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Deutsch-Französische Hochschule

2nd German-French Summer School on noncontact atomic force microsccopy

Universität Osnabrück

September 12th to 16th 2016

Organisers: Clemens Barth and Michael Reichling

Website

www.root-1.de/2nd_nc-AFM_school

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Adam Foster	Aalto University Helsinki (FI)
Sébastien Gauthier	CEMES Toulouse (FR)
Benjamin Grévin	CEA-CNRS-UJF Grenoble (FR)
Angelika Kühnle	Johannes Gutenberg-Universität Mainz (DE)
Jeppe Lauritsen	Aarhus University (DK)
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Laurent Nony	IM2NP Marseille (FR)
Steffen Porthun	RHK Technology (US)
Philipp Rahe	University of Nottingham (UK)
Michael Reichling	Universität Osnabrück (DE)
André Schirmeisen	Justus-Liebig Universität Gießen (DE)
Alexander Schwarz	Universität Hamburg (DE)
Ralf Bechstein	Johannes Gutenberg-Universität Mainz (DE)

Practical Training

Matthias Temmen and Fabian Schlage (Universität Osnabrück, DE)

Virtual AFM Training

Filippo Federici Canova and John Tracey (Aalto University Helsinki, FI)

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Program

	Sunday	Monday	Tuesday	Wednesday	Thursday	Friday
08:30 – 09:00	Arrival	Registration				
09:00 – 10:30		Reichling Introduction	Schirmeisen Force sensors	Gauthier Imaging molecules	Nony Kelvin probe force microscopy	practical training
10:30 – 11:00		coffee	coffee	coffee	coffee	coffee
11:00 – 12:30		Bechstein Imaging modes	Rahe Methods in force measurements	Kühnle Imaging in liquids	Grévin Photovoltaic materials	practical training
12:30 – 14:00		lunch	lunch	lunch	lunch	Departure
14:00 – 15:30		Foster Simulation	Lauritsen Oxides	Porthun Lock-In, PLL and control loops	practical training	
15:30 – 16:00		coffee	coffee	coffee	coffee	
16:00 – 17:30		Foster Virtual AFM	Schwarz Magnetic force microscopy	Mélin Electrostatic force micrsoscopy	practical training	
17:30 – 19:30		snacks and virtual AFM training	snacks and posters	snacks and posters	dinner	
19:30 – 23:00					NC-AFM award Party	

Lectures

Non-contact atomic force microscopy - an introduction

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Non-contact atomic force microscopy (NC-AFM) is a dynamic technique for exploring the field of forces by a sharp tip oscillating above a surface. Although, the forces measured are always of electromagnetic nature, the details of the tip-surface interaction may be very different and allow the measurement of many properties like the surface atomic structure, nanostructure, charge and polarisation, chemical affinity and magnetic interactions. A clear identification and quantitative description of the measured quantities, however, always requires a combination of experimental results with rigorous modelling of the forces acting between the tip and the surface as well as a precise characterisation of the force probe. Meaningful and accurate results are obtained in experiments with a tip well suited for the respective task and a measurement and control system optimised in its transfer functions for the pre-set experimental parameters, the probe dynamics and the tip-surface interaction.

The basic idea of NC-AFM is to keep the tip mounted on an elastic probe system in constant oscillation and to periodically probe the tip-sample interaction over a certain range of tip-surface distances. For a probe system of sufficient stiffness, the restoring force will always be larger than any adhesive force and the tip will not snap into contact to the surface. This allows the experimentalist to precisely position the tip by the proper choice of cantilever-surface distance and oscillation amplitude and to probe the tip-sample interaction either over a large range of the tip-sample interaction curve or differentially at a certain point above the surface. For high resolution imaging, it is advantageous to choose a working point close to the minimum of the tip-sample force where short range interactions between tip and surface atoms can best be separated from the background of longer range tip-surface interactions. The interaction between tip and sample introduces a slight anharmonicity in the otherwise harmonically oscillating probe system. This anharmonicity can be measured by various methods. The most common method is to stabilise the oscillation amplitude by a feedback control loop and measuring the cantilever resonance frequency f_{int} as a function of the tip-sample interaction while alternatively the interaction-induced change in amplitude of the probe system excited to oscillation at a fixed frequency close to the resonance frequency can be measured.

The basic principles, components and parameters relevant in NC-AFM are introduced and a rational approach towards "best practice" NC-AFM imaging and force mapping is discussed.

The Master Equations of Dynamic AFM

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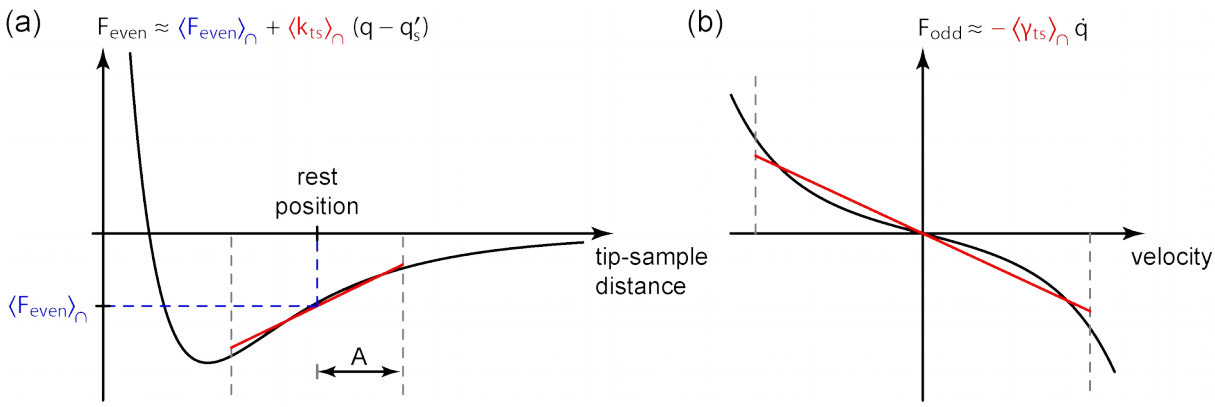
Atomic force microscopy in the dynamic mode has developed into an extremely useful technique in the three decades since the first images with atomic resolution. Today, a wide variety of dynamic atomic force microscopy modes are employed in the field of surface science. These modes are often adjusted to particularly suit the investigation of a specific sample property.
Summarizing the existing literature [1-10] on atomic force microscopy data evaluation, we introduce a general set of three equations [11] to analyse data obtained in any singlefrequency operation mode. Hereby, only the harmonic approximation is needed. The resulting **Master Equations of Dynamic AFM** connect the observables excitation force, excitation frequency, amplitude, phase shift and static deflection with the three aspects of the tip-sample force accessible within the harmonic approximation (see figure). This comprehensive set of equations allows for a quantitative determination of the tip-sample force, regardless of the specific mode used. The validity of the harmonic approximation – the most common in modern dynamic AFM data analysis – is checked comparing analytical results provided by the master equations with virtual AFM simulations. We will discuss advantages and limitations of most common dynamic AFM modes. The equivalence of various dynamic AFM modes will be verified by comparing high-resolution data obtained in amplitude modulation and frequency modulation mode.



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Accuracy and uncertainty in simulations of atomic force microscopy

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As surface science has increasingly moved to the nanoscale over the past decade, it has entered a realm that is also accessible to highly accurate computational approaches. Simulations have become a key partner in many studies, with the interplay between theory and experiment being the critical element in real understanding. This is especially true in Scanning Probe Microscopy (SPM), where joint experimental and theoretical studies are common [1].

In this lecture, I will try to introduce the most popular tools used in computational surface science, with particular emphasis on quantum approaches, along with examples highlighting their interaction with experiment. I will also show examples where common methods fail, and point out the consequences of some "short-cuts" often hidden in the technical details. From this, I will walk through the stages of building a simulation of SPM, with the details mostly relevant to modelling of noncontact Atomic Force Microscopy (AFM).

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Fabrication, characterization and modelling of force sensors and tips

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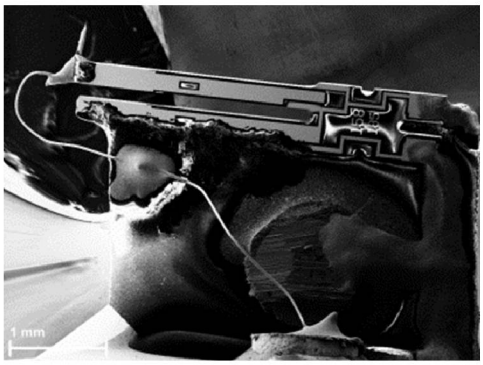
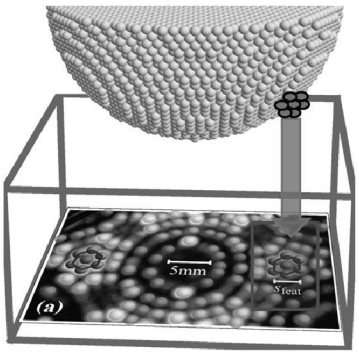
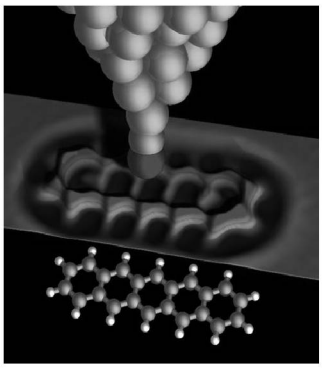
Non-contact atomic force microscopy allows measurement of the force interaction between a sharp tip and a sample surface with atomic scale precision. Usually, the surface atom identities as well as their positions are known from the high resolution surface scan. Further, the exact force interaction curves can be obtained by force spectroscopy techniques, i.e. measuring the frequency shift as a function of tip sample distance. However, interpretation of those force curves depends critically not only on the surface atoms, but equally on the exact tip structure and tip atom termination. This information is usually unknown making image contrast interpretation ambiguous. Secondly, quantitative force curves rely on force sensor calibration, which is a recurring issue in the nc-AFM community.

