

## O 73: Organic Molecules on Inorganic Substrates V: Adsorption, Growth and Networks

Time: Wednesday 15:00–18:15

Location: TRE Phy

O 73.1 Wed 15:00 TRE Phy

**Comparison of the adsorptions of ethanol and azobenzene molecules on single-layer hexagonal boron nitride on Rh(111)** — ●KRISZTIÁN PALOTÁS<sup>1,2,3</sup>, ARNOLD FARKAS<sup>3,4</sup>, ÁDÁM SZITÁS<sup>3</sup>, DÁNIEL JURDI<sup>3</sup>, RICHÁRD GUBÓ<sup>3,4</sup>, TIBOR PÁSZTOR<sup>3</sup>, LÁSZLÓ ÓVÁRI<sup>3,4</sup>, JÁNOS KISS<sup>3</sup>, ANDRÁS BERKÓ<sup>3</sup>, and ZOLTÁN KÓNYA<sup>3</sup> — <sup>1</sup>Budapest University of Technology and Economics, Budapest, Hungary — <sup>2</sup>Wigner Research Center for Physics, Budapest, Hungary — <sup>3</sup>University of Szeged, Szeged, Hungary — <sup>4</sup>ELI-ALPS, Szeged, Hungary

The nanomesh structure of single-layer hexagonal boron nitride (hBN) on various metal surfaces can be used as a nanotemplate for molecular adsorption. Possible applications can be molecular electronics, heterogeneous catalysis, sensing, or light harvesting. We investigate the adsorption properties of ethanol and azobenzene molecules on the hBN/Rh(111) surface by density functional theory calculations and experimental methods. We find high selectivity of the nanomesh structure for the azobenzene adsorption, but no selectivity for the ethanol adsorption. The latter finding is in line with experimental observations of a very weak interaction between ethanol and the hBN/Rh(111) substrate. Finally, we analyze the trans- and cis-azobenzene adsorption and azobenzene-azobenzene interactions in great details by using theoretical means. These results contribute to the understanding of the behavior of photo-switching molecules on nanotemplated surfaces.

O 73.2 Wed 15:15 TRE Phy

**Boron-doping Induced States in Single Graphene Nanoribbons Probed in Transport Measurements** — ●NIKLAS FRIEDRICH<sup>1</sup>, PEDRO BRANDIMARTE<sup>2</sup>, JINGCHENG LI<sup>1</sup>, THOMAS FREDERIKSEN<sup>2</sup>, ARAN GARCIA-LEKUE<sup>2</sup>, DANIEL SÁNCHEZ-PORTAL<sup>3</sup>, and J.I. PASCUAL<sup>1</sup> — <sup>1</sup>CIC nanoGUNE, San Sebastian (Spain) — <sup>2</sup>Donostia International Physics Center, San Sebastian (Spain) — <sup>3</sup>Centro de Física de Materiales, San Sebastian (Spain)

Bottom-up synthesized graphene nanoribbons (GNRs) are a versatile playground for engineering electronic properties of low-dimensional systems. Numerous predictions state that certain GNR shapes carry zero energy states hosting an even number of electrons. Despite their large potential for spintronics, the synthesis and observation of magnetism in graphene-based structures is so far very limited.

Here, we show that a spin-polarized state can be induced in 7-armchair GNRs by substitutional Boron-doping of two central Carbon atoms. Electronic transport measurements through a B-doped GNR suspended between the Au(111) substrate and the tip of scanning tunneling microscope reveal a zero-bias Kondo resonance, attributed to the induced spin-polarization. Density functional theory simulations confirm an emerging spin-polarization in the GNR upon detachment of the dopant from the surface.

Simulations also reveal strong kinetic exchange interactions between doping sites within the same GNR, which modifies the net spin-polarization of the ribbon. Our experimental transport results confirm the presence of such a non-conventional spin texture.

**Invited Talk**

O 73.3 Wed 15:30 TRE Phy

**1.\*Real-space investigation of the influence of polar species on ice structure** — ●KARINA MORGENSTERN — Physikalisches Chemie I, Ruhr-Universität Bochum, Germany

The interaction of water with solid surfaces is crucial in several scientific disciplines as diverse as environmental science, solvation science, biophysics, and astrochemistry. In these disciplines, there are several major water ice-related challenges that require a molecular-level understanding and description of water. In particular atmospheric chemistry, where most reactions in the atmosphere proceed on ice-covered nanoparticles poses a large variety of unanswered questions with respect to ice surfaces. Thereby, natural water was and is never as pure as distilled water, but contains air, salts, dust, organics, bacteria and so forth. Appropriate answers of relevance to real systems thus require a fundamental understanding of the structure of ice, not only in its purest, but in particular in its more realistic contaminated state. We explore how contaminants, in particular organic molecules and cations, alter the structure of ices on the (111) faces of the coin metals using low-temperature scanning tunneling microscopy. The systems discussed in this talk are azobenzene [1,2] and carbene [3] as proto-

types for polar molecules and lithium and cesium ions as prototypes for cations. Moreover, we will present an example, how the structure of ice influences the reactivity of a photo-induced reaction [4].

