

O 42: Poster: Organic-Inorganic Hybrid Systems and Organic Films

Time: Tuesday 18:15–20:30

Location: Poster A

O 42.1 Tue 18:15 Poster A

Intermolecular Repulsion at Metal/Organic Interfaces: A Quantitative TPD Study — ●STEFAN RENATO KACHEL, BENEDIKT P. KLEIN, MAIK SCHÖNIGER, MARK HUTTER, MARTIN SCHMID, and J. MICHAEL GOTTFRIED — Fachbereich Chemie, Philipps-Universität Marburg, Germany

Understanding the interaction of π -conjugated organic molecules with metal surfaces is crucial for the development of modern organic electronic devices. Recently we showed how the topology of the π -system influences the surface chemical bond using the example of the structural isomers azulene and naphthalene on Ag(111) and Cu(111) investigated by TPD and DFT calculations. On Cu(111), azulene has a much higher desorption temperature (520 K) than naphthalene (340 K) in the limit of low coverage, while the difference is smaller on Ag(111). With increasing submonolayer coverage, all systems show substantial peak broadening towards lower temperatures. This effect is most pronounced for azulene on Cu(111), where the monolayer signals spread over almost 300 K, and reveals strong intermolecular repulsion. Two different approaches towards obtaining information about the desorption energy spreading over a monolayer and the strength of the repulsion are presented. Both the Persson model and the inverted Polanyi-Wigner equation are in good agreement with constant-coverage methods like heating-rate variations in the low-coverage range. These studies provide zero-coverage desorption energies of 170 kJ/mol for azulene and 100 kJ/mol for naphthalene, both on Cu(111). Nearest-neighbor repulsion energies for the four systems will be reported.

O 42.2 Tue 18:15 Poster A

Benzene on Ag(111) and Cu(111): A quantitative TPD study — ●JANIK A HOCHSTRASSER, LUKAS HELLWEG, STEFAN RENATO KACHEL, MARTIN SCHMID, and J. MICHAEL GOTTFRIED — Fachbereich Chemie, Philipps-Universität Marburg, Germany

The quantitative understanding of metal-organic interfaces is an important prerequisite for the further rational improvement of organic electronic devices, in which these interfaces occur at the electrode/semiconductor contacts. One of the most important single parameter for the quantitative characterization of the metal-organic interaction is the adsorption energy, which can be determined by precision temperature-programmed desorption (TPD) experiments via the desorption activation energy. Such energies represent valuable benchmark data for comparison with computational studies. Here, we focus on benzene as an aromatic model compound and study its interaction with Ag(111) and Cu(111) surfaces. Using an advanced TPD setup with a cryoshroud housing around the mass spectrometer enables us to detect exclusively molecules with a direct line-of-sight path between sample and ion source. The highly precise desorption energies obtained with this setup will be compared with previous experimental and theoretical results.

O 42.3 Tue 18:15 Poster A

Modification of aromatic self-assembled monolayers by electron irradiation: basic processes, related applications, and electric transport properties — CAN YILDIRIM¹, ERIC SAUTER¹, ANDREAS TERFORT², and ●MICHAEL ZHARNIKOV¹ — ¹Applied Physical Chemistry, Heidelberg University, 69120 Heidelberg, Germany — ²Institut für Anorganische und Analytische Chemie, Universität Frankfurt, 60438 Frankfurt, Germany

The effect of electron irradiation on aromatic thiolate self-assembled monolayers (SAMs) with oligophenyl, acene, and oligo(phenylene ethylene) backbones was studied, with emphasis on the basic irradiation-induced processes, performance of these films as negative resists in electron lithography, and electric transport properties. All films exhibited similar behavior upon the irradiation, with clear dominance of cross-linking. The cross-sections for the modification of the SAM matrix, the damage of the SAM-substrate interface, and irradiation-induced cross-linking were derived. Limitations for lithographic applications of these films were considered. The electric transport properties of the SAMs were found to be affected strongly by electric irradiation, with their resistance increasing progressively, by 2–3 orders of magnitude, upon irradiation with doses up to 40 mC/cm². This increase stemmed predominantly from a change of the contact resistance which, in its turn, was predominantly attributed to progressive irradiation-promoted ad-

sorption of airborne molecules at the SAM-ambient interface. Based on the transition voltage spectroscopy, the behavior of the HOMO-LUMO gap upon irradiation was monitored.