In this lecture I will review the current state of force spectroscopy techniques, from point spectroscopy to full 3D force field acquisition [1]. Force curve interpretation with respect to different force contributions from dispersion forces, electrostatic forces and chemical forces is discussed. The two mainly used force sensors, i.e. cantilever beams and quartz crystal tuning forks, are introduced, as well as the corresponding force calibration methods with recent modelling approaches. In the last part, I will focus on current strategies to resolve the unknown tip atom problem from the experimental point of view. One possibility is to use field ion microscopy, which allows atomic scale tip imaging and interpretation of sharp metal tips [2]. A further approach is to pick-up surface atoms or molecules of known identity, and use those functionalized tips for imaging and force curve acquisition. In particular the latter method has revolutionized imaging of surface molecules, making nc-AFM a powerful tool for studying surface confined chemical reactions mechanisms.







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Methods in Force Measurements

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The measurement of tip-sample interaction forces with pico Newton resolution is one of the key capabilities of atomic force microscopy. Joined with the ability to also spatially resolve forces at the pico metre scale, the non-contact atomic force microscope (NC-AFM) is now established as one of the most important surface science tools [1]. The force measurement capability was already swiftly exploited during the early days of NC-AFM by, for example, measuring the formation of a single chemical bond [2], and was soon pushed towards the acquisition of two- and three-dimensional volume data sets [3]. Also, the experimental [4] as well as theoretical [5] framework necessary to perform and analyse dense force volume data has been developed over the last decade.

This lecture will discuss critical aspects of quantitative force measurements using the NC-AFM technique. Starting from fundamental considerations of the relation between frequency shift, force, and potential, the numerical back conversion to forces from measured signals [5,6] will be introduced together with practical considerations. Furthermore, suitable approaches for experimental challenges faced in force spectroscopy experiments will be discussed and methods to determine system parameters necessary for a quantitative force calculation introduced. Finally, an outlook will be given on data analysis steps often taken after calculating the vertical interaction forces.

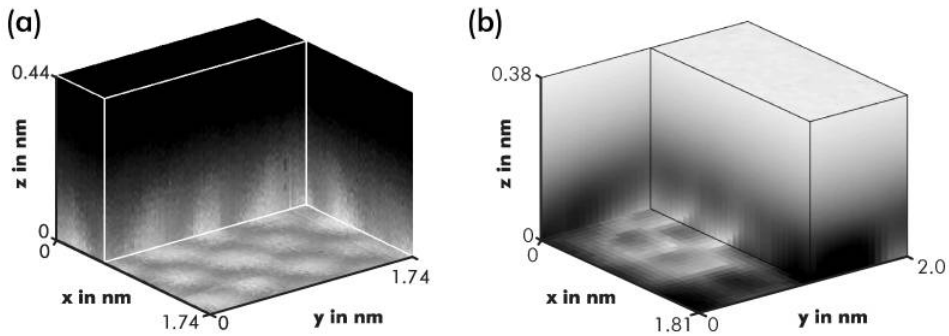

Figure 1: Frequency shift Δf data mapped along three spatial directions on (a) calcite(104) at room temperature [7] and (b) at 77K on an NTCDI molecule adsorbed on Ag:Si(111)-(√3×√3) R30° [8].

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NC-AFM imaging of metal oxide surfaces

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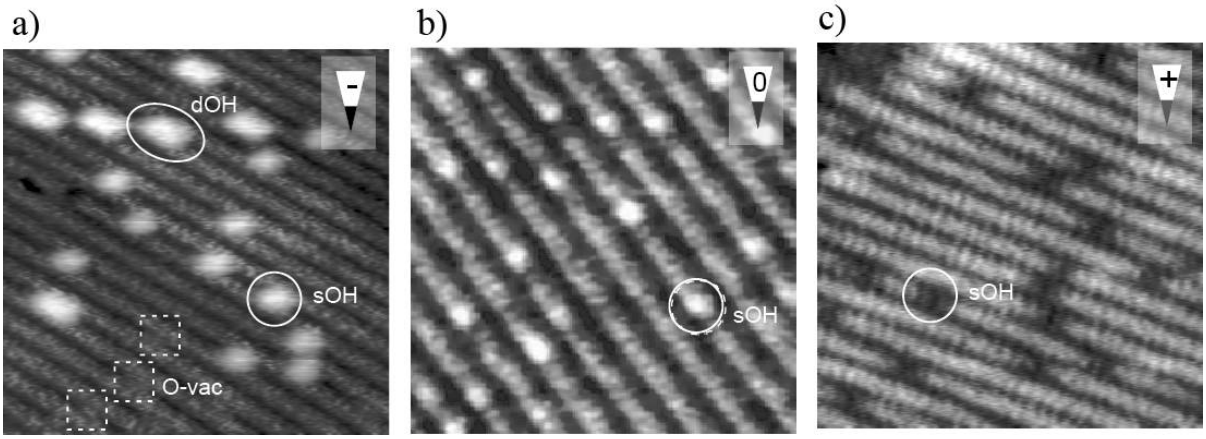
In materials science and technology, many insulating oxides play an essential role. NC-AFM is so far one of the only techniques with the ability to address their atomic-scale surface structure. A distinct advantage of NC-AFM imaging is for example the access to defects and single adsorbates on such surfaces. One such application of NC-AFM is in fundamental studies of heterogeneous catalysis. A heterogeneous catalyst typically consist of an active metal nanoparticles dispersed on a high-surface are oxide support. The role of oxide supports has often been seen as structural stabilizer of the metal nanoparticles, but we now know that the situation is often much more complex. Nevertheless, not much is understood for such systems, which motivates the use of NC-AFM provide information on the properties of the clean oxide surfaces and their interaction with metals and adsorbates.

Against this background I will in my lecture present NC-AFM studies of important insulating or poorly conducting oxide surfaces [1,2]. I will discuss the general challenges associated with the preparation and imaging of oxides. I will also show how subtle NC-AFM contrast variations due to AFM tip termination can be give rise to widely different images of TiO_2 surfaces, and how such information can be used to analyse atomic defects in the surface region. In extension of this, I will then show how mapping of oxide surfaces in different contrast modes could be used to determine the surface structure of the "spinel" $MgAl_2O_4(001)$ surface and its prevalent surface defects. In this connection, I will also discuss the concept of polar oxide surfaces [3].



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Magnetic Sensitive Force Microscopy

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Magnetism is an intriguing and, from a technological perspective, an extremely important phenomenon. Its existence is long known to mankind and nowadays still essential for data storage and sensing in, e.g., automobiles or consumer electronic products. Miniaturization asks for tools to investigate magnetic structures with high resolution and high sensitivity. Force microscopy provides two tools to study magnetism on the nanometer down to the atomic scale: magnetic force microscopy (MFM) [1], introduced already 1987 just one year after atomic force microscopy has been invented, and magnetic exchange force microscopy (MExFM), which could be realized in 2007 [2].

After a general introduction to magnetism, its origin and the relevant energy contribution, which fundamentally determine the magnetic state of a system, both microscopy techniques will be described in detail: tip preparation, separation of magnetic forces from other forces, imaging as well as spectroscopic modes, etc. Thereafter, some examples will be presented to demonstrate the capabilities of both techniques: imaging ferromagnetic domains, visualization of flux line lattice in superconductors, mapping antiferromagnetic spin structures with atomic resolution, determining magnitude and distance dependence of the magnetic exchange interaction. Finally, the issue of thorough data analysis will be discussed, as this is very important to avoid false interpretation of contrast patterns.

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High resolution molecular imaging, spectroscopy and manipulation

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I will try to identify and discuss the specificities of imaging molecules in the non-contact AFM mode and the factors that limit the resolution that can be reached in different cases.

A major difficulty in imaging molecules in nc-AFM stems from the relatively weak adsorption energies (especially on insulators) and weak diffusion barriers that they exhibit. The resolution is usually limited by the maximal force that the molecules can support without being laterally displaced or picked up by the tip. Imaging and manipulation are both sides of the same experiment.

The usual strategy that experimentalists employ to get the best resolution possible consists usually in increasing the tip-substrate interaction (by increasing the absolute value of the frequency detuning set value $|\Delta f|$ in the constant Δf mode or by reducing the tip-surface distance in the constant height mode) until "something" happens.