[1] J. Am. Chem. Soc. 136, 13341 (2014); [2] Angew. Chem. Int. Ed. 57, 1266-1270 (2018); [3] Angew. Chem. Int. Ed. 57, 16334-16338 (2018); [4] Phys. Rev. Lett. 121, 206001 (2018)

O 73.4 Wed 16:00 TRE Phy

**STM Investigation on Structural Transformation of Terphenylthiol Self-Assembled Monolayers Induced by Electron Irradiation** — ●PATRICK STOHHMANN, SASCHA KOCH, YANG YANG, CHRISTOPHER DAVID KAISER, XIANGHUI ZHANG, and ARMIN GÖLZHÄUSER — Physics of Supramolecular Systems and Surfaces, Bielefeld University, 33615 Bielefeld, Germany

Carbon Nanomembranes (CNMs) are two-dimensional sheets with tailored physical and chemical properties. They are prepared via electron irradiation induced cross-linking of aromatic self-assembled monolayers (SAMs). However, the molecular structure of CNMs and the underlying mechanisms of the cross-linking process are not fully understood. Here, the structural transformation of a pristine terphenylthiol (TPT) SAM on Au(111) was studied with a scanning tunneling microscope (STM) combined with a scanning electron microscope (SEM). STM images of the initial steps of irradiation exhibit depressive spots in the SAM, which is analogous to nucleation sites and could be correlated with radical chain reactions connecting up to 40 molecules. The chain reactions could be initiated by 6 eV (secondary) electron attachment and potentially terminated by steric hindrance. The electron irradiation was carried out by employing a low-energy flood gun emitting 50 eV electrons for a comparative study.

O 73.5 Wed 16:15 TRE Phy

**Solvation of Large Organic Molecules in Two Dimensions - Imaging Single Cage Precursor Molecules in Chloroform Supported on Ag(111)** — ●MARVIN QUACK<sup>1</sup>, KARINA MORGENSTERN<sup>1</sup>, HAERI LEE<sup>2</sup>, and GUIDO CLEVER<sup>2</sup> — <sup>1</sup>Physical Chemistry I, Ruhr-University of Bochum, Germany — <sup>2</sup>Chair for Bioinorganic Chemistry, TU Dortmund, Germany

Exploring the solvation of molecules is of utmost importance for the basic understanding of chemical processes, since the interaction of solvent and solute determines reaction pathways as well as the structure of the solute. However, the investigation of solvated molecules in the liquid phase is restricted to averaging methods or theory due to the dynamic nature of solvation processes. In order to overcome this problem, we present the formation of a two dimensional solvent layer supported on a metal substrate, enabling us to study the structure of solvated molecules in real space by the means of low-temperature scanning tunneling microscopy (STM). To understand the interaction of single molecules with its solvent, we coadsorbed the bidentate ligand molecule C<sub>75</sub>H<sub>51</sub>N<sub>3</sub>O and chloroform on a Ag(111) single crystal surface by the means of atomic layer injection, followed by cooling to 5 K. The STM results reveal the molecule in three different conformations embedded within the 2D chloroform layer. In addition, the structure of the solvent layer is disturbed compared to the ordered structure of pure chloroform on Ag(111). The significance of these results with regard to solvation will be discussed in this contribution.

O 73.6 Wed 16:30 TRE Phy

**Pentamers-like molecules forming a self-assembled monolayer onto a FCC(111) surface: a theoretical study** — ●EDUARDO CISTERNAS<sup>1,2</sup>, GONZALO DOS SANTOS<sup>3</sup>, MARCOS FLORES<sup>2,4</sup>, EUGENIO VOGEL<sup>1,5</sup>, and ANTONIO RAMÍREZ-PASTOR<sup>6</sup> — <sup>1</sup>Universidad de La Frontera, Temuco, Chile — <sup>2</sup>Millennium Nucleus MultiMat — <sup>3</sup>Universidad de Mendoza, CONICET Mendoza, Argentina — <sup>4</sup>Universidad de Chile, Santiago, Chile — <sup>5</sup>Center for the Development of Nanoscience and Nanotechnology (CEDENNA), Santiago, Chile — <sup>6</sup>Universidad Nacional de San Luis, CONICET San Luis, Argentina

In the aim to understand the formation of a self-assembled monolayer when 2-thiophene molecules are adsorbed on a Au(111) surface, we studied the deposition of rigid straight pentamers onto a FCC(111) surface. Thus, by combining density functional theory calculations and Monte Carlo simulations we have found that for a certain value of the chemical potential there exists an isotropic-nematic phase transition

which can explain the formation of a self-assembled monolayer. An order parameter is defined to characterize the transition which presents a step-like behavior at a critical chemical potential value. The possible nature of the nematic transition is discussed as future work by means of statistical physics techniques.