O 42.4 Tue 18:15 Poster A

Investigation of Metal-Organic Interfaces by Adsorption Calorimetry — ●MAIK SCHÖNIGER, MARTIN SCHMID, and J. MICHAEL GOTTFRIED — Fachbereich Chemie, Philipps-Universität Marburg

Measuring heats of adsorption and reaction by desorption-based techniques such as temperature-programmed desorption (TPD/TDS) is more challenging than it might seem at first view, because even small organic molecules such as benzene decompose before they desorb from reactive surfaces such as Pt(111). In these cases, where irreversible adsorption occurs, TPD fails. Instead, direct calorimetric measurements of the heats released during adsorption have to be performed. The same is true for adsorption processes which have an activation barrier. With our adsorption calorimeter, heats of adsorption and reaction can be determined directly for a large variety of systems, including the adsorption of metals and organics on metal surfaces or the reaction of metals with organic films. Metal-organic interface energies are of special importance for the design and development of future organic electronic devices such as organic light-emitting diodes (OLEDs) or organic solar cells (OSCs). Here, we discuss interfaces of low work function electrode metals such as Ca with organic semiconductors. Besides the interface energies, we also obtained data on the transmittance of thin metal films for IR radiation.

O 42.5 Tue 18:15 Poster A

Metal-Phthalocyanines on Noble Metal Surfaces: A Systematic Investigation With Respect to Strong Correlation Effects — ●MANUEL GRIMM, DENNIS HEIN, CHRISTIAN METZGER, MARTIN GRAUS, ACHIM SCHÖLL, and FRIEDRICH REINERT — Exp. Physik 7, Universität Würzburg, 97074 Würzburg, Germany

Metal-organic interfaces provide an ideal playground to study fundamental interaction mechanisms. In particular cases, these can lead to electronic correlations which cannot be described within a single particle picture. In case of some adsorbate/substrate combinations the LUMO of molecules in the first layer is partially occupied due to charge transfer from the metal substrate. As a result such samples, e.g. NTCDA or CuPc on Ag(111) [1,2] show a sharp Kondo resonance at the Fermi energy in high resolution photoelectron spectroscopy (PES) experiments. Here we present a systematic study of these resonance features. We analyze the influence of sample temperature and vary the bonding strength and charge transfer at the interface by changing the adsorbate and the orientation of the substrate surface. While we observe a Kondo scenario for NiPc and CuPc on Ag(111) which is explained within a Single Impurity Anderson model (SIAM), a more complicated behavior occurs on Ag(100) and Ag(110) surfaces. In the latter cases the NiPc and CuPc LUMO is still partially filled at room temperature, but starts to shift to larger binding energies upon cooling. This also leads to a shift of the sharp resonance peak away from the Fermi energy, which demands for an explanation beyond the SIAM.

[1] Schoell *Science* 329, 303 (2010) [2] Ziroff *PRB* B85 (2012)

O 42.6 Tue 18:15 Poster A

Photoisomerization characteristics of azobenzene-functionalized SAMs/Au(111) — ●WIBKE BRONDSCH, LARISSA BOIE, THOMAS MOLDT, JAN BÖHNKE, BEATRICE ANDRES, DANIEL PRZYREMBEL, CORNELIUS GAHL, and MARTIN WEINELT — Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin

Self-assembled monolayers (SAMs) of azobenzene-functionalized alkanethiols form molecular ensembles with preferential orientation and significant excitonic coupling among the azobenzene chromophores. It has been under debate if the excitonic coupling influences the *trans-cis* photoisomerization of the azobenzene units in the ensemble. In this contribution we use the sensitivity of the sample work function on the density of *trans* and *cis* isomers [1] to investigate this question by means of two-photon-photoemission. The photon-energy dependence of the photostationary state and the effective isomerization cross-sections in SAMs with different azobenzene content allows for disentangling dif-

ferent excitation pathways. It turns out that predominantly localized excitations contribute to photoswitching while the contribution of intermolecular coupled and thus delocalized excitonic states is minor [2].

