O 46: Organic molecules on inorganic substrates: electronic, optical and other properties – Poster

Time: Tuesday 14:00–16:00 Location: P2

O 46.1 Tue 14:00 P2

Investigation of chiral helicene molecules on the superconducting substrate Pb(111) — •Melvin Grumser[1], Rahel Specht[1], Vincent Herzog[1], Wenhui Niu[2], Narcis Avarvari[3], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany — [3]University of Angers, Angers, France

Chiral molecules have recently garnered a lot of attention for their ability to partially spin polarize currents running through them, which is of interest for the emerging field of spintronics. Chirality induced spin selectivity (CISS) typically manifests itself in experiments in which a current passes through a chiral molecule, as has been done down to the single-molecule scale using scanning tunneling microscopy [1]. However, recent studies suggest that the adsorption of chiral molecules might already lead to magnetization in the surface layer which could locally interact with the Cooper-pairs of a superconducting substrate [2]. Here, we investigate the effect of adsorbed chiral molecules on the elemental superconductor Lead. For this, [7]-Helicene and [6]-Helicene derivatives were evaporated onto a Pb(111) surface and investigated via STM and AFM. The molecules form ordered islands with different orientations of the molecules. In addition, we use scanning tunneling spectroscopy and identified the energy of the HOMO and LUMO. However, we do not observe any signatures of an alteration of the local superconducting behavior.

[1] Safari, Mohammad Reza, et al. Small 20.22 (2024): 2308233.

[2] Shapira, Tamar, et al. Phys. Rev. B 98.21 (2018): 214513.

O 46.2 Tue 14:00 P2

On-Surface Reaction of Naphthothiadiazole Derivatives on Au(111) — •Mohsen Ajdari[1], Jakob Steidel[1], Larissa Winkelmann[1], Felix Landwehr[1], Jakob Sawatzki[1], Jakob Roth[1], Christian Huck[1], Hendrik Hoffmann[2], Uwe H. F. Bunz[2], and Petra Tegeder[1] — [1]Institute for Physical Chemistry — [2]Institute for Organic Chemistry, Heidelberg University, Germany

Naphthothiadiazole (NTD) and its halogenated derivatives (NTD-Br/Cl) are promising electron acceptor candidates for use in (opto)electronic applications.

In a multi-technique approach, this study utilizes scanning tunneling microscopy, two-photon-photoemission spectroscopy, and temperature-programmed desorption to identify on-surface reactions of adsorbed NTD-Br/Cl on Au(111).

Our findings suggest that the halogenated molecules undergo temperature (NTD-Br) and photo-induced (NTD-Br/Cl) dehalogenation reactions. As a result, we found work function changes, differences in the energy-level alignment as well as changes in the adsorption structure.

O 46.3 Tue 14:00 P2

Second Harmonic Generation in Thin Films of Chiral Organic Molecules — •Martin Richter[1], Gayani Liyanage[1], Marjan Krstic[2], Erik Misselwitz[3], Milan Kivala[3], Carsten Rockstuhl[2], and Petra Tegeder[1] — [1]Institute for Physical Chemistry, Heidelberg University, Germany — [2]Institute of Theoretical Solid-State Physics, Karlsruhe Institute of Technology, Germany — [3]Institute of Organic Chemistry, Heidelberg University, Germany

Nonlinear optical (NLO) techniques enable increased sensitivity to chiroptical features. In contrast to linear circular dichroism (CD), second harmonic generation (SHG) chiroptical features can be explained within the dipole approximation. This includes electric as well as magnetic dipolar contributions. The latter are usually much weaker and specific measurement schemes are required to detect them. Here, we investigated thin films of chiral organic molecules using SHG-CD and SHG-ORD (optical rotatory dispersion) to probe the nonlinear CD and optical rotation. Continuous rotation of a quarter-wave plate generates circular and elliptical light to gain insights into the relative amplitudes of the second-order susceptibilities from electric χ^{eee} and magnetic (χ^{mee} and χ^{eem}) dipolar contributions. Our theoretical modelling allowed us to disentangle electric and magnetic dipole contributions.

O 46.4 Tue 14:00 P2

Electronic structure of spiro-bridged N-heterotriangulenes on Au(111) — •Jakob Roth[1], Jakob Sawatzki[1], Christian Huck[1], Angelina Jocic[2], Milan Kivala[2], and Petra Tegeder[1] — [1]Institute for Physical Chemistry — [2]Institute of Organic Chemistry, Heidelberg University

N-heterotriangulenes are versatile p-type organic semiconductors combining enhanced planarity with sterically defined bridges, enabling highly stable amine-centered radical cations, making them promising candidates for semiconducting and energy storage applications.

