

O 49: Poster: Nanostructures on Surfaces I

Time: Tuesday 18:15–20:30

Location: Poster A

O 49.1 Tue 18:15 Poster A

Ullmann Coupling of 1,3-Dibromoazulene — •CLAUDIO K. KRUG, QITANG FAN, FLORIAN FILLSACK, JOHANNES GLOWATZKI, NICOLE TREBEL, MARTIN SCHMID, and J. MICHAEL GOTTFRIED — Department of Chemistry, Philipps-Universität Marburg, Germany, Hans-Meerwein-Str. 4, 35032 Marburg

The surface-confined Ullmann coupling reaction is a well-established strategy for creating covalent bonds between formerly halogenated aromatic molecules on coinage metal surfaces. So far, the focus has been on benzoid carbon backbones with alternant topologies. Here, we report the first Ullmann coupling involving a non-alternant aromatic hydrocarbon backbone. Specifically, the reaction of 1,3-dibromoazulene (DBAz) on Cu(111) was studied by means of scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS) under ultrahigh vacuum (UHV) conditions. Upon room temperature deposition of DBAz on Cu(111), long regioirregular chains are formed. The organometallic character suggested by the lattice constant is confirmed by XPS. Annealing to 440 K transforms the chains to cyclic organometallic hexamers with high yield. We have investigated the formation of these hexamers depending on the surface coverage. At low coverages, only isolated hexamers are observed because of lateral repulsive interactions. Increasing the coverage yields larger islands of Cu-DBAz cyclic hexamers. Annealing to higher temperatures results in the formation of regioregular covalent chains.

O 49.2 Tue 18:15 Poster A

Vibrational eigenmodes of the Sn-($\sqrt{3} \times \sqrt{3}$)/Si(111) reconstruction observed by surface Raman spectroscopy — •BENEDIKT HALBIG, UTZ BASS, and JEAN GEURTS — Universität Würzburg, Experimentelle Physik III, Würzburg, Germany

Adatoms on semiconductor surfaces, like Si(111), may reconstruct as two-dimensional layers leading to novel properties. For our subject Sn-($\sqrt{3} \times \sqrt{3}$)/Si(111), effects like a row-wise antiferromagnetic spin ordering [1] and a temperature-induced metal-insulator-transition were reported, but no phase transition [2,3]. Structure determination via surface sensitive Raman spectroscopy was successfully shown for surface adlayers [4].

We report on polarization dependent *in situ* Raman spectra of Sn-($\sqrt{3} \times \sqrt{3}$)/Si(111) at 300 K and ≈ 20 K. In contrast to the unreconstructed surface, new Raman peaks arise, the strongest ones at 184 and 383 cm^{-1} . Upon sample cooling, no significant changes in the Raman spectra were observed. In accordance with literature, we therefore acknowledge no phase transition.

In particular we observe a theoretically predicted mode at 81 cm^{-1} [3]. Unlike in the reports for Sn/Ge(111), this mode is not softening with decreasing temperature and not responsible for a change of the surface reconstruction, in agreement with theory prediction for Sn/Si(111) [3].

[1] G. Li et al., nat. comm. **4**, 1620 (2013) [2] S. Modesti et al., PRL **98**, 126401 (2007) [3] R. Pérez et al., PRL **86**, 21 (2001) [4] M. Liebhaber et al., PRB **94**, 235304 (2016).

O 49.3 Tue 18:15 Poster A

Self-assembly & optoelectronic properties of bis- & tetra-pyridil functionalized pyrene molecules — •DOMENIK ZIMMERMANN¹, KNUD SEUFERT¹, LUCA DORDEVIC², TOMAS MARANGONI², DAVIDE BONIFAZI³, and WILLI AUWÄRTER¹ — ¹Physik-Department E20, Technische Universität München, Germany — ²Department of Chemical and Pharmaceutical Sciences, University of Trieste, Italy — ³Department of Chemical and Pharmaceutical Sciences, University of Trieste, Italy

Pyridil functionalized pyrenes have shown well defined self-assembled structures on Ag(111). Dependent on the number and geometric positioning of the substituents, one-dimensional coordination chains, two-dimensional arrays and chiral, porous kagomé-type networks have been tailored in UHV and were investigated by STM[1].

However, to address the photoactivity of these polycyclic aromatic hydrocarbons an electronic decoupling from the metallic support is mandatory and achieved here by using an insulating layer of h-BN on Cu(111)[2]. On this electronically nanopatterned but topographically weakly corrugated substrate the molecules form self-assemblies reminiscent of the Ag case but show a distinct band gap between promi-

nent HOMO/LUMO states. STS shows a decrease of this gap upon increasing the number of substituents of the pyrene core. This result is confirmed by gas phase DFT calculations and UV-Vis spectra in solution.

