O 66: Poster: Scanning Probe Microscopy with Quartz Sensors

Time: Wednesday 18:00–20:00 Location: P2/EG

O 66.1 Wed 18:00 P2/EG

Atomically Precise Synthesis and Characterization of Heptauthrene with Triplet Ground State — Xuelei Su[1], Can Li[2], •Qingyang Du[1], Kun Tao[3], Shiyong Wang[2], and Ping Yu[1] — [1]School of Physical Science and Technology, ShanghaiTech University, 201210 Shanghai, China — [2]Key Laboratory of Artificial Structures and Quantum Control (Ministry of Education), Shenyang National Laboratory for Materials Science, School of Physics and Astronomy and Tsung-Dao Lee Institute, Shanghai Jiao Tong University, Shanghai 200240, China — [3]Key Lab for Magnetism and Magnetic Materials of Ministry of Education, Lanzhou University, 730000 LanZhou, China

Heptauthrene, one of the most well-known structures, is a benzene-fused bisphenalenyls in mirror symmetry with triplet ground state. However, it is difficult to synthesize heptauthrene without any substituents due to its high activity. Owing to the development of on-surface synthesis, it is possible to obtain highly active species with properly-designed precursors. Here, we combined in-solution and on-surface synthesis to achieve unsubstituted heptauthrene, whose chemical structure can be characterized with bond-resolved atomic force microscopy. Its triplet ground state is clearly confirmed by the Kondo resonance around zero bias in dI/dV spectra. The response of this Kondo peak to external magnetic field is also detected to verify the high-spin state. We also engineered its spin-state through hydrogen atom addition or dissociation by tip manipulation. Our work provides access to phenalenyl-based structures with high-spin ground states, potentially useful in constructing spin networks.

O 66.2 Wed 18:00 P2/EG

Novel image interpretation methods for high-resolution STM — •Lauri Kurki[1], Niko Oinonen[1], Ondrej Krejci[1], and Adam S. Foster[1,2] — [1]Department of Applied Physics, Aalto University, 00076, Espoo, Finland — [2]WPI Nano Life Science Institute, Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan

Scanning tunnelling microscopy (STM) functionalized with a CO molecule on the probe apex is a method capable of capturing sub-molecular level detail of the electronic and physical structure of a sample[1]. However, the produced images are often difficult to interpret due to the convoluted nature of the signal. We propose image interpretation tools to extract physical and electronic information directly from STM images using machine learning.

In recent years, there has been rapid development in image analysis methods using machine learning, with particular impact in medical imaging. These concepts have been proven effective also in SPM in general and in particular for extracting physical features from atomic force microscopy (AFM) images[2]. We build upon these models and show that we can extract atomic positions and electrostatics directly from STM images. We further explore how the accuracy of these predictions varies with the use of a simultaneous AFM signal and ultimately establish the limits of the approach in an experimental context.

[1] Shuning Cai, Lauri Kurki, Chen Xu, Adam S. Foster, and Peter Liljeroth. JACS 144 (44), 20227-20231 (2022)

[2] Niko Oinonen, Lauri Kurki, Alexander Ilin, and Adam S. Foster. MRS Bulletin 47, 895-905 (2022)

O 66.3 Wed 18:00 P2/EG

Distance dependence of s- and p-wave contributions in CO-tip STM — •Leonard-Alexander Lieske, Fabian Paschke, Florian Albrecht, and Leo Gross — IBM Research Europe - Zürich, Säumerstrasse 4, 8803 Rüschlikon, Switzerland

Funtionalized tips are frequently used in high-resolution AFM, particularly CO terminated tips, to facilitate atomic resolution [1]. CO functionalized tips can also enhance contrast in STM measurements of ionic resonances, mapping orbital densities [2,3]. For CO tips both s- and p-wave character of the tip contribute to the contrast [3,4,5]. Here, we study the contributions of s- and p-wave character of CO tips as a function of tip height, bias voltage and tunneling current.