Here, we investigated the adsorption and electronic structure of two model systems - dimethylmethylene-bridged N-heterotriangulene (TN) and spirofluorene-bridged N-heterotriangulene (FTN) - deposited on Au(111). The spiro-annulated fluorenyl groups of FTN are expected to elevate the molecular core and hence reduce the electronic coupling strength to the metal substrate. Scanning tunnelling microscopy reveals that both species form well-ordered monolayers. Two-photon photoemission spectroscopy quantitatively resolves occupied and unoccupied electronic (transport levels) as well as excitonic states (optical gaps). These results highlight how molecular design controls surface coupling and electronic level alignment in Triphenylamine-based materials.

O 46.5 Tue 14:00 P2

Deprotonation of quinacridone on Ag(100) - an NIXSW/XPS study of the phase transition — Lucas Hirschfeld[1], Morris E. L. Mühlpointner[1], Anna J. Kny[1], Sergey Subach[2], and •Moritz Sokolowski[1] — [1]Clausius Institute for Physical and Theoretical Chemistry, University of Bonn, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, Germany

Quinacridone (QA) forms two different phases on the Ag(100) surface. When QA is deposited at room temperature, the formation of the α-phase with a point-on-line (*pol*) structure is observed. After annealing, the commensurate β-phase is irreversibly formed [1]. The mechanism, involving the loss of intermolecular hydrogen bonds, was not disclosed so far. Thus we have performed a detailed Normal Incidence X-ray Standing Waves (NIXSW)/XPS study.

The N1s XPS spectra exhibit a second peak shifted by 2.2 eV to lower binding energies when going from the α- to the β-phase. This reveals that the irreversible reaction from the α- to the β-phase is explained by a deprotonation of 50 % of the amine groups. The deprotonated N-atoms form stronger bonds to the Ag(100) surface, indicated by a drastic approach of the respective N adsorption height from 4.3 Å in the α-phase to 3.4 Å in the β-phase. These results show that the reaction is driven by the energy gain related to N/Ag interfacial bonds, which overcompensate the loss of intermolecular hydrogen bonds.

Support by Diamond Light Source is acknowledged.

[1] JPCC 124.45 (2020), 24861-24873.

O 46.6 Tue 14:00 P2

Fluorescence Spectroscopy of Quinacridone Molecules on thin Epitaxial KCl(100) films. — •Morris E. L. Mühlpointner and Moritz Sokolowski — Clausius-Institut für Physikalische und Theoretische Chemie der Universität Bonn, Germany

Quinacridone forms one-dimensional chains on metal surfaces and thin epitaxial KCl films grown on Ag(100) [1]. TD-DFT predicts the transition dipole moment in the direction of chain growth. The resulting J-like coupling suggests superradiance which can be enhanced by chemical modifications that increase the inter-chain distance. However, no data on the optical properties of QA on KCl surfaces exist.

We have measured the fluorescence at cryogenic temperatures (7 K) of quinacridone (QA) and its fluorinated derivative (FQA) on ultrathin KCl films grown on Ag(100). Isolated QA molecules on KCl have a 0-0 transition at 20200 ± 200 cm^{-1}. The spectral lines have asymmetric shapes with large line widths (400 to 700 cm^{-1}). We relate the broadening to the weak bonding interactions of the molecule and the substrate.

Upon forming a 2D aggregate on the surface, we observe a significant red shift by 1600 cm^{-1} for QA and FQA. This can be understood by the attractive of the transition dipoles.

[1] JPCC **127** (2023): 23814-23826.

Acknowledgements: We thank the DFG for support via the research training group 2591, Mohammad Al Dubel and Sigurd Höger for kindly providing FQA molecules and Harshita Malik and Thomas Bredow for DFT calculations.

O 46.7 Tue 14:00 P2

On-Surface Coupling of Feringa-Type Molecular Motors — •David Le[1], Grant J. Simpson[1], Matthew J. Timm[1], Dongdong Liu[2], James M. Tour[2], and Leonhard Grill[1] — [1]University of Graz, Austria — [2]Rice University, Houston, USA

Artificial molecular motors are fundamental components of nanoscale machines that convert external energy into uni-directional motion. On metallic surfaces, their operation can be probed with sub-molecular precision, allowing observation of rotational pathways and intermediates. In nanomachines, it could be advantageous to have not only one, but several motor units incorporated. However, the synthesis of such complex molecules is very challenging. Here, we studied whether individual Feringa-type motor units can be coupled covalently directly on a Au(111) surface to form bimotors, thus avoiding the complex synthesis and difficult deposition of molecules that contain more than one motor unit. Using low-temperature scanning tunnelling microscopy (STM) under ultrahigh vacuum conditions, we identified individual bimotor molecules after the coupling and could resolve distinct conformations. Moreover, conformational transitions and lateral translation could be induced by STM tip manipulation. The results for bimotors are compared with the mono-motors, i.e. before the coupling. Our results demonstrate controlled reactions and manipulation of molecular motors on a metallic surface, supporting the development of more complex nanomachines.