[1] Kaposi et al, ACSNano **10**, 7665 (2016)

[2] Joshi et al, Nano Letters **12**, 5821 (2012)

O 49.4 Tue 18:15 Poster A

Efficient anchoring of molecular end groups via electric field driven chemical reaction — •TOMASZ MICHNOWICZ¹, BOGDANA BORCA^{1,2}, REMI PETUYA³, MARCEL PRISTL¹, VERENA SCHENDEL¹, IVAN PENTEGOV¹, ULRIKE KRAFT¹, HAGEN KLAUK¹, PETER WAHL^{1,4}, ANDRES ARNAU^{3,5}, UTA SCHLICKUM¹, and KLAUS KERN^{1,6} — ¹Max Planck Institute for Solid State Research, Germany — ²National Institute of Materials Physics, Romania — ³Donostia International Physics Centre, Spain — ⁴University of St Andrews, United Kingdom — ⁵Basque Country University CSIC-UPV/EHU, Spain — ⁶Ecole Polytechnique Federale de Lausanne, Switzerland

One of the challenges of single molecule electronics is to form a stable bond of the desired molecule to the metal electrodes, providing low resistance at the molecule-metal interfaces. One of the tools allowing both controlled manipulation of single molecules and probing their properties, including the electric conductance, is Scanning Tunneling Microscopy (STM). We show that a direct desulfurization reaction of a single thiophene unit embedded in a tetracenothiophene molecule on a Cu (111) surface can be driven by an electric field present in the STM tip-sample junction. This controlled, atomically precise reaction leads to the formation of covalent bonds between two carbon and two copper surface atoms. The enhanced coupling leads to 50% increase of the electric conductance measured by precisely contacting the molecules at the desired atomic positions and forming a molecular bridge between the metallic STM tip electrode and the metallic surface electrode.

O 49.5 Tue 18:15 Poster A

2D Nanoporous Chiral Supramolecular Networks Steered by Two σ -hole Interactions of S-Br & Br-Br. — •LINGBO XING¹, ZHICHAO HUANG¹, JINGXIN DAI¹, ZHAOHUI WANG², and KAI WU¹ — ¹College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China — ²Key Laboratory of Organic Solid, Chinese Academy of Sciences, Beijing 100190, China.

A variety of weak interactions such as hydrogen bonds, dipole-dipole interactions, van der Waals interactions, and metal-ligand coordination have been employed to assemble 2D nanoporous supramolecular networks at surfaces. σ -hole bond is a noncovalent interaction between a covalently-bonded atom of Groups IV-VII and a negative site, e.g. a lone pair of a Lewis base or an anion. Halogen bonding is a subset of σ -hole interactions. In this study, self-assembly behaviors of 3,10-dibromo-perylo[1,12-b,c,d]thiophene (2BPET) on Ag(111) will be discussed by means of scanning tunneling microscopy (STM) and density functional theory (DFT) calculations. For the first time, S-Br σ -hole interactions act as the driven force of molecular assembly on metal surfaces. Three types of porous chiral assembly phases can be fabricated under different coverage and deposition temperature steered by S-Br and Br-Br. Combined with DFT calculations, it turns out that S-Br is more thermodynamic stable.

O 49.6 Tue 18:15 Poster A

A Family of Hierarchical Molecular Fractal Porous Networks Constructed by a Small Molecule at Surface — •JINGXIN DAI, JIAN SHANG, WENHUI ZHAO, LINGBO XING, and KAI WU — SKLSCUSS, BNLMs, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China.

By using B3PB as the precursor, standalone molecular fractals (Sierpiński triangles, ST-n, n = 0, 1, 2, 3, 4, etc.) consisting of B3PB were constructed on Ag(111). The B3PB-ST-n fractals further formed new building motifs that self-assembled into a whole series of hierarchical two-dimensional molecular networks via a unified assembling pattern (rhombus unit cell containing two opposite chiral structures of the ST-n series). This unique hierarchical molecular self-assembly involved both fractal features and hierarchical features at the same time, and could provide new possibilities towards novel and complex hierarchical assemblies.

O 49.7 Tue 18:15 Poster A

Adsorption and Assembly of Photoelectronic TiOPc Molecules on Coinage Metal Surfaces — ●WENHUI ZHAO, HAO ZHU, and KAI WU — College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China

The adsorption and assembly of individual and sub-monolayered TiOPc on Ag(111), Cu(111) and Au(111) has been investigated by STM and STS. High-resolution STM imaging and dI/dV and I - z measurements reveal that TiOPc adsorbed on Ag(111) possesses two configurations, i.e., O-up and O-down configurations. Dipole-dipole interactions drive the TiOPc molecules to form a highly ordered checkerboard assembly structure on Ag(111) with alternating rows of the O-up and O-down adsorption conformations. The restricted surface mobility and diffusivity due to the strong interaction between the Cu(111) substrate and the TiOPc molecules and the templating effect of the reconstructed Au(111) herringbone structure result in no assemblies of the TiOPc molecules on these surfaces. Instead, the experimentally observed molecular dimers on both Au(111) and Cu(111) as well as the molecular aggregates on Au(111) indicate that the intermolecular dipole-dipole attraction and weak hydrogen bonding play an important role in dictating the adsorption and steering the assembly of the TiOPc molecules on the coinage metal surfaces.