Beyond this crude approach, there are several ways to improve the imaging resolution:

- Optimizing the control parameters (feedback loops settings, oscillation amplitude, bias voltage,…)
- Adapting the system if possible (use another substrate or equip the molecule with grafting groups to enhance the adsorption energy)
- Modifying the tip

A major breakthrough was achieved with this last option by functionalizing the tip with small molecules (especially CO) [1]. Atomic and intra-molecular bond resolution is now routinely obtained on –generally- flat molecules at low temperature ($T \lesssim 10K$) and with tuning forks, in the qPlus configuration. These experiment are performed at constant height.
This approach has still not been used at higher temperature, because these small molecules are not stable enough on the tip. But there are examples in the literature that display similar resolution with unintentionally functionalized tips, suggesting that the technique could be generalized.

After a brief historical introduction, the presentation will be organized around the two main and relatively distinct approaches that structure the literature:

- The imaging of molecules on bulk insulators -meaning that STM cannot be used- mainly with cantilevers and at room temperature.
- The imaging of molecules with functionalized tips and at low temperature, mainly with tuning forks and very often coupled to STM.

Afterwards, a few examples of lateral and vertical molecular manipulations will be presented and discussed.
Finally some perspectives on this domain will be given.

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Dynamic AFM in Liquids

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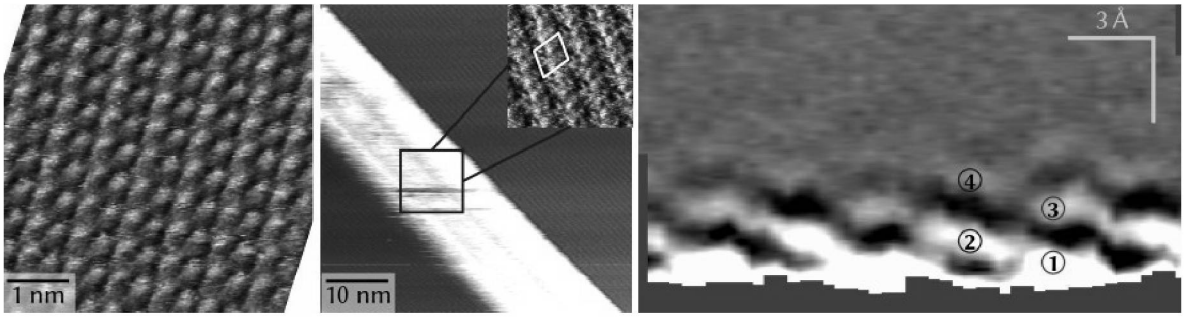
Solid-liquid interfaces play a decisive role in a wide range of natural and technological processes. For example, mineral dissolution, growth and weathering are pivotal within geochemistry and environmental science [1]. Molecularly controlled nucleation and growth at the solid-water interface govern biomineralisation and biomimetic crystallisation; processes that are known to result in highly sophisticated, tailor-made materials [2]. Moreover, interfacial reactions are at the heart of many industrial fields such as catalysis and corrosion protection [3].

For understanding, controlling and predicting processes at the solid-liquid interface, a detailed knowledge of the atomic structure, potential surface rearrangements and the solvation structure is mandatory. In the last decade, dynamic atomic force microscopy (AFM) has been developed into a most powerful tool for investigating the interfacial structure and reactivity in real space and at the atomic level.

In this lecture, main challenges of dynamic AFM in liquids and their technical solutions will be presented. Besides increasing the signal-to-noise ratio [4], a direct excitation of the cantilever is needed to avoid the "forest of peaks" [5]. Nowadays, dynamic AFM provides atomic-resolution imaging at the solid-liquid interface on a routine basis, which is used for investigating molecular self-assembly and molecule-induced surface restructuring [6, 7]. State-of-the-art applications include three-dimensional solvation layer mapping [8, 9], revealing the solvent structure at the interface. Finally, an outlook will be given addressing promising solutions for Kelvin probe force microscopy measurements in electrolyte solutions.



Examples for dynamic AFM in liquids: (*left*) Atomic resolution imaging on the dolomite (10.4) surface in water, (*middle*) a self-assembled stripe of Congo Red molecules on calcite with molecular-scale resolution as inset and (*right*) a vertical slice of a 3D hydration layer map acquired at the calcite-water interface.

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Lock-In, Phase Locked Loop and Proportional-Integral Controllers

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Best results in NC-AFM measurements can be achieved when the operator knows the technology of the microscope and the function of basic components well and is confident in its operation. Starting out from the basic principles of the Lock-In technique, Phase Locked Loop (PLL) and Proportional-Integral (PI) Controllers, this presentation will explain the basics of non-contact AFM detection electronics, discuss some of the design choices made for the RHK R9 controller and make us aware of some common pitfalls in NC-AFM controller design and how to avoid them. Furthermore, it will be shown how, using "elementary" NC-AFM technology building blocks, complex measurement schemes like Kelvin Probe Force Microscopy (KPFM) can be built up.

Principles of Electrostatic force microscopy and applications

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This lecture will be devoted to the basics of electrostatic force sensing, and to an introduction to the different techniques used for this purpose: electrostatic force microscopy (EFM), in which one wants to directly measure electrostatic forces; and Kelvin probe force microscopy (KPFM) techniques, in which one wants to compensate/nullify electrostatic forces, by the application of a suitable dc bias.

Implementations for these techniques will be presented - mostly in the long-range regime for electrostatic forces - and discussed through examples taken in ambient air and/or vacuum. Measurement limitations, in term of resolution, sensitivity, temporal resolution, will be described. A special focus will be devoted to the achievement of quantitative results, beyond quantitative imaging. Common practical imaging artifacts or tricks will be described as well.

This lecture should also consist in an introduction to part of the lectures of L. Nony (KFPM techniques in UHV) and B. Grévin (KPFM applied to electronic and photovoltaic devices).

Principles of KPFM and applications

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Kelvin Probe Force Microscopy (KPFM) is a technique aiming at the detection and compensation of electrostatic forces arising between a nanoprobe (the tip of the microscope) and a surface (hereafter referred to as the electrodes) when they are biased. The origin of these forces differs upon the distance between the electrodes [1]. At large distance (>1nm), electrostatic forces can be quantitatively connected to the Contact Potential Difference (CPD) between the electrodes, i.e. the difference between their work functions. Thus the technique gives a quantitative CPD map of the surface on the local scale [2]. When measured closer to the surface (in the range of 0.5-1 nm), short-range electrostatic forces start to get involved in the imaging process. Then, a KPFM image with atomic-scale resolution can be achieved [3]. However, in this situation, the origin of the KPFM signal rather reflects atomic-scale properties of the surface, among which its local polarizability. The ability for the technique to provide access to the CPD and other properties down to the atomic-scale makes KPFM widely used in surface science nowadays. In the 1990's, the KPFM technique has been coupled with noncontact-AFM [1]. The possibility to perform experiments where structural and electronic properties become jointly accessible made the couple KPFM/nc-AFM attractive and intensively developed and used in numerous research labs (see fig.1, after [4]).

The goal of this lecture will be to discuss experimental (technical implementation, modes, time constants considerations, artefacts…) and theoretical aspects (long-/short-range electrostatic forces) of the KPFM technique when coupled with nc-AFM and to illustrate these by means of examples taken from recent literature [4, 5].

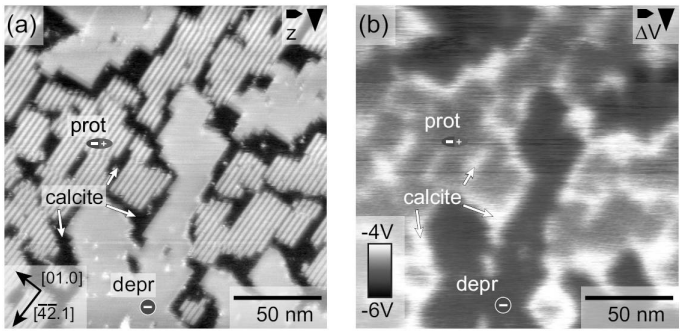

Figure 1: nc-AFM topographical (a-) and related CPD (b-) images of 2.5-dihydroxybenzoic acid molecules on a calcite substrate.

