O 35: Organic molecules on inorganic substrates: Adsorption and growth II

Time: Tuesday 10:30–12:15 Location: HSZ/0401

O 35.1 Tue 10:30 HSZ/0401

Phophangulenes on Au(111): comparing the influence of the environment on single molecule rotation — •Wyatt Highland[1], Sajjan Mohammad[1], Paul Philip Schmidt[1], Roberto Robles[2], Milan Kivala[3], Nicolas Lorente[2], Meike Stöhr[1,4], and Sabine Maier[1] — [1]Department Physik, FAU Erlangen-Nürnberg, Erlangen, Germany — [2]CFM/MPC (CSIC-UPV/EHU), Donostia-San Sebastian, Spain — [3]Institute of Organic Chemistry, Heidelberg University, Heidelberg, Germany — [4]University of Applied Sciences of the Grisons, Switzerland

Bowl-shaped phosphangulenes represent a promising class of rotor molecules for molecular energy-storage applications on surfaces, owing to their fixed rotational axis defined by the central phosphorus atom, which simultaneously serves as the anchoring group on gold substrates. For low coverge, the phosphangulenes stay isolated on Au(111). We examined their adsorption configurations and subsequently, the possibility for rotational motion using both the STM tip and thermal activation as external triggers. At higher coverage, phosphangulenes form compact self-assemblies that suppress their rotational motion. To overcome this, we employ porous, hydrogen-bonded trimesic-acid networks to isolate individual phosphangulenes at the surface. Comparing their rotational dynamics inside and outside the pores allowed to directly reveal the influence of the immediate surroundings on the rotational motion.

O 35.2 Tue 10:45 HSZ/0401

Self-assembly and electronic properties of functionalized norbornadiene photoswitches on Au(111) and graphene/Ir(111) — •Shreya Garg[1], Roberto Robles[2], Pedro Ferreira[3], Kasper Moth-Poulsen[3], Nicolas Lorente[2], Meike Stöhr[1,4], and Sabine Maier[1] — [1]Department of Physics, Friedrich Alexander University Erlangen-Nürnberg, Germany — [2]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), Donostia-San Sebastián 20018, Spain, SanSebastián, Spain — [3]Universitat Politecnica de Catalunya, Barcelona, CT, Spain — [4]University of Applied Sciences of the Grisons, Switzerland

The norbornadiene/quadricyclane (NBD/QC) system represents a notable class of photoswitches, in which the low-energy NBD isomer can be transformed into its metastable QC isomer upon exposure to external energy. Here, we investigate the self-assembly and electronic properties of a benzoic acid-functionalized NBD on Au(111) using STM, STS, and DFT. Two distinct adsorption conformations are identified; nevertheless, the overall structure of the self-assembled layers remains governed by hydrogen bonding between the carboxyl groups. To further elucidate molecule-substrate coupling effects, we examined NBD derivatives on graphene/Ir(111), which offers a reduced density of states near the molecular levels, thereby providing partial electronic decoupling. This approach revealed differences in electronic properties compared to Au(111), emphasizing the critical influence of the substrate and contributing to the optimization of their switching performance in future electronic systems.

O 35.3 Tue 11:00 HSZ/0401

Validation of the Rotational Degrees of Freedom in Azobenzene Subphthalocyanine — •Dominik Volavka[1], Wyatt Highland[1], Bartosz Szczefanowicz[1], Rebecci Samuele[1], Roberto Robles[2], Nicolas Lorente[2], Meike Stöhr[1,3], and Sabine Maier[1] — [1]Department of Physics, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — [2]Centro de Física de Materiales (CSIC-UPV/EHU), Donostia-San Sebastián, Spain — [3]University of Applied Sciences of the Grisons, Switzerland

Azobenzene mounted on Subphthalocyanine (Azo-SubPC) via a single covalent oxygen bond is predicted to exhibit interesting rotational and switching properties due to the single bonding character of the boron-oxygen-carbon. Recent attempts at observing these rotational actions through scanning tunneling microscopy were hindered because of the self-assembling nature of Azo-SubPC when deposited on Au(111) and Ag(111). In each case, one-dimensional arrangements of Azo-SubPC formed, wherein molecules were neighbored by additional Azo-SubPC molecules on both sides. The resulting configuration of the molecules thusly led to a high steric hindrance and ultimate restriction of Azo-SubPC's anticipated rotational degree of freedom. Alternative preparation methods of Azo-SubPC are herein proposed and evaluated in the attempt of depositing and identifying isolated Azo-SubPC molecules with preserved rotational freedom. Isolated Azo-SubPC molecules can give insight into the underlying principles dictating the mechanisms of rotation in rotor molecules.

O 35.4 Tue 11:15 HSZ/0401

TPD/R Investigations of Metal-Substrate Interactions of Polyfluorinated Molecules on Au(111) — •Stefan R. Kachel, Evelyn Versok, Leonard Neuhaus, Kassandra Zoltner, and J. Michael Gottfried — Fachbereich Chemie und mar.quest, Philipps-Universität Marburg, Germany.