[1] L. Gross, F. Mohn, N. Moll, P. Liljeroth and G. Meyer, Science, 325(5944), 1110-1114 (2009).
[2] J. Repp, G. Meyer, S. M. Stojković, A. Gourdon and C. Joachim, Physical Review Letters, 94(2) 026803 (2005).
[3] L. Gross, N. Moll, F. Mohn, A. Curioni, G. Meyer, F. Hanke and M. Persson, Physical Review Letters, 107(8), 086101 (2011).
[4] N. Pavliček, I. Swart, J. Niedenführ, G. Meyer and J. Repp, Phys. Rev. Lett. 110, 136101 (2013).
[5] A. Gustafsson and M. Paulsson, Phys. Rev. B, 93, 115434 (2016).

O 66.4 Wed 18:00 P2/EG

Atomic-scale imaging of individual cyclic oligosaccharides with non-contact atomic force microscopy — •Márkó Grabarics[1,3], Benjamin Mallada Faes[2,3], Alejandro Jiménez-Martín[2], Pavel Jelínek[2], Bruno de la Torre[2], and Stephan Rauschenbach[1] — [1]University of Oxford, Department of Chemistry, United Kingdom — [2]Institute of Physics of Czech Academy of Sciences, Czech Republic — [3]These authors contributed equally.

Carbohydrates, also referred to as saccharides, are a major class of biopolymers that are essential to all known living organisms. While important in a range of biological processes, the structural complexity of carbohydrates poses a challenge to conventional analytical techinques, which often fail to provide unambiguous structural assignment.

We aim to overcome this challenge by imaging single, surface-adsorbed carbohydrate molecules using high-resolution SPM. For these proof-of-concept experiments, β-cyclodextrin was chosen as model compound, a cyclic oligosaccharide consisting of seven glucose units linked together *via* α-1,4-glycosidic linkages. Incompatible with thermal evaporation, the molecules were deposited in ultrahigh vacuum onto close-packed noble metal surfaces using electrospray deposition. STM and non-contact AFM with CO-functionalized tips revealed two distinct adsorption geometries, with the individual glucose units clearly resolved within the macrocycles.

Our results demonstrate the potential of high-resolution SPM for the structural characterization of carbohydrates, opening up novel ways for the analysis of this important class of biomolecules.

O 66.5 Wed 18:00 P2/EG

observation and definition of lipid raft in live MCF-7 cell by AFM — •Hsiang-Ling Chuang[1], Yu-Chen Fa[2], Chun-Hsien Chen[1], Lli-Chen Wu[3], and Ja-An Ho[1,2] — [1]department of chemistry, National Taiwan University, Taiwan 10617. — [2]department of biochemical science and technology, National Taiwan University, Taiwan 10617. — [3]department of applied chemistry, National Chi Nan University, Nantou, Taiwan 54561.

Lipid rafts are composed of cholesterol, sphingolipid, and proteins. Previous studies indicated that resveratrol and fibrinogen can bind to the receptor on alpha-v beta-3 integrin. Through the protein-lipid or protein-protein interactions, drug-bound integrins will aggregate into larger raft blocks with unbound integrins. Due to the limitation of optical microscopy and complicated sample preparation, the techniques on lipid rafts observation have shortages of real-time and original state information. In this study, we explore the application of in-situ atomic force microscope (AFM) for the observation of lipid rafts on the cell surface and the response upon the administration of chemicals in real time. We obtained AFM images of morphology and stiffness of live breast cancer cells (MCF-7) in phosphate buffered saline (PBS), resveratrol and fibrinogen solutions to identify the location, drifting and aggregation of lipid rafts. Via cross-comparison of AFM images, the regions are higher and stiffer than the surrounding cell membranes resemble the characteristics of lipid rafts. The developed method may be applicable to identify the location of lipid rafts in real-time and allow us to elucidate complex biological systems at the molecular level.