O 49.8 Tue 18:15 Poster A

Hong-Ou-Mandel interference on dielectric metasurfaces — ●PHILIP CHRISTIAN GEORGI¹, KAI HONG LUO¹, FABIAN MEYER¹, GUIXIN LI², CHRISTINE SILBERHORN¹, and THOMAS ZENTGRAF¹ — ¹University of Paderborn, Paderborn, Germany — ²Southern University of Science and Technology, Shenzhen, China

Metasurfaces enable a spatial phase and amplitude manipulation of light, which makes them a powerful and versatile tool for all kinds of optical applications, especially holography. In contrast to their plasmonic counterparts, dielectric metasurfaces are inherently lossless and in recent years they gained an increased popularity in the research community due to the achievement of high operational efficiencies. This property makes them interesting for quantum optical application. As an initial step in this direction we present a recreation of the Hong-Ou-Mandel experiment based on a dielectric metasurface.

O 49.9 Tue 18:15 Poster A

2D self-assembly of TPT on noble metal surfaces — ●SEBASTIAN BECKER^{1,2}, LU LYU¹, SINA MOUSAVION¹, MANIRAJ MAHALINGAM¹, MARKUS GERHARDS², BENJAMIN STADTMÜLLER^{1,3}, and MARTIN AESCHLIMANN¹ — ¹Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern — ²Department of Chemistry, University of Kaiserslautern, Erwin-Schrödinger-Str. 52, 67663 Kaiserslautern — ³Graduate School Materials Science in Mainz, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern

Interfacial properties of organic films on noble metal surfaces are determined by a delicate balance between different interactions at the interface. Here, we investigate the geometric and electronic structures of TPT (2,4,6-triphenyl-1,3,5-triazine) on three (111) different noble metal surfaces with different surface reactivity using LT-STM and LEED. On Cu(111), TPT forms a long range ordered honeycomb-like metal-organic network with Cu adatoms in which the nitrogen atoms of the triazine ring adsorb on top of the Cu atoms[1]. In contrast, a close packed herringbone structure is observed for TPT on the less reactive Ag(111) and Au(111) surfaces at RT. Most interestingly, for TPT/Ag(111), we find a temperature-driven structural phase transition from the herringbone structure at RT to a honeycomb-like cavity structure at LT which was not observed for the other surfaces. Our findings will be correlated to the surface reactivity and the corresponding molecule-substrate interaction of each adsorbate system. [1] PRB 95, 094409 (2017)

O 49.10 Tue 18:15 Poster A

Formation of Metal-Organic Coordination Networks on a Bulk Insulator Surface — ●LUKAS SCHÜLLER¹, MD TAIBUR RAHMAN¹, RALF BECHSTEIN¹, and ANGELIKA KÜHNLE² — ¹Institute of Physical Chemistry, Johannes Gutenberg University Mainz, Duesbergweg 10-14, 55128 Mainz, Germany — ²Department of Chemistry, Bielefeld University, Universitätsstraße 25, 33615 Bielefeld, Germany

Metal-organic coordination networks (MOCNs) are a class of two-dimensional compounds with potentially interesting electronic, magnetic and catalytic properties. A variety of MOCNs have been created

on metal surfaces. However, an underlying insulator surface is beneficial for the electronic decoupling of structure and surface. To this end, we demonstrate the self-assembly of organic linker molecules and the formation of MOCN precursor structures in the presence of iron nanoclusters at room temperature. Our study of biphenyl-4,4'-dicarboxylic acid (BPDCA) in presence of iron on calcite (10.4) unravels two important findings: First, the deposition order plays a vital role in the formation of MOCNs. Second, a strong templating effect of the underlying surface is decisive for the direction, in which the MOCN is more extended. Currently, we vary the size of the linker molecule in order to match the surface unit cell size. Terephthalic acid (TPA), a homologue of BPDCA with one phenyl ring less, is examined in presence of iron, as well as 1,1':4',1''-terphenyl-4,4''-dicarboxylic acid (TPDCA), i.e., the homologue of BPDCA with one phenyl ring more. With this work, we explore the formation of an extended MOCN on an application-relevant bulk insulator surface.

O 49.11 Tue 18:15 Poster A

Simulation of reversibly interlocked SWCNTs — ●SEBASTIAN GSÄNGER and BERND MEYER — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

In chemical functionalization of single-walled carbon nanotubes (SWCNTs), usually one has to compromise between altering the structure of the nanotube via covalent attachment of the adsorbates or by forming rather fragile supramolecular complexes. An alternative, which combines having only non-covalently bound species but leads to very stable structures, is the concept of mechanically interlocking the CNT inside the adsorbate molecule. Specifically, we explore adsorbates which allow for a reversible ring closure in the rotaxane-forming step, therefore promising greater yields and a better control of the target structure. By combining classical molecular dynamics with DFT and metadynamics in a QM/MM approach we shed light on the adsorption behavior and the ring-closure reaction in different environments.