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High resolution KPFM investigations of photovoltaic materials and interfaces

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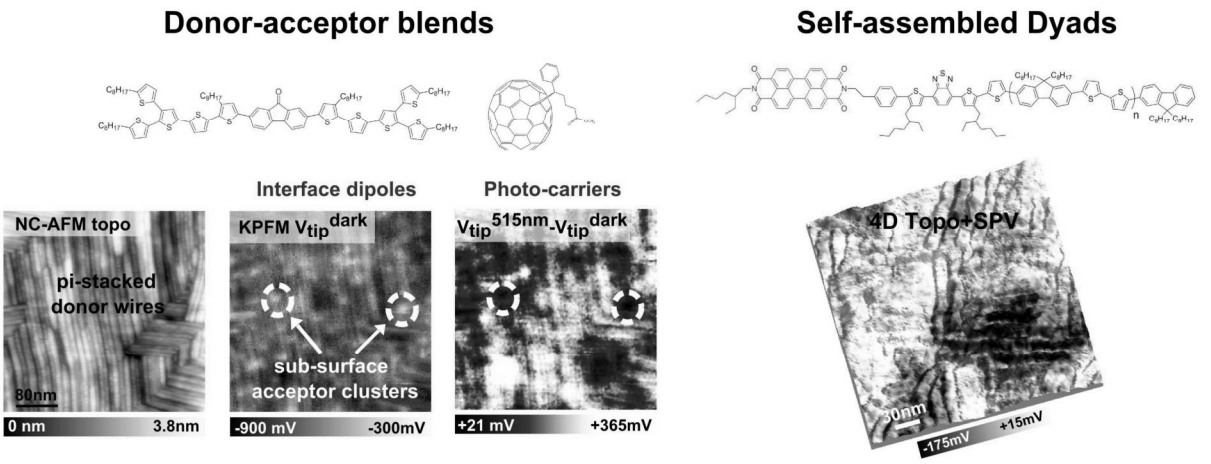
Nowadays, Kelvin Probe Force Microscopy (KPFM) is a well-established technique in the field of organic, hybrid and inorganic photovoltaics. Several reports have already demonstrated that the local surface photovoltage (SPV) of photoactive thin films and devices can be mapped by analyzing the surface potential (SP) shift upon illumination. Besides, SP images recorded in dark can be used to investigate the permanent charges, electrostatic dipoles and band bending effects at various interfaces and defects, such as the grain boundaries in polycrystalline materials or the donor-acceptor interfaces in organic bulk heterojunctions. However, imaging the surface potential and SPV with a sub-10nm resolution remains often a challenge even in the case of investigations carried out in ultrahigh vacuum (UHV) by non-contact AFM (nc-AFM). This is especially true in the case of complex materials such as nano-phase segregated organic donor-acceptor bulk heterojunctions (BHJ).
In this lecture, we will show how nc-AFM/KPFM can be used to investigate photoactive organic self-assemblies and organic solar cells at the relevant scales. First, an introduction to the basic concepts of charge generation at donor-acceptor interfaces, electronic transport and recombination mechanisms in organic solar cells will be given. In a second part, nc-AFM/KPFM technical issues/hints will be discussed, including: illumination setup geometry, cantilever calibration, artifacts, SPV images calculation and lateral resolution. In a third part, we will review the recent literature and will present our recent achievements on BHJ thin films[1] and self-assembled donor-acceptor dyads[2]. Last, beyond the current state of the art, we will introduce ongoing and future developments towards time resolved imaging of the photo-carrier dynamics, yielding a direct access to the charge generation, trapping and recombination mechanisms at the nanometer scale.



[1] F. Fuchs, F. Caffy, R. Demadrille, T. Mélin, B. Grévin ACS Nano **10**, 739, (2016).
[2] B. Grévin, P.O. Schwarz, L. Biniek, M. Brinkmann, N. Leclerc, E. Zaborova, and S. Méry, Beilstein J Nanotechnol. **7,** 799, (2016).

Posters

NC-AFM and KPFM study of monoatomic Au islands on AlN(0001)

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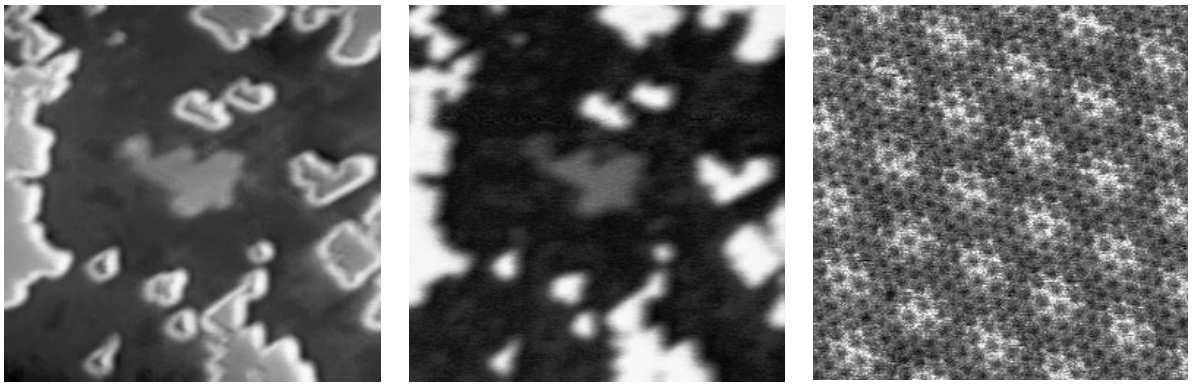
We are looking for a substrate that would allow the electrical connection of a nanoscale object such as a single molecule between contact pads in a planar configuration. This objective requires to use an insulating substrate on which conductive islands can be grown. These islands should be as flat and wide as possible in order to allow the AFM imaging of the connected object and the connection of these metallic pads to the external world with for instance a 4 probe scanning tunneling microscope. AlN is a suitable candidate for this purpose with its 6.2 eV wide band gap. We have investigated the growth of a few metals (Mg, In, Ag, Au) on the AlN(0001)-(2x2)-N reconstructed surface. We report here the results for Au, which satisfy the requirements mentioned above.

AlN does not exist in nature, but can be elaborated on different substrates by a few methods. It exhibits outstanding properties making it a useful material for power and RF electronics and light emitting devices. Our samples are made by molecular beam epitaxy in the form of thick (100 nm) films on 4H-SiC substrates. They are fully insulating and cannot be imaged by STM. Gold is deposited at high temperature on the (2x2) reconstructed surface and then examined by RT or LT (5 K) nc-AFM.

The morphology of a ≈0.3 ML deposit is illustrated in Fig. a. Disconnected, monolayer thick islands, with extensions in the 100 nm range can be observed. The Au monolayer presents a hexagonal structure and is slightly disoriented relative to the AlN(0001) crystallographic axes. This configuration produces a moiré pattern that is observed on atomically resolved nc-AFM images (Fig. c), allowing a precise comparison with the results of DFT calculations. These calculations show that some of the gold atoms form a chemical bond with the surface nitrogen atoms of the AlN-c(2x2) reconstruction, while the other gold atoms are only physisorbed on the AlN substrate. As shown in the KPFM images (Fig. c), these islands can be charged in both polarities, by applying suitable voltage pulses above them. The charge retention times range from seconds to days, depending on the experimental conditions.



(a) Topography and (b) Kelvin potential nc-AFM images of Au islands on AlN(0001). The central island has been *positively* charged by a voltage pulse. Size: 400nm x 400nm, T = 300 K. (c) High resolution nc-AFM image on an Au island. Size: 6 nm x 6 nm, T = 5 K.

Acknowledgements: This work has been supported by the European Commission within the PAMS project (Contract N°. 610446).

Controlling the growth of Bi films and particles on an insulating substrate

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Nanostructured ultrathin bismuth films [1,2] have attracted a lot of interest as they reveal exotic functional properties that do not exist in bulk. The material properties are advantageous for the realization of e.g. spin based electronic devices, magnetoresistance effects and topological properties [3]. Due to a wide variety of potential applications in biomedical, optical, and electronic fields, the controlled fabrication of nanoparticles (NP) is currently an area of intense scientific research. Therefore nanosized Bi structures, anticipated to reveal exotic functional properties, have high potential for both fundamental research and technological applications. Especially growth on an atomically well defined insulating substrate is essential for future electronic applications as well as to get a deeper understanding of its controllability.

In this study we demonstrate by Surface X-ray Diffraction (SAXS) the controlled growth of thin Bi(110) and Bi(111) films on such a substrate: atomically smooth insulating sapphire (α-Al_2O_3(0001)). The preparation of (110)-oriented Bi films, a rather exotic orientation, is a difficult task. At temperatures as low as 40K, we are able to slow down kinetics and thereby controlling the growth of Bi towards Bi(110), stable up to 400K. By annealing the Bi(110) films beyond, they can be transformed towards stable Bi(111) films. Melting these films, recrystalization into Bi(110) NPs is studied by combining Surface X-ray Diffraction (SXRD) and Reflective High Energy Electron Diffraction (RHEED). By the use of Atomic Force Microscopy (AFM) and Kelvin Probe Force Microscopy (KPFM) we determine the NP size and their distribution. We demonstrate the ability to tune the NP size by controlled heating and growth.

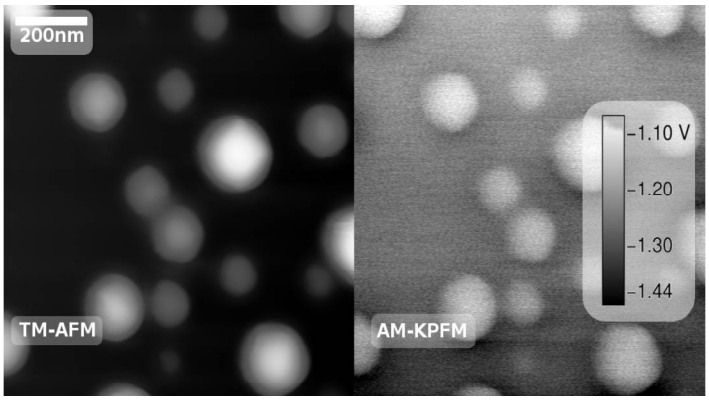

Illustration 1: Tapping-Mode Atomic Force Microscopy (left) and Amplitude Modulation Kelvin Probe Force Microscopy (right) image of Bi nanoparticles on a sapphire substrate.