[1] W. Bronsch, D. Przyrembel, L. Boie, C. Gahl and Martin Weinelt, *Fast optical work-function tuning at an organic/metal interface*, Appl. Phys. Lett. **111**, 081601 (2017)

[2] W. Bronsch, T. Moldt, L. Boie, C. Gahl and Martin Weinelt, *Delocalized versus localized excitations in the photoisomerization of azobenzene-functionalized alkanethiolate SAMs*, J. Phys.: Condens. Matter **29**, 484002 (2017)

O 42.7 Tue 18:15 Poster A

STM investigation of organic molecules on a Dy-Ag surface alloy — ●SINA MOUSAVION, JOHANNES SEIDEL, LU LYU, BENJAMIN STADTMÜLLER, and MARTIN AESCHLIMANN — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany

One of the great goals in the field of molecular adsorbates is to control the electronic and geometric structure at metal-organic interfaces. While most studies so far focused on modifications of the organic film to tune the interfacial properties, we have started to tailor metal-organic interfaces by surface alloying [1].

Here, we extend this approach to new surface alloy consisting of silver and lanthanide metal, Dysprosium grown on a silver crystal. The lateral order of the bare Dy1Ag2 surface alloy is characterized by LEED and STM and reveals a $\sqrt{3}\times\sqrt{3}$ structure with an additional Moiré pattern. Subsequently, the structure formation and lateral order of PTCDA and the single molecular magnet Sc3N@C80 are investigated. We find a clear correlation between the local arrangement of the molecular adsorbates and the Moiré pattern of the surface alloy.

[1] Phys. Rev. Lett. **117** 096805 (2016)

O 42.8 Tue 18:15 Poster A

Towards Computational Structure Prediction of Organic Thin Films and Multilayers: TCNE on Cu(111) — ●ALEXANDER T. EGGER, LUKAS HÖRMANN, ANDREAS JEINDL, MICHAEL SCHERBELA, and OLIVER T. HOFMANN — Institute of Solid State Physics, Graz University of Technology, Austria

Organic thin films often crystallize in peculiar, surface-induced phases, which exhibit physical properties that are superior to the bulk structures. However, resolving the surface-induced thin film phases remains a huge challenge, in particular for first-principle calculations. While efficient structure determination strategies exist for isolated molecules or bulk crystals - and to a limited extend also molecular monolayers - none of these are efficiently applicable to multilayer structures or organic thin films.

In this contribution, we demonstrate a strategy to fill this gap. Using the SAMPLE approach, which combines coarse-graining of the potential energy surface with machine learning, we start from an energetically optimized first layer. Subsequently, we predict energetically favorable positions for a single molecule in the second layer. Using these positions as "building blocks", we create a new discretized PES to predict structure of higher layers.

Here, we demonstrate the applicability of this approach on TCNE (tetracyanoethene) on Cu(111). Specifically, we investigate whether, at high coverage, the system will undergo a phase transition from a densely packed, face-on geometry to upright standing molecules, or whether - and in which structure - a TCNE bilayer forms.

O 42.9 Tue 18:15 Poster A

Molecular dynamics simulation of transport and nucleation of conjugated organic molecules on inorganic surfaces — MILA MILETIC, JOACHIM DZUBIELLA, and ●KAROL PALCZYNSKI — Institut für Weiche Materie und Funktionale Materialien, Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner Platz 1, 14109 Berlin, Germany

In our study we analyze the influence of polarity on the surface transport and nucleation of conjugated organic molecules on the inorganic amorphous SiO₂ and ZnO surfaces by means of all-atom molecular dynamics simulations. In particular, we thoroughly investigate the effects of partial fluorination of the popular para-sexiphenyl (*p*-6P) molecule with chemical modifications of one head group (*p*-6PF2) or both head and tail (*p*-6PF4). Even though the chemical modifications do not lead to significant changes in the molecular structure, the effect of the fluorination on the diffusion process on the ZnO substrate is considerable, leading to a difference in the diffusion barriers of one order of

magnitude between *p*-6P and *p*-6PF4. However, in case of the amorphous SiO₂ substrate, the difference in the diffusion barriers between *p*-6P and *p*-6PF2 is negligible. To fully understand the effects that control the diffusion mechanisms, our aim is to investigate the relation between the surface barriers and the underlying surface dynamics, as well as to characterize substantial contributions of entropy to the effective diffusion barriers. Furthermore, we employ molecular dynamics simulations to identify the sources of nanometer-scale disorder in organic crystal structures on inorganic substrates.

