O 3: Scanning probe techniques: Method development I

Time: Monday 10:30–12:15 Location: HSZ/0204

O 3.1 Mon 10:30 HSZ/0204

Single-Molecule Insights into On-Surface C-C Bond Formation: Radical Control via Sequential Dehalogenation — Qigang Zhong[1], Daniel Kohrs[2], Jannis Jung[3], Daniel Ebeling[1], Doreen Mollenhauer[3], Hermann Wegner[2], and •Andre Schirmeisen[1] — [1]Institute of Applied Physics, Justus-Liebig University Giessen, Giessen, Germany — [2]Institute of Organic Chemistry, Justus Liebig University Giessen, Giessen, Germany — [3]Institute of Physical Chemistry, Justus Liebig University Giessen, Giessen, Germany

On-surface synthesis through dehalogenative coupling provides a powerful route to construct carbon-carbon bonds with atomic precision. Using a combination of scanning tunneling microscopy (STM), atomic force microscopy (AFM), and density functional theory (DFT), we investigated the radical intermediates and coupling pathways of brominated polyaromatic precursors, specifically BBPN and BPIN, on Ag(111). Controlled thermal and tip-induced dehalogenation enabled the selective generation of phenyl and naphthyl radicals, which were subsequently characterized at the single-molecule level. Statistical analysis of tip-induced reactions reveals that cyclization leading to C-C bond formation occurs preferentially when the first dehalogenation takes place at the naphthyl group. Computational modeling demonstrates that radical alignment and flexibility govern the feasibility of C-C coupling. These findings highlight the interplay between precursor structure, radical generation sequence, and surface interactions in steering on-surface coupling chemistry.

O 3.2 Mon 10:45 HSZ/0204

Scanning probe microscopy investigation on cyclocarbons — •Jakob Eckrich[1], Lisanne Sellies[1], Marco Vitek[3], Yueze Gao[2], Fabian Paschke[1], Florian Albrecht[1], Leonard-Alexander Lieske[1], Harry L. Anderson[2], Igor Rončević[3], and Leo Gross[1] — [1]IBM Research Europe - Zurich, Rüschlikon, Switzerland — [2]Oxford University, Oxford, UK — [3]University of Manchester, Manchester, UK

I will discuss our recent investigations of cyclocarbons by means of scanning tunneling microscopy (STM) and atomic force microscopy (AFM). Cyclocarbons, molecular carbon allotropes consisting of a ring of two-fold coordinated carbon atoms, have been synthesized on surface using tip-induced chemistry [1-3], and the formation of larger cyclocarbons by dimerization of precursors was shown [3]. This talk will focus on the generation and investigation of large cyclocarbons.

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

O 3.3 Mon 11:00 HSZ/0204

Machine Learning Models Tailored for Scanning Probe Microscopy Topographic Data — •Lovis Hardeweg, Johanna Matusche, Johannes Schwenk, Christoph Sürgers, Wolfgang Wernsdorfer, and Philip Willke — Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany

Modern machine learning methods have great potential to automate processes in scanning probe microscopy (SPM). An important step for any automated operation of SPM is the accurate extraction of meaningful information, such as the position and type of adsorbates, from topographic data. Existing frameworks, that localize and identify adsorbates on the surface [1], often rely on large models developed by the traditional computer vision community. Therefore, their application to SPM topographies has certain drawbacks.

Here, we present two machine learning architectures that are adapted specifically for their application to high-resolution low-temperature SPM data. The first model predicts a semantic segmentation on samples with heterogeneous surface material, Ag(001) and MgO/Ag(001) in particular. The second model is trained to identify adatoms, molecules and possible clusters adsorbed on the surface. Both models achieve high accuracy. Additionally, due to their reduced size, they require fewer resources during training and application than models, that have not been purpose-built for their respective tasks.

[1] J. Am. Chem. Soc, 147, 39, 35232-35243 (2025)

O 3.4 Mon 11:15 HSZ/0204

Exploring Dissipation in Single-Molecule Manipulation — •Norio Okabayashi[1], Alfred J. Weymouth[2], Sophia Schweiss[2], Thomas Frederiksen[3,4], and Franz J. Giessibl[2] — [1]Kanazawa University, Ishikawa 920-1192, Japan — [2]University of Regensburg, Regensburg D-93053, Germany — [3]Donostia International Physics Center, San Sebastián 20018, Spain — [4]Basque Foundation for Science, Bilbao 48013, Spain

Single-molecule manipulation with scanning probe microscopy (SPM) offers a well-defined platform for studying nanoscale friction. While previous work has focused mainly on the forces driving molecular motion [1], the corresponding dissipation processes remain less explored. Here, we investigate a single CO molecule on Cu(110) using STM, AFM, LFM, and DFT at low temperatures. DFT identifies the preferred adsorption sites and the switching pathway (top-bridge-top), which are confirmed experimentally by IETS and by dissipation signals during AFM and LFM oscillations. In AFM [2], dissipation appears only along specific manipulation paths, whereas in LFM it also arises along trajectories associated with molecular switching. The switching rate is evaluated from STM as a function of lateral tip position, giving the manipulation probability per LFM oscillation cycle. Combining this cycle-resolved rate with the measured dissipation per cycle allows us to quantify the energy dissipated per manipulation event. [1] M. Ternes et al., Science 319, 1066 (2008); [2] N. Okabayashi et al., PRL 131, 148001 (2023).