[1] E.I. Rogacheva, et al. Appl. Phys. Lett. **82**, 2628 (2003)
[2] Y.W. Wang, et al. Appl. Phys. Lett. **88**, 143106 (2006)
[3] Koroteev et al. Phys. Rev. B, **77**, 045428 (2008)

Studies of stability of *para*-hexaphenyl structures grown on ion beam modified $TiO_2(110)$

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Organic electronics has been a subject of studies for a long time. Molecular structures grown on metal oxide surfaces drawn considerable attention over the years. We have investigated the growth and stability of molecular ultra-thin films, consisting of rod-like semiconducting para-hexaphenyl (6P) molecules vapor deposited on ion beam modified $TiO_2(110)$ surfaces. The ion bombarded $TiO_2(110)$ surfaces served as growth templates exhibiting nm-scale anisotropic ripple patterns with controllable parameters, like ripple depth and length. Imaging of the developed molecular structures has been performed with non-contact atomic force microscopy (NC-AFM) and kelvin probe force microscopy measurements (KPFM) in UHV, and tapping-mode atomic force microscopy (TM-AFM) at ambient conditions.

It has been found that the highly anisotropic substrate pattern influence the shape of grown 6P islands composed of "standing up" molecules. The island's elongation is directly correlated with the ripples' long axis direction as an effect of 6P's anisotropic diffusion [1]. Also, we have observed the formation of wetting layer, of lying molecules, on rippled $TiO_2(110)$ surfaces. The specimen exposure to air leads to formation of new structures between the already existing 6P islands. A similar behavior was already observed in the case of 6P growth on atomically flat $TiO_2(110)$ [2]. Contact potential difference (CPD) measurements revealed different electronic properties of the 6P islands and the wetting layer.

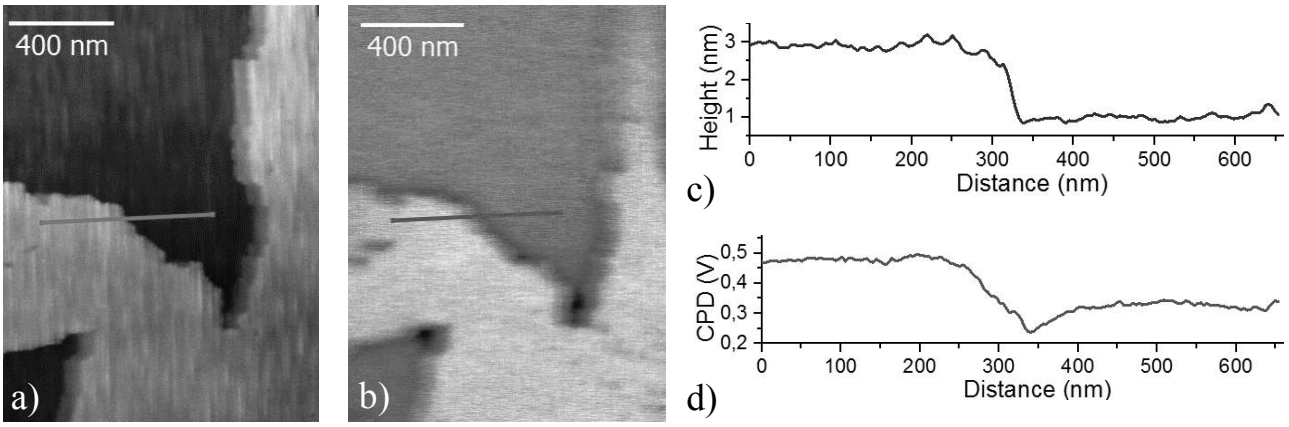

Figure 1: a) NC-AFM and b) KPFM images of *para*-hexaphenyl islands on rippled $TiO_2(110)$ surface with c) TOPO and d) CPD profiles.

[1] M. Kratzer, D. Wrana, Phys. Chem. Chem. Phys., 16, 26112-26118, (2014)
[2] D. Wrana, M. Kratzer, J. Phys. Chem. C, 119, 17004-17015, (2015)

Molecular Self-Assembly Versus Surface Restructuring at the Calcite-Water Interface

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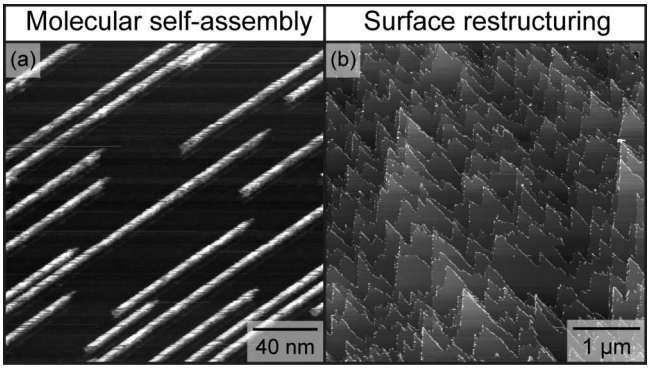
Water-soluble, organic additives at the mineral-water interface are known to exhibit a decisive influence on dynamic processes like, for example dissolution, growth and mineral replacement [1, 2]. Furthermore, organic molecules can self-assemble into ordered structures on the surface significantly affecting the resulting materials' properties by altering, e.g., the crystal morphology and mechanical characteristics [3]. Here, we study the interaction of the two constitutional isomers Eriochrome Black T (EBT) and Eriochrome Black A (EBA) with the calcite (10.4) cleavage plane using *in-situ* high-resolution atomic force microscopy [4]. Despite the difference in their structures, we find that in the presence of each molecule the calcite surface is restructured in a similar way. Characteristic etch pits - observed on the surface in the absence of the additives - retreat, resulting in a surface that discloses step edges exclusively along the crystallographic [010] and [48-1] direction. Interestingly this surface reorganization is independent of the pH. In sharp contrast, we are able to control the structure formation of EBA assemblies by adjusting the pH to a very narrow pH window at a pH value of around 3.6. Formation of molecular stripes is observed along the crystallographic [42-1] direction in addition to the restructuring process. Summarized, these finding might indicate that the self-assembly of well-defined molecular structures requires more precise properties of the additive - including specific protonation states - as compared to additive induced surface restructuring processes which was revealed to be indeed molecule and pH independent.



In-situ AFM images of the calcite (10.4) surface in the presence of the molecule EBA. (a) Illustrating molecular self-assembly of EBA on the calcite surface. (b) Demonstrating surface restructuring and step edge stabilization.

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[2] C. V. Putnis, E. Ruiz-Agudo, Elements. **9**, 177 (2013).
[3] M. Ricci et al., Langmuir **31**, 7563 (2015).
[4] M. Nalbach et al., *in preparation*.

Atomic resolution of mica with qPlus sensors in ambient and liquid environments

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We set up an AFM with qPlus sensors to operate in ambient conditions as well as in liquid environments and measured on muscovite mica. For measurements in liquids we immerse the sample in liquid and use long tips, only submerging the tip apex.
Atomic resolution of muscovite mica was achieved both in ambient conditions and in liquid. The liquid we used was a Ham's Medium which is a biological solution used for cell growth, containing a range of salts, amino acids, vitamins and other solutes.
We discuss the decrease of the Q-factor as a function of the penetration depth of the tip in liquid. The high stiffness of our qPlus sensors allows us to keep this Q value above 140 during measurements.

Enantiopure supramolecular motifs of self-assembled chiral molecules

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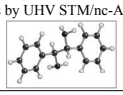
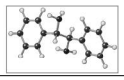
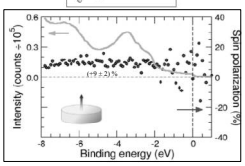
Introduction

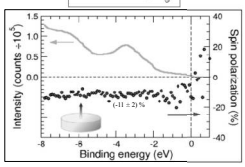
Chiral molecular recognition plays a pivotal role in pharmacology, chemistry, catalysis, non-linear optical devices, sensors, smart coatings[1-3] and relevant because of the optical activity with polarized light. Understanding how the chirality of a single molecule is transferred to different hierarchical levels of organization on a surface is particularly important in the context of molecular self-assembly, biomineralization and for the design of novel chiral nanostructured materials.[4]

Motivation

We study the self-assembly of two enantiomers R-R and S-S of the molecule Diphenylethylenediamine (RR-DPEDA and SS-DPEDA, respectively) deposited on Cu(100) under Ultra High Vacuum (UHV). The structure at the molecular level has been investigated for different surface coverages by UHV STM/nc-AFM.

(1S,2S)-(-) DPEDA  $[C_6H_5CH(NH_2)]_2$  *(1R,2R)-(+)* DPEDA

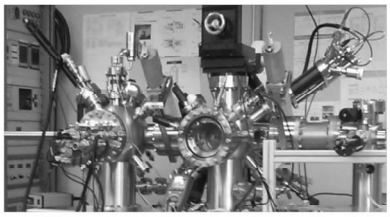


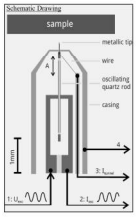


The influence of chirality on the spin polarization of extracted electrons has been studied for the two enantiomers. For each enantiomer, the spin polarization is out of the plane but opposite direction.

