaction (ORR) [4] in a home-built setup optimized for single crystalline samples.



a *Structural formulas.* **b**,**c** *nc-AFM image of triazine- and heptazine based supramolecular structures on Cu(111).* **d** *DFT-simulation showing a lifted copper atom and illustration of the oxygen reduction reaction.* **e** *Cyclic voltammograms proving the electrochemical performance.*

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Poster 31

Workflow for prediction of hydration layers on surfaces

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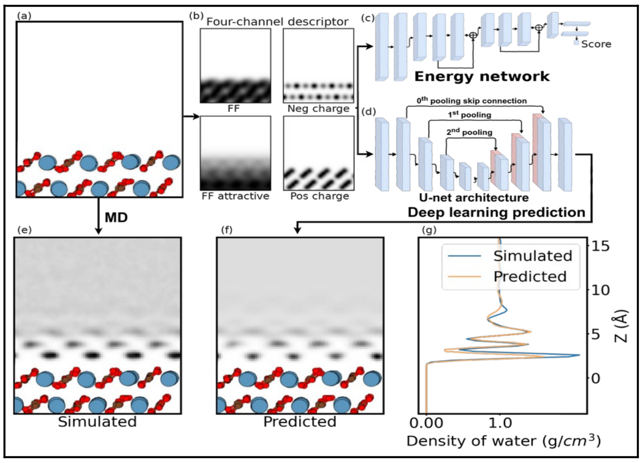
At solid-liquid interfaces, water forms hydration layers of varying densities at the interface. This interface has wide applications in technological and natural processes, which makes it crucial to study. These are governed by the nano-scale interactions at the interface. Atomic Force Microscopy (AFM) has gained prominence at understanding such interactions. However, AFM images need computationally intensive molecular dynamics (MD) simulation of accurate solid-liquid interfaces to complement the analysis. In previous work, we showed that machine-learning this interaction at the interface can lead to quick generation of hydration-layer densities for new surface topologies[1]. However, that method was limited to calcium, carbon and oxygen atom based surfaces. In this work, we introduce deep-learning methods to get an element-agnostic approach to predict the hydration surface. Further, we introduce energy-networks to estimate the errors the predicted hydration network would give on a hitherto unseen surface.

Figure 1: *Schematic for workflow for prediction of hydration layers over calcite surface. Blue, red and brown spheres are calcium, oxygen, and carbon atoms respectively.*



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Poster 33

Investigating UV-Induced Polymerization of Pre-Assembled Supramolecular Layers on Ionic Crystal Substrates

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On-surface polymerization is of growing interest for many applications in nanotechnology. A wide variety of chemical reactions have already been demonstrated to work on surfaces, however, mostly on metal substrates and by thermal activation of the covalent bond formation (for an overview, see [1]). On insulating substrates, only few work has been presented so far, the most promising use UV-illumination to activate the polymerization process [2-4] since thermal annealing does mostly result in desorption of the organic molecules.

In this work, we use the knowledge of a previous work [5] on the control of the supramolecular self-assembly of specially designed organic molecules. We present results on how the formation of radicals induced by UV-illumination in pre-assembled supramolecular layers influences the subsequent polymerization process and the re-organization of the structures formed. Molecules used are designed with halogen- as well as vinyl- endgroups.

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https://doi.org/10.1002/admi.201400414

Poster 35

Automated and highly accurate adjustment of a fibre interferometer for NC-AFM displacement detection

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Interferometry is a highly sensitive method for measuring the cantilever displacement in an NC-AFM. It is usually accomplished by placing the end of an optical fibre in a well-defined mean distance d to the cantilever back side so that both together form an optical cavity. As the cantilever oscillates, the light power returned by the fibre varies periodically yielding a time trace consisting of periods exhibiting inversion symmetry with respect of the signal inflection point for a perfectly aligned interferometer (Fig. 1(a)). If, however, the zero point of the cantilever oscillation is not exactly placed in the inflection point of the optical response function, the interferometer signal exhibits some asymmetry (Fig. 1(b)).

We introduce the automatic correction of any misplacement d_{err} of the cantilever oscillation zero position with a proportional/integral (PI) control loop. As the Fourier spectrum of the response of the perfectly aligned interferometer contains only odd harmonics, the second harmonic signal present for a misaligned interferometer is the perfect error signal for the control loop. The error signal is derived from the X output of a Lock-In detector locked to the second harmonic of the cantilever oscillation. The X output signal is processed by the loop operated at a set-point of zero signal and providing the output voltage acting on the piezo element controlling the fibre-cantilever distance d. As an example, Fig. 2 shows the error signal, the associated quadrature signal and the controller output voltage recorded over a period of 55.5 hours. The control loop compensates for thermal drift induced effects reflecting short term fluctuations, the day/night cycle and the long term temperature development with an accuracy in the d_{err} correction better that 1 nm. The residual error signal exhibits only a minute deviation from zero.

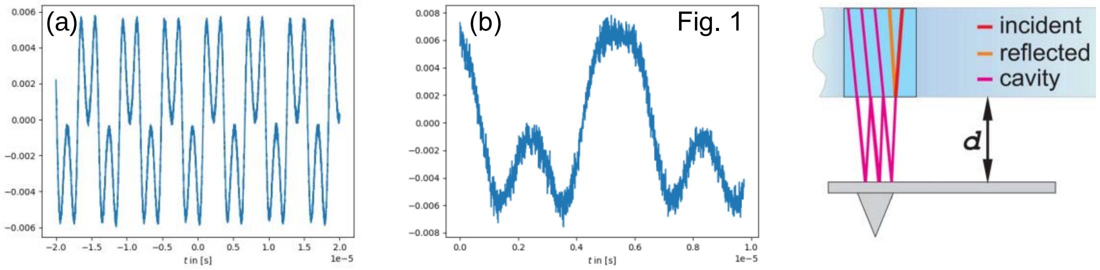

Fig. 1

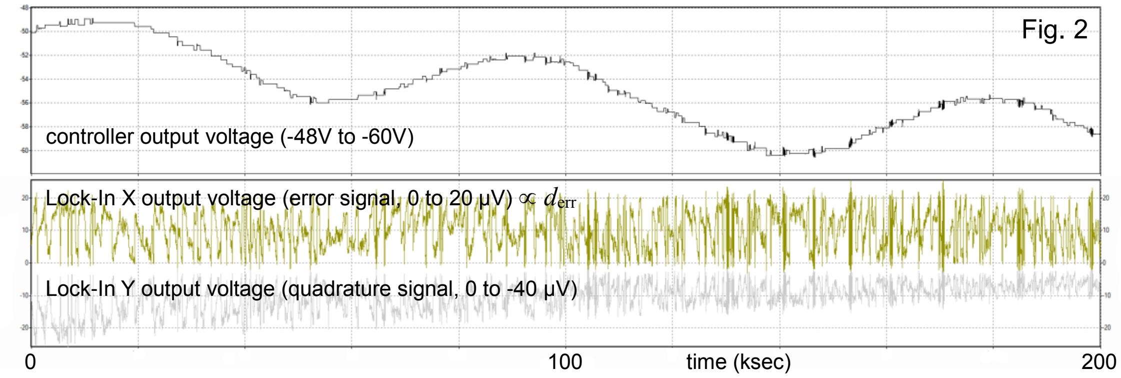

Fig. 2

Poster 37

Epitaxial Growth of Ultraflat Bismuthene with Large Topological Band Inversion Enabled by Substrate-Orbital-Filtering Effect

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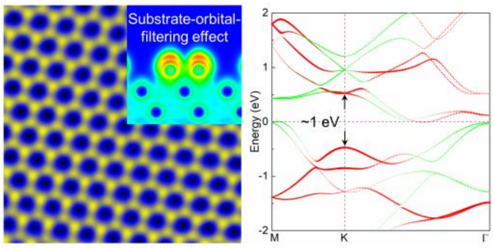
Quantum spin Hall (QSH) systems hold promises of low-power-consuming spintronic devices, yet their practical applications are extremely impeded by the small energy gaps. Fabricating QSH materials with large gaps, especially under the guidance of design principles, is essential for both scientific research and practical applications. Here, we demonstrate that large on-site atomic spin-orbit coupling can be directly exploited via the intriguing substrate-orbital-filtering effect to generate large-gap QSH systems and experimentally realized on the epitaxially synthesized ultraflat bismuthene on Ag(111). Theoretical calculations reveal that the underlying substrate selectively filters Bi pz orbitals away from the Fermi level, leading pxy orbitals with nonzero magnetic quantum numbers, resulting in large topological gap of ~1 eV at the K point. The corresponding topological edge states are identified through scanning tunneling spectroscopy combined with density functional theory calculations. Our findings provide general strategies to design large-gap QSH systems and further explore their topology-related physics.[1]



Ultraflat bismuthene on Ag(111)

Large topological band inversion

Figure 1: *Ultraflat bismuthene monolayer on Ag(111) with large topological band inversion.*

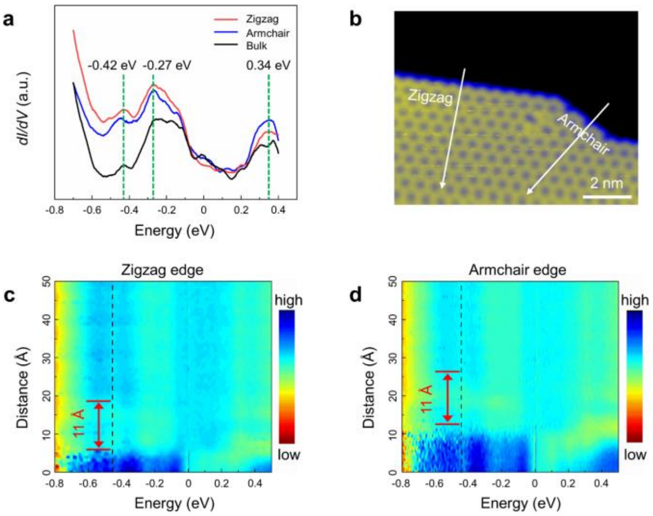


Figure 2: *STS measurements of the corresponding topological edge states.*

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Poster 39

Characterization of one-dimensional silicene structures on Au (110) by atomic force microscopy.

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Since the mechanical exfoliation of a single graphene layer from graphite [1], analogous nanoelemental 2D materials, generically termed Xenes, have attracted much interest in recent years [2]. Among them, silicene is structurally similar to graphene as it constitutes a two-dimensional honeycomb structure made of silicon atoms [3]. In contrast to graphene however, it is subject to a prominent atomic buckling depending on the underlying substrate [4]. To date, silicene was grown on Ag(111) [4] and on Ag(110) [5].

In this work, we explore the growth of silicon structures on Au(110) by means of scanning tunneling microscopy (STM) and atomic force microscopy (AFM). The adsorption of Si atoms on Au(110) below one monolayer (ML) leads to the formation of an extended alloy (Fig. 1a). Subsequent depositions above 1 ML then induce a restructuring of the surface into well-aligned silicon nanoribbons (Fig. 1b). AFM imaging is employed to characterize their structure with atomic precision.

