

O 75: Poster Session VI: Organic molecules on inorganic substrates: electronic, optical and other properties II

Time: Wednesday 13:30–15:30

Location: P

O 75.1 Wed 13:30 P

Temperature induced conformational changes in phospholipid monolayers studied by sum-frequency spectroscopy — DAMIAN FIRLA, •TIM LÄMMERZAHN, MATTHIAS LINKE, and ECKART HASSELBRINK — Universität Duisburg-Essen, Germany

Phospholipids are a major component in cell membranes because they form bilayers due to their amphiphilic character. This was exploited to prepare monolayers on glass substrates using the Langmuir-Blodgett technique to study them by sum frequency spectroscopy (SFS). The main goal was to observe structural changes upon raising the temperature. SFS probes the local centrosymmetry of the methylene groups because of its inherent selection rules. Therefore, conformational disorder of the alkyl chains due to the increased temperature, and thus breaking of the local centrosymmetry, can be directly observed. Typically, *gauche* defects are observable by an increase of the intensities of CH₂ vibrational modes. Different types of phospholipids and mixtures of phospholipids with varying chain lengths were studied. Monolayers prepared using a single phospholipid species showed only changes of the intensity of CH₃ vibrational modes with rising temperatures. Furtheron, mixtures of phospholipids with different chain lengths were studied. In these cases CH₂ modes were observed as well, consistent with the larger space being available for conformational changes. The thermal stability of phospholipid monolayers was also examined. We found that monolayers of single phospholipid species were more stable than monolayers of phospholipid mixtures. Divalent cations also increased the thermal stability of these monolayers.

O 75.2 Wed 13:30 P

Rotation of Ethoxy and Ethyl Moieties on a Molecular Platform on Au(111) — TORBEN JASPER-TÖNNIES¹, MANUEL GRUBER¹, SVEN JOHANNSEN¹, THOMAS FREDERIKSEN², ARAN GARCIA-LEKUE², TORBEN JÄKEL³, FYNN ROEHRICHT³, RAINER HERGES³, and •RICHARD BERNDT¹ — ¹Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität, 24098 Kiel — ²Donostia International Physics Center, E-20018 Donostia-San Sebastián; IKERBASQUE, Basque Foundation for Science, E-48013 Bilbao — ³Otto-Diels-Institut für Organische Chemie, Christian-Albrechts-Universität, 24098 Kiel

Molecular rotors have attracted considerable interest for their prospects in nanotechnology. However, their adsorption on supporting substrates, where they may be addressed individually, usually modifies their properties. Here, we investigate the switching of two closely-related three-states rotors mounted on platforms on Au(111) using low-temperature scanning tunneling microscopy and density functional theory calculations. Being physisorbed the platforms retain important gas-phase properties of the rotor. This simplifies a detailed analysis, and permits, for instance, the identification of the vibrational modes involved in the rotation process. The symmetry provided by the platform enables active control of the rotation direction through electrostatic interactions with the tip and charged neighboring adsorbates. The present investigation of two model systems may turn out useful for designing platforms that provide directional rotation and for transferring more sophisticated molecular machines to surfaces.

O 75.3 Wed 13:30 P

Magnetic Coupling in Clusters of Rhombus-Shaped Nanographenes — •NILS KRANE¹, XUELIN YAO², QIANG CHEN², KRISTJAN EIMRE¹, CARLO A. PIGNEDOLI¹, KLAUS MÜLLEN², PASCAL RUFFIEUX¹, AKIMITSU NARITA^{2,3}, and ROMAN FASEL^{1,4} — ¹nanotech@surfaces Laboratory, Empa - Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland — ²Department of Synthetic Chemistry, Max Planck Institute for Polymer Research, Mainz, Germany — ³Organic and Carbon Nanomaterials Unit, Okinawa Institute of Science and Technology Graduate University, Okinawa, Japan — ⁴Department of Chemistry and Biochemistry, University of Bern, Bern, Switzerland

The exact tailoring of open-shell nanographenes (NGs) with non-trivial magnetic ground states opens a pathway towards carbon-based molecular spintronics. The synthesis of these NGs remains challenging, due to their high reactivity. Embedding the NGs into a non-magnetic molecular network on the surface could allow for a passivation and

more controlled growth.