Experimental

STM/nc-AFM system in UHV at Room Temperature (RT): SPM - Aarhus 150 controlled by Nanonis electronic using KolibriSensors™. f_0~1MHz, Q~25000, A~200pm, collecting simultaneously the topography (z), tunneling current (I_t), frequency shift (Δf_{shift}) and dissipation channels.



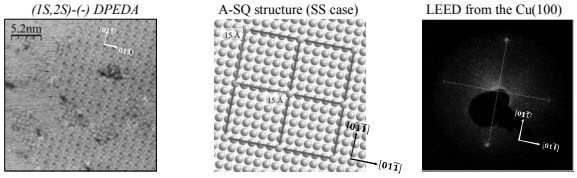


The Cu(100) substrate was prepared by repeated argon sputtering and annealing cycles. Molecules were deposited keeping the substrate at RT.

Morphology and structure

Submonolayer coverage

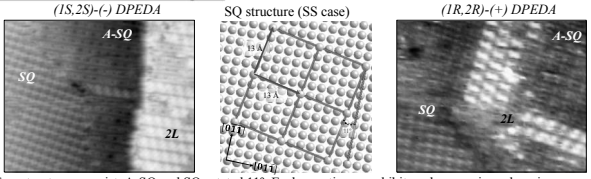
(1S,2S)-(-) DPEDA — A-SQ structure (SS case) — LEED from the Cu(100)



Below the monolayer, molecules are ordered in a square aligned lattice with the main directions of Cu (100).

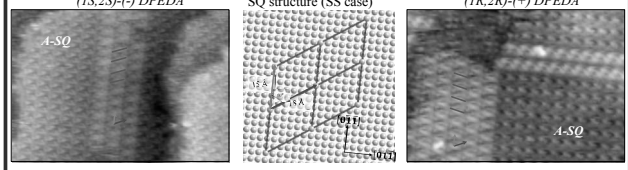
Above the monolayer

(1S,2S)-(-) DPEDA — SQ structure (SS case) — *(1R,2R)-(+) DPEDA*



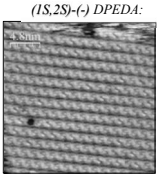
Two structures coexist: A-SQ and SQ rotated 11º. Each enantiomer exhibits only one mirror domain. A second layer is also observed (2L).

(1S,2S)-(-) DPEDA — SQ structure (SS case) — *(1R,2R)-(+) DPEDA*



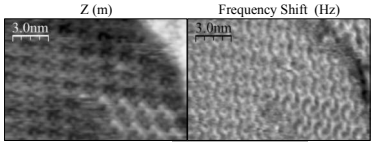
The second layer grows only on top of the A-SQ structure and, with a clear chiral arrangement, exhibits an oblique unit cell where one direction coincides with one of the directions of the A-SQ.

(1S,2S)-(-) DPEDA:



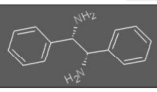
Large chiral domains (>200nm)

Z (m) — Frequency Shift (Hz)

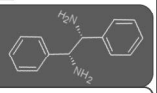


STM images for *(1S,2S)-(-) DPEDA:*

Summary and conclusions

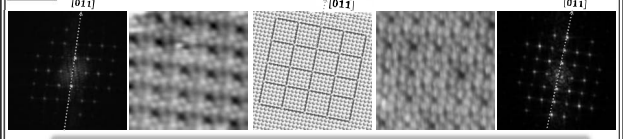


(S,S)-DPEDA (R,R)-DPEDA



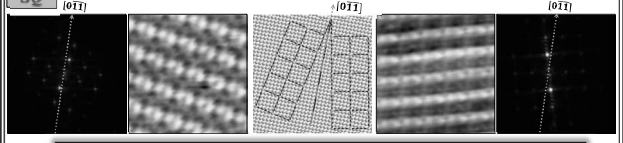
The chirality of DPEDA enantiomers is transferred at different levels of molecular organization. Below the monolayer completion, each enantiomer orders in a square lattice aligned with the principal crystallographic directions of the substrate (A-SQ) forming two-dimensional (2D) domains. The intrinsic chirality of the molecule is only manifested within the unit cell (lack of mirror-symmetry). For increasing coverage, this A-SQ structure coexists with 2D domains of a square lattice (SQ) rotated ≈ ±11º with respect to the principal direction of the Cu(100) substrate (organizational chirality). Chirality is also transferred to the second layer (2L) grown on top of the A-SQ structure.

A-SQ



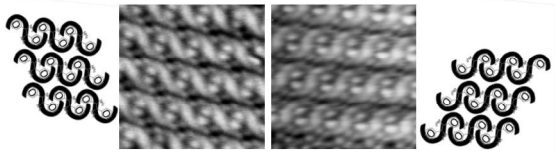
A-SQ: a square lattice aligned with the principal crystallographic directions **(local point chirality)**

SQ



SQ: Mirror-like structure for each enantiomer **(global organisational chirality)**

2L



Chirality is transferred to a second layer (2L) grown on top of the A-SQ structure, the chiral supramolecular order is unambiguously reflected in the helicity observed for each enantiomer

References:

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[2] A. Kühnle *et al.*, Nature, 415, 891-893 (2002)

[3] M. Ortega *et al.*, Nature, 404, 376-379 (2000)

[4] R. Raval, Chem. Soc. Rev., 38, 707-721 (2009)

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Underlying mechanism of time dependent surface properties of calcite

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Abstract

The increasing number of reports on the influence of wettability on oil recovery and waterflood performance recognizes wettability of porous surfaces within reservoir rocks as the key factor that affects the success of water flooding processes. Unfortunately, a conclusive and satisfactory understanding of all the factors affecting the wettability of the reservoir rocks is still elusive. This is mainly due to the complexity of the intrinsic properties affecting the rock surface and due to the lack of techniques with sufficient spatial resolution necessary to assess the wettability at the pore scale. Using both macro- and microscopic analytical techniques, an idealized flat surface of mineral composition representative for carbonate type formation i.e. calcite ($CaCO_3$), is studied to provide a baseline for future investigation of the underlining mechanisms influencing reservoir wettability. The development of heterogeneities on different calcite planes when exposure to the atmosphere is responsible for the transition in the observed wettability behavior. This work fills the absence of a baseline for the wettability of calcite and provides a reference for future

Illustration of the method

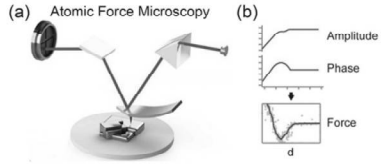

Figure1. (a) A scheme showing the basic set-up of an AFM. (b) Amplitude, phase versus distance (APD) curves were recorded in order to reconstruct the tip-sample interaction forces.

Results and discussions

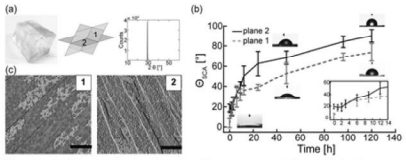

Figure 2. (a) An illustration for the representation of 2 cleavage planes. (b) Time dependent SCAs for plane 1 and plane 2. (c) AFM phase image for 2 calcite cleavage planes. Scale bar: 500 nm.

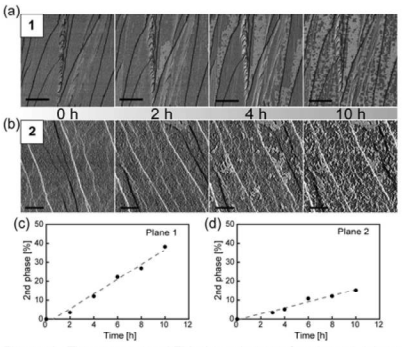

Figure 3. Time sequence AFM phase images for plane 1 (a) and plane 2 (b). (c) and (d) show the percentage of 2nd phase growing with time. Scale bar: 500 nm for (a) and 200 nm for (b).

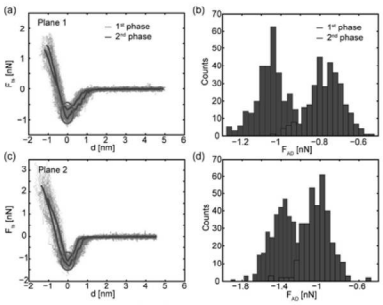

Figure 4. (a) Force profiles for both phases on plane 1. (b) Histogram of F_{AD} for the 1st and 2nd phase one plane 1. (c) Reconstructed force curves on plane 2. (d) F_{AD} histogram for both phases on plane 2. Blue and green dots represent for experimental data while the continuous lines stand for averaged force curves.

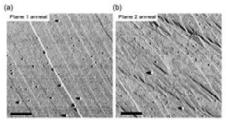

Figure 5. The AFM phase image of annealed calcite plane 1 (a) and plane 2 (b) samples. Scale bar: 200 nm.