O 42.10 Tue 18:15 Poster A

Interfaces of solution processable doped organic transport layers with metals and conductive oxides — ●PATRICK REISER^{1,2}, ERIC MANKEL^{1,2}, and WOLFRAM JAEGERMANN^{1,2} — ¹Institute for Materials Science, Technische Universität Darmstadt — ²InnovationLab GmbH Heidelberg

Employing printing and solution processing of organic films has the potential to reduce manufacturing costs and to enable large scale flexible organic devices. A key to maintain high performance is given by proper interface engineering of printed layer towards the electrode material. Buffer layers or doped organic transport layers are used to create Ohmic contacts, which generally improves device performance. Here, we investigated the energetic and electrochemical properties of a doped hole transport material like P3HT and Spiro-OMeTAD towards electrodes like ITO or Silver by means of Photoelectron Spectroscopy. We further compare vacuum and solution processed films as well as the deposition sequence.

O 42.11 Tue 18:15 Poster A

Towards accurate prediction of ground state charge transfer with Fermi-Löwdin orbital self-interaction corrected DFT — ●TORSTEN HAHN¹, SIMON LIEBING¹, MARTIN KNUFFER², MARK PEDERSON³, and JENS KORTUS¹ — ¹TU Freiberg, Institute for Theoretical Physics, Germany — ²IFW Dresden, Electronic and Optical Properties Department, Germany — ³Johns Hopkins University, Department of Chemistry, USA

Organic charge transfer (CT) compounds are a class of materials that allow tuning of electronic and optical properties by controlling the amount of charge that is transferred between a donor and acceptor molecule. Accurate predictions of properties of CT materials based on calculations within the density functional theory (DFT) framework are challenging and often result in unsystematic failures.

The application of the recently proposed Fermi-Löwdin orbital self-interaction correction [1,2,3] scheme (FLO-SIC DFT) to CT compounds containing TCNQ and related acceptor molecules leads to significant improvements of the theoretical results compared to experimental data.

[1] M. R. Pederson et al., J. Chem. Phys., vol. 140, 121103 (2014)

[2] M. R. Pederson, J. Chem. Phys., vol. 142, 064112 (2015)

[3] T. Hahn et. al., J. Chem. Phys., vol- 143, 224104 (2015)

O 42.12 Tue 18:15 Poster A

Orbital Imaging of Non-Planar Molecules Beyond the Free Electron Finalstate Approximation — ●CHRISTIAN METZGER, MANUEL GRIMM, MARTIN GRAUS, ACHIM SCHÖLL, and FRIEDRICH REINERT — Julius-Maximilians-Universität Würzburg, Experimentelle Physik VII, 97074 Würzburg, Germany

It has been shown that the imaging of molecular orbitals is possible by angle-resolved photoelectron spectroscopy (ARPES). For planar aromatic molecules the approximation of the photoemission final state by a simple plane wave allows for a particularly straightforward interpretation of the experimental data. Here we present a combined experimental and theoretical study on the angular intensity distribution of photoelectrons from non-planar molecules. The ARPES data of a single layer of C60 on Ag(110) was acquired by a momentum microscope which enables the efficient detection of photoelectrons emitted into the entire hemisphere above the sample. The symmetry of the recorded photoelectron momentum maps (PMM) immediately demonstrates that the molecules adsorb with a single specific alignment and do not rotate even at room temperature. On the theoretical side, a simple plane-wave approximation of the finalstate is bound to fail due to the 3D geometry of C60. A more suitable description can be realized within the framework of independent atomic centers (IAC), where the finalstate can be assembled by the composite contributions of the individual atoms inside the molecule. We demonstrate that this IAC approach provides a very good simulation of the experimental PMM and thus allows the assignment of different initialstate orbitals.

O 42.13 Tue 18:15 Poster A

Interactions in Hybrid Nanocomposite Systems studied by Laser-Induced Photoemission Electron Microscopy —•KEVIN OLDENBURG¹, CHRISTIAN VÖLKNER¹, JOHANNES A. A. W. ELEMANS², KARL-HEINZ MEIWES-BROER¹, SYLVIA SPELLER¹, and INGO BARKE¹ — ¹University of Rostock, Institute of Physics, 18059 Rostock, Germany — ²Radboud University Nijmegen, Institute for Molecules & Materials, NL-6525 AJ Nijmegen, The Netherlands