In this work, we passivated 5-rhombenes [1] with p-terphenyl linkers, creating one-dimensional non-magnetic backbones in which the NGs are embedded. Scanning tunneling spectroscopy and inelastic electron tunneling spectroscopy reveal the antiferromagnetic ground state with a large magnetic coupling constant to be preserved upon passivation. Furthermore, magnetically coupled dimers of 5-rhombenes embedded in the phenyl backbone have been investigated.

[1]: Mishra et al.: <https://arxiv.org/abs/2003.03577> (2020)

O 75.4 Wed 13:30 P

Decoupled or not decoupled? Investigation of charge transfer in organic/2D insulator/metal interfaces — •MAXIMILIAN SCHAAL¹, ILIYAN KARADZHOV¹, TAKUMI AIHARA², MARCO GRUENEWALD¹, FELIX OTTO¹, JARI DOMKE¹, ROMAN FORKER¹, HIROYUKI YOSHIDA², and TORSTEN FRITZ¹ — ¹Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — ²Graduate School of Engineering, Chiba University, 1-33, Yayoi-cho, Inage-ku, Chiba 263-8522, Japan

2D materials like hexagonal boron nitride (h-BN) are widely used as interlayer to decouple organic molecules from metallic surfaces. Nevertheless, there are also indications for a significant hybridization which results in a perturbation of the intrinsic molecular properties. This raises the question: what are the specific conditions under which an h-BN monolayer is sufficient to efficiently decouple organic molecules? In this work we deal with this question by comparing the electronic and optical properties as well as the lateral structure of about one monolayer 3,4,9,10-perylene-tetracarboxylic dianhydride (PTCDA) and tetraphenylidibenzoperiflanthene (DBP) on h-BN/Ni(111). Therefore, we combined *in situ* differential reflectance spectroscopy, ultraviolet photoelectron spectroscopy, low energy electron diffraction and low temperature scanning tunnelling spectroscopy. Our results reveal that an integer charge transfer happens for PTCDA on h-BN/Ni(111). In contrast, the DBP molecules on h-BN/Ni(111) are well decoupled from the metal substrate, and no charge transfer occurs.

O 75.5 Wed 13:30 P

Adsorption site dependent gating of C60 on h-BN/Rh(111) — •MAX BOMMERT and OLIVER GRÖNING — Empa Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland

Epitaxial, single layered hexagonal Boron Nitride (h-BN) on a metal substrate provides numerous interesting properties as it can be used as a template organizing the adsorption of organic molecules due to the substrate dependent Moiré pattern formation [1] as well as decoupling said molecules from the underlying metal preventing orbital hybridization [2]. In this project we use the topographic and electronic corrugation of the h-BN/Rh(111) Moiré pattern to form [3] and electrostatically gate specific C60 molecules in regular frameworks. Our experimental approach consists of two parts; in a first step, we use low-temperature scanning tunneling microscopy (STM) to analyze the C60 adsorption configuration. In a second step, we use scanning tunneling spectroscopy (STS), Kelvin probe force microscopy (KPFM) as well as non-contact atomic force microscopy (nc-AFM) to investigate the adsorption-site dependent gating effect of the on surface electric field on the C60 molecules. The combination of STS and KPFM grants insight into single molecular charging events. We can use the on surface electric field and the electric field of the STM tip to operate the C60 molecules as single molecular transistors. We will show how the molecular orbital level alignment and the site-dependent gating are related. [1]M. Iannuzzi et al., PCCP, 16 (2014), [2]L. Liu et al., ACS Nano, 9 (2015), [3]M. Corso et al., Science, 203 (2004)

O 75.6 Wed 13:30 P

Force Spectroscopy of Iron Tetraphenylporphyrin Molecules with Cl Tips — KATHARINA SCHEIL¹, •MANUEL GRUBER^{1,2}, MARTIN ONDRÁČEK³, and RICHARD BERNDT¹ — ¹Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — ²Faculty of Physics, University of Duisburg-Essen, D-47057 Duisburg, Germany — ³Institute of Physics,