Summary

1. Freshly cleaved calcite surfaces would undergo wettability transition when exposed to the atmosphere.
2. Chemistry heterogeneity on calcite surfaces developed upon exposure.
3. The developed films can be removed by annealing.

1. Sheng, J. J. Enhanced Oil Recovery Field Case Studies, 1 ed.; Gulf Professional Publishing: Waltham, MA, 2013.
2. Rodriguez-Navarro, C.; Ruiz-Agudo, E.; Luque, A.; Rodriguez-Navarro, A. B.; Ortega-Huertas, M. Thermal Decomposition ofCalcite: Mechanisms of Formation and Textural Evolution of Cao Nanocrystals. Am. Mineral. 2009, 94, 578–593
3. Lai, C.-Y., et al., *Underlying Mechanism of Time Dependent Surface Properties of Calcite (CaCO3): A Baseline for Investigations of Reservoirs Wettability.* The Journal of Physical Chemistry C, 2015. **119**(52): p. 29038-29043

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ADNOC

In situ investigation of 2D materials after ion irradiation

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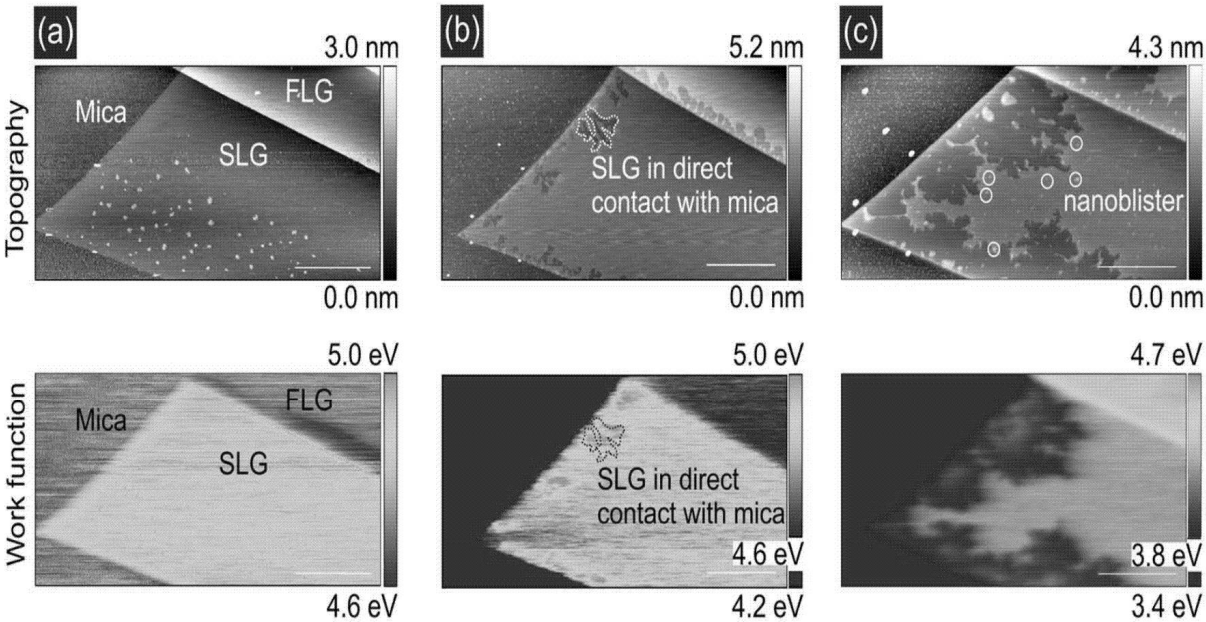
We are interested in investigating the properties of pristine and defective 2D materials in detail, and therefore several irradiation experiments were done. As we could show via KPFM measurements, graphene can be doped e.g. by intercalated water as well as by ion irradiation [1]. In addition, NC-AFM measurements were performed, to characterize defects in 2D materials caused by highly charged ion (HCI) and swift heavy ion (SHI) irradiation. For the latter, characteristic foldings of the monolayers were observed for different 2D materials. These foldings obviously are facilitated by intercalated water [2]. To the avoid the influence of intercalated water our SPM-setup was optimized. The new setup allows us to irradiate 2D materials and investigate the resulting defects in situ.



Topography and work function of graphene on mica. a) Continuous intercalated water layer (IWL) beneath graphene and mica. b) Map after heating to 180 °C for 1 hour. IWL is not continuous anymore and the graphene is in contact with the substrate. c) Map after heating to 600 °C for 19 hours. Further removing of IWL [3].

[1] O. Ochedowski et. al., Appl. Phys. Lett., **102**, 153103 (2013)
[2] O. Ochedowski et. al., Nucl. Instr. Meth. Phys. Res. B, **340**, 39-43 (2014)
[3] O. Ochedowski et. al., Sci. Rep., **4**, 6003 (2014)

Study of 2D-crystalline conjugated oligomer layers for FET application

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Ordering of conjugated molecules via crystallization for enhanced charge transport is a hot topic of interest. We study the crystallization processes of an 2,5-dialkoxy-phenylene-thienylene based oligomer (5TBT). The monomer unit consists of a benzene with thiophene rings on each side, giving it a conjugated backbone and thus making it a promising candidate for high conductivity in supramolecular charge transport systems [1], both along the backbone and the π-stacking direction.
In this study, we prepare quasi-two-dimensional crystals of 5TBT through appropriate thermal treatment of spin coated thin films on various substrates.

Atomic force microscopy revealed the organization of the molecules to be in layers with discrete thickness (~2nm), according to the size of the molecules when oriented edge on. In agreement with the orientation of the dipole moment deduced from microscopy with crossed polarizers, we conclude that both the backbone and the π-stacking are oriented parallel to the substrates. Such an orientation of the molecules favours lateral charge transport and hence provides a good basis for realizing an organic quasi-2D-crystalline field effect transistor. Preliminary conductive AFM measurements support the high lateral conductivity. As the molecules are known to be sensitive to DNT, such structures could be applied as chemical sensors.

Further studies are in progress, using qPlus, a technique combining NC-AFM with scanning tunnelling microscopy (STM) within a single tip in ultra high vacuum (UHV), in order to investigate the interconnections between the molecules. Four-point-probe measurements are planned in order to quantify the conductivity of the crystals.

[1] R. Shokri *et al.*, J. Am. Chem. Soc., **135**, 15, (2013).

Towards Autonomous Scanning Probe Microscopy

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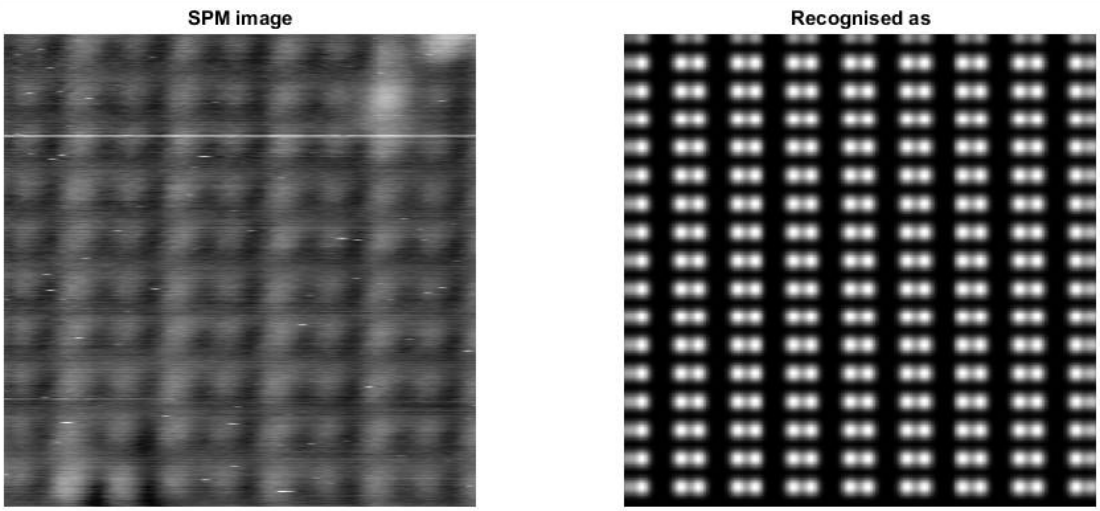
Saoirse.Freeney@gmail.com

Automatic acquisition of scanning probe images with atomic resolution is an extremely attractive prospect for nanoscience research. Ultimately the aim of this on-going project is to create a set of computer programs that obtain SPM images, ascertain the type of surface and resolution present, and reactively reconfigure the state of the probe tip in response to poor quality scans. This would save researchers huge amounts of time and remove the tedious task of manually acquiring good images.

This particular work was focused on using image processing techniques for image registration and recognition. A database of hydrogen-passivated Si(100)c(4×2) surface images were used. Analysis of noise in the images was carried out by calculating the signal-to-noise ratio. Noise removal was applied where necessary for further image analysis. Fourier and Mutual Information methods were used for image alignment/rotation. Model images of the surface were created as a means to compare the real images. Principal Component Analysis and Mutual Information were explored as techniques to categorise and recognise images of different types, comparing them to the model images. Density Functional Theory programs were used to model tip-surface interactions, which can act as another way to identify real SPM images.

