O 87: Focus Session: Scanning Probe Microscopy with Quartz Sensors III

Time: Thursday 15:00–17:30 Location: TRE Ma

Topical Talk O 87.1 Thu 15:00 TRE Ma

Quartz-sensor detection for single-electron tunneling spectroscopy — •Jascha Repp — Department of Physics, University of Regensburg, 93040 Regensburg, Germany

We exploit the high sensitivity of qPlus-based [1] atomic force microscopy (AFM) to perform scanning tunneling microscopy (STM) and spectroscopy on molecules in absence of any conductance of the underlying substrate. Thereby, we gain access to out-of-equilibrium charge states that are out of reach for conventional STM [2]. Extending this technique by electronic pump-probe spectroscopy [3], we measured the triplet lifetime of an individual pentacene molecule on an insulating surface [4] and lifetime quenching by nearby oxygen molecules. Combined with radio-frequency magnetic-field driving we introduce AFM-based electron spin resonance and spin manipulation showing long spin coherence in single molecules.

References: [1] F. J. Giessibl, Appl. Phys. Lett. 73, 3956 (1998). [2] L. L. Patera et al., Nature 566, 245 (2019). [3] S. Loth et al., Science 329, 1628 (2010). [4] J. Peng et al., Science 373, 452 (2021).

O 87.2 Thu 15:30 TRE Ma

molecular diffusion studied by multidimensional cantilever-based UHV AFM — •Zuned Ahmed[1,2], Hao Liu[1,2], Manfred Parschau[1], and Hans Josef Hug[1,2] — [1]Empa (Swiss Federal Laboratories for Materials Science and Technology), Dübendorf , Switzerland — [2]University of Basel, Switzerland

Scanning probe microscopy permits a characterization of the diffusion of atoms or molecules on surfaces, which is governed by diffusion energy barrier and entropy difference between ground and excited states. With our home-built, cantilever based UHV, low temperature scanning force microscope [1], we studied the diffusion of benzene-based molecules with flexible and rigid hydrocarbon chains, namely,1,3,5-Triethylbenzene (TEB) and 1,3,5-Trimethylbenzene (TMB), respectively, measured at temperatures between 6.38 and 10.68 K on Cu (111). An Arrhenius analysis revealed that the molecule with the flexible hydrocarbon arms (TEB) showed an enhanced diffusion rate which we can attribute to its higher configurational entropy of its ethyl chains. Moreover, we used multidimensional AFM to map the vertical and lateral forces required to manipulate both molecules. Compatible with the lower diffusion energy barrier of the TEB molecule, the force required to manipulate the TEB was much smaller than that of the TMB molecule. In addition, the measured flexural and torsional frequency shift data permitted a detailed analysis of the manipulation process.

[1] Liu et al. Beilstein J. Nanotechnol. 2022, 13, 1120-1140

O 87.3 Thu 15:45 TRE Ma

Flexible Superlubricity Unveiled in Snake-Like motion of Individual Chains — •Guilherme Vilhena[1,2], Rémy Pawlak[1], Philipp D'Astolfo[1], Xunshan Liu[3], Enrico Gnecco[4], Marcin Kisiel[1], Thilo Glatzel[1], Rúben Pérez[2], Robert Häner[3], Silvio Decurtins[3], Alexis Baratoff[1], Giacomo Prampolini[5], Shi-Xia Liu[3], and Ernst Meyer[1] — [1]University of Basel, Switzerland — [2]Universidad Autónoma de Madrid, Spain — [3]University of Bern, Switzerland — [4]Jagiellonian University, Poland — [5]Consiglio Nazionale delle Ricerche, Italy

A combination of low-temperature atomic force microcopy and molecular dynamic simulations demonstrates that soft designer molecules realize a sidewinding motion when dragged over a gold surface. Exploiting their longitudinal flexibility, pyrenylene chains are indeed able to lower diffusion energy barriers via on-surface directional locking and molecular strain. The resulting ultralow friction reaches values on the order of tens of pN reported so far only for rigid chains sliding on an incommensurate surface. Therefore, we demonstrate how molecular flexibility can be harnessed to realize complex nanomotion while retaining a superlubric character. This is in contrast with the paradigm guiding the design of most superlubric nanocontacts (mismatched rigid contacting surfaces).

O 87.4 Thu 16:00 TRE Ma

Machine learning for high-resolution AFM image interpretation — •Niko Oinonen[1], Lauri Kurki[1], Chen Xu[1], Shuning Cai[1], Markus Aapro[1], Alexander Ilin[2], Peter Liljeroth[1], and Adam Foster[1,3] — [1]Department of Applied Physics, Aalto University, Finland — [2]Department of Computer Science, Aalto University, Finland — [3]WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Japan

State-of-the-art non-contact atomic force microscopy (AFM) setups operating in vacuum at low temperatures are able to resolve features on the scale of individual atoms in molecules [1]. However, 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]. Our recent work refines the geometry prediction task by predicting the molecule graph of the sample using a model based on graph neural networks [3]. The current challenge is in generalizing from simulated training data to experimental test data, where we find that the choice of the training data becomes very important.

[1] L. Gross et al., Science, vol. 325, no. 5944, pp. 1110–1114, 2009.
[2] N. Oinonen et al., ACS Nano, 16, 1, 89–97, 2022.
[3] N. Oinonen et al., MRS Bulletin 47, 895–905, 2022.

