O 46: Poster Organic Molecules on Inorganic Substrates: Electronic, Optical and Other Properties

Time: Tuesday 18:00–20:00 Location: P2

O 46.1 Tue 18:00 P2

Electronic Properties of Interfaces between N-Heterotriangulene Donors and Strong Tetracyanoquinodimethane Acceptors — •Mohsen Ajdari[1], Jakob Roth[1], Ronja Pappenberger[1], Christian Walla[2], Ina Michalsky[3], Friedrich Maass[1], Milan Kivala[3], Andreas Dreuw[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut — [2]Interdisziplinäres Zentrum für Wissenschaftliches Rechnen — [3]Organisch-Chemisches Institut, Heidelberg University

N-Heterotriangulenes (N-HTAs) are promising functional molecules with significant potential for optoelectronic applications, in particular, as electron donors in donor/acceptor (D/A) systems. This study explores the electron-donating properties of two N-HTAs, N-HTA 550 and N-HTA 557, at interfaces with well-known tetracyanoquinodimethane acceptors, TCNQ and F4TCNQ. Using high-resolution electron energy loss spectroscopy (HREELS) combined with quantum chemical calculations, we investigated the electronic properties of D/A interfaces adsorbed on Au(111) [1]. For all D/A combinations, low-energy electronic transitions ($E<2.5$ eV) associated with charge transfer (CT) states are identified. Quantum chemical calculations rule out the formation of ground-state CT complexes. Instead, CT in the excited state, in which an electron-stimulated CT from the N-HTAs to TCNQs is the underlying process, is proposed. The energies of the CT states are determined by the values of the ionization potential and electron affinity of the involved donor and acceptor.
[1] M. Ajdari et al., J. Phys. Chem. C, 128, 14399-14406 (2024)

O 46.2 Tue 18:00 P2

Self-assembly of magnetic complex on Cu (111) using scanning tunneling spectroscopy: probing Kondo resonance and decomposition effects — •Behzad Mortezapour[1], Torben Adam[2], Eike Kuhlemann[2], Felix Tuczek[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany — [2]Institut für Anorganische Chemie, Christian-Albrechts-Universität zu Kiel, Germany

The spin-crossover complex bis-(hydro-tris-(3-methyl-pyrazolyl)-borat)-Iron(II) on Cu (111) at ambient temperature was investigated with a scanning tunneling microscope (STM) under ultrahigh-vacuum conditions at a temperature of 4.6 K. The three-dimensional molecules self-assemble into ordered two dimensional arrays while some decomposition also occurs. The STM images of the intact molecules exhibit a significant dependence on the bias voltage and spectra of the differential conductance (dI/dV) show a zero-bias resonance that we tentatively attribute to the Kondo effect. Time series of the current reveal abrupt transitions that possibly are linked to spin switching. In addition, negative differential resistance is observed from decomposed molecules.

O 46.3 Tue 18:00 P2

stochastic spin-state switching of a Fe(II) complex on Cu (111) — •jasmeen jasmeen[1], sujoy karan[1], karl ridier[2], gaël reecht[1], and manuel gruber[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, 47057 Duisburg, Germany — [2]LCC, CNRS and Université de Toulouse, UPS, INP, 31077 Toulouse, France

Spin-crossover (SCO) molecules exhibit different spin states that make them attractive for nanoscale memory applications. Using scanning tunneling microscopy (STM) at 4.5 K, we studied the [Fe(HB(1,2,4-triazolyl)3)2] complex adsorbed on a Cu (111) surface, focusing on the spin-state switching dynamics. Time traces of the tunneling current revealed switching in the order of milliseconds, which we investigated under a range of bias voltages and currents, providing insights into the stochastic response of this system.

Controlled switching of individual molecules induced by voltage pulses was successful, but also drove a pronounced neighborhood effect: switching a target molecule simultaneously influenced adjacent ones. These events suggest an intermolecular interaction acting on the neighboring molecules due to the conformational changes of the target molecule.

These findings help improving the understanding of electron-induced switching of SCO molecules. Funding from the CRC 1242 is acknowledged.