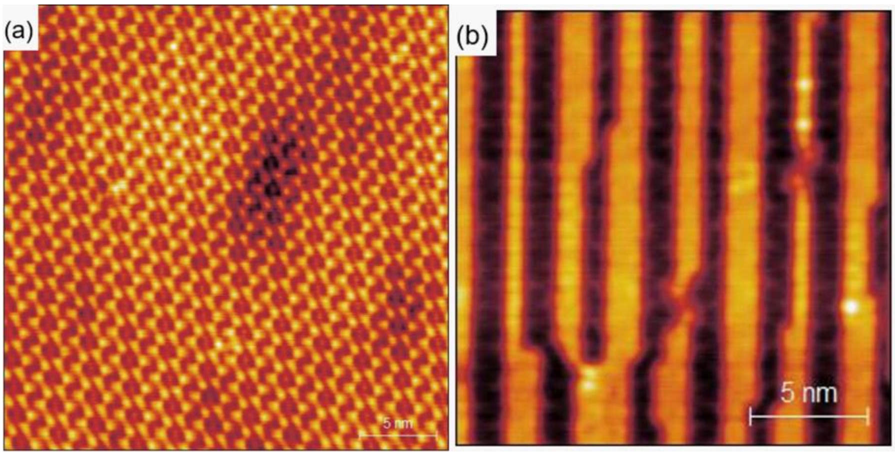

Figure 1: Atomic structure of silicene on Au (110). **a,** Atomically resolved filled-states STM image recorded at 0.2 monolayer of Si. **b**, High-resolution STM image showing the structure of the Si nanoribbons upon deposition above one monolayer coverage.

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Poster 41

Applications of the tuning fork planar probe: on-tip magnetic SPM sensor in UHV

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[1] Molecular Materials and Nanosystems - M2N – Eindhoven University of Technology - Netherlands
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A novel scanning probe microscopy (SPM) sensor is developed by Çiftçi *et al* [1,2] and introduce a large mass functionalized tip-on-chip called the planar probe for scanning probe microscopy (SPM). This approach offers a combination of multiple integrated tip functionalities such as local heating [3] and magnetic field sensing, see figure 1A. It also offers a future development platform for even more specific multifunctionalities possible for luminescent SPM or spin-polarized STM. With especially AFM developments towards combining multiple tip functionalities, transitioning away from the conical sharp tip and to a planar design offers more surface area to integrate these functionalities and materials near the tip end, yet still offering high resolution imaging. However, previous reported large mass tips have inevitable reduced the sensitivity (Q-factor) in AFM force sensing when combined with the self-sensing quartz tuning fork [1,2]. To go beyond these limitations mass balancing was combined with electrical retuning of the tuning fork, enabling the restoring of sensor sensitivity close to those of non-modified tuning forks [1,2]. An example of successful high resolution imaging with the planar probe of the 6R3 reconstruction of SiC graphene is given in figure 1B. This image was taken with the planer probe in NC-AFM in UHV. In this work we show functionalization of the tip-on-chip by incorporating electrically controllable magnetic field polarity in the tip-end. Furthermore, we will demonstrate a custom scan head modification for a commercial UHV SPM system which allows the integration of extra tip functionalization's. The tip-on-chip consists of an atomically sharp cleaved wafer which is functionalized with a magnetic layer that offers electrically and *in vacuo* control of the tip magnetic field. Image 1C shows imaged (MFM) magnetic layer variations on the tip as electrically controlled with a current pulse. Current applications of the planar probe are focused on studying the magnetic properties of transition metal oxide perovskites, see figure 1D. Strain engineering and atomically sharp layer thickness control are valuable tools in modifying the magnetic properties for example of LaMnO [4]. We study the morphology dependent magnetic properties of these materials in UHV with the planar probe.

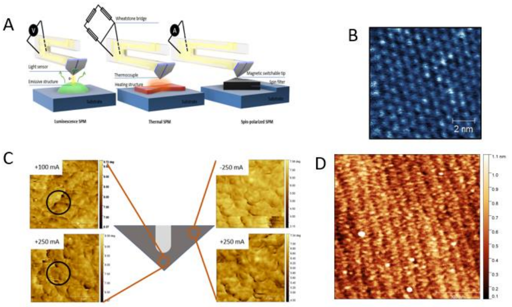

Figure 1: A. Proposed applications of the tip-on-chip planar probe especially for local heating and controlling magnetic interactions. **B**. High resolution NC-AFM image of SiC graphene in UHV. **C**. Electrical control of the magnetic layer in the tip imaged with MFM. **D**. Resolved transition metal oxide perovskite step-edges in UHV.

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Poster 45

Surface resistivity evaluated by frequency modulation atomic force microscopy through Joule heat energy dissipation

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It is beneficial that the conservative and non-conservative (dissipative) force interactions between a tip and a sample in proximity can be simultaneously examined by frequency modulation atomic force microscopy (FM-AFM). The frequency shift (Δf) of a cantilever oscillating at its resonance, measured in the FM-AFM, is approximately proportional to the derivative of conservative forces with respect to the tip–sample separation. Meanwhile, the non-conservative interactions are evaluated from the change in the cantilever excitation signal as dissipation energy under the constant oscillation amplitude (A) of the cantilever. The detected dissipation energy has been chiefly ascribed to Joule heat via displacement current [1] and to the hysteresis of forces between tip approach and retraction [2]. We had previously reported that the dissipation energy (D_J) due to Joule heat was proportional to the resonance frequency shift (Δf_{ele}) due to the long-range electrostatic force, independently of the tip–sample separation z and bias voltage V; these terms can be eliminated from the equation expressing its proportionality [3], as below:

$$D_J = -16\pi^3 \varepsilon_0 k A^2 \times R_J \times \Delta f_{ele}, \qquad (1)$$

where ε_0 is the permittivity of vacuum, k is the spring constant of the cantilever, and R_J is the resistance responsible for Joule heat. Figure 1 shows a typical example, independent of the bias polarity. From its proportional coefficient, the resistance R_J could be evaluated. The experimentally measured values were so high as of the order of GΩ for Si(111)-(7×7) using a Si tip. Recently, we reported that the proportionality held for metal films using a metal-coated Si tip, as well as thin dielectric films covering a metallic substrate [4]; in eq.1, the term of R_J was replaced by ($R_J + r_m \sin^2\delta$), where r_m is the resistance of the dielectric film, parallel to the capacitance in an equivalent circuit, and δ is the phase difference of the complex dielectric function of the dielectric film. This indicates that the proportionality for the dielectric films was partly coupled to dielectric energy loss; the evaluated values of the resistance were also high. The high values for the metal films would originate from inelastic scattering at the surfaces and interfaces, where the charge was moved by the tip approach and retraction with a fast relaxation time of 10^{-19} sec. At present, there is still room for consideration of the high values; whether were the measured surface resistances the same as those measured by contact probes or not? In the present study, we will reconsider the measured dissipation energy due to Joule heat, and discuss the surface resistances evaluated by the FM-AFM.

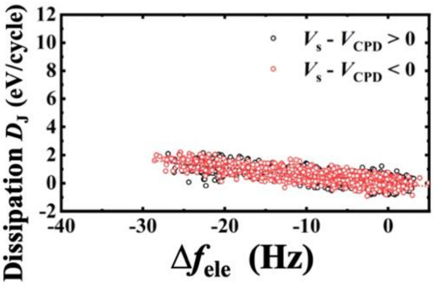

Figure 1: Linear relationship between D_J and Δf_{ele} for an Ir-thin film measured with a Pt Ir-coated Si

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[4] M. M. Hasan, T. Arai, and M. Tomitori, Jpn. J. Appl. Phys. published online (2022).

Poster 47

In-situ characterization of atomic friction of pristine and Nitrogen-doped graphene in ultrahigh vacuum

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Graphene, as a two-dimensional material, offers a unique frictional property and has shown exciting applications in micro- and nanoelectromechanical systems (MEMS/NEMS) [1]. Atomic-level chemical doping can significantly alter the frictional properties of graphene [2,3]. After the deposition of a C_{60} nano-flake as a mask on graphene/Ir(111) surface by thermal evaporation, the sample was exposed to a nitrogen radical flux produced by a remote RF plasma source. Nano-patterned N-doped and pristine graphene surface was obtained. By the means of high-resolution ultrahigh vacuum atomic force microscopy, in-situ comparison between pristine graphene and N-doped graphene on Ir(111) surface has been revealed in both contact and bimodal mode.

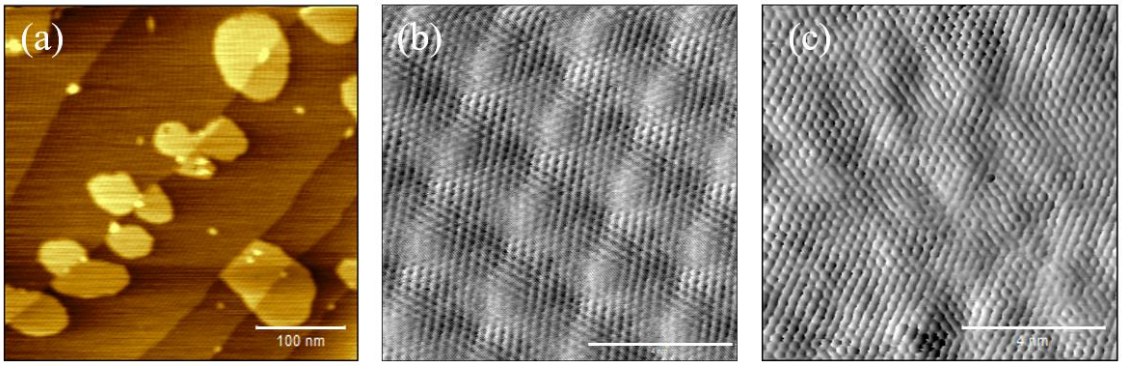

Figure 1: *(a) Large-area non-contact AFM topography image of C60 molecules absorbed on graphene/Ir(111) surface, (b) atomic-resolution lateral force map of pristine graphene on Ir(111), (c) atomic-resolution lateral force map of N-doped graphene. The scale bar corresponds to 100 nm, 4 nm, 4 nm, respectively.*

[1] A. K. Geim, et al., Nature **499**, 419-425 (2013)
[2] L. S. Panchakarla, et al. Adv. Mater. **21**, 4726–4730 (2009)
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Poster 49

Oscillatory behavior of dissipation energy in hydration layers at the interface between a nanometer-thin water film and a KBr(100) surface observed by frequency modulation atomic force microscopy

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High-resolution observations of water–solid interfaces using frequency modulation atomic force microscopy (FM-AFM) have successfully revealed the structures of hydration layers with molecular-level resolution [1]. Therein the eigenfrequency shift of a cantilever oscillating at its resonance was utilized, which corresponds to the conservative force interactions between a tip and a sample. Meanwhile, the FM-AFM can simultaneously detect the nonconservative force interactions through the measurement of dissipation energy of the oscillation cantilever; this would shed light on the different viewpoints for such dynamic nanomechanical analysis of hydration structures [2]. We found that nanometer-thick water films (NWFs) were formed on hydrophilic solid surfaces in high-humid environments and the hydration layers were formed at the interface between the NWF and the solid surface, similarly to solid-water interfaces in bulk water, although the separations between hydration layers in the NWF were narrower than those in bulk water. The narrower separations indicate that they would be rigidly bonded [3,4]. In the present study, an NWF was formed on a cleaved KBr(100) surface at a high humidity of about 70%, the interface between the NWF and the KBr surface was scanned two-dimensionally in a Z-X plane, where Z and Z denote the vertical and horizontal axes to the surface, respectively, and 2D maps of the force and dissipation energy were simultaneously depicted. We discuss the dynamical behaviors of the hydration structures in the NWF using the tip pushing the film.