Topical Talk O 87.5 Thu 16:15 TRE Ma

Application of atomic force microscopy with quartz sensors to quantum states in graphene and related twisted heterostructures — •Joseph Stroscio — National Institute of Standards and Technology, Gaithersburg, MD, USA.

Atomic force microscopy (AFM) with quartz sensors pioneered by Franz Giessibl has opened many applications in quantum nanoscience where AFM measurements can be made simultaneously and conveniently with scanning tunneling microscopy measurements (STM). In this presentation I will review our work using combined AFM/STM measurements to give a microscopic view of the quantum states in single layer graphene and in twisted graphene heterostructures. In single layer graphene, electrostatic pn junction boundaries provide a convenient geometry for the examination of quantum Hall edge states with microscopic probes. For a graphene Hall bar device defined and tunable by dual gates, we carry out simultaneous AFM, STM, and electrical transport measurements in the system which we developed for detailed measurements of two-dimensional devices in-operando at mK temperatures and in magnetic fields up to 15 T. The AFM, operated in the Kelvin probe force microscopy (KPFM) mode, detects the chemical potential transitions when Landau levels are being filled or emptied as a function of back gate potential with the same fidelity as the scanning tunneling spectroscopy measurements. With KPFM we can map the dispersion of the Landau levels across the quantum Hall edge boundary as a function of density and spatial position.

O 87.6 Thu 16:45 TRE Ma

On the origin and elimination of cross coupling between excitation and tunneling current in scanning probe experiments that utilize the qPlus sensor — •Michael Schelchshorn — Institute of Experimental and Applied Physics, University of Regensburg, Universitätsstraße 31, 93053 Regensburg

The qPlus sensor is a stiff quartz cantilever that facilitates high-resolution combined STM/AFM [1]. Both a tunneling current and the deflection signal resulting from the forces at the tip are measured simultaneously; however, unwanted cross coupling between the tunneling current signal and the excitation of the sensor oscillation can occur. At one bias polarity, this cross coupling acts as an excitation of the oscillation, in the opposite bias it appears as a damping.

This unwanted effect has been observed since the early years of combined STM/AFM experiments using qPlus sensors, but was difficult to explain. Here, we present a new theory that explains this phenomenon, supported by experiments and supplemented by verified measures on how to prevent or at least minimize cross talk. [2]

[1] F.J. Giessibl, The qPlus sensor: a powerful core for the atomic force microscope, Rev. Sci. Instrum. 90, 011101 (2019).

[2] M. Schelchshorn, On the origin of cross coupling between excitation and tunneling current in combined STM/AFM qPlus experiments, University of Regensburg, B.Sc. thesis (2022)

O 87.7 Thu 17:00 TRE Ma

Fe adsorbates and their effect on the surfaces of topological insulators $TlBiSe_2$ and Bi_2Se_3 — •Adrian Weindl, Christoph Setescak, Emma Grasser, Alexander Liebig, and Franz J. Giessibl — University of Regensburg, Regensburg, Germany

Can one tailor the properties of the topological surface state (TSS) of topological insulators (TIs) by magnetic doping of the TI material? Here, we study the effect of magnetic adatoms on TI surfaces by combined scanning tunneling microscopy (STM) and atomic force microscopy (AFM). Two archetypical TIs, Bi_2Se_3 and $TlBiSe_2$, are analyzed, which both have relatively large band gaps with their Dirac points well isolated and far from bulk states. Magnetic impurities, in this case single Fe adatoms, and their influence on the local density of states (LDOS) of the two TIs are investigated by scanning tunneling spectroscopy. We detect resonances in the LDOS for both surfaces that arise due to the scattering of electrons in the TSS at these impurities. The position and shape of these resonances are a function of the exact adsorption position of the adatoms, which can be determined by atomically-resolved AFM measurements. In addition, we detect a relaxation of surface atoms due to the presence of Fe adatoms on Bi_2Se_3. The charge state of the Fe adatoms is determined by Kelvin probe force spectroscopy.

O 87.8 Thu 17:15 TRE Ma

The (2x1) reconstruction of calcite(104) — Jonas Heggemann[1], Yashasvi Ranawat[2], Ondřej Krejčí[2], Adam S. Foster[2], and •Philipp Rahe[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49076 Osnabrück, Germany — [2]Department of Applied Physics, Aalto University, Helsinki FI-00076, Finland

Calcite 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 CO2 [2]. Despite intensive studies, however, there is still serious ambiguity regarding the properties of this surface due to conflictive conclusions for the so-called row-pairing [3] and (2x1) reconstruction [4].

Here, we use a combination of non-contact atomic force microcopy (NC-AFM) with CO-functionalized tips at 5K, density functional theory with state-of-the-art dispersion corrections, and NC-AFM image simulations to clarify the microscopic geometry of calcite(104). A (2x1) reconstruction and a glide plane symmetry is consistently found in the NC-AFM data and DFT results. Most importantly, we identify two different adsorption positions for CO molecules within the (2x1) unit cell. These findings are most critical for future studies where processes on calcite(104)-(2x1) are influenced by the surface geometry.

[1] L. Addadi, S. Weiner, Angew. Chem. Int. Ed. Engl. 31, 153 (1992). [2] P. A. E. Pogge von Strandmann, et al., Nat. Commun. 10, 1983 (2019). [3] A. L. Rachlin, et al., Am. Mineral. 77, 904 (1992). [4] S. L. S. Stipp, et al., Geochim. Cosmochim. Acta 58, 3023 (1994).