O 46.4 Tue 18:00 P2

STM Investigation of Molecular Double Motors — •Ken Kolar[1], Grant Simpson[1], Ben Feringa[2], and Leonhard Grill[1] — [1]Dept. of Physical Chemistry, University of Graz, Austria — [2]Stratingh Institute for Chemistry, University of Groningen, Netherlands

A molecular motor is a molecule with stator and rotor chemical groups which undergo directional motion relative to each other. They represent potential building blocks for nanoscale machinery and their motion on surfaces is of particular interest. With high-resolution imaging from a scanning tunnelling microscope (STM), we revealed distinct appearances of different conformers of a molecule containing two motor units. Furthermore, motion induced by voltage pulses from the STM tip was studied in detail, investigating unidirectionality. Finally, double motors with additional alkane chains attached to them were deposited, showing distinguishable appearances. The experiments showed that the alkane chain conformation can impact the motion of the molecules.

O 46.5 Tue 18:00 P2

Excited state alignment of molecular orbitals on the ferroelectric WTe2 bulk crystal — •Jannis Lessmeister[1], Ralf Hemm[1], Joohyung Park[2], Martin Aeschlimann[1], Oliver L.A. Monti[2], and Benjamin Stadtmüller[3] — [1]Rheinland-Pfälzische technische Universität Kaiserslautern-Landau and Research center OPTIMAS, Kaiserslautern, Germany — [2]University of Arizona, Tucson, USA — [3]Universität Augsburg, Augsburg, Germany

The interaction between organic molecules and ferroelectric domains on WTe$_2$ offers a promising pathway for tuning the electronic properties of hybrid systems. WTe$_2$, a layered transition metal dichalcogenide, exhibits ferroelectricity in its few-layer form due to broken inversion symmetry, resulting in switchable polarization domains. When organic molecules are deposited onto the surface, the local electronic environment created by these ferroelectric domains significantly influences molecular adsorption and electronic coupling.

Utilizing real- and momentum-space photoemission electron microscopy, we investigate how the ferroelectric properties of WTe$_2$ modulate the alignment of excited state energy levels at the FePc/WTe$_2$ interface. Our study elucidates the charge transfer behavior and interaction strength, exploring the role of local electric polarizations for tuning the energy level alignment in molecule-2D material heterostructures.

O 46.6 Tue 18:00 P2

Momentum space signatures of molecular orbitals on a ferromagnetic surface — •Martin Anstett[1], Lu Lyu[1], Martin Aeschlimann[1], and Benjamin Stadtmüller[1,2] — [1]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

The integration of organic molecules with ferromagnetic surfaces is a promising approach to advance spintronic applications. The spin functionalities depend not only on the molecular properties, but also on the energetics and spin polarization of so-called hybrid interface states, which arise due to the hybridization between molecular orbitals and substrate states.

This work focuses on momentum space imaging of the adsorption-induced modification of molecular orbitals on ferromagnetic surfaces at room temperature. This is challenging due to the lack of ordered or aligned molecules on highly reactive magnetic substrates, which is required for momentum space imaging using ARPES. This limitation can be overcome by using ultrathin cobalt films on Au(111) as a ferromagnetic platform. On this surface, we prepare long-range ordered superstructures using iron phthalocyanine molecules. We combine spin- and momentum-resolved photoemission spectroscopy with photoemission orbital tomography to study the characteristic emission pattern of the orbitals of the adsorbed molecules. Our analysis reveals how the molecules arrange on the cobalt surface, producing distinct photoemission signatures associated with individual molecular orbitals.

O 46.7 Tue 18:00 P2

Thermal-Driven Coordination Effect for Structural and Electronic Tailoring of a Metal-Organic Network — •Jonas Gödde[1], Lu Lyu[1,2], Benjamin Stadtmüller[2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — [2]Experimentalphysik II, Institute of Physics, Augsburg University, Universitätsstraße 2, 86159 Augsburg, Germany

Two-dimensional metal-organic porous networks (2D-MOPNs) have emerged as a unique material platform for designing structural tessellations and emergent electronic states on surfaces. The metal centre in a 2D-MOPN plays a vital role in bridging network and substrate. In this study, we investigate the cobalt-coordination effects in cyano-functionalized hexaaza-triphenylene-hexacarbonitrile (HATCN) on Ag(111). Scanning tunnelling microscopy (STM) reveals that HATCN self-assembles into a well-ordered porous network. A partially occupied LUMO state observed by angle-resolved photoemission spectroscopy (ARPES), indicates charge transfer from the substrate to the molecules. After cobalt deposition, the robust equilibrium, between intermolecular and substrate interactions, preserves the porous structure and molecular orbital states of HATCN, while trapping cobalt in the low-potential pores. Upon post-annealing the molecules coordinate with cobalt atoms, inducing a structural transition and creating distinct energy and momentum states. These results provide insights into tailoring 2D-MOPNs for applications in electronics and spintronics.