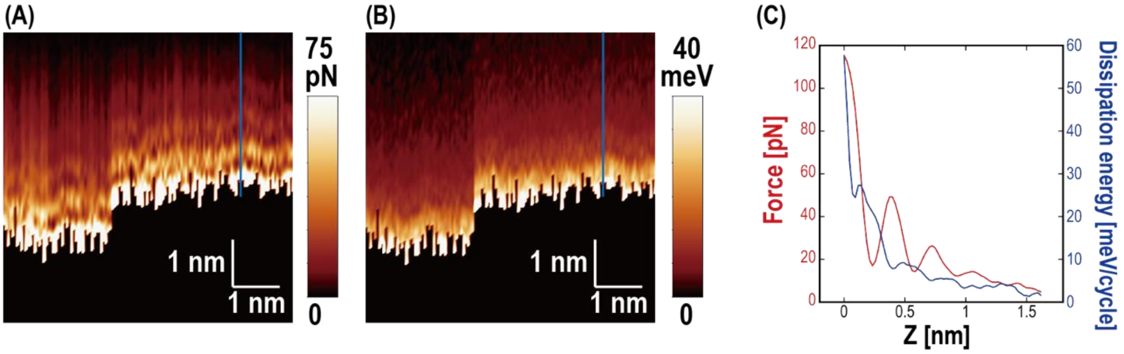

Figure 1: *(A) and (B) Z-X plane maps of the force and the dissipation, respectively, for the hydration layers at the interface between the NWF and the KBr(100) surface, at a humidity of 73% and the oscillation amplitude of 100 pm. (C) Cross-sectional line profiles along the blue lines in (A) and (B). Both profiles exhibited oscillatory behaviors.*

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[2] K. Umeda, K. Kobayashi, T. Minato, and H. Yamada, Phys. Rev. Lett. **122**, 116001 (2019).
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Poster 51

Development of a low-temperature scanning probe microscopy setup to study atomic-scale magnetism in 2D materials

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A few or single layers of van der Waals materials have attracted huge interest in the past years. Many of these 2D materials host a wealth of different quantum phases, e.g., novel types of charge and spin orders at the atomic scale that are often driven by electron correlations. Metallic and semiconducting van der Waals materials have been studied a lot over the past years down to a single material layer using scanning probe techniques (STM and nc-AFM). Recently, layered magnetic materials have also raised high interest as they show interesting properties such as 2D ferromagnetism [1] and switching of the magnetism via electric fields [2]. However, layered magnetic materials have been scarcely investigated so far at the atomic scale, especially regarding their magnetic properties. One reason may be that, in contrast to graphene or some transition metal dichalcogenides, layered magnetic materials are highly reactive and it is challenging to create clean surfaces. In addition, these materials are often poorly conducting which makes their magnetic properties inaccessible to the routinely-used spin-polarized STM method. To this end, magnetic exchange force microscopy (MExFM) [3] would be advantageous as it does not require a conducting material and it can resolve non-collinear magnetic ground states at the atomic scale [4].

Here, we present the design of a home-built combined STM/nc-AFM setup working at 1K based on a JT-stage with 4He, operating in a 3T out-of-plane magnetic field. The goal of the setup is to independently study the geometric, electronic and magnetic structure in insulating quantum phases of 2D materials, as well as at phase transitions to conducting phases, utilizing nc-AFM, KPFM and MExFM. A gating stage will allow to study 2D materials in a device geometry. The setup will be optimized for fast sample turnaround times and will allow for single-atom deposition at cryogenic temperatures.

[1] C. Gong, *et al.,* Nature **546**, 265-269 (2017).
[2] B. Huang, *et al*., Nat. Nanotechnol. **13**, 544-548 (2018).
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[4] N. Hauptmann *et al*., Nat. Commun. **11**, 1197 (2020).

Poster session B, Tuesday, August 2nd 2022

P02 **Hapala, Prokop** *Integrated simulation package for on-surface chemistry and SPM*

P04 **Nicolini, Paolo** *Ultra-low friction and edge-pinning effect in large-lattice-mismatch van der Waals heterostructures*

P06 **Yogi, Priyanka** *Manifestation of intermolecular interaction of hydrogen with a single VOPc molecule on the Au(111) surface*

P08 **Navarro, Gema** *Nanographene on surface: Direct electrospray deposition compared to on surface cyclodehydrogenation from precursor molecule*

P10 **Pawlak, Rémy** *Coupling quantum states engineered in nanoporous molecular networks to an atomic force microscope*

P12 **Gisbert, Victor G.** *Nanomechanical Mapping of Ultrathin Interfaces with Bimodal Atomic Force Microscopy*

P14 **Duan, Sisheng** *High-Chern-Number Topology in a Two-dimensional Kagome Ferromagnet*

P16 **Weindl, Adrian** *Characterization of defects in the topological insulator* Bi_2Se_3 *at the picometer scale*

P18 **Heile, Daniel** *Measuring the charge state of a metal nanoparticle by the charge compensating bias method*

P20 **Guevara Parra, Jose Maria** *How covalent chemistry affects the surface dipole of metallic nanostructures*

P22 **Bustamante, José** *Electrostatic Force Microscopy to study single dopant atoms encapsulated in Silicon*

P24 **Suvachintak, Netaji** *Scanning Probe Force Microscopy on GaN/AlGaN based Nanowire*

P26 **Ritz, Christian** *Three-dimensional photoinduced force microscopy and its interpretation*

P28 **Choi, Hyoju** *Capillary Force Microscopy: A Novel Non-Contact Imaging Method*

P30 **Laflör, Linda** *Mapping the axial interaction forces with a carboxylic acid dimer*

P32 **Boisvert, Catherine** *Single Electron Spectroscopy on Metalloenzymes*

P34 **Koall, Maximilian** *Towards characterisation, exploration, and manipulation of molecules on surfaces with haptic feedback*

P36 see Tuesday, 10:00.

P38 **Lotze, Christian** *Resolution of Intramolecular Dipoles and a Push-Back Effect of Individual Molecules on a Metal Surface*

P40 **Vennema, Hester** *Performance of an electrically driven q-plus sensor in a commercial Joule Thomson STM*

P42 **Kumar, Saravana** *Does the electrostatic decay length in highly concentrated electrolytes increase with concentration?*

P44 **Godey, Sylvie** *Modification by electrical stimuli of molecular assemblies composed of azobenzene derivatives*

P46 **Liu, Danyang** *Cobalt nano-island growth on* $Cu_3Au(111)$

P48 **Kangül, Mustafa** *Open Source SPM Controller*

P50 **Zutter, Marco** *Analysis of Force Volume Data gathered with the Intermodulation AFM Method at Cryostatic Temperatures with a Tuning Fork*

Poster 2

Integrated simulation package for on-surface chemistry and SPM

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On-surface chemistry complemented with scanning probe microscopy (SPM) opens a completely new area of single-molecular organic synthesis and nano-fabrication. But this unparalleled level of atomic control and insight can be achieved only by close collaboration between SPM experiments with simulations. Currently these simulations are often unnecessarily costly and laborious due to lack of optimized software. Therefore, we are developing a new integrated package dedicated to autonomous search for absorption geometries of molecules on substrate and simulation of respective AFM images (https://github.com/ProkopHapala/FireCore). We aim to (1) streamline and speed-up these simulations to enable high throughput screening of chemical reactions and molecular architectures on surface and (2) to simplify the simulations to such a degree which allows it to be used by non-experts and experimentalists. Significant speed-up necessary for this goal is achieved by combination of density functional theory with classical force-fields in QM/MM manner, and by extensive use of GPU acceleration.

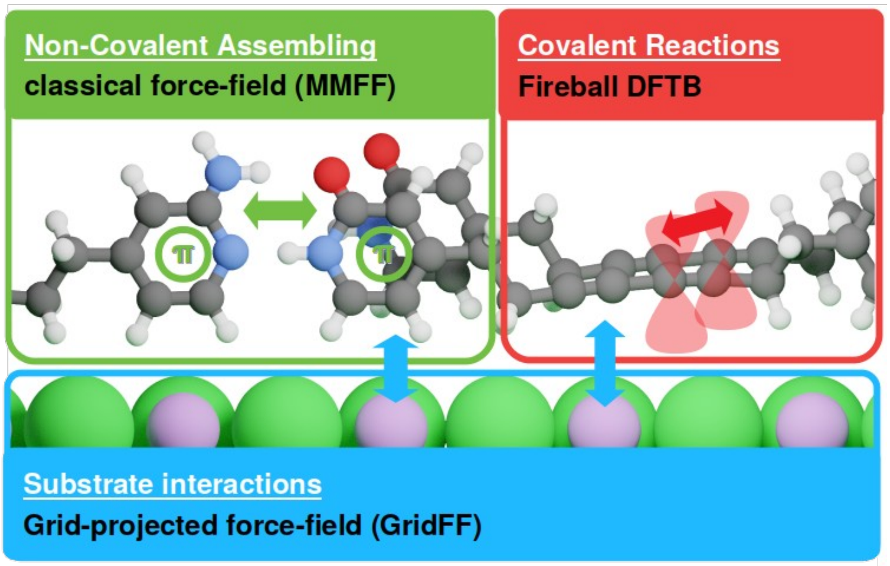

***Figure 1** : Schematic illustration of different aspects of on-surface chemistry simulations, and methods used for their efficient description.*

Poster 4

Ultra-low friction and edge-pinning effect in large-lattice-mismatch van der Waals heterostructures

Mengzhou Liao,[1,2] **Paolo Nicolini**,[2,3,*] Luojun Du,[1,4] Jiahao Yuan,[1,5] Shuopei Wang,[1,6] Hua Yu,[1,5] Jian Tang,[1,5] Peng Cheng,[7] Kenji Watanabe,[8] Takashi Taniguchi,[8] Lin Gu,[1,5] Victor E. P. Claerbout,[2] Andrea Silva,[9] Denis Kramer,[9,10] Tomas Polcar,[2,9] Rong Yang,[1,6], Dongxia Shi,[1,5,6] Guangyu Zhang,[1,5,6]

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[3] Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic
[4] Department of Electronics and Nanoengineering, Aalto University, Tietotie, Finland
[5] School of Physical Sciences, University of Chinese Academy of Sciences, Beijing, China
[6] Songshan Lake Materials Laboratory, Dongguan, China
[7] Oxford Instruments (Shanghai) Co. Limited, Shanghai, China
[8] National Institute for Materials Science, Tsukuba, Japan
[9] National Centre for Advanced Tribology (nCATS), Department of Mechanical Engineering, University of Southampton, Southampton, United Kingdom
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Heterostructures made up of two-dimensional materials are excellent platforms to achieve twist-angle-independent ultra-low friction due to their weak interlayer van der Waals interactions and natural lattice mismatches. However, for finite-size interfaces, the domain edges can still play a role on the friction process, and their overall effect remains still unclear. In a recent publication[1], we reported on the superlubricity phenomenon and on the edge-pinning effect for the MoS_2/graphite and the MoS_2/h-BN heterostructures (two prototypical 2D materials). By means of atomic force microscopy experiments, we found that the coefficients of friction of such interfaces can be below 10^{-6}. The relevance of our findings is at least twofold: on the one hand we have proved that the contribution to friction coming from the contact area is basically vanishing for van der Waals heterostructures (the value of coefficient of friction that we estimate is the lowest reported in the literature so far), but on the other hand we have shown that a non-vanishing component of friction (which scales with the flake's perimeter) is still present. The latter aspect (and in particular the supporting computational study) is the main focus of this contribution. In fact, molecular dynamics and static simulations corroborate the experimental findings, and help to clarify the role of domain edges and interface steps in the friction process. Thanks to a detailed structural and energetic analysis, it was possible to highlight the contribution of sulfur atoms placed at the edge of the flakes. They turned out to present enhanced distortions (with respect to the atoms in the center of the flake) and they are more prone to get locked into locally commensurated structures. This then leads to the above-mentioned edge-pinning effect, and ultimately brings a greater contribution to the final friction force. The results provide more information on the sliding mechanism of finite low-dimensional structures, which is vital to understand the friction process of laminar solid lubricants.

[1] M. Liao, P. Nicolini *et al.*, *Nat. Mater.*, **21**, 47-53 (2022).