Utilizing the plasmonic properties of metal nanoparticles to locally create excitons in organic semiconductors is a promising pathway to transfer energy from a defined starting point over long distances. By means of spatially and energetically resolved Photoemission Electron Microscopy (PEEM) we study two nanocomposite systems consisting of mass-selected silver nanoparticles (≈ 15 nm diameter) on top of Cu porphyrin [1] and of tetracene aggregates, respectively. In case of Cu porphyrin we observe an enhancement of the photoemission signal in the direct vicinity of the nanoparticles. Contributions of electrons from particles versus dye can be clearly distinguished, based on spectral information. In tetracene an additional long lived state is populated which shows both enhanced and decreased population nearby different nanoparticles. The results are discussed in view of particle-molecule aggregate coupling (see also [2]). Open questions concern the dynamics and possible exciton migration as well as annihilation.

[1] H. Hartmann et al., J. Phys. Chem. C 120, 16977 (2016)

[2] K. Stallberg et al., J. Phys. Chem. C 121, 13833 (2017)

O 42.14 Tue 18:15 Poster A

Steering the growth of multiple ordered heteromolecular phases by utilizing intermolecular repulsion — CAROLINE HENNEKE, JANINA FELTER, F. STEFAN TAUTZ, and •CHRISTIAN KUMPF — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany and Jülich Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology

Metal-organic interfaces and their structural, electronic, spintronic and thermodynamic properties have been investigated intensively, aiming to improve and develop future electronic devices. In this context, heteromolecular phases add new design opportunities simply by combining different molecules. However, controlling the desired phases in such complex systems is a challenging task. Here, we report an effective way of steering the growth of a bimolecular system composed of adsorbate species with opposite intermolecular interactions, repulsive and attractive, respectively. The repulsive species forms a two-dimensional lattice gas, the density of which controls which crystalline phases are stable. Critical gas phase densities determine the constant-area phase diagram that describes our experimental observations, including eutectic regions with three coexisting phases. We anticipate the general validity of this type of phase diagram for binary systems containing two-dimensional gas phases, and also show that the density of the gas phase allows engineering of the interface structure.

O 42.15 Tue 18:15 Poster A

Analysis of normal incidence X-ray standing wave data considering non-dipolar effects — MARKUS FRANKE, GERBEN VAN STRAATEN, GIUSEPPE MERCURIO, FRANÇOIS C. BOQUET, SERGUEI SOUBATCH, F. STEFAN TAUTZ, and •CHRISTIAN KUMPF — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany and Jülich Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology

Normal incidence x-ray standing wave (NIXSW) is the most established technique for determining the vertical structure at interfaces and surfaces with sub-Ångström accuracy and chemical sensitivity. However, non-dipolar contributions to the photoemitted electron yield are an issue, in particular since normal incidence conditions are in practice never met. An angle-dependent data analysis is indispensable. In the absence of user-friendly and well-documented software we developed the program "Torricelli" for analyzing NIXSW data. It is open-source, python-based and has an easy-to-use graphical user interface. Data output in an Argand-diagram is included.

O 42.16 Tue 18:15 Poster A

Structural investigation of highly ordered incommensurate monolayer domains of C₆₀ on Ag(111) — •MARCO GRUENEWALD, PHILIPP MÜLLER, FALKO SOJKA, JARI DOMKE, ROMAN FORNER, and TORSTEN FRITZ — Institute of Solid State Physics, Friedrich Schiller University Jena

We structurally investigated monolayers of C₆₀ on Ag(111), which have

been prepared by annealing of multilayers, by means of low energy electron diffraction (LEED) and scanning tunneling microscopy (STM). We find that depending on the annealing temperature either the well-known commensurate ($2\sqrt{3} \times 2\sqrt{3}$)R30° structure [E. I. Altman and R. J. Colton, Phys. Rev. B 48, 18244 (1993)] or previously unknown incommensurate phases are formed. More precisely, a whole family of differently rotated structures could be observed for the latter with domain angles quasi-continuously ranging from 0° to 13.2° while the other unit cell parameters are essentially unaltered compared with the commensurate phase. By means of STM we find that the molecules appear differently rotated on the surface, most likely owing to their inequivalent adsorption sites.