O 46.8 Tue 14:00 P2

Optical properties of pi conjugated molecule on insulator films supported by metal surface — •harshita malik — Clausius Institute for Physical and Theoretical Chemistry , University of Bonn,Bonn,Germany

Quinacridone (QA) is a pi-conjugated molecule whose optical properties are strongly influenced by hydrogen bonding and by its local environment. To establish consistent reference data, we determined the gas-phase and solution-phase excitation energies of QA using CCSD, TDDFT, and GW-BSE, and compared the results with available experimental spectra. These calculations provide reliable values for the ionization potential, the lowest singlet excitation, and the main vibronic features.

We then examined several structural variants of QA, including tautomers, substituted derivatives, and solid-state polymorphs. Their different packing motifs lead to measurable shifts in excitation energies, which we quantified using periodic GW-BSE.

To investigate QA on insulating surfaces, we used machine-learning potentials (MACE) combined with Bayesian optimization (BOSS) to identify stable adsorption geometries on KCl(100). The monomer and dimer structures obtained from this approach agree with DFT benchmarks and serve as starting points for further excited-state calculations on KCl films supported on Ag(100). I am currently working on computing excitons and other optical properties for QA adsorbed on these KCl/Ag surfaces to understand how substrate screening and adsorption geometry modify its electronic and optical response.

O 46.9 Tue 14:00 P2

Photoemission intermittency from organic quasi-one-dimensional crystals coupled with silver nanoparticles — •Moha Naeimi[1,2], Waqas Pervez[1,2], Frithjof Harmsen[1,2], Ingo Barke[1,2], and Sylvia Speller[1,2] — [1]Institute of physics, University of Rostock — [2]Department of life, light & matter, University of Rostock

Organic, quasi-one-dimensional crystals are suitable platforms for triplet exciton migration, latter only requiring minimal orbital coupling [1]. In organic molecules, triplet excitons can be generated via singlet fission, where excited singlet states convert into two long-lived triplet states [2]. We recently prepared long quasi-one-dimensional rubrene crystals on silicon substrates with a native thin silicon oxide layer (SiO2) [3]. After depositing Ag nanoparticles, we observe strong photoemission intermittency (blinking) at the interface sites and weak blinking on the rod crystal itself. In this work, we characterize the blinking in terms of its time traces and time-of-flight electron spectra. The blinking is consistent with exciton propagation that becomes trapped at nanoparticle-containing interface sites, where apparent electron binding energies shift to lower values. These molecule-nanoparticle systems offer promising pathways for directed energy transport and guided exciton migration.

[1] S. R. Yost et. al., J. Phys Chem C 116, 17369 2012. [2] T. Zhu et. al., J. Phys. Chem. Lett. 9, 6502 - 6510 2018. [3] Naeimi et. al, Adv. Opt. Mater., 2025 (DOI:10.1002/adom.202502744).

O 46.10 Tue 14:00 P2

Tip-induced hysteretic switching in copper-coordinated bipyridine (BIPY) thin films — •Sunny M P Gautam, Ankita Jaiswal, Thiruvancheril G Gopakumar, and Sandeep Verma — Indian Institute of Technology, Kanpur, India

In this work, we present a rationally designed hypoxanthine-based ligand, 1,9-bis(pyridine-2-ylmethyl) hypoxanthine (BIPY), specifically tailored for constructing functional surface-confined metal-organic networks (SMONs). The ligand integrates a π-conjugated purine core with flexible pyridyl donor arms, creating a nitrogen-rich, tridentate coordination environment ideal for forming robust 2D frameworks. Its conformational adaptability around metal centers enables dynamic metal*ligand interactions, offering a pathway toward SMON-based molecular switching driven by electronic-state transitions rather than geometric changes. Such electronically mediated bistability provides enhanced stability and potentially faster switching compared to conventional conformational molecular switches. Our results highlight BIPY as a promising platform for developing adaptive, switchable SMON architectures with potential applications in sensing, spintronics, data storage, and molecular logic systems.

O 46.11 Tue 14:00 P2

Monolayers of Thiols with Very High Dipole Moments Show Surprisingly Small Work Function Changes — Michael Gärtner[1], Andreas Terfort[1], and •Michael Zharnikov[1,2] — [1]Institut für Anorganische und Analytische Chemie, Johann Wolfgang Goethe Universität Frankfurt, 60438 Frankfurt am Main, Germany — [2]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

The recently introduced concept of distributed dipoles in molecular self-assembly was combined with the standard dipolar tail group decoration in the context of electrostatic engineering of surfaces and interfaces by self-assembled monolayers (SAMs). To this end, thiol-anchored molecules, containing dipolar 2,5-bipyrimidine units within their molecular backbones, were decorated with either nitrile or dimethylamino tail groups and assembled on Au(111). The directions of the distributed and tail group dipoles were aligned either upwards or downwards to the anchor to achieve the maximum effect on the work function (WF) of the substrate. Despite a dense molecular packing and an upright molecular orientation, the decoration of the bipyrimidine thiols with the tail groups not only provided no WF gain but even had a detrimental effect in the dimethylamino case. This behavior is explained by the upside-down orientation of a part of the molecules in the SAMs, driven by the minimization of the energy associated with the strong dipole-dipole interaction between the SAM-forming molecules.