O 66.6 Wed 18:00 P2/EG

Balanced trolling quartz-based sensor with high quality factor used for atomic force microscopy in the liquid — Rui Lin, •Yingzi Li, Jianqiang Qian, and Peng Cheng — School of Physics, Beihang University, Beijing, China

Quartz tuning fork (QTF) has been widely used in atomic force microscopy (AFM) due to its self-sensing property, high quality factor, and high frequency stability. However, owing to the bulky structure and exposed surface electrode arrangement of QTF, the application of quartz-based AFM sensor in the liquid imaging is limited. One way to solve this problem is to coat the QTF with an insulating layer and immerse it into the liquid. However, it would result in a sharp drop of the quality factor and lead to reduction of force detection sensitiv-

ity. Here, a high quality factor AFM sensor based on balanced trolling QTF is proposed. Both prongs of the QTF are glued with same tips to make sure high symmetry of QTF, while only one tip is immersed in the liquid. In this configuration, the hydrodynamic interaction can be reduced so that the quartz-based sensor can maintain a high quality factor, which will improve the sensitivity of force detection in the liquid. A theoretical model is presented to analyze the sensing performance of the balanced trolling quartz-based sensor in the liquid. Then, the sensing performance of the sensor is estimated through experimental tests. Finally, the proposed sensor is applied in AFM imaging on different samples in the liquid. The results validate the high quality of the proposed balanced trolling quartz-based sensor and its feasibility of liquid imaging of AFM.

O 66.7 Wed 18:00 P2/EG

AFM characterization of surface metal oxides with an O-terminated copper tip — •Philipp Wiesener, Bertram Schulze-Lammers, Harald Fuchs, and Harry Mönig — Westfälische Wilhelms-Universität, Münster, Germany

Previously we invastigated the performance of various tip terminations, namely Cu-, Xe-, CO-, and O-terminated Cu-tips (CuOx-tips), on the Cu(110)O(2x1) surface with non contact AFM. A direct comparison of the imaging and force-spectroscopy capabilities by these different tip terminations shows, that only for the CuOx-tip a significantly selective force interaction between metal and oxygen atoms can be observerd.

In this work we want to generalize the idea of chemical selective imaging by analyzing a broad spectrum of metal oxide systems with CuOx-tips. We perform constant height measurements over an extendend range of tip sample distances and analyze surfaces that posses varying relative heights of metal and oxygen atoms to probe possible effects on the chemical selectivity. For an additional contrast analysis we investigate various defects of the metal oxide surfaces and complement our site-selective microscopy with force-spectroscopy measuerements on the observerd metal and oxygen atoms.

The performed measurements can be seen as a first step of developing CuOx-tip AFM imaging as an efficient tool for the surface characterization of metal oxide materials. Subsequently, we want to extend our methodology to more complex surface- and bulk metal oxide systems and relate them with complementary DFT calulations and AFM simulations.

O 66.8 Wed 18:00 P2/EG

On-Surface Synthesis of C144 Hexagonal Coronoid with Zigzag Edges — •Xujie Zhu, Yanan Liu, Weiwen Pu, Fang-Zi Liu, Zhijie Xue, Zhaoru Sun, Kaking Yan, and Ping Yu — School of Physical Science and Technology, ShanghaiTech University, 201210 Shanghai, China

Coronoids as polycyclic aromatic macrocycles enclosing a cavity and they can be also regarded as nanoporous graphene molecules whose electronic properties are critically dependent on the size and topology of their outer and inner peripheries. However, because of their synthetic and characteristic challenges, the extended hexagonal coronoids with zigzag outer edges have not been reported yet. Here, we report the on-surface synthesis of C144 hexagonal coronoid with outer zigzag edges on a designed precursor undergoing hierarchical Ullmann coupling and cyclodehydrogenation on the Au(111) surface. The chemical and electronic structure is unambiguously characterized by bond-resolved non-contact atomic force microscopy and scanning tunneling spectroscopy measurements. In combination with the density functional theory calculations, the result is shown that the HOMO-LUMO energy gap oscillates with the size of the central cavity. Moreover, the values of the harmonic oscillator model of aromaticity suggest that the molecular structure is ideally represented by Clars model. Our results provide approaches toward realizing a hexagonal coronoid with zigzag edges, potentially inspiring fabrication of hexagonal zigzag coronoids with multiple radical characters in the future.