O 42.17 Tue 18:15 Poster A

Thermal stability and interlayer exchange processes of MePc-PTCDA heterostructures on Ag(111) — •SEBASTIAN THUSSING and PETER JAKOB — Fachbereich Physik, Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany

The growth and thermal stability of organic heterolayers containing PTCDA and either CuPc or TiOPc have been investigated. Thereby the adsorption geometry and layering of individual species is derived from IR absorption spectroscopy. Information regarding long range order is obtained from SPA-LEED data. Throughout all processing a parallel orientation of the π -conjugated backbone of the deposited molecules is found. Thermal stability of the original layering and the produced organic-organic interface depends crucially on the nature and sequence of deposited species. Heterolayer interfaces involving PTCDA contact layers show excellent stability due to the favorable adsorption energy per unit area for PTCDA in comparison to the phthalocyanines [1]. Another key observation is that all layers comprising double layers of the face-to-face oriented TiOPc species display particular high resistance with respect to thermal annealing, i.e. regarding interlayer exchange and desintegration of the double layer membrane.

[1] S. Thussing and P. Jakob, J. Phys. Chem. C 121 (2017) 13680-13691.

O 42.18 Tue 18:15 Poster A

Morphology and luminescence of tetracene micro- and nanostructures — •CORDELIA HORNS, CHRISTIAN VÖLKNER, MOHAMMADRAZA BAHRAMI, KEVIN OLDENBURG, REGINA LANGE, SYLVIA SPELLER, and INGO BARKE — University of Rostock, Institute of Physics, 18059 Rostock, Germany

Tetracene is a promising material for long-range exciton transport [1, 2, 3]. We are interested in the transport and coupling of excitons in nanostructured molecule materials. Since fluorescence is one of the possible channels for exciton decay, spatial mapping of fluorescence is a valuable approach for the analysis of excitation pathways. In this work we report on the morphology and luminescence of mesoscopic and nanoscopic tetracene aggregates created by drop-casting on a variety of substrates such as sapphire and glass. We use a correlative approach where the morphology is measured by Atomic Force Microscopy at the same location as fluorescence images within a single microscope, thus avoiding sample transfers. The aggregates exhibit different shapes including morphologies with distinct heights of ~ 30 nm and ~ 100 nm, showing different fluorescence intensity and polarization. By analyzing the images possible reasons and mechanisms for the dependence of fluorescence on the local environment are discussed.

[1] SR Yost, E Hontz, S Yeganeh, T Van Voorhis, J. Phys Chem C, 116, 17369 (2012)

[2] GM Akselrod, PB Deotare, NJ Thompson, J Lee, WA Tisdale, MA Baldo, VM Menon, V Bulovic, Nature Comm. 6, 1 (2014)

[3] X Xie, H Ma, ChemistryOpen, 5, 201 * 205 (2016)

O 42.19 Tue 18:15 Poster A

Multiscale Modeling of ion-sensitive sensor devices — •JÖRG BUCHWALD, LEONARDO MEDRANO SANDONAS, AREZOO DIANAT, RAFAEL GUTIÉRREZ, and GIANAURELIO CUNIBERTI — Institute for Materials Science and Max Bergmann Center of Biomaterials Dresden University of Technology, 01069 Dresden, Germany

For the purpose of ion-sensing we want to apply the concept of a reservoir computer. Main part of this device will constitute a network of sensors, that are in contact with the ionic solution (reservoir). To understand the properties of the reservoir computer, knowledge about individual IV characteristics of each sensor is needed. A good candidate for such a sensor is the ion-sensitive field effect transistor (ISFETs). The ISFET can be considered as a FET in which the gate is in contact with an ionic solution and covered by a self-assembled monolayer

of biomolecules that are able to bind to specific kinds of ions. The number of bound ions determines the gate potential and the current of the FET. It is assumed to be a function of ion concentration and controlled by binding kinetics.

A good candidate for SAM molecules constitutes the neuropeptide oxytocin, which is able to bind to different types of divalent metal ions. We will employ Molecular Dynamics as well as DFT calculations to scrutinize conformational changes and kinetic stability upon ion binding. From these information we are able to develop a sensor model in which the conformational changes determine the maximum response of the FET gate.