O 73.7 Wed 16:45 TRE Phy

**Polymorphism of 6,13-Pentacenequinone on Ag(111) in the monolayer regime** — ●JARI DOMKE, FALKO SOJKA, ROMAN FORKER, and TORSTEN FRITZ — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Pentacene and its derivatives have been studied extensively and with great interest in the last decades due to their potential and actual application in organic electronics. For devices utilizing those molecules an understanding of the layer growth on a distinct substrate is of fundamental importance, as this can be strongly affected by introducing functional groups – for example – to promote hydrogen bonds.

We structurally investigated 6,13-pentacenequinone (P2O) on Ag(111) in monolayer and sub-monolayer regimes using distortion-corrected low-energy electron diffraction (LEED) and low-temperature scanning tunneling microscopy (STM). Accordingly, several coverage-dependent structures were found, most of them exhibiting an on-line epitaxy. Additionally, a phase consisting of many line-shaped nano domains was observed for annealed samples in STM, yielding a consistent model for LEED patterns that would otherwise suggest a commensurate structure incompatible with the molecular size of P2O.

O 73.8 Wed 17:00 TRE Phy

**Self-assembly, metalation and oxidation of a novel macrocyclic compound on Ag(111)** — ●FELIX HAAG<sup>1</sup>, PETER DEIMEL<sup>1</sup>, RAPHAEL LAUENSTEIN<sup>2</sup>, MANUEL KASPAR<sup>2</sup>, JOHANNES BARTH<sup>1</sup>, CORINNA HESS<sup>2</sup>, and FRANCESCO ALLEGRETTI<sup>1</sup> — <sup>1</sup>Physics Department E20, Technical University Munich, Germany — <sup>2</sup>Chemistry Department, Technical University Munich, Germany

We report the first experimental study of the adsorption of the free-base macrocyclic biquinazoline (H-mabiq) on a model solid surface. This tetraaza-macrocyclic offers two potential coordination sites combined with multi-electron transfer capacity - properties reaching beyond the well-studied surface-confined metallo-porphyrins and -phthalocyanine systems. Those coordination sites can be occupied by different metal atoms, rendering adsorbed mabiq complexes promising candidates for photocatalytic applications as well as epoxidation reactions.

Here, we report on the bonding and self-assembly of H-mabiq on Ag(111) by using X-ray photoelectron spectroscopy (XPS), low-energy electron diffraction (LEED) and temperature programmed desorption (TPD). We confirm the molecular integrity and establish protocols for well-ordered single layers and controlled metalation with Co atoms. A number of long-range ordered structures are identified, depending critically on molecular and metal coverage. Furthermore, reversible cycling between different phases is observed by tuning the H-mabiq surface density and the temperature. Finally, the interaction of adsorbed H-Mabiq and Co-mabiq with dioxygen is compared.

O 73.9 Wed 17:15 TRE Phy

**2D molecular Self-assembly of C8-BTBT on metallic surfaces** — ●SEBASTIAN BECKER<sup>1,2</sup>, LU LYU<sup>1</sup>, SINA MOUSAVION<sup>1</sup>, MANIRAJ MAHALINGAM<sup>1</sup>, BENJAMIN STADTMÜLLER<sup>1</sup>, and MARTIN AESCHLIMANN<sup>1</sup> — <sup>1</sup>Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — <sup>2</sup>Department of Chemistry, University of Kaiserslautern, Erwin-Schrödinger-Str. 52, 67663 Kaiserslautern, Germany

Owing to a unique high mobility, [1]Benzothieno[3,2-b]benzothiophene (BTBT) based organic semiconductors (OSCs) have an enormous potential for photonic and spintronic applications. Here we systematically investigate the self-assembly of 2,7-Diethyl-BTBT (C8-BTBT) molecules on Cu(111), Cu(001) and Co/Cu(001) surfaces. In the first monolayer, C8-BTBT molecules adopt a flat lying geometry on these surfaces due to dominant molecule-metal interactions. Depending on sample temperature, various C8-BTBT phases with different unit cells are found on Cu(111), in which the molecular C8-arms rotate into different orientations. On the more reactive surface of a Co thin film on Cu(100), a chemical desulfurization is observed in the first layer of C8-BTBT in contrast to the adsorption of C8-BTBT directly on Cu(001). The desulfurization reaction blocks the electron transfer across the in-

terface. Our findings will provide new insight into the structural and electronic properties of BTBT-derivatives on metallic surfaces