O 66.9 Wed 18:00 P2/EG

Setup of a quartz needle sensor-based nc-AFM/STM operating at millikelvin temperatures — •Sven Just[1,2], Taner Esat[1,2], Denis Krylov[1,2], Peter Coenen[1,2,3], Vasily Cherepanov[1,2,3], Bert Voigtländer[1,2,3], Stefan Tautz[1,2], and Ruslan Temirov[1,2,4] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology — [3]mProbes GmbH, 52428 Jülich, Germany — [4]Institute of Physics II, University of Cologne, 50937 Cologne, Germany

A non-contact (nc) atomic force microscope (AFM) is developed for operation in ultra-high vacuum at a base temperature of 300 mK. The AFM is based on an ultra-compact quartz needle sensor oscillating at 1 MHz with a 7.5 μm thick tungsten tip glued to one end of the needle allowing for simultaneous operation of AFM and STM [1]. Nanopositioners with resistive readout and a scanner with a large low-temperature scan range of $30 \times 30\,\mu m^2$ are used. Additionally, HF wiring for an antenna and a capillary for supply of gases, both close to the junction, are provided. The AFM setup is mounted on a removable insert (mK-stick) for usage in an existing millikelvin system based on adiabatic demagnetization refrigeration (ADR) [2]. Due to the modularity of the mK-sticks a quick exchange is possible without any need for warming up the LHe cryostat.

[1] I. Morawski et al., Rev. Sci. Instrum. **81**, 033703 (2010)
[2] T. Esat et al., Rev. Sci. Instrum. **92**, 063701 (2021)

O 66.10 Wed 18:00 P2/EG

Electrostatic Discovery Atomic Force Microscopy — Niko Oinonen[1], •Chen Xu[1], Benjamin Alldritt[1], Prokop Hapala[2], Filippo Federici Canova[1,3], Fedor Urtev[1,4], Shuning Cai[1], Ondřej Krejčí[1], Juho Kannala[4], Peter Liljeroth[1], and Adam S. Foster[1,5] — [1]Department of Applied Physics, Aalto University, 00076 Aalto, Espoo, Finland — [2]FZU - Institute of Physics of the Czech Academy of Sciences, 182 21 Prague 8, Czechia — [3]Nanolayers Research Computing Ltd., London N12 OHL, United Kingdom — [4]Department of Computer Science, Aalto University, 00076 Aalto, Espoo, Finland — [5]WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan

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.

O 66.11 Wed 18:00 P2/EG

Building up atomically-precise topological heterostructures in one-dimensional conjugated polymers — •Alejandro Jiménez-Martín[1,2,3], Shayan Edalatmanesh[1,2], Benjamin Mallada[1,2], Héctor González-Herrero[4], David Ecija[5], Pavel Jelínek[1,2], and Bruno de la Torre[1,2] — [1]Czech Advanced Technology and Research Institute (CATRIN), Palacký University, Olomouc, Czech Republic — [2]Czech Academy of Sciences, Prague, Czech Republic — [3]Czech Technical University, Prague, Czech Republic — [4]Universidad Autónoma, Madrid, Spain — [5]IMDEA Nanoscience, Madrid, Spain

The discovery of topological phases in acene-based π-conjugated polymers has been one of the most exciting developments in the field of on-surface synthesis [1]. We recently demonstrated that the topological phase transition can be precisely controlled by the length of the polymer [2], where topologically protected zero-mode states forms at the boundary between two interfaces.

In this contribution, we use such new design criteria for engineering the quantum phase to place edge-gap states at specific sites within a single polymer. We investigate the electronic properties and level of hybridization in close enough topological states depending on their separation by Scanning Tunneling Microscopy and non-contact Atomic Force Microscopy. The results presented here could serve as a blueprint for creating topologically protected quantum spin chains.

[1] B. Cirera, et al., Nano letters 14, (2014).
[2] H. González-Herrero, et al., Advanced Materials 33, (2021)