Poster 6

Manifestation of intermolecular interaction of hydrogen with a single VOPc molecule on the Au(111) surface

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Non-contact atomic force microscopy (NC-AFM) with functionalized tip mostly by carbon monoxide molecule have achieved sub-atomic resolution of chemical structures of molecules. Recently, hydrogen molecule (H2) also can be used to improve spartial resolution of a single molecule on NC-AFM. However, the dynamic behavior of hydrogen molecule interacting with molecule underneath needs further investigation at atomic scale. In the present study, Vanadyl Phthalocyanine (VOPc) molecules were deposited on Au (111) surface, resulting on sitting mostly at the kink sites of Herringbone structure with oxygen atom up or down from the surface.To understand the dynamic behavior of H2, random telegraphic noise (RTN) in tunneling current using STM were measured by placing the tip on the VoPc molecule. The tunneling spectra shows switching between two states with different tunneling conductance as a function of sample bias voltage and RTN measured near transition voltage between the two states. Spatial variation of the RTN indicates that the two-state fluctuation depende on the atomic-scale interaction of H2 with VOPc molecule. AFM was used to investigate dynamic behavior of hydrogen molecule, which can be trapped and released between a tip and a VOPc molecule junction depending on bias voltages. The trapped hydrogen molecule can be used to image inter-molecular structure, which cannot be achieved by normal STM and AFM imaging. Figure 1 shows the AFM images of VOPc molecules using bias voltages of 60 mV (without hydrogen) and 10 mV (with trapped hydrogen), which clearly visualize the internal molecular structure with hydrogen. Theoretical calculation shows that a H2 molecule trapped by a combination of a tip-induced electrostatic potential well and the potential formed by a VOPc underneath. Present study suggests the origin of two-state noise as transition of H2 between minima in these potentials with barrier height of 20–30 meV.

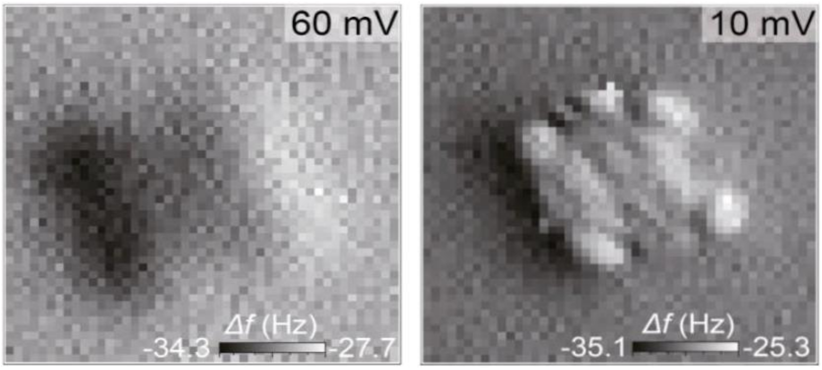

Figure 1: *AFM images of a single VOPc molecule with bias voltage of 60 mV (left) and 10 mV (right) configurations on gold. Image size:* $(3\text{nm})^2$

Poster 8

Nanographene on surface: Direct electrospray deposition compared to on surface cyclodehydrogenation from precursor molecule

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On-surface synthesis is a well established technique to obtain very large covalently bounded structures on surfaces, from a specifically designed small precursor molecule. Specially, it is a well advanced method to obtain atomically precise graphene nanoribbons [1]. On-surface cyclodehydrogenation can also be used as an efficient alternative approach to synthesize nanographenes (NGs) that cannot be obtained in solution because of stability and/or solubility issues. In particular, when it is combined with an high vacuum electrospray deposition (HV-ESD) setup [2], the on surface reaction process can be applied to high-molecular-weight compounds such as dendritic polyphenylene precursors (PPs) [3].

In the present work, we study the adsorption of the nanographene C_{96}-$6C_{12}$ molecule (Fig. 1a) on the Au(111) surface after its deposition via high vacuum electrospray deposition. We performed nc-AFM imaging at room temperature to characterize the molecular assemblies (see topography image in Fig. 1b). On the other hand, a second path to form this nanographene is also investigated, by the deposition of the precursor molecule preC_{96}-$6C_{12}$ (Fig. c). Our goal is to characterize the precursor, before and after annealing of the surface to reveal structural changes and possible on-surface cyclodehydrogenation reaction leading to the formation of the C_{96}-$6C_{12}$ nanographene.

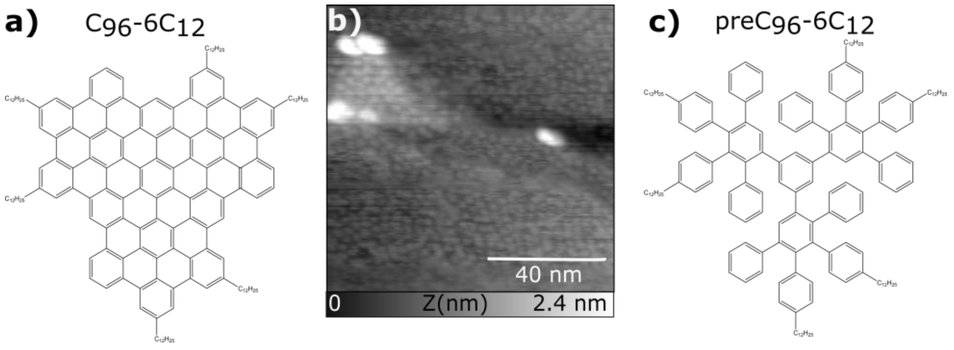

Figure 1: *a) Molecular structure of the nanographene* C_{96}-$6C_{12}$ *molecule. b) Low resolution non-contact AFM image of* C_{96}-$6C_{12}$*/Au(111). c) Structure of the compound pre*C_{96}-$6C_{12}$*.*

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[2] S. Scherb et al., Commun Mater **1**, 1 (2020).
[3] I. C.-Y. Hou, A. Hinaut, Chem. Asian J., e202200220 (2022).

Poster 10

Coupling quantum states engineered in nanoporous molecular networks to an atomic force microscope

Philipp D’Astolfo,[1] Xing Wang,[2] Xunshan Liu,[2] Marcin Kisiel,[1] Carl Drechsel,[1] Alexis Baratoff,[1] Ulrich Aschauer,[2] Silvio Decurtins,[2] Shi-Xia Liu,[2] **Rémy Pawlak,[1,*]** Ernst Meyer[1,*]

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Periodic confinement of surface electrons in atomic structures or extended nanoporous molecular networks is the archetype of a two-dimensional quantum dot (QD) superlattice [1]. Yet, an electrical control of such an artificial lattice by external gating has never been demonstrated. In work, we show the mechanical coupling between an atomic force microscope (AFM) and quantum states engineered in highly crystalline nanoporous molecular networks on Ag(111). We characterize local density of states (LDOS) using scanning tunneling microscopy (STM). Low-temperature force spectroscopy reveals force/dissipative responses at threshold voltages that arise from charging/discharging of the superlattice’s eigen-states under the local electric field of the tip. We infer the quantum capacitance and resonant tunneling rates, opening new avenues in the characterization of exotic phenomena in designer quantum materials via a nanomechanical oscillator.

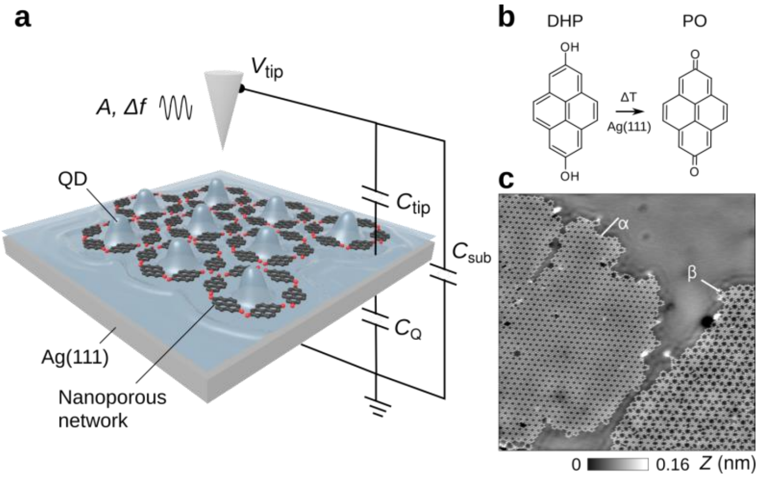

Figure 1:* *a, *Schematic of the experiment: An oscillating AFM probe is capacitively coupled to the confined state of surface electrons in a nanoporous molecular network.* C_{tip} *and* C_{sub} *refers to the capacitance of tip and substrate, respectively.* C_Q *is the quantum capacitance of the ”minibands” emerging in the artificial superlattice.* ***b,*** *Surface oxidation of 2,7-dihydroxypyrene (DHP) into pyrene-2,7-dione (PO).* ***c,*** *STM overview of the α- and β-assemblies of PO molecules on Ag(111).*

[1] M. F. Crommie, C.P. Lutz, and D.M. Eigler. Science 262, 218–220 (1993).
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Poster 12

Nanomechanical Mapping of Ultrathin Interfaces with Bimodal Atomic Force Microscopy

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Accurate nanoscale measurement of the mechanical properties of interfaces and thin layers is of great importance in materials science and biology. Bimodal AFM [1] is one of the most advanced nanoscale techniques for the measurement of the elastic modulus of interfaces. In nanometer-thin materials, the bottom effect [2-4], this is the influence of the rigid support, produces an overestimation up to a 10-fold factor during the determination of the nanomechanical properties. This makes semi-infinite models inappropriate to describe the mechanical response of thin samples such as lipids and proteins when the indentation is comparable to the thickness of the material. Here we develop a bottom-effect correction for bimodal AFM that measures the real Young's modulus value of thin films independent of its thickness [5-6].

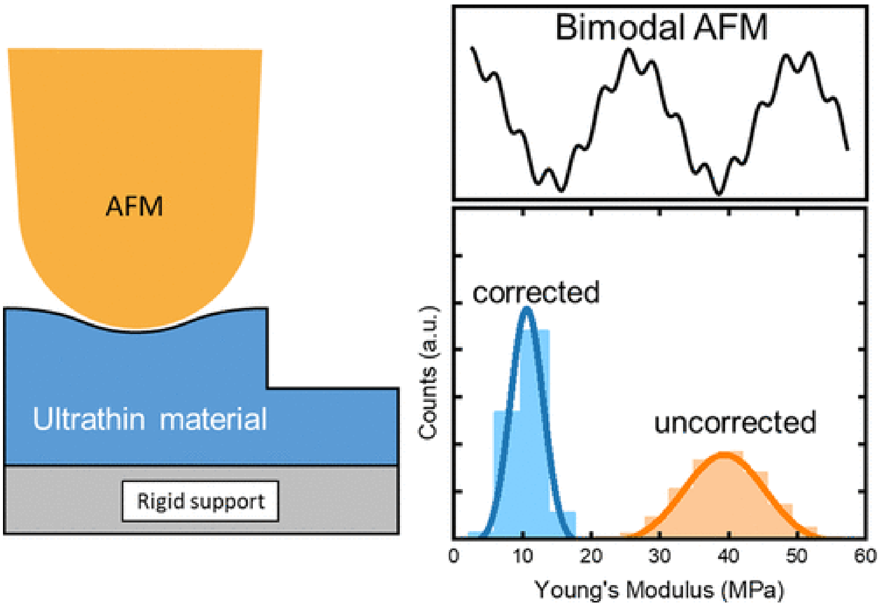

Figure 1: *Scheme of a tip, ultrathin-layer and solid support interface. The bimodal AFM measurement of the nanomechanical properties of such a system yields an overestimation of the Young's modulus due to the bottom effect. With the bottom effect correction, the corrected value of the Young's modulus is measured.*

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[4] S. Chiodini, S. Ruiz-Rincón, P. D. Garcia, S. Martin, K. Kettelhoit, I. Armenia, D. B. Werz, P. Cea, *Small* **16,** 2000269 (2020).
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Poster 14

High-Chern-Number Topology in a Two-dimensional Kagome Ferromagnet

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The interplay between ferromagnetic order and nontrivial topology provides fertile ground for developing novel quantum phases, such as quantum anomalous Hall effect (QAHE) and axion insulator states. Whereas the two-dimensional (2D) materials with intrinsic ferromagnetism and nontrivial topology are rare. Here, we report the epitaxial growth of single-layer iron germanide (FeGe) kagome nanoflakes with room-temperature ferromagnetism and high Chern number topology. Using the scanning tunneling microscopy/spectroscopy and non-contact atomic force microscopy, we reveal that the edge states residing on the nanoflakes originate from nontrivial band structures with Chern number |C| = 3. Meanwhile, the X-ray magnetic circular dichroism (XMCD) measurements confirm a ferromagnetic ground state with a Curie temperature above 300 K in the atomically thin FeGe, which is verified by density functional theory and Monte Carlo simulations. Apart from the intrinsic magnetic topological states hosting chiral edge modes, the realization of kagome magnets in the 2D limit also holds promise for future studies of geometric frustration.