It was found that there is a drastic difference between the calculated signal-to-noise ratio and the human perception of how noisy an image is. Using Fourier methods to correct the rotation of images yielded a 67% success rate. Principal Component Analysis sorted images into categories and was successful 69% of the time, while Mutual Information was successful only 46% of the time. The main obstacles are the huge diversity of the types of images that can be obtained, even from just one surface, and the fact that humans are not consistent with categorising images. An ideal solution would be the implementation of machine learning algorithms.



An SPM image and its closest matching model image, found using Principal Component Analysis.

Local information

Meeting site

The meeting is held on the **Campus Westerberg** in the **Bohnenkamp-Haus** of the **Universität Osnabrück botanical garden**.

To access the meeting site from the central train station or the city by bus, use

- bus 21 in **direction Atterfeld**; get off at **stop Hochschulen Westerberg**
- bus 22 in **direction Campus Westerberg/ICO**; get off at **stop Hochschulen Westerberg**
- bus 11, 12 or 13 in **direction Eversburg-Büren**; get off at **stop Sedanplatz**.

Bus tickets are available from the bus driver (mention your destination) at some bus stops also from machines. We recommend to use discounted 4-Fahrten-Karten (tickets for four rides) or a weekly ticket. The latter is not available from the bus driver but at the Mobilitätszentrum der Stadtwerke Osnabrück Am Neumarkt 9-10, 49074 Osnabrück (link, location).

Luncheon and lunch break

Meals will be served at lunchtime in the **Mensa**. Work and relax during the lunch break or after the talks in sunshine in front of the Mensa, in the **Cafeteria** or in the lobby of **building SL** (see map on previous page).

To have lunch in the Mensa, use the **luncheon vouchers (one for each day)** that you receive upon registration. A luncheon voucher is valid for a meal comprising a main dish or hotpot, a soup or salad, a side dish, a dessert and a drink. You can choose from any of the Mensa offers except the special employee's meal (Bedienstetenessen). **Please put the luncheon voucher well visible on your tray at the cashier**; the voucher will be collected.

Summer School farewell party

The party will be held on Thursday, September 15th at 7:30 pm in the Botanical Garden.

Meeting site WiFi connection

The meeting site and other facilities of the Universität Osnabrück are covered by an **eduroam** WiFi connection. The university has completely abandoned all other WiFi systems. For those not having access to eduroam, we set up an alternative WLAN network. Access information is given below.

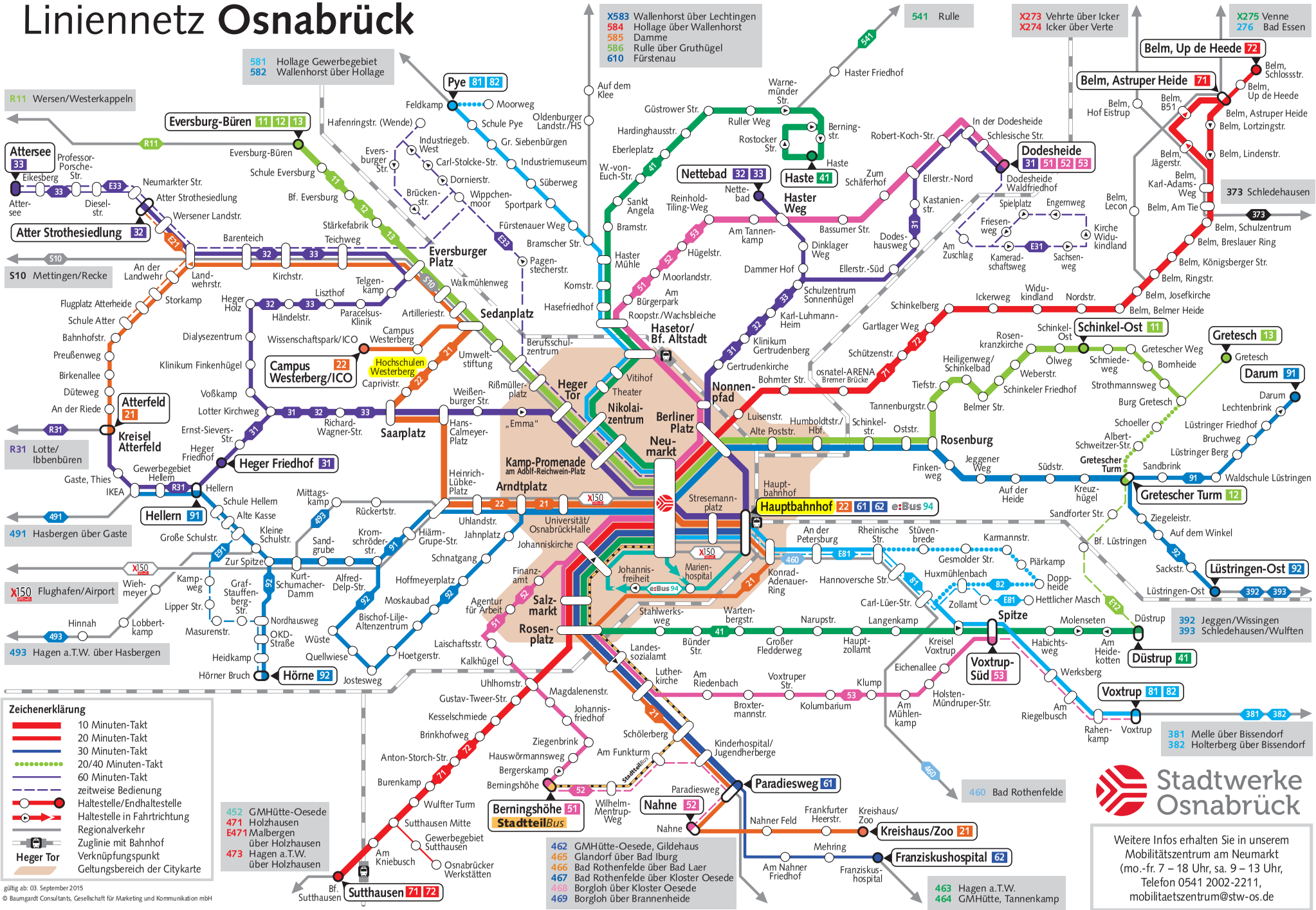
SSID: NCAFM

Password: BinnigRohrer

Security: WPA2

WiFi NCAFM Summer School

Liniennetz **Osnabrück**



21: Neumarkt - Hauptbahnhof - Iburger Staße - Nahne - Kreishaus/Zoo

22: Campus Westerberg/ICO - Hochschule Westerberg - Neumarkt - Hbf.

Stadtwerke Osnabrück

	Montag bis Freitag						Samstag			Sonn- u. Feiertag	
Std.	**Minuten**						**Minuten**			**Minuten**	
5	12	42					27	57			
6	12	42					27	57			
7	03	23	43				27	57		27	
8	03	13Ⓝ A	23	33Ⓝ A	43	53Ⓝ A	27	57		27	57
9	03	13Ⓝ A	23	33Ⓝ A	43	53Ⓝ A	27	41		27	57
10	03	13Ⓝ A	23	33Ⓝ A	43	53Ⓝ A	11	41		27	57
11	03	13Ⓝ A	23	33Ⓝ A	43	53Ⓝ A	11	41		27	57
12	03	13Ⓝ A	23	33Ⓝ A	43	53Ⓝ A	11	41		27	57
13	03	13Ⓝ A	23	33Ⓝ A	43	53Ⓝ A	11	41		27	57
14	03	13Ⓝ A	23	33Ⓝ A	43	53Ⓝ A	11	41		27	57
15	03	13Ⓝ A	23	33Ⓝ A	43	53Ⓝ A	11	41		27	57
16	03	13Ⓝ A	23	33Ⓝ A	43	53Ⓝ A	11	41		27	57
17	03	13Ⓝ A	23	33Ⓝ A	43	53Ⓝ A	11	31	57	27	57
18	03	12Ⓝ A	27	57			27	57		27	57
19	27	57					27	57		27	57
20	27	57					27	57		27	57
21	27	57					27	57		27	57
22	27	57					27	57		27	57
23	42						42			42	

gültig ab 03.09.15

Ⓗ **Hochschulen Westerberg**

ausgewählte Haltestellen

21	22	Haltestelle
●	●	Hochschulen Westerberg
○	○	Caprivistraße
○	○	Saarplatz
○	○	Hans-Calmeyer-Platz
○	○	Heinrich-Lübke-Platz
○	○	Uhlandstraße
○	○	Arndtplatz
○	○	Uni/OsnabrückHalle
○	○	Neumarkt
○	○	Stresemannplatz
○	○	Hauptbahnhof
○		Konrad-Adenauer-Ring
○		Rosenplatz
○		Landessozialamt
○		Lutherkirche
○		Schölerberg
○		Kinderhospital/Jugendhbg.
○		Paradiesweg
○		Nahne
○		Nahner Feld
○		Frankfurter Heerstraße
○		Kreishaus/Zoo

A : Linie 22

Ⓝ : NICHT vom 23.12.15 - 03.01.2016 + 23.06. - 03.08.2016

ohne Zeichen Linie 21