O 73.10 Wed 17:30 TRE Phy

**Adsorption Behaviour of Benzohydroxamic Acid on TiO<sub>2</sub>(110)** — ●JULIA KÖBL, ELMAR KATAEV, DANIEL WECHSLER, LISA-MARIE AUGUSTIN, HANS-PETER STEINRÜCK, and OLE LYTKEN — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, D-91058

We are aiming for a deeper understanding of basic interactions between organic molecules and oxide surfaces, as these interfaces are apparent in many electronic devices, such as dye-sensitized solar cells and organic field effect transistors. Thus, we studied the adsorption properties of the model system benzohydroxamic acid on rutile TiO<sub>2</sub>(110)-(1x1) as a function of coverage and temperature. This molecule is an interesting candidate for anchoring larger organic molecules like porphyrins on oxide surfaces. Using Synchrotron Radiation Photoelectron Spectroscopy (SRPES), we studied the bonding mechanism and thermal stability of benzohydroxamic acid, which was deposited by evaporation. From SRPES, we can identify different species in the N 1s spectra. The results are compared to our previous studies on phosphonic acid. Supported by the DFG through FOR 1878 (funCOS).

O 73.11 Wed 17:45 TRE Phy

**Molecular arrangement discloses intermolecular interactions: The case of 1D structure formed by 3-hydroxybenzoic acid on calcite(10.4)** — ●MAXIMILIAN VOGTLAND<sup>1</sup>, CHRISTOPH SCHIEL<sup>2</sup>, JONAS STAUDE<sup>1</sup>, JULIA NEFF<sup>1</sup>, HAGEN SÖNGEN<sup>1</sup>, PHILIPP MAASS<sup>2</sup>, RALF BECHSTEIN<sup>1</sup>, and ANGELIKA KÜHNLE<sup>1</sup> — <sup>1</sup>Universität Bielefeld, Deutschland — <sup>2</sup>Universität Osnabrück, Deutschland

Molecular self-assembly constitutes a convenient way to create molecular structures at surfaces. In the past, the focus of controlling the structure has been on attractive interactions, while repulsive interactions have been explored only rarely. Our group has investigated the self-assembly of benzoic acid derivatives with dynamic atomic force microscopy (AFM) at room temperature on calcite (10.4). Here, we focus on 3-hydroxybenzoic acid (3-HBA) that forms a 1D (striped) structure. The obtained next-neighbour stripe distance distributions differ substantially from what is expected for randomly placed, non-interacting stripes. These distance distributions have been explained by a long-range repulsion of adsorption induced dipoles. On the other hand, the stripe length distribution is a result of short-range attractive and long-range repulsive forces. We show how to extract the strength of repulsive and attractive interactions between the 3-HBA molecules by combining the information from length and distance distributions. In the future, we want to compare with other 1D structures, e.g., 3-aminobenzoic acid on calcite(10.4). We believe that tuning repulsive interactions is a powerful tool to influence molecular structure formation on bulk insulator surfaces.

O 73.12 Wed 18:00 TRE Phy

**Multi-method study of trans-DBPen on coinage metal (111)-surfaces** — ●FELIX OTTO, MAXIMILIAN SCHAAL, TOBIAS HUEMPFNER, FALKO SOJKA, MARCO GRUENEWALD, ROMAN FORKER, and TORSTEN FRITZ — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Several polycyclic aromatic hydrocarbons (PAHs) become superconducting after the intercalation of alkali metal atoms. The number of promising candidates has increased in the last few years. Among them, K<sub>3,45</sub>1,2:8,9-dibenzopentacene (trans-DBPen, C<sub>30</sub>H<sub>18</sub>) is the one with the highest critical temperature reported so far. Nevertheless, the microscopic mechanisms of superconductivity in K-doped PAHs are still under debate. One open question is, for example, the effect of structural order in bulk materials as well as two-dimensional layers.

Our work deals with the growth of trans-DBPen on Ag(111), Au(111), and Cu(111) in the monolayer (ML) regime. The self-assembled thin films were prepared using organic molecular beam epitaxy. The structure was characterized by means of low energy electron diffraction (LEED). In the sub-ML range, we observe a 2D gas-like behavior, whereas the first MLs on the different substrates are characterized by highly ordered structures. Photoelectron spectroscopy (PES) including photoelectron momentum maps (PMMs) was used to study the interaction of the molecules with the substrate as well as the influence of the second ML on the electronic structure. The investigated systems exhibit notable differences according to the different interaction strengths with the substrate.