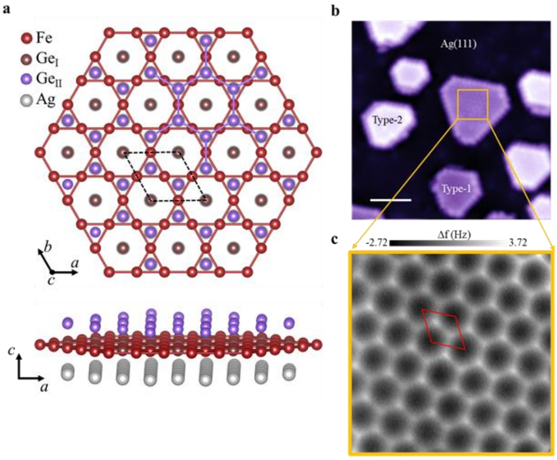

Figure 1: Atomic-scale structure of FeGe nanoflakes on Ag(111). *a) Top view and side view of the atomic model. The FeGe unit cell highlighted by a dashed rhombus corresponds to a (√3×√3)R30° supercell of the underlying Ag(111) surface. b) STM topographic image (set point: Vs = -0.30 V, I = 100 pA) shows two different FeGe nanoflakes observed on Ag(111), namely type-1 and type-2. Scale bar, 40 Å. c) Atomically resolved nc-AFM image captured in the orange square in (b) shows a honeycomb lattice formed by GeII atoms. Scale bar, 6 Å. The red rhombus indicates the FeGe unit cell corresponding to the dashed one in (a).*

Poster 16

Characterization of defects in the topological insulator Bi_2Se_3 at the picometer scale

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Topological insulators are a class of materials that are semiconducting or insulating in their bulk but possess topologically-protected gapless states at their boundaries. Bi_2Se_3 is a promising material for applications due to its large bulk band gap and single surface state Dirac-cone. Pure electric conduction exclusively via the topological surface state is, however, hampered due to an n-type doping caused by the presence of native point defects, especially Se vacancies.

Here, we apply high-resolution atomic force microscopy for real-space imaging and determination of the polarity of surface defects in Bi_2Se_3. We observe surface defects ranging from a single missing Se atom to defects composed of multiple missing Se atoms in the surface layer and find a positive polarity for all Se vacancies confirming them as electron donors. Our work establishes AFM as a powerful method for atomic-scale studies of topological insulator surfaces, opening the possibility to more precisely determine the physical properties of defects in topological insulators.

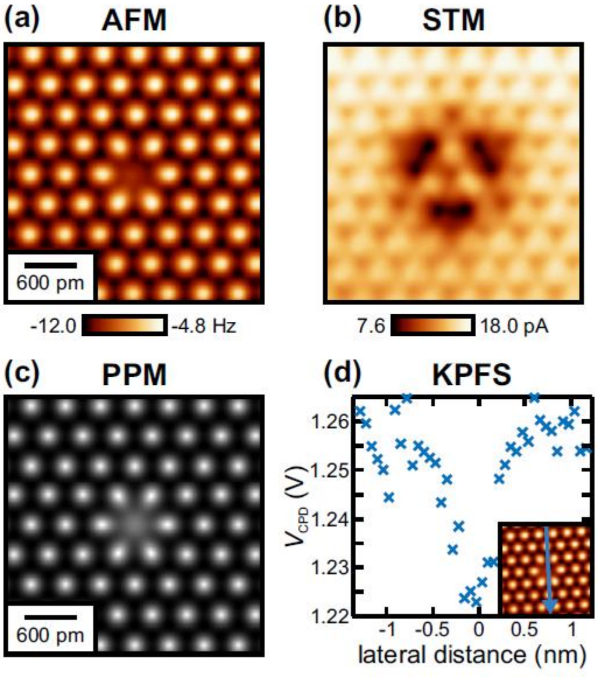

Figure 1: *Single-atom Se surface vacancy. (a) Constant height Δf image of a single Se vacancy in the surface layer of Bi_2Se_3. (b) Simultaneously recorded tunnelling current map at V_b = -200mV. (c) Simulated image of a surface Se vacancy using the Probe Particle Model. (d) Kelvin probe force spectroscopy data recorded across the surface vacancy (see inset).*

Poster 18

Measuring the charge state of a metal nanoparticle by the charge compensating bias method

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We introduce a two-step procedure for quantitative nanoscale charge measurements with the charge compensating bias method (CCB) that is similar to Kelvin probe force microscopy (KPFM) and utilises recently introduced protocols for precisely measuring force curves [1]. First, distance-dependent data of the capacitance signal (measured at twice the modulation frequency) is used to determine system parameters for the electrostatic model [2]. Second, the KPFM weight function for charges [3] is calculated from these parameters at each given point charge position. The circular symmetry of the problem allows the radial projection of each charge position surrounding the tip onto one linear axis. For a fit of the model to the experimental data, surrounding charges are combined to effective charges $q_\mathrm{i}^\mathrm{eff}$ reducing the overdetermined parameter space (Figure 1a). The fit of distant-dependent CCB data yields the magnitude of the central charge q_0 below the tip and estimates for the surrounding effective charges $q_\mathrm{i}^\mathrm{eff}$ and contact potential difference V_CPD (Figure 1b).

We demonstrate the capability of this approach by measuring charge states of gold nanoclusters supported by a $CeO_2(111)$ substrate. The CCB voltage $V_\mathrm{Bias}^\mathrm{COMP}$ is systematically measured as a function of the tip-sample distance for a set of oscillation amplitudes and post-processed by the presented two-step procedure. We determine the charge magnitude of the central Au cluster $q_0 = (22 \pm 3)e$ as the main result (Figure 1c), and estimates for the contact potential difference V_CPD (Figure 1d) as well as the magnitudes of the surrounding effective charges (Figure 1e) with little variation for the data obtained at different amplitudes.

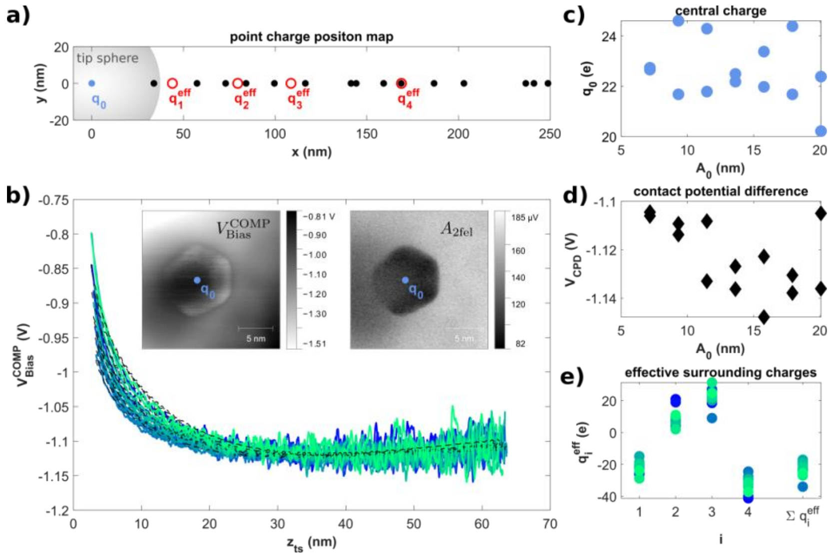

Figure 1: *Charge quantification by the CCB method with a two-step procedure.*

[1] D. Heile *et al.*, Phys. Rev. B **103**, 075409 (2021).
[2] A. Sadeghi *et al.*, Phys. Rev. B. **86**, 075407 (2012).
[3] H. Söngen *et al.*, J. Appl. Phys **119**, 025304 (2016).

Poster 20

How covalent chemistry affects the surface dipole of metallic nanostructures

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Scanning probes experiments often encounter nanostructures of undercoordinated metal atoms, either as the investigated system or, quite generally, at the tip apex. While the electrostatic properties of extended planar surfaces are textbook material, the interaction of metal adatoms with the surface and with each other opens an interesting playground in which local electrostatic potential can be designed. At the same point, our intuition for the covalent chemistry of such metal structures is limited.

Here we investigate Ag and Au nanostructures, namely adatoms, monoatomic chains and small clusters, on the Ag (111) surface using quantum dot microscopy (SQDM) [1, 2]. We image the electrostatic potential above these nanostructures (Fig. 1) and quantify the respective surface dipoles. The two species of adatoms behave antagonistic, as the surface dipoles are positive for Ag and negative for Au structures. Moreover, for Ag structures, the dipole magnitude per atom decays asymptotically when lengthening the structures, while it stays constant for Au.

The measured dipoles are in excellent agreement with density functional theory calculations. We disentangle the influence of individual adatoms-surface and adatom-adatom bonds down to individual atomic orbitals.

As a mean of extending the SQDM method to a wide variety of nanoscale systems, we also present a recently developed sample holder, which supports independent preparation but simultaneous loading of two different samples into the SPM

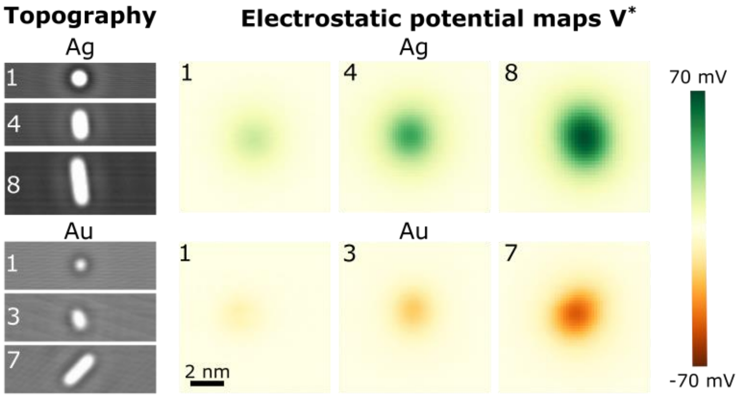

Figure 1: Topography and SQDM electrostatic potential images of monoatomic Ag and Au chains on the Ag (111) surface.

[1] C. Wagner, et al. Phys. Rev. Lett. **115**, 026101 (2015)
[2] C. Wagner, et al. Nat. Mater. **18**, 853-859 (2019)

Poster 22

Electrostatic Force Microscopy to study single dopant atoms encapsulated in Silicon

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[2] London Centre for Nanotechnology, University College London, London WC1H 0AH, U.K.
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Atomic scale position control of single dopant atoms in silicon, using Scanning Tunneling Microscopy (STM) and hydrogen resist lithography, has enabled the fabrication of prototype devices for future classical and quantum computing. In the fabrication process, phosphorus or arsenic atoms are positioned with atomic precision on the surface of pure silicon and encapsulated with an additional layer of silicon [1]. This technique allows to reach the limit of single dopant atom devices [3], with promising advantages for Quantum Information Technology. Several questions remain unanswered about the properties of single dopant atoms encapsulated in silicon. For instance, how is their energy level structure affected by the environment? How far do single dopants diffuse in a silicon crystal? How does the coherence time of two entangled dopants change as a function of environmental variables? Electrostatic force microscopy, with single electron sensitivity (eEFM) is a technique that could offer answers to these questions. eEFM has been used to study metal nanoparticles, semiconductor quantum dots and single molecules, but never an engineered nanostructure [2]. We have built a new Atomic Force Microscope, tailored to investigate electrically contacted single electron transistors defined by a single dopant atom as well as the coupling between individual dopant atoms. I will present an overview of the project and preliminary results on the performance of our new instrument.