O 49.12 Tue 18:15 Poster A

Radiation pattern of the third harmonic emission generated in metal nanoantennas — ●TORSTEN STIEHM, JOHANNES KERN, ROBERT SCHMIDT, MARIUS JÜRGENSEN, STEFFEN MICHAELIS DE VASCONCELLOS, and RUDOLF BRATSCITSCH — Institute of Physics and Center for Nanotechnology University of Münster, 48149 Münster, Germany

Plasmon resonances in metallic nanoantennas give rise to strong field enhancements. This drastically boosts the nonlinear light-matter interaction in the metal and enables efficient third harmonic generation. We measure the angular distribution of the third harmonic emission of gold nanoantennas [1]. Single and multiple nanoantennas with resonances in the infrared [2] are excited by ultrashort laser pulses. The third harmonic emission is analyzed with back focal plane imaging using a high numerical aperture objective lens. Our experimental findings are in excellent agreement with numerical calculations.

1. T. Stiehm, J. Kern, M. Jürgensen, S.M. de Vasconcellos, R. Bratschitsch, Appl. Phys. B 122, 1 (2016)

2. T. Stiehm, J. Kern, R. Schmidt, S.M. de Vasconcellos, R. Bratschitsch, Appl. Phys. B 123, 150 (2017)

O 49.13 Tue 18:15 Poster A

Material sensitive reconstruction of nanostructures based on finite-element simulations of complementary X-rays measurements — ●VICTOR SOLTWISCH, ANALIA FERNANDEZ HERRERO, PHILIPP HÖNICKE, MIKA PFLÜGER, BURKHARD BECKHOFF, and FRANK SCHOLZE — Physikalisch-Technische Bundesanstalt, Berlin

In order to model visible light scattering, rigorous calculations of the near and far field by numerically solving Maxwell's equations with a finite-element method are well established. The application of this technique to X-rays is still challenging, due to the discrepancy between the incident wavelength and the discretization size. We show that a rigorous calculation of the near and far field is still suitable for grazing incidence techniques e.g. grazing incidence small angle X-ray scattering (GISAXS) or grazing incidence X-ray fluorescence (GIXRF) and 2D periodic nanostructured surfaces. The flexibility of the finite-element approach in combination with statistical evaluations allows for parameter reconstruction of the surface shape with sub-nm uncertainty. This combined toolset of scattering and fluorescence measurements with rigorous simulations paves the way for a versatile

characterization of nanoscale structured surfaces.

O 49.14 Tue 18:15 Poster A
Reactivity of CO on Sulfur-Passivated Graphene-Supported Platinum Nanocluster Arrays — FABIAN DÜLL, UDO BAUER, FLORIAN SPÄTH, PHILIPP BACHMANN, JOHANN STEINHÄUER, HANS-PETER STEINRÜCK, and •CHRISTIAN PAPP — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany

Poisoning of heterogeneous catalysts, in particular platinum, by sulfur and its oxides is of a hot topic in catalysis for decades.

Utilizing the intrinsic Moiré pattern of graphene on Rh(111) as a template and chemically inert support, Pt nanocluster arrays were grown.[1] They were then poisoned with sulfur via thermal reduction of SO₂. To understand the changes that occur upon sulfur poisoning, the adsorption and desorption of the probe molecule CO were investigated. The changes in the adsorption behavior for several preadsorbed sulfur coverages were studied with in situ high-resolution XPS. Three different CO species can be distinguished: top and bridge bonded CO on terrace sites and CO at step sites. Sulfur blocks those adsorption sites to different degrees. While on-top and step sites are highly affected, bridge sites are affected to a lower degree. These results will be compared to measurements on the stepped Pt(322) and Pt(355) surfaces.[2] Upon annealing, a displacement of sulfur from step to terrace sites by CO occurs around 330 K, which is reversed after desorption of the CO. Such a behavior was also found on stepped platinum crystals.

[1] K. Gotterbarm et al., ACS Catal. (2015) 2397-2403.

[2] R. Streber et al., Chem. Phys. Lett. 452 (2008) 94-98.

O 49.15 Tue 18:15 Poster A
Studying surface interactions of molecular polyoxovanadate species for new electronic nanodevices — •MARCO MOORS¹, OLIVER LINNENBERG², MARIA GLÖSS^{1,2}, ALEKSANDAR KONDINSKI², and KIRILL MONAKHOV^{1,2} — ¹Forschungszentrum Jülich — ²RWTH Aachen

Polyoxovanadates (POVs) have already been for a long time in the focus of several experimental and theoretical studies due to their synthetic accessibility, versatile structural chemistry, and intriguing electronic and magnetic properties. The possible applications for POVs cover many different fields of interest ranging from catalysis to nanoelectronics. A very promising approach is hereby their implementation as redox active centers in resistive switching memory cells. However, one of the most important challenges for a technological integration of such molecular systems in real devices is the controlled deposition of single POVs on surfaces and their individual contacting.

In our recent study we investigate the deposition of [V18O42]5- on Au(111) by droplet deposition from different solvents and by thermal deposition from the solid phase. This mixed-valent superkeggin-type POV is a perfect candidate for molecular switching experiments due to its several and easily addressable vanadium redox states. Depending on the deposition technique and parameters we are able to control the particle size on the surface ranging from small agglomerates over single molecules up to molecular fragments, which tend to recombine on the metallic substrate leading to new low-valent vanadium-oxo species.