O 46.8 Tue 18:00 P2

Spectroscopic study of the interface between organic molecules and platinum telluride thin films — •Lorenz Klein, Hibiki Orio, Romana Ganser, Muthu P. T. Masilamani, Maximilian Ünzelmann, and Friedrich Reinert — Universität Würzburg, Experimentelle Physik VII & Würzburg-Dresden Cluster of Excellence, Würzburg, Germany

Van der Waals heterostructures of organic molecules and transition metal chalcogenides (TMCs) represent excellent model systems for the study of weak molecule-substrate interactions.

Here, we use two phases of metallic platinum telluride, which both host spin-polarized surface states in their electronic surface band structures. Using those as substrates, we deposit copper phthalocyanine (CuPc) and study the resulting atomic and electronic interface structure by means of x-ray (XPS) and angle-resolved photoemission spectroscopy (ARPES) as well as low-energy electron diffraction (LEED). On that basis, we discuss the differences in surface ordering, work function, and the binding energies of the observed molecular features.

O 46.9 Tue 18:00 P2

Fluorescence spectroscopy of linear trans-quinacridone (QA) on KCl/Ag(100): The influence of KCl layer thickness — •Morris E. L. Mühlpointner and Moritz Sokolowski — Clausius-Institut für Physikalische und Theoretische Chemie der Universität Bonn, Germany

The organic dye-molecule linear QA has attracted interest as a fluorescent probe molecule in STM luminescence (STM-LE) experiments [1]. We have performed fluorescence spectroscopy of multilayers on the bare Ag(100) surface and highly diluted layers of QA on an epitaxially grown thin KCl film on Ag(100) under UHV.

We find spectra that are reminiscent of solid state spectra for multilayers of QA on Ag(100). In addition, we see blue-shifted spectra for highly dilute QA layers (0.0005 ML – 0.1 ML) with a multitude of spectral features. We find that the stability of these spectral features under laser illumination varies depending on the thickness of the underlying KCl layer. Spectra are stable at 13 K for QA on 3-4 layers of KCl. However, on 6-8 layers of KCl, a spectral red-shift and a loss of FL-intensity is induced upon laser illumination at 13 K. We attribute these findings to a diffusion barrier of QA on KCl films that is dependent on the KCl-film thicknesses because the long-range interactions with the Ag(100) substrate are relevant [2].

[1] Phys. Rev. Lett. 2023, **130** (12), 126202.

[2] J. Phys. Chem. C 2023, **127** (49), 23814-23826.

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O 46.10 Tue 18:00 P2

Field driven crossover of bonding and antibonding states in excitonic aggregates — •Amandeep Sagwal[1,2], Rodrigo Cezar De Campos Ferreira[1,3], Petr Kahan[1], Tomáš Neuman[1], and Martin Švec[1,3] — [1]Institute of Physics, Czech Academy of Sciences — [2]Faculty of Mathematics and Physics, Charles University; Czech Republic — [3]Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences

The present study aims to examine the effect of an electric field on the excitonic states of chromophore aggregates confined in optical nanocavity of a low-temperature SPM. Utilizing an optical configuration intended for near-field spectroscopies, tip-enhanced photoluminescence (TEPL) is used to investigate PTCDA molecules, deposited on a thin decoupling layer of NaCl on Ag(111) surface. A different energy shift is observed consistently between the bonding and antibonding excitonic emission lines in the spectra of dimer, trimer, and tetramer aggregates, in some cases even leading to a crossover. Typically, the antibonding states manifest a larger blue shift with increasing positive bias voltage applied on the gate electrode (substrate). We discuss the phenomenon using TD-DFT simulations and many-body state diagrams.