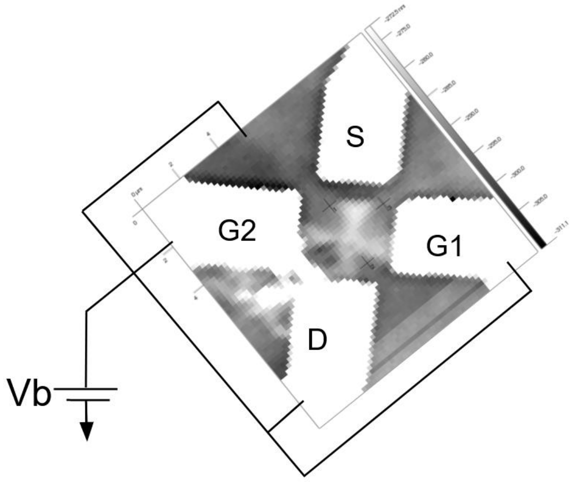

Figure 1: *Topography scan of the contacts of a quantum dot Single Electron Transistor built with hydrogen resist lithography. The indicated Souce (S), Drain(D) and two gates (G1,G2) are metal regions that connect to encapsulated dopant atom contacts leading to the SET.*

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[3] X. Jehl, Y. Niquet and M. Sanquer, *J. Phys.: Condens. Matter* **28**, 10 (2016).

Poster 24

Scanning Probe Force Microscopy on GaN/AlGaN based Nanowire

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GaN/AlGaN based nanoscale devices have witnessed immense growth in the recent past owing to their properties like faster switching speed, higher thermal conductivity and lower on state resistance etc. With the feature size of these devices getting smaller, understanding the changes in the properties becomes much more important than ever. As the device dimensions get into the nanoscale domain, the analysis of carrier transport becomes a lot more difficult as it starts to depend on a number of effects which don’t play a significant role in the micro-scale domain. Hence, in our study, we have tried to map the properties of a GaN/AlGaN based nanowire (NW) e.g. the local resistance, surface potential, tunneling current, surface topography and piezoelectric properties. We have also mapped the change in the properties of the nanowire with the change in the dimension of the contacts. Kelvin Probe Force Microscopy (KPFM) has been performed to map the potential profile along the nanowire and to estimate quantitatively the no. of surface states and traps in the nanowire. Scanning Thermal Microscopy (SThM) has been performed to map the heat profile and Conductive Atomic Force Microscopy (CAFM) has been performed to get the current-voltage characteristics of the nanowire.

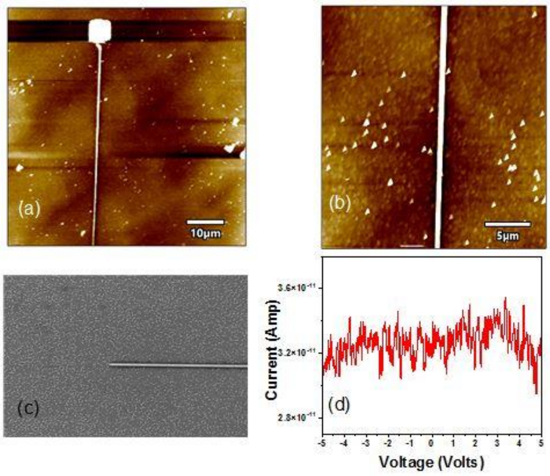

Figure 1 : *Some typical images for the nanowire : (a) AFM image of the NW with contact (b) NW AFM image (c) SEM image of the NW (d) Current-voltage characteristics of the NW*

[1] Clement Marchat, et al., Nanoscale. Res. Lett.**14**, 398 (2019).

[2] Sarah R. McKibbin, et al., Nano Lett. **20**(2), 887-895 (2019).

[3] Shujie Wang, et al., Nanoscale Res. Lett**. 6**, 541 (2011).

[4] Mengchen Huang, et al., APL Mater. **1**, 052110 (2013).

Poster 26

Three-dimensional photoinduced force microscopy and its interpretation

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Photoinduced force microscopy (PiFM) is an emerging field of AFM and aims to measure local light-matter interactions. Spectral data from IR-based experiments generate chemical maps. It is widely accepted that IR-induced signals originate from tip-enhanced absorbance and subsequent thermal vibration of the sample. In the region of visible wavelengths, the contrast is usually explained by changes in the refractive index and by dipole-dipole forces. The exact origin, however, remains disputed and depends on sample and setup [1].

Measurements of the three-dimensional (3D) force field bring clarity to this matter. Our 3D method uses frequency-modulated AFM [2] and is applicable for well-controlled heterodyne PiFM [3]. Our method provides stable and reliable measurements of the force field directly above the sample and can be used for fast scans on samples with difficult topography.

A 3D scan of a gold nanoparticle is shown in Fig. 1. A vertical slice through the scan at the line indicated in (a) shows similarities between the PiFM signal (b) and the derivative of the simultaneously measured force gradient (c). This suggests a vibration-induced origin of the force. The signal depends on the local curvature of the sample, the sample material, the tip geometry, and, most of all, the tip–sample distance. This can lead to a misinterpretation of PiFM signals when only classic 2D scans are considered. Topography- and material-induced crosstalk through the second gradient can be misinterpreted as a plasmonic effect where none is present.

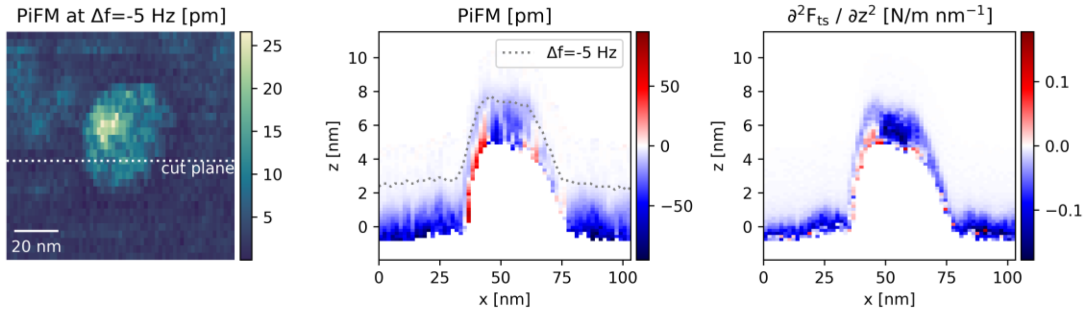

Figure 1: *Three-dimensional PiFM measurement of a gold nanoparticle. (a) PiFM signal extracted at a virtual setpoint of Δf = -5 Hz; (b) PiFM signal and (c) second gradient of the overall force field as a vertical slice through the 3D measurement at the line indicated in (a).*

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Poster 28

Capillary Force Microscopy: A Novel Non-Contact Imaging Method

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Atomic force microscopy (AFM) very often causes damage to the tip and the sample due to the tip scanning in nanometric proximity to the sample surface. While there exist several methods of the non-contact operations, exploiting the dynamic characteristics of cantilevers [1, 2], it is still a challenge to achieve true non-contact, non-destructive imaging in AFM in ambient air. Here, we present a novel method for noncontact imaging, ‘capillary force microscopy’. We use a quartz tuning fork-based, shear-mode atomic force microscope and utilize a nanometric water bridge naturally formed between the tip and the sample [3, 4]. Prior to the scanning, we form the capillary bridge between the etched gold tip and the sample surface, and then we set the amplitude setpoint for the feedback to be a value of amplitude that is changed only by the capillary interaction without the tip-sample mechanical hard-contact. The resolution of the new mode is limited by the thermodynamics of capillary bridge; the bridge grows or evaporates depending on tip’s lateral speed and vertical position, and the z-feedback fluctuates accordingly, around 3 nm in our experiments. The capillary force microscopy could offer true non-contact, non-destructive imaging method in ambient air.

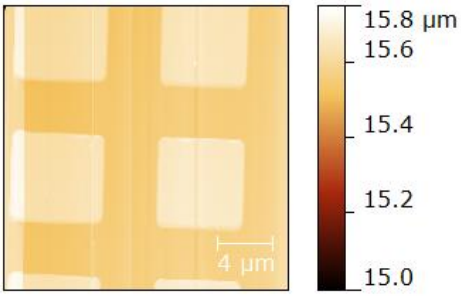

Figure 1: *Capillary force microscopy of a standard sample with rectangular columns.*

[1] R. Garcia and R. Perez, Surf. Sci. Rep. **47**, 197 (2002).
[2] Franz J. Giessibl, Rev. Mod. Phys. **75**, 949 (2003).
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Poster 30

Mapping the axial interaction forces with a carboxylic acid dimer

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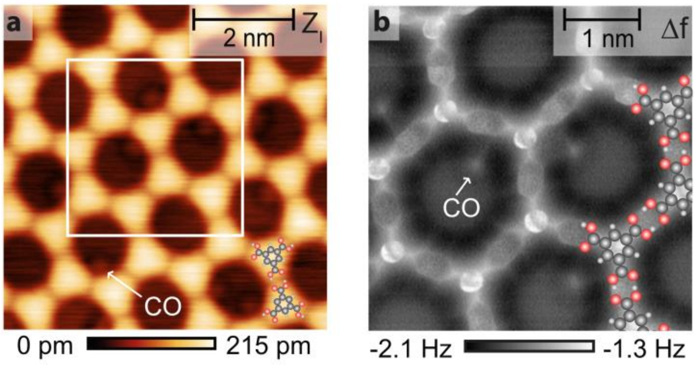
The description of hydrogen bonds clarified the understanding of biochemical structures and processes, including the DNA as life's basic building block or the catalytic activity of enzymes [1]. On surfaces, the imaging of hydrogen bonds with NC-AFM has intensively been discussed [5-7] after the observation of bond-like features at a hydrogen bond position [2-4] opposed reports of apparent bonds [8].
Here, the force field axial to a carboxylic acid dimer is mapped within the hydrogen-bonded honeycomb network (HON) of trimesic acid (TMA) on Au(111). The HON consists of a self-assembled pore structure stabilised by carboxylic acid dimers. Due to the large pore size [9], the carboxylic acid dimers are rather isolated from each other. Systematic force mapping experiments are conducted and force curves are analysed at different positions of this sample system including the hydrogen bond area, the trimesic acid molecule, and the pore area. Force curves acquired within the void pores allow the subtraction of site unspecific forces. At all positions, comparably small attractive short-range forces with a maximum of around 50 pN are observed. Repulsive forces are strongest at the benzene centre and weakest at the hydrogen bond position. Mapping the axial interaction forces allows comparing experimental results with the theoretical concepts of high resolution NC-AFM.