O 49.16 Tue 18:15 Poster A
Silver clusters in ionic liquids of different viscosity - stabilisation and aggregation — •PHILIPPE POULET, FLORIAN LIPPERT, ALEXANDER KONONOV, STEFANIE ROESE, and HEINZ HÖVEL — Fakultät Physik/DELTA, Technische Universität Dortmund, 44227 Dortmund, Germany

Due to their low vapor-pressure, enabling cluster deposition to liquids, Ionic Liquids (IL) gained interest for vacuum application [1]. Due to the relatively high viscosity of the IL at low temperature the aggregation of deposited clusters is significantly slowed down and the clusters stay separated. However, during cluster deposition a high viscosity hinders the mixing of the clusters into the volume of the IL.

For ILs with high viscosity Ag-clusters are deposited by temperatures higher than room-temperature to decrease the viscosity of the ILs and the temperature is decreased afterwards for storage. Via UV/vis-spectroscopy the aggregation of clusters is measured in-situ and ex-situ for different storage-temperatures.

Therefore the refractive indices depending on the wavelength are measured via Fabry-Pérot-Interferometry for the ILs [BMIM][PF₆], [BMIM][BF₄], [BMIM][TF₂N], [BMIM][DCA], [OMIM][BF₆] and [EMIM][FAP].

Additionally the temperatures for the glass transition of the above

mentioned ILs are determined by measuring transmission.

[1] D. C. Engemann, S. Roese, H. Hövel, J. Phys. Chem. C **120**, 6239, (2016)

O 49.17 Tue 18:15 Poster A
Chemical Analysis of engineered Nanomaterials using Time of Flight Secondary Ion Mass Spectrometry (ToF-SIMS) — •MARKUS RENNHAKE, THOMAS HEINRICH, and WOLFGANG E. S. UNGER — Bundesanstalt für Materialforschung und -prüfung, Fachbereich 6.1 Oberflächenanalytik und Grenzflächenchemie, Unter den Eichen 87, 12205 Berlin

The analysis of nanomaterials is current an important task - especially in case of risk assessment, as the properties of these material class are not well understood currently. The rather high surface area of these objects renders their interactions significantly different to their corresponding bulk. Thus, the surfaces chemical composition has to be investigated to get a better understanding and prediction of the nanomaterials' behavior. ToF-SIMS has proven as a powerful tool to determine said chemical composition. Its superior surface sensitivity allows us to study mainly the utmost atomic layer and therefore gives us an idea of the interactions involved. Here, we show first result from the validation of the method for the analysis of polystyrene and gold nanoparticles. ToF-SIMS will be compared to other methods like XPS, T-SEM or REM. Furthermore, principle component analysis (PCA) will be used to detect the influence of different sample preparation performed by an innovative microfluidic device. ToF-SIMS imaging is desired to be implemented for single particle detection as well.

O 49.18 Tue 18:15 Poster A
Temperature-dependent stabilization of silver nanoparticles in BMIM PF₆ — •STEFANIE ROESE, ALEXANDER KONONOV, FLORIAN LIPPERT, and HEINZ HÖVEL — Technische Universität Dortmund, Dortmund, Germany

The storage of nanoparticles (NPs) is one of the most challenging tasks. It is indispensable to prevent the NPs from aggregation to larger agglomerates after production. Many groups report that the NPs are electrostatically stabilized without additional agents by ionic liquids (ILs). A detailed review is given by Dupont and Scholten[1]. In addition, due to their low vapour pressure, ILs are ideally suited for vacuum applications. We investigated the temperature-dependent aggregation of preformed 2 nm silver NPs, which were produced by supersonic nozzle expansion and were deposited in a BMIM PF₆ IL[2]. With the help of the UV/VIS spectroscopy measurements and the analysis of the theoretically calculated spectra based on the Generalized Mie Theory for various shapes of aggregates, we were able to explain the stability of the samples with the temperature dependence of the viscosity of BMIM PF₆[3]. The same approach was also applied to samples produced by sputtering, to investigate the aggregation process. In this case the size distribution of the NPs is not fixed, as the formation of NPs by sputtering is likely to occur on the surface or in the first layer of the IL during and after the sputter deposition. [1] J. Dupont, J. D. Scholten, Chem. Soc. Rev. **39**, 1780, (2010). [2] D. C. Engemann, S. Roese, H. Hövel, J. Phys. Chem. **120**, 6239, (2016). [3] S. Roese, A. Kononov, J. Timoshenko, A. I. Frenkel, H. Hövel, submitted (2017).