O 3.5 Mon 11:30 HSZ/0204

A direct measurement of weak lateral trapping over a C_6 ring — •Alfred John Weymouth[1], Maximilian Titl[1], Shinjae Nam[1], Lukas Hörmann[2], Oliver Hofmann[3], and Franz J. Giessibl[1] — [1]University of Regensburg, Germany — [2]University of Warwick, U.K. — [3]TU Graz, Austria

Six-membered carbon rings (C_6 rings) can be found in a multitude of systems from graphite to organic molecules. Graphitic surfaces are so flat that they have been used to explore superlubricity, where one important aspect of their frictional response is the trapping of a single atom in an individual C_6 ring. This trapping also plays a role in the lateral movement of adsorbates on these surfaces. However, studies investigating trapping on these surfaces often focus only on strongly-bound adsorbates. We experimentally measure the trapping of a weakly-bound single atom asperity using lateral force microscopy with a CO-tip and simulate this system with DFT-based methods. Surprisingly, we observe a uniform lateral spring constant within individual C_6 rings over heights of tens of picometers for a range of systems. To precisely determine the surface trapping, we re-evaluate the lateral spring constant of the CO at the tip apex. With this value, we determined a very weak lateral spring constant of a particle within a C_6 ring.

O 3.6 Mon 11:45 HSZ/0204

Atomic scale energy dissipation as a function of temperature measured with LFM — •Sophia Schweiss[1], Lukas Hörmann[2], Franz Giessibl[1], and Alfred Weymouth[1] — [1]University of Regensburg, Regensburg, Germany — [2]University of Vienna, Vienna, Austria

One method of studying atomically resolved surfaces and adsorbates is small amplitude FM-AFM. With this technique, the conservative (frequency shift, Δf) and non-conservative (dissipated energy, E_{diss}) components of the tip-sample interaction are measured. Lateral force microscopy (LFM) is a related technique in which the tip oscillates laterally. Tip preparation for standard FM-AFM experiments at low temperature often includes the pickup of a CO molecule at the tip apex, which results in an inert tip with enhanced imaging properties. [1] These tip preparation techniques are also available for LFM. Over individual chemical bonds, LFM yields a measurable E_{diss} signal which we interpret as the CO snapping over the bond. [2]

Here, a CO-terminated tip is used to investigate the bonds of PTCDA molecules deposited on a Cu(111) surface with LFM. E_{diss} is measured for different temperatures in the range of 5.3 K to 6.5 K. Certain bonds exhibit a distinct T-dependence, whereas others do not.

[1] Gross et al., Science, 325, 1110 (2009)

[2] Weymouth et al., Phys. Rev. Lett., 124, 196101 (2020)

O 3.7 Mon 12:00 HSZ/0204

Bond-resolved STM with density-based methods — Emiliano Ventura-Macias[1], Jose Martinez-Castro[2], Guillermo Haas[1,3], •Jara Trujillo-Mulero[1], Pablo Pou[1], Markus Ternes[2], Ruslan Temirov[2], Frank Stefan Tautz[2], and Rubén Pérez[1] — [1]Departamento de Física Teórica de la Materia Condensada and Instituto de Física de la Materia Condensada (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425, Jülich, Germany — [3]Grenoble INP-Phelma, 3 Parv. Louis Néel, 38000 Grenoble, France

Bond-resolved STM (BRSTM) combines scanning tunneling microscopy with the intramolecular resolution of CO-functionalized ncAFM. We introduce a simple, broadly applicable method for simulating BRSTM images and apply it to new measurements of PTCDA on Ag(111) acquired with unprecedented tip-sample control (~10 pm). Our approach integrates the Full-Density-Based Model (FDBM) for high-resolution AFM with Chen's derivative approximation, capturing both σ and π tunneling channels while accounting for CO-tip deflection. It accurately reproduces experimental images of PTCDA/Ag(111) and TOAT/Cu(111), including subtle distance-dependent features. We also show that substrate-induced changes in orbital occupation and CO relaxation significantly influence BRSTM contrast.