Academy of Sciences of the Czech Republic, 182 21 Prague, Czech Republic

Cl ions are bidirectionally transferred between Fe tetraphenylporphyrin (FeTPP) molecules adsorbed on Au(111) and the tip of a low-temperature scanning probe microscope. This controlled transfer is used to switch between metal- and Cl-terminated tips. Both tips are employed to probe the forces and conductances upon contacting the Au(111) substrate, FeTPP and chlorinated FeTPP. The force spectroscopy of a Cl tip on Au(111) may be modeled by a point charge of $-0.3 e$ at the Cl ion interacting with its image charge in the substrate. Such Cl tips, beside modifying electrostatic interactions and thereby the force spectra acquired over molecules, turned out useful for high-resolution imaging at small molecule-sample distances [1]. Density function theory calculations reproduce important aspects of the experimental data. [1] Scheil et al., *J. Phys. Chem. C* 124, 26889 (2020)

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O 75.7 Wed 13:30 P

Uni-directional rotation of molecular motors on Cu(111) — ●MONIKA SCHIED¹, DEBORAH PREZZI², DONGDONG LIU³, PETER JACOBSON¹, ELISA MOLINARI², JAMES M. TOUR³, and LEONHARD GRILL¹ — ¹Department of Physical Chemistry, University of Graz, Austria — ²Nanoscience Institute of CNR, S3 Center, Modena, Italy — ³Department of Chemistry, Rice University, USA

Artificial molecular motors that convert external energy into controlled motion have seen great developments in the last decades [1]. While many studies exist in solution, little is known how such functional molecules behave on a surface. However, such a solid support can be advantageous as it offers fixed points of reference as well as confinement in two dimensions, making it easier to study the directionality of their motion.

We have studied single molecules with a so-called Feringa motor [2,3] on a Cu(111) surface by low-temperature scanning tunnelling mi-

croscopy (STM). It was found that rotations of individual molecules can be induced over rather long distances by voltage pulses with the STM tip. Importantly, these rotations show high directionality (clockwise or anticlockwise), which will be discussed in view of their specific chemical structure and adsorption.

- [1] W. R. Browne and B. L. Feringa, *Nat. Nanotech.* 1, 25 (2006)
 [2] T. Kudernac et al., *Nature* 479, 208 (2011)
 [3] A. Saywell et al., *ACS Nano* 10, 10945 (2016)

O 75.8 Wed 13:30 P

Light-assisted charge propagation in organic semiconductor networks on hexagonal boron nitride — ALEKSANDAR MATKOVIC¹, JAKOB GENSER², ●MARKUS KRATZER¹, DANIEL LÜFTNER³, ZHONGRUI CHEN⁴, OLIVIER SIRI⁴, PETER PUSCHNIG³, CONRAD BECKER⁴, and CHRISTIAN TEICHERT¹ — ¹Institute of Physics Montanuniversität Leoben Franz Josef Strasse 18, Leoben 8700, Austria — ²Institute of Solid State Electronics, Technische Universität Wien, Gußhausstraße 25-25a, 1040 Vienna, Austria — ³Institute of Physics Karl-Franzens-Universität Graz NAWI Graz Universitätsplatz 5, Graz 8010, Austria — ⁴Aix Marseille University CNRS CINaM UMR 7325 Campus de Luminy 13288, Marseille cedex 09, France

Electrostatic force microscopy is utilized to track charge propagation in organic semiconductor nanoneedles. As model system, crystalline dihydro-tetraazaheptacene needles epitaxially grown on ultrathin hexagonal boron nitride was investigated. Due to light exposure, the specific resistivity of the crystallites changed by two orders of magnitude. Exploiting the highly anisotropic optical properties of the organic nanoneedles, selective charge propagation along the crystallites was achieved by matching the incident light's polarization direction with the direction of the molecular backbones in the crystals. Thus, it was possible to guide charge propagation along desired paths in self-assembled crystallite networks. This way, polarized light can be used as a "light gate" to control charge propagation.