O 46.11 Tue 18:00 P2

Near-field spectroscopy of vibronic states of molecular aggregates — •Sidhartha Nayak[1], Fulu Zheng[2], and Alexander Eisfeld[1] — [1]MPIPKS, Dresden, Germany — [2]Department of Physics, Ningbo University, Ningbo, China

Strong dipole-dipole interactions between molecules give rise to delocalized electronic excited states in molecular aggregates, which determine their optical properties such as absorption. In near-field spectroscopy, the absorption spectrum of an aggregate is obtained when the molecules interact with electromagnetic radiation that is inhomogeneous across the length of the aggregate. Theoretically, by considering the near-field radiation from the apex of a metallic tip as a source of a localized field, it has been shown that the spectra of the aggregate reveal it's purely electronic states that are inaccessible through traditional far-field methods [1, 2]. In this contribution, we study aggregates composed of molecules with internal vibrational modes that are strongly coupled to electronic excitations, leading to non-Markovian phenomena. Using a local field method, which is numerically inexpensive, we observe that the vibronic states of aggregates are revealed in the near-field spectra and the spectra are comparable to those obtained by using a more accurate but computationally intensive method [3].

[1] X. Gao and A. Eisfeld, *J. Phys. Chem. Lett.* 9, 6003 (2018)

[2] S. Nayak, F. Zheng and A. Eisfeld, *J. Chem. Phys.* 155, 134701 (2021)

[3] D. Suess, A. Eisfeld and W. T. Strunz, *Phys. Rev. Lett.* 113, 150403 (2014)

O 46.12 Tue 18:00 P2

The Luminescence of Rylene Derivatives — •Petr Kahan[1], Rodrigo Ferreira[1,2], Amandeep Sagwal[1], Jiří Doležal[2], and Martin Švec[1,2] — [1]Institute of Physics, Czech Academy of Sciences — [2]Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences

The exploration of single-molecule luminescence using scanning tunneling microscopy (STM) is a vividly developing area of research. A number of works using STM-PL/EL and TERS techniques addressing the photophysics at the true single-molecule limit have employed rylene dyes for their known luminescent properties [1,2]. However, up to this point, a thorough comparison investigating the absorption and luminescent characteristics of molecules that share similar rylene-based configurations has not been carried out. This study presents a comparative analysis with the tip-enhanced spectromicroscopy in STM nanocavity on isolated molecules such as NTCDA, PTCDA, and DBP [3]. The findings reveal surprisingly distinct characteristics of each species; notably of their photoluminescence (PL) fingerprints and photocurrent maps. This shows the versatility of chemically related species, which holds promise for tailoring custom optoelectronic functionality in molecular aggregates.

[1] Doležal, J. et al. ACS Nano 16, 1082*1088 (2022). [2] Kimura, K. et al. Nature 570, 210*213 (2019). [3] Kröger, J. et al. Nano Lett. 18, 3407*3413 (2018).

O 46.13 Tue 18:00 P2

Spin Hall Magnetoresistance as a Probe for Chiral-Induced Spin Selectivity — •Simon Sochiera[1], Ashish Moharana[1], Yael Kapon[2], David Anthofer[1], Fabian Kammerbauer[1], Akashdeep Akashdeep[1], Shira Yochelis[2], Mathias Kläui[1], Yossi Paltiel[2], and Angela Wittmann[1] — [1]Institute for Physics JGU, Mainz, Germany — [2]Hebrew University of Jerusalem, Jerusalem, Israel

Chiral molecules have gained significant attention in the spintronics community due to their ability to polarize electron spin angular momentum without any heavy metal atoms via the chiral-induced spin selectivity (CISS) [1] effect. Several optical and electrical methods confirmed the CISS effect. However, despite numerous theoretical approaches, the fundamental mechanisms of the CISS effect are still an open question. A recent experiment [2] reported a significant modulation of spin-to-charge conversion with chiral molecules in a spin-pumping experiment. Building on this result, we create a hybrid structure by combining a well-established spin Hall magnetoresistance (SMR) experiment with chiral molecules. The SMR relies on the reflection and absorption of spin currents at interfaces adjacent to a layer exhibiting an (inverse) spin Hall effect, such as a heavy metal. This allows for direct probing of the spin-to-charge conversion modulation by chiral molecules. Combined with the results established in the spin-pumping experiment, this paves the path toward designing new chiral-molecule-based spin-torque devices.

[1]: R. Naaman et al., Nat. Rev. Chem. 3, 250 (2019)
[2]: A. Moharana et al., arXiv:2402.19246 (2024)