O 42.20 Tue 18:15 Poster A

On the inner structure of porphyrin nanoaggregates revealed by luminescence polarization — ●JANNIS BECKER, MOHAMMADREZA BAHRAMI, SVEN KRAFT, CHRISTIAN VÖLKNER, KEVIN OLDENBURG, INGO BARKE, and SYLVIA SPELLER — University of Rostock, Institute of Physics, 18059 Rostock, Germany

For studying exciton pathways in molecule nanostructures we prepared copper-based porphyrin aggregates on various surfaces by self-assembly from a solution [1,2]. Apart from the morphology also the inner structure of such aggregates is of interest, particularly for the interpretation of optical and electronic properties in the context of first-principles theory. We address this topic by mapping the luminescence polarization directions of such aggregates. This provides information on the orientation of the transition dipoles and thereby on the orientation of the molecules within the aggregates. We find a pronounced orientation preference for lengthy, tree-like structures, while for more isotropic island morphologies the degree of order is lower. Based on the results we discuss possible structural motifs for the tree-like aggregates.

[1] Hartmann et al., J. Phys. Chem. C 120, 16977 (2016).

[2] Bahrami et al.: Correlative Microscopy of Morphology and Luminescence of Cu porphyrin aggregates, submitted.

O 42.21 Tue 18:15 Poster A

A versatile facility for time-resolved multidimensional spectroscopy of few-layer surface systems in a nanostructured environment — ●SEBASTIAN PRES¹, BERNHARD HUBER¹, EMANUEL WITTMANN², DANIEL FERSCH¹, LYSANNE DIETRICH¹, JULIAN LÜTTIG¹, VICTOR LISINetskii¹, MATTHIAS HENSEN¹, EBERHARD RIEDLE², and TOBIAS BRIKNER¹ — ¹Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — ²Lehrstuhl für BioMolekulare Optik, Ludwig-Maximilians-Universität, Oettingenstraße 67, 80538 München,

Germany

We present here a surface spectroscopy setup which combines aberration-corrected photoemission electron microscopy (AC-PEEM), enabling sub-5 nm spatial resolution, with a widely tunable high-repetition-rate (up to 1 MHz) laser source. Organic and inorganic few-layer systems can be directly prepared and characterized in-situ by low-energy electrons (LEEM, LEED) and ex-situ by scanning fluorescence microscopy. Tuning of the optical excitation from 900 nm down to 230 nm at sub-25 fs pulse duration allows a precise spectral addressability of sample specific resonances. The laser pulses, used in collinear time-interferometric scanning schemes like two-colour pump-probe techniques, reveal surface dynamics in 2D materials, e.g., WSe₂. Further, the usage of amplitude- and phase-shaped pulse sequences permits the investigation of transport processes between and within individual molecules in organic-inorganic hybrid systems by space- and time-resolved multidimensional spectroscopy.

O 42.22 Tue 18:15 Poster A

III/V-on-Si(100) heterointerfaces and single-domain virtual substrates — ●OLIVER SUPPLIE¹, BENJAMIN BORKENHAGEN², OLEKSANDR ROMANYUK³, TOMA SUSI⁴, MATTHIAS M. MAY⁵, SEBASTIAN BRÜCKNER¹, AGNIESZKA PASZUK¹, ANDREAS NÄGELEIN¹, PETER KLEINSCHMIDT¹, MICHAEL RIENÄCKER², GERHARD LILIENKAMP², WINFRIED DAUM², and THOMAS HANNAPPEL¹ — ¹Institute of Physics, TU Ilmenau, Germany — ²Institute of Energy Research and Physical Technologies, TU Clausthal, Germany — ³Institute of Physics, ASCR Prague, Czech Republic — ⁴Faculty of Physics, University of Vienna, Austria — ⁵Chemistry Department, Cambridge University, UK

Pseudomorphic virtual GaP/Si substrates are attractive for III/V-on-Si integration. Adequate preparation of the GaP/Si(100) heterointerface is of particular interest since its atomic and electronic structure highly impacts crystal quality. Here, we present experimental results regarding the formation of the GaP/Si(100) heterointerface from optical in situ studies during metalorganic vapor phase epitaxy and in system photoelectron spectroscopy. These are discussed with respect to recent results from density functional theory [PRB 94:155309 (2016); PRL 118:237403 (2017)]. Specific changes in the MOVPE process routes enable modifications of the atomic structure at the heterointerface. In particular, we study the influence of As and Ga. We correlate these experiments to reference experiments, where Si surfaces are exposed to Ga and P in UHV and the impact on the surface structure is studied in situ with low energy electron microscopy (LEEM).