

O 51: Nanostructures at Surfaces: 1D and 2D Structures and Networks

Time: Tuesday 18:30–20:30

Location: P1C

O 51.1 Tue 18:30 P1C
growth of covalently bonded Sierpiński triangles up to the second generation — GAOCHEN GU, NA LI, and YONGFENG WANG — key laboratory for the physics and chemistry of nanodevices, department of electronics, Peking University, Beijing, China.

Growth of covalently bonded Sierpiński triangles (CB-STs) on metal surfaces was investigated by scanning tunneling microscopy (STM). Three synthetic strategies (namely, dehydration condensation, cyclotrimerization coupling and Schiff-base reactions