O 49.19 Tue 18:15 Poster A
Topographic and Phase Measurements of Embedded Gold Nanoparticles using Atomic Force Microscopy — •ANNIKA BERGMANN, SVEN KRAFT, REGINA LANGE, SYLVIA SPELLER, and INGO BARKE — University of Rostock, Institute of Physics, 18059 Rostock, Germany

For functional mapping of nanoscale samples a clear distinction between topographic effects and the signal of interest is inevitable. In atomic force microscopy (AFM) phase images do not only reveal material contrast but they may also contain topographic information [1], which is sometimes referred to as topographic crosstalk. Here we study the phase contrast between gold-nanoparticles and a PMMA environment using AFM. In order to obtain largely "pure" phase images we aim at creating a planar surface by embedding the nanoparticles into the polymer matrix. To achieve this, two different approaches are taken: first, heating of the sample which enables the nanoparticles to sink into the PMMA layer [2]; and secondly, spin-coating an additional PMMA layer on top of the sample. Our results show phase contrasts which have been detected for both approaches. Residual topographic effects are discussed, as well as the possibility of phase detection on fully embedded nanoparticles.

[1] García, Ricardo; Pérez, Rubén. Surf. Sci. Rep. 47, 197 (2002)

[2] M. Hanif, R. Juluri, M. Chirumamilla, V. Popok. J. Polym. Sci. B 54, 1152 (2016)

O 49.20 Tue 18:15 Poster A

Low-temperature STM measurements on the stable phase of $\text{Ge}_1\text{Sb}_2\text{Te}_4$ grown by MOVPE — ●PHILIPP KÜPPERS¹, CHRISTIAN HOLL¹, MARCUS LIEBMANN¹, ALBERT RATAJCZAK², DETLEV GRÜTZMACHER², HILDE HARDTDEGEN^{2,3}, and MARKUS MORGENSTERN¹ — ¹II. Physikalisches Institut B, RWTH Aachen — ²Peter-Grünberg-Institut 9, Forschungszentrum Jülich — ³Ernst Ruska-Centrum für Mikroskopie und Spektroskopie mit Elektronen 2, Forschungszentrum Jülich

$\text{Ge}_1\text{Sb}_2\text{Te}_4$ is a phase change material, similarly used in DVDs and random access memory. It exhibits a metastable and a stable crystalline phase which differ only by their stacking sequence. Here, we study the stable phase of $\text{Ge}_1\text{Sb}_2\text{Te}_4$, grown by metalorganic vapor phase epitaxy (MOVPE) using scanning tunneling microscopy (STM) and spectroscopy at 6 K. We present atomically resolved flat and defect-free terraces as large as $30 \times 30 \text{ nm}^2$ revealing a Te termination. Local density of states (LDOS) measurements show subsurface defects as triangular features in LDOS maps. While contacting the sample with a Cr (W) tip such that the resistivity decreases to $\approx 10^4 \Omega$, we observe an additional sharp drop in resistivity by an order of magnitude after ramping the voltage to 0.8 V (1.1 V). The process is reversible by removing and recontacting the tip at the same position. Possible explanations of the switching process are discussed.

O 49.21 Tue 18:15 Poster A

Controlling telegraph noise in a few donor system by laser illumination — ●OLE BUNJES, PHILIPP KLOTH, JUDITH VON DER HAAR, and MARTIN WENDEROTH — IV. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Extending a low-temperature Scanning Tunneling Microscope with optical excitation, we have investigated the effect of laser-induced minority charge carriers on temporal charge fluctuations within the tip-induced space charge region (SCR) on the (110) surface of n-doped GaAs. Discrete charging events in GaAs cause the tunneling current to switch abruptly between well-defined values [1], a signature referred to as telegraph signal. We investigated the temporal characteristic of the underlying single-electron charging events with a spatial resolution on the atomic scale by recording a time series of the tunneling current at every tip position. We studied the variation of the telegraph signal in the presence of laser-induced free charge carriers in the SCR. Reduction of the current's noise originating in the telegraph signal is found for small but non-vanishing hole concentrations, using the tunneling current as control parameter [2]. We attribute the reduction of the telegraphic step height to the photo-generated low-density hole gas that homogenizes the potential landscape at the sample surface. We acknowledge the financial support by the SFB1073 C04. [1] K. Teichmann et al., Nano Lett. 11, 3538-3542 (2011) [2] P. Kloth et al., Nat. Commun. 7, 10108 (2016)

O 49.22 Tue 18:15 Poster A

Nanosecond laser-induced periodic surface structures on fused silica dependent on additional confinement layer stacks — MARTIN EHRHARDT^{1,2}, ●PIERRE LORENZ², SHENGYING LAI², FRANK FROST², BING HAN¹, and KLAUS ZIMMER² — ¹Advanced Launching Co-innovation Center, Nanjing University of Science and Technology, 200 Xiaolingwei, 210094 Nanjing, Jiangsu, China — ²Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstr. 15, 04318 Leipzig, Germany

Laser-induced periodic surface structures (LIPSS) are generated in semiconductor, polymer, metal and dielectric surfaces irradiated with short and ultra-short laser pulses. LIPSS generation with nanosecond laser pulses shows a dependency of the periodicity and the ripple orientation on the wavelength as well as the polarization of the laser beam. In the present study, LIPSS formation on fused silica surfaces covered by a layer stack system was studied. The layer stack system consist, start from the fused silica surface, of a polymer or semiconductor interface layer, a metal absorber layer and a photoresist confinement layer. The resultant LIPSS structures were analyzed by atomic force (AFM) and scanning electron microscopy (SEM). It was found that the LIPSS periodicity and height is dependent on the thickness and the material properties of the layers.