(a) Scanning tunnelling microscopy (STM) and (b) constant-height NC-AFM images of TMA on Au(111) assembled in the HON structure. Molecular models of TMA are included to scale. Imaging parameters STM: I*=5 pA,* U_s*=50 mV. NC-AFM:* f_0*=26172 Hz,* U_s*=0 V.* T_s*=5 K.*

[1] S. Schreiner, J. Indian Inst. Sci. **100**, 61 (2020)
[2] M. Ellner, et al. Nano Lett. **16**, 1974 (2016).
[3] M. Ellner, et al. ACS Nano **13**, 786 (2019).
[4] P. Hapala, et al. Phys. Rev. B **90**, 085421 (2014).
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Poster 32

Single Electron Spectroscopy on Metalloenzymes

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Single-electron electrostatic force microscopy (e-EFM) has been a useful method for probing nanoscale systems and extracting quantum properties. With this AFM technique, we can mobilize and probe single-electron transfers in structures with discrete electronic states. By monitoring the frequency shift and dissipation of our oscillating conductive cantilever, we induce electron tunneling events and determine quantum dot density of states, measure single electron tunneling rates, and observe transitions between quantized nuclear vibronic states at the single-molecule level [1-3]. Recently, e-EFM has been of great interest to understand redox energetics and electron transfer rates of metalloenzymes, two fundamentally quantum derived processes that underpin catalytic activity. Specifically, we would like to use our home-built low-temperature atomic force microscope (LT-AFM) to image single-electron transfers in single- and multi-redox site metalloenzymes. With e-EFM, we will be able to determine Franck-Condon factors associated with redox transitions, measure energetic offsets, and map electronic coupling between redox centers [3,4]. This will allow us to understand and engineer the catalytic activity of metalloenzymes in an effort to develop sustainable energy solutions [5].

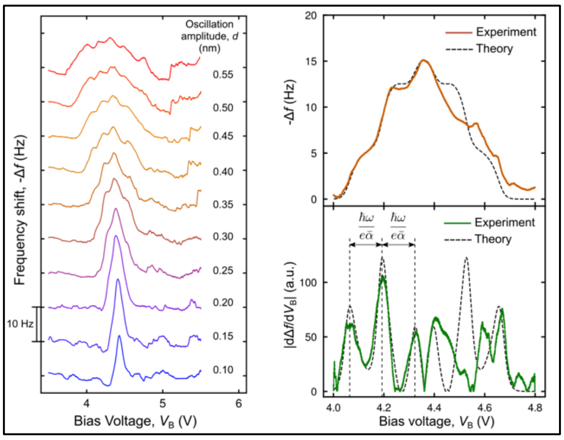

Figure 1: *Frequency shift as a function of bias spectroscopy (Ferrocene molecule). Vibronic energy and tunnelling rate can be extracted from the derivative of the frequency shift response [1].*

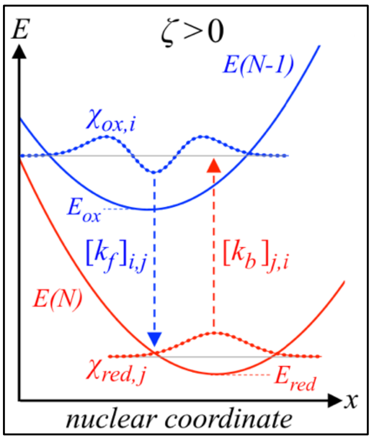

Figure 2*: Energy picture of electron transfer to a molecule. Nuclear wavefunctions can be seen for oxidized and reduced states, and their associated Franck-Condon factors [3].*

[1] A. Roy-Gobeil, Y. Miyahara, K. H. Bevan, P. Grütter, Nano Lett **19**, 6104-6108 (2019).
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Poster 34

Towards characterisation, exploration, and manipulation of molecules on surfaces with haptic feedback

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Modern experiments with scanning probe microscopy (SPM) demand both an intuitive tip positioning with picometer precision and an intuitive access to picometer resolved physical data acquired in the three-dimensional space above a sample. However, the overly exact control in an actual heuristic situation on the one hand and the interpretation of the tip and surface state basically resting on time-consuming two-dimensional data on the other hand slows down experiments substantially. One would prefer to directly control the tip position by macroscopically moving the hand within the three dimensional space and have the tip following the position of the hand at the microscopic scale several orders of magnitude below the haptic dimensions. Along these lines, approaches have already been presented where virtual reality techniques have been adapted to control scanning probe experiments [1,2].

Additionally, it is desirable to have an immediate feedback from the measurement signals that reflect the interaction of the tip with the sample. An instantaneous reaction of the experimenter to the measurement observables would both reveal critical situations for the probing tip and enable novel manipulation and measurement protocols. Both aspects are difficult to achieve in most classically controlled situations, not only because of complicated user interfaces often hindering immediate reactions, but also due to the inherent projection on two dimensions of the underlying three-dimensional problem.

Here, we introduce an approach to interface the data analysis work station as well as the scan controller with a haptic device for both exploring pre-recorded data and controlling the tip. While the setup can on the one hand be used for exploring pre-recorded three-dimensional data, the system shows its strength best when the hand-controlled motion of the haptic device is directly translated into the motion of the tip, in both cases with the device providing tactile feedback depending on the data at the tip position. Conductivity landscapes and force fields of pristine and adsorbate-covered surfaces can be explored physiologically by hand and accelerated tip preparation processes or atom manipulation procedures are possible.

We present the *“offline”* implementation for pre-recorded two- and three-dimensional data in a complete virtual environment (Unity), allowing for an improved intuitive understanding of the data recorded of the well-studied system PTCDA on Ag(111) [3]. Furthermore, we discuss the approach to interface this system with the scan controller for *“online”* experiments. A 3D Systems Touch X device is used to provide tip control and haptic feedback. The physical observable (i.e. tunnelling current, frequency shift, damping, force, or others) at the tip position in the recorded data is translated into a haptic feedback consisting of either a force guiding the device or a vibration with adjustable intensity. Various transfer functions translating the physical observables to haptic feedback are developed and investigated for their usability in the laboratory. After investigating the parameter space for the implemented haptic transfer functions, useful setups could be identified that promise to unravel the great potential for a simplification and acceleration of the work flow in SPM experiments.

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Poster 38

Resolution of Intramolecular Dipoles and a Push-Back Effect of Individual Molecules on a Metal Surface

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Molecules consisting of a donor and an acceptor moiety can exhibit large intrinsic dipole moments. Upon deposition on a metal surface, the dipole may be effectively screened and the charge distribution altered due to hybridization with substrate electronic states. We study Ethyl-Diaminodicyanoquinone molecules on a Au(111) surface with scanning tunnelling microscopy (STM) and non-contact atomic force microscopy (nc-AFM). By mapping the local contact potential difference (LCPD) over the flat lying molecules we show that the intrinsic dipole moment of the molecules persists upon adsorption on the Au(111) surface. Density functional theory calculations reveal that the dipole moment is even increased on the metal substrate as compared to the gas phase. Overall, the LCPD value is decreased by several tens of meV with respect to the bare metal as a consequence of the so-called push-back or cushion effect [1].

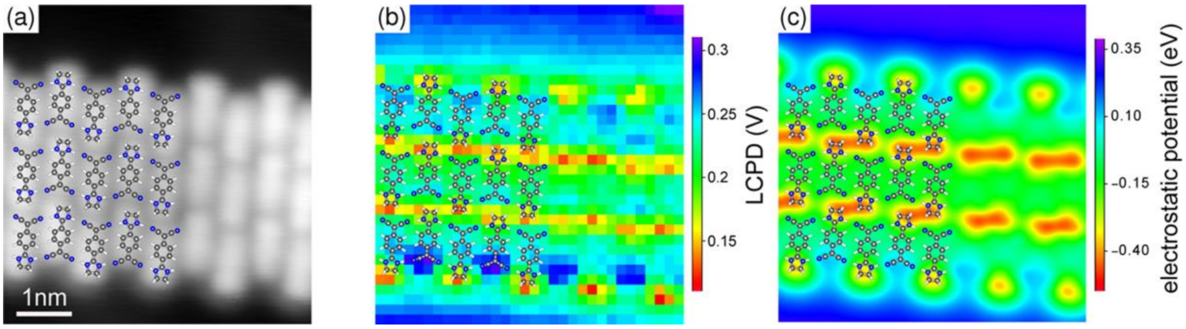

Figure 1: (a) STM topography of a three-molecule-wide chain ethyl-DADQ adsorbed on a Au(111) surface (b) LCPD values extracted from a grid of spectra along the same area as in (a). (c) Calculated electrostatic potential of a three-molecule-wide chain.

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Poster 40

Performance of an electrically driven q-plus sensor in a commercial Joule Thomson STM

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The q-plus sensor is a wide-spread tool for performing combined STM-AFM measurements in ultra-high vacuum at cryogenic temperatures. Commercial JT-STMs are typically equipped for specific cantilever designs operating at very high frequencies [1]. Replacing broken or outdated sensors with original components tends to be costly and time consuming. In order to gain flexibility we decide to implement the use of q-plus sensors in a JT-STM. Contrary to other set-ups in which q-plus sensors are used, we do not drive our sensor mechanically, via an excitation of the Z-piezo, but electrically, with the excitation signal directly sent to the tuning fork.

In order to characterize the performance of our homemade q-plus sensors we develop a set-up to test their response to an electrical drive in ambient conditions. Following M. Lee et al. [2], we can disentangle the mechanical and electrical response of the sensors to the driving signal. After transfer into the JT-STM we demonstrate the possibility to use electrically driven q-plus sensors for combined STM-AFM measurements: with a Q factor around 20000 we can control the amplitude of the oscillation to be as low as 70 pm. Our first principle measurements are performed on a $CuCl_2$/Cu(100) surface. We are able to move single Cl vacancies to create vacancy patches similarly to what is done with an STM tip that doesn't vibrate [3]. We investigate with local contact potential difference (LCPD) measurements the local change of work function that leads to the confinement of field emission resonances above such vacancy patches.

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Poster 42

Does the electrostatic decay length in highly concentrated electrolytes increase with concentration?

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Abstract

The interaction between charged surfaces is important in many industrial applications as well as a wide variety of fields such as colloidal science, biology, geology, renewable energy etc... DLVO theory successfully explains the long-range interaction between charged surfaces in low electrolyte concentrations. DLVO theory is expected to break down when the Debye length (λ_D) becomes smaller than the size of electrolytes. However, the general consensus was that the decay length of the electrostatic interactions decreases with increasing concentration even beyond the regime in which DLVO theory is strictly valid. Recent studies[1-3] report that the decay length of electrostatic interaction forces at solid-electrolyte interface exhibit a non-monotonic behaviour. While in the low concentration regime, the decay length agrees with the Debye length and decreases with concentration, the opposite trend follows for concentrations whose $a/\lambda_D > 1$, where a is the average ion diameter. In this work, we conduct an independent study, where interaction forces are measured between silica surfaces in alkali-halide salt solutions over three orders of magnitude of concentration(1mM to 5M). We find that the decay lengths do not increases with increasing concentration in highly concentrated electrolytes for different temperatures, pH and ion size. Our experiments are complemented by DFT calculations using a primitive model, where the electrolytes are modeled as charged hard-spheres in a bulk medium.

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Poster 44

Modification by electrical stimuli of molecular assemblies composed of azobenzene derivatives

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In recent years, molecular switches such as azobenzene adsorbed on metal surfaces have attracted considerable attention due to their potential use in nanotechnology, information storage or molecular electronics [1,2]. In particular, the 3,3',5,5'-tetra-tert-butylazobenzene (TBA) molecule is a promising candidate for such studies, due to the four lateral tert-butyl-groups which act as "spacer leg" to reduce the electronic coupling between the active part of the molecule (azobenzene) and the metal surface. This azobenzene derivative switches reversibly between the two isomeric states (*trans*-TBA and *cis*-TBA; Fig. 1a). This isomerization has already been demonstrated by STM using either the electric field induced by the STM tip [3] or by exposure to UV or blue light [4].