Interfaces between organic molecules and metal surfaces are crucial in heterogeneous catalysis, organic electronics, and related nanotechnological and sensing applications. Molecules with large dipole moments are particularly relevant, as dipole enhancement through tailored fluorination can strongly influence adsorption geometries, adsorbate-substrate interactions, and thus the electronic properties of molecule-metal interfaces. Among nonionic, saturated compounds, all-cis-hexafluorocyclohexane (HFCH) exhibits the highest known polarity (μ = 6.2 D). Here, we use temperature-programmed desorption and reaction (TPD/R) to investigate the desorption kinetics and energetics of HFCH and two reference compounds, perfluoromethylcyclohexane and cyclohexane, on Au(111). The polar HFCH shows markedly stronger interactions with the substrate than the two reference compounds, and all systems display desorption behavior that deviates substantially from structurally related aromatic species. The pronounced polarity and stacked packing motif of HFCH render it a promising model system for studies in supramolecular chemistry and organic materials research, including potential applications in organic ion-conducting materials.

O 35.5 Tue 11:30 HSZ/0401

TPD Studies on LOHC-relevant Cycloalkanes and Aromatics on Au(111) — •Kassandra Zoltner, Leonard Neuhaus, Stefan R. Kachel, and J. Michael Gottfried — Fachbereich Chemie and mar.quest, Philipps-Universität Marburg, Germany

Liquid organic hydrogen carriers (LOHCs), such as the decalin/tetralin pair, are promising compounds for hydrogen storage, yet their (de)-hydrogenation cycles are limited by catalyst-induced side reactions. In this context, molecule–surface interactions fundamentally determine adsorption strength and reactivity, thereby controlling catalytic selectivity and activity. This work presents surface analytical studies using temperature-programmed desorption (TPD) to investigate the desorption kinetics and energetics of decalin, perhydroazulene, and (partially) dehydrogenated analogues on Au(111). The study focuses on how the degree of hydrogenation, structural motifs including ring connectivity, and configurational isomerism as well as electronic properties influence substrate and intermolecular interaction strengths. The results reveal distinct differences in desorption characteristics: aromatic molecules (naphthalene, azulene, tetralin) exhibit stronger adsorption to the metal substrate and repulsive intermolecular interactions, arising from their π-electron system, whereas saturated hydrocarbons (decalin, perhydroazulene) show weaker substrate binding and intermolecular attraction. The findings provide molecular-level insights into LOHC adsorption properties on metal surfaces and contribute to the development of improved hydrogen storage–catalysis systems.

O 35.6 Tue 11:45 HSZ/0401

MAD-SURF: a general Machine-Learning Potential for molecular adsorption on metal surfaces — •Manuel González Lastre[1], Joakim S. Jestilä[2], Rubén Pérez[1], and Adam S. Foster[2] — [1]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Spain — [2]Department of Applied Physics, Aalto University, 00076, Espoo, Finland.

Predicting how organic molecules adsorb, assemble and interact on metal surfaces is central to surface chemistry, molecular electronics and scanning probe microscopy. Yet, the application of first-principles simulations to interfaces is hampered by the computational cost for evaluating the electronic structure for the large number of atoms typically involved. Here we present MAD-SURF, a general Machine-Learning Interatomic Potential tailored for molecular adsorption on metal sur-

faces. Trained on a broad dataset spanning diverse molecules, adsorption motifs, surfaces, molecular dynamics and non-covalent aggregates, MAD-SURF achieves near quantum-mechanical accuracy while enabling simulations that are orders of magnitude faster than Density Functional Theory. The model reliably reproduces energies, forces and adsorption geometries across different surfaces. We demonstrate its versatility by capturing experimentally observed systems, ranging from organic monolayers and polycyclic aggregates to flexible biomolecules and long-range metal surface reconstructions. By combining accuracy, speed, and generalizability, MAD-SURF offers a practical framework for accelerating atomistic simulations in surface science.

O 35.7 Tue 12:00 HSZ/0401

Using Machine Learning to predict molecular conformations from STM images — •Tim J. Seifert[1], Dhaneesh Kumar[2], Stephan Rauschenbach[3], Klaus Kern[2], Markus Etzkorn[1,4], Kelvin Anggara[2], and Uta Schlickum[1,4] — [1]Institute of Applied Physics, TU Braunschweig, Braunschweig — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]Department of Chemistry, Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom — [4]Laboratory for Emerging Nanometrology LENA, Braunschweig

Single-molecule imaging of biologically essential building blocks such as saccharides and peptides by scanning tunneling microscopy (STM) holds immense promise, enabling key insights into their structure and biological functions. However, automatic structural analysis remains bottlenecked by the lack of available experimental training data. We overcome this fundamental limitation through a novel workflow that rapidly generates vast datasets of high-fidelity synthetic STM images from geometric molecular models. We train a custom Machine Learning architecture on this synthetic data to predict atomic coordinates directly from STM images, enabling fully automated reconstruction of molecular conformations. Validated on two distinct organic systems - glycans and polypeptides - the method achieves atomic positional accuracies below 4 Å and 2 Å, respectively, with unsupervised conformer classification of polypeptides exceeding 97% accuracy. The trained models transfer robustly to experimental STM data, delivering visually convincing structural predictions.