O 49.23 Tue 18:15 Poster A

Charge distribution within nanostructures of molecular dipoles on Au(111) — ●SERGEY TRISHIN¹, DANIELA ROLF¹, PHILIPP RIETSCH², CHRISTIAN LOTZE¹, SIEGFRIED EIGLER², and KATHARINA J. FRANKE¹ — ¹Freie Universität Berlin, Fachbereich Physik — ²Freie Universität Berlin, Institut für Chemie und Biochemie

Donor-acceptor molecules have been investigated widely, because they offer suitable electronic characteristics for a possible use in electronic devices, such as single-molecule diodes or transistors. When deposited on a surface, the charge distribution within the molecule may change significantly due to screening and hybridization effects. Here, we investigate the N_2 -ethane-tetracyano-quino-dimethane molecule on a Au(111) surface, which exhibits a large dipole moment in gas phase. On the Au(111) substrate, the molecules form ordered self-assembled chains of varying width. Employing non-contact AFM at low temperature, we measure the local contact potential difference (LCPD). We show that the molecules still exhibit a distinct dipole character on the substrate. The dipole moment depends on the width of the molecular chains.

O 49.24 Tue 18:15 Poster A

Ion beam induced surface patterns - All coefficients for the equation of motion from Monte Carlo simulations — ●HANS HOFSSÄSS, OMAR BOBES, and ALRIK STEGMAIER — II. Physikalisches Institut, Universität Göttingen, Germany

Linear theories of surface pattern formation typically consider curvature dependent effects related to the 1st order moments of the erosion, redistribution and implantation crater functions. Smoothing of a surface is described by either thermal surface diffusion or ion-induced viscous flow. The equation of motion (EOM) of the surface $h(x,y,t)$ then consists of 1st and 2nd order spatial derivatives and a 4th order term related to smoothing. Using the Monte Carlo simulation codes SDTrimSP we calculate all crater function moments (erosion, redistribution and implantation) up to 4th order and derive all coefficients for the EOM up to 4th order, including the non-linear coefficients. The calculation is applicable to almost any ion-target combination up to ion energies of several 10 keV, any ion incidence angle, and may include dynamic changes of the target stoichiometry. Higher order crater function moments give rise to a wavelength dispersion of the ripple propagation velocity and contributions similar to a diffusion term. Non-linear coefficients related to derivatives $(dh/dx)^2, (dh/dx)^3, (dh/dy)^3, (dh/dx)(dh/dy)^2$ give rise to amplitude saturation and terrace formation. We calculate the complete set of coefficients using SDTrimSP for several model cases, which are then used as input for a software package that allows the simulation of dynamics for arbitrary, nonlinear EOMs.

O 49.25 Tue 18:15 Poster A

Transport-based single-atom STM electron-spin resonance: a cotunneling description — ●JOSE REINA¹, NICOLAS LORENTE¹, and FERNANDO DELGADO² — ¹Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU, Manuel de Lardizabal 5, E-20018 San Sebastián, Spain. — ²Departamento de Física, Universidad de La Laguna, Instituto de estudios avanzados (IUdEA), Avda. Astrofísico Francisco Sánchez, S/N 38203 La Laguna (Tenerife), Spain

Electron spin resonance (ESR) has recently overcome its main limitation, reaching the single atom detection limit[1]. In its new form, magnetic resonance is observed as a variation of the current flowing through a scanning tunneling microscope tip positioned over a magnetic adatom while applying an ac. voltage of different frequencies. Although several theoretical origins of the ESR signal have been proposed [2], it is still unclear how the time-varying bias voltage couples to the localized spin, with marked discrepancies with the experimental observations. Here we show that this signal is associated to the variation of the potential energy felt by the electrons on its occupation of the adatom energy levels. Thus, by using a time-dependent cotunneling description of the transport, we estimate the STM-ERS driving strength and its dependence with the main control parameters of the ERS setup, making a close comparison with the experimental findings.

[1] S. Baumann et al., Science 350, 417 (2015)

[2] P. Berggren and J. Fransson, Sci. Rep. 6, 25584 (2016). J.L. Lado, A. Ferrón, and J. Fernández-Rossier, Phys. Rev. B 96, 205420 (2017)

O 49.26 Tue 18:15 Poster A

Controlled soft-landing electrospray ion-beam deposition on freestanding graphene for high resolution transmission electron microscope characterization of molecules — ●SUMAN SEN,

NILESH VATS, STEPHAN RAUSCHENBACH, SABINE ABB, WILFRIED SIGLE, MARKO BURGHARD, PETER VAN AKEN, and KLAUS KERN — Max Planck Institute for Solid State Research, Heisenbergstr.1, 70569 Stuttgart Germany