Here we report an other effect of electric field for one monolayer TBA coverage on Au(111). After the TBA evaporation, molecules are organized on the Au(111) surface in the *trans* isomer with four lobes corresponding to the 4 "legs", with an apparent height of 0.25 ± 0.02 nm (Fig. 1b 1c 1e). STM imaging at 77K reveals domains only visible in negative polarity; by scanning theses TBA assemblies at -2V (Fig. 1b) bright spots appear, with an apparent height of 0.36 ± 0.05 nm confirmed by nc-AFM. These spots are usually associated to the formation of *cis*-TBA molecules, induced by the *trans*-TBA to *cis*-TBA isomerization under the presence of an electric field[3]. For domains imaged by STM with both polarities, an in plane rotation of TBA network is observed in STM and nc-AFM images, after scanning at a negative polarity (-1V). The origin of this in plane rotation will be discussed. These results show how crucial are the intramolecular and molecular-substrate forces control and understanding in the perspective of molecular electronics.

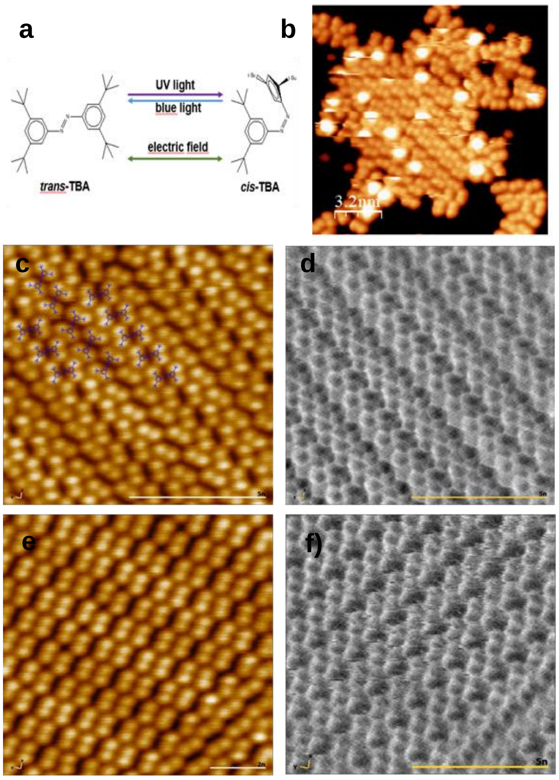

Figure 1: a) Isomerization of the TBA molecule with light or electric field between the two isomers *trans*-TBA and *cis*-TBA; b) STM image of TBA on Au(111), V = -2.0 V, I = 20 pA showing bright spots corresponding to cis isomers; c) e) STM images (+1V- 3pA) and d) f) constant height nc-AFM images of the same TBA domain before and after scanning in STM mode at -1V (3pA) respectively.

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Poster 46

Cobalt nano-island growth on $Cu_3Au(111)$

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The growth of thin films and nanostructures on solid surfaces is governed by the substrate structural properties and lattice matching. In this respect, an interesting alternative to conventionally utilized pure metal substrates are metallic alloys, mainly due to a larger flexibility in the effective lattice parameter. One of the candidates is the binary alloy Cu3Au, recently employed to grow large insulating copper-nitride islands [1]. Cu3Au is also a classical example of a system that undergoes a first order order–disorder phase transition that alters its electronic structure due to the emergence of new Brillioune zone boundaries. [2]

In our work, we investigate the structural and electronic properties of Cu3Au(111) surface employing STM and nc-AFM. Employing a novel multi-frequency lock-in amplifier (MLA) technique [3] for dIdV mapping and making use of CO molecules as scattering centers, we probe and compare the surface state dispersion on the ordered and disordered phase. Furthermore, we demonstrate the crystal's potential as a substrate for the growth of cobalt islands as an alternative to Co/Cu(111) [4]. One of the main assets is the possibility to grow the islands at elevated substrate temperatures up to 350 ºC without significant alloying of cobalt with the Cu_3Au. We explore structure of the islands and characterize their magnetic properties with conventional STS and nickelocene-terminated tip [5].

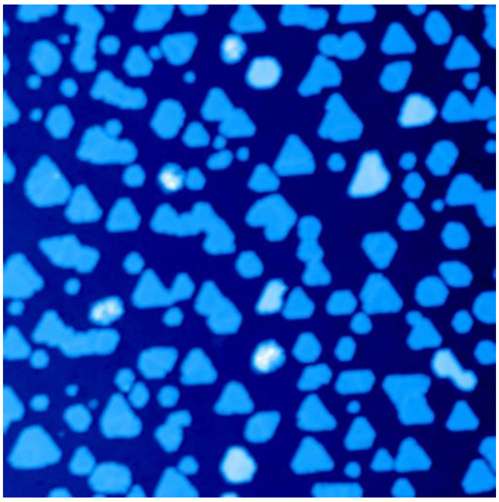

***Figure 1:** Growth of magnetic cobalt nano-islands on $Cu_3Au(111)$ substrate. ($100x100\ nm^2$)*

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Poster 48

Open Source SPM Controller

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By the nature of research and development, custom needs that cannot be solved by off-the-shelf products often arise. As we are working on new Scanning Probing Microscopy (SPM) techniques we didn’t want to be limited by the commercial instruments. This has brought us to develop our own home-built modular SPM controller.

The control electronics (Fig. 1a) consists of a real time FPGA controller (NI-7856R), interconnect boards to implement digitally controlled signal conditioning such as filters, gain, and offset stages, and a microscope adapter board to easily customize the controller for the interested microscope. The microscope is controlled through a custom software suite developed in the graphical programming language LabView (Fig. 1c). This platform has already been adapted to control different SPMs such as contact mode AFM, AM-AFM, high-speed off-resonance tapping mode AFM [1][2], scanning ion microscopy [3], correlative AFM/SEM [4], and STM.

We have experienced that our scientific and industrial collaborators are interested in our controller to adapt and use in their own systems. Hence, we have decided to share our controller platform in an open-source fashion. While developing our SPM controller, we aimed to improve the accessibility, mainly through additional documentation efforts and supporting resources such that adopting the platform becomes easier for new users and developers. For the electronic and mechanical components, the documentation comprises design files, manufacturing guides, and assembly notes. The provided design files are schematics, layouts, bill of material (BOM), functional descriptions for the electronics, and 3D CAD and production drawings for the mechanics. By nature, software development requires a different documentation strategy. Documentation explaining the functionality of the real-time controller is provided, while the user interface side of the software is documented with user guides.

Here we report an FPGA based open source SPM controller platform built in a modular fashion at hardware and software levels. It is not only an inexpensive yet high-performance SPM controller alternative but also a solution for the custom needs of researchers by providing user control over the modules of the platform.

Figure 1: *Open source SPM controller consists of an FPGA-based modular controller electronics (a), a high voltage amplifier (b), a software suite with the real-time controller and the user interface (c).*

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Poster 50

Analysis of Force Volume Data gathered with the Intermodulation AFM Method at Cryostatic Temperatures with a Tuning Fork

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We like to present here the analysis of the force volume data which we can acquire within a single scan pass using mixing products of different tones. The limitation for the acquisition of force volume data were already addressed by us with the development of an advanced measurement method that uses multiple drive tones and their mixing products [1-3].

The data gathered from these intermodulation AFM measurements is multidimensional in nature and everything is stored within the frequency space from the measurement. Therefore, multiple analysis steps are necessary to change the measured raw data into a model that explains the force interactions between the tip of our tuning fork and the sample. To correctly gauge the force volume data, the intermodulation AFM measurements need to be compared with traditional frequency shifts z-spectroscopies which can be analysed using the well known Sader-Jarvis method. The force volume data is then further fitted with a model containing a combination of the different interaction forces to correctly describe the tip-sample interaction and learn more about any given sample.

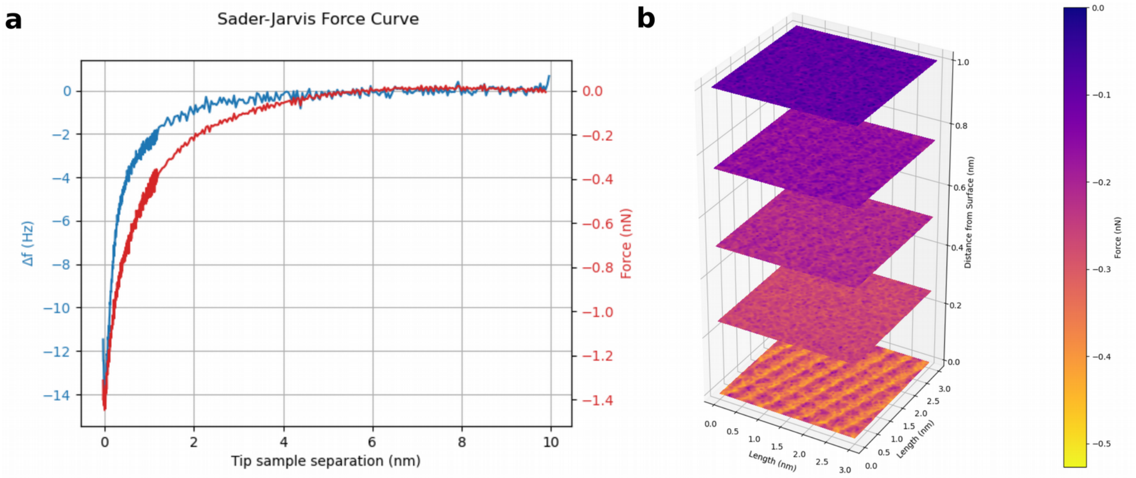

***Figure 1. a:** z-spectroscopy force curve analysed with the Sader-Jarvis method used as a guideline to further analyse the 3-dimensional force volume data form intermodulation AFM measurements. **b:** Multiple cuts through the 3-dimensional force volume above a 3 nm by 3 nm NaCl sample surface with a total z-height of 1 nm between the highest and lowest measurement point.*

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	Sunday Jul 31st	Monday Aug 1st	Tuesday Aug 2nd	Wednesday Aug 3rd	Thursday Aug 4th	Friday Aug 5th
09:00 – 09:20		Registration	Priante	Setvín	Wrana	Scherb
09:20 – 09:40			Brown	Glatzel	Sokolović	Laflör
09:40 – 10:00			Yamamoto	Miyazaki	Heggemann	Liu
10:00 – 10:20			Jugade	Cowie	Li, Y.-J.	Pawlak
10:20 – 10:40		Coffee				
10:40 – 11:00						
11:00 – 11:20		**Welcome**	Sellies	Pérez	Telychko	de Campos Ferreira
11:20 – 11:40		Ebeling	Martin Jimenez	Vilhena	Gou	Sekatskii
11:40 – 12:00		Schwarz, U.	Sugawara	Gallardo	Behn	Khachatryan
12:00 – 12:20		Štich	Heile	Henry	Spiegelberg	**Closing remarks**
12:20 – 12:40		Lunch				
12:40 – 13:00						
13:00 – 13:20						
13:20 – 13:40						
13:40 – 14:00					**Excursions** (13:40–16:00)	
14:00 – 14:20		Zahl	da Lisca	Nam		
14:20 – 14:40		Eftekhari	Hoffmann-Vogel	Ollier		
14:40 – 15:00		Oinonen	Navarro Rodriguez	Song		
15:00 – 15:20		Coffee				
15:20 – 15:40						
15:40 – 16:00						
16:00 – 16:20	**Welcome reception** Fort Boven-Lent	Schwarz, A.	Su	Ihle		
16:20 – 16:40		Giessibl	Gisbert	Ventura-Macias		
16:40 – 17:00		Weiss	Siretanu	Loppacher		
17:00 – 17:20		Stilp	Ikarashi	Li, C.		
17:20 – 17:40						
17:40 – 18:00		Poster session A	Poster session B			
18:00 – 18:20					**Conf. photo** (18:15)	
18:20 – 18:40					**Dinner** Landgoed Brakkesteyn (18:30–22:30)	
18:40 – 19:00						
19:00 – 19:20						
19:20 – 19:30						