Electrospray ion-beam deposition (ES-IBD) has evolved as a pivotal technique for studying molecules in ultra-high vacuum (UHV) condition to attain single molecular resolution [1]. In this work, we deposited and learned about absorption properties of phosphotungstic acid (PTA) on single-layer graphene (SLG). We have demonstrated how large poly-oxo-metallate (POM) anions can be deposited in a controlled way with different landing energies on SLG in UHV. We showed that, PTA molecules have higher affinity to absorb onto amorphous impurity present on graphene compared to pristine SLG. Furthermore, atomic scale resolution of the PTA molecule absorbed on SLG using low-voltage (80 kV) aberration-corrected, high-resolution TEM was performed. Our study provides first detailed learning about the soft landing, absorption and characterization of individual POM anions on SLG. This can give insight into fabrication of two-dimensional materials involving graphene and POM species. [1] Rauschenbach, S. et al., *Small*, 2, 540-547, (2006)

O 49.27 Tue 18:15 Poster A

Self-assembly and charging of molecules on insulating films — PHILIPP SCHEUERER and •JASCHA REPP — University of Regensburg, Regensburg, Germany

Thick insulating films and bulk insulators enable the charging of adsorbates and have been used in studies to investigate charge transfer between individual molecules[1] and multiple charging of ensembles of molecules[2]. Self assembly on insulating films[3] allows one to investigate charging phenomena in ordered structures.

Here, we study self-assembled Perylenetetracarboxylic dianhydride (PTCDA) islands on a few layers of NaCl on Au(110). From AFM imaging with submolecular contrast, as well as dI/dV- and KPFS-measurements, we conclude that individual molecules in self assembled PTCDA islands can be charged. Furthermore, charges can be controllably transferred to neighboring molecules within a PTCDA island.

[1] W. Steurer et al., *Nature Communications* 6, 8353 (2015)

[2] P. Rahe et al., *Nano Letters* 16, 911 (2016)

[3] S. Burke et al., *Nature Communications* 6, 8312 (2015)

O 49.28 Tue 18:15 Poster A

Field emission investigations on flat polycrystalline Cu and Nb samples after argon-ion bombardment and pulsed laser treatment — •SÜLEYMAN SOYKARCI, HENDRIK BÜRGER, VITALI PORSHYN, PAVEL SERBUN, DIRK LÜTZENKIRCHEN-HECHT, and GÜN-

TER MÜLLER — Bergische Universität Wuppertal, Gaußstr. 20, 42119 Wuppertal

In the present work, systematic investigations of polycrystalline Cu and Nb surfaces before and after Ar⁺ irradiation at 5 keV as well as laser treatments at different energies (300 uJ-2000 uJ) with a varying number of pulses (20-200) were performed by means of optical profilometry, atomic force microscopy and high-resolution scanning electron microscopy. In addition, local FE measurements were performed using a tungsten truncated cone needle anode in a field emission scanning microscope [1]. The results of ion bombardment indicated that the first detectable changes of the Cu and Nb surfaces occurred already after 3 min of ion bombardment. A reduction of the β -factors of sharp emitters was observed, resulting in an increase of the onset field values. The measurements on laser treated Nb samples showed an increase of the initial surface roughness values, however local field emission measurements ($\phi_a = 30 \text{ um}$, $z = 11 \text{ um}$) showed that the onset field for FE shifted to $E > 700 \text{ MV/m}$. Detailed results will be presented and discussed at the conference. The work is funded by BMBF project 05H2015. [1] D. Lysenkov and G. Müller, *Int. J. Nanotechnology* 2, 239 (2005).

O 49.29 Tue 18:15 Poster A

Ultrahigh vacuum piezo-based mask aligner for shadow mask evaporation with sub-100 nm precision — •PRIYAMVADA BHASKAR, SIMON MATHIOUDAKIS, TIM OLSCHESKI, FLORIAN MUCKEL, JAN RAFAEL BINDEL, MARCUS LIEBMANN, and MARKUS MORGENSTERN — II. Institute of Physics B, RWTH Aachen University, 52056 Aachen, Germany

Realizing nanostructures in ultrahigh vacuum (UHV) could be beneficial for many experiments including the STM investigation of lateral interfaces or quantum transport experiments employing a 4-tip STM. Another example is to realize a clean interface for the detection of Majorana fermions, where in-situ evaporation of superconductors with pierced holes onto a topological insulator $(\text{Bi}_{x-1}\text{Sb}_x)_2\text{Te}_3$ is a controllable setup. Using three piezo-drivers on the mask aligner and three capacitive sensors on the shadow mask, the sample-mask distance can be controlled with a sub-100 nm precision and the mask can be aligned parallel to the sample surface. Mask and sample can be exchanged in-situ and the sample can be moved laterally with respect to mask using an additional piezo motor. The precise control of the mask-sample distance allows to minimize the penumbra of evaporated regions and improves the quality of the lateral interface. We demonstrate μm -sized patterns of Au on Si(100) with penumbra as low as 90 nm and show that the penumbra increases with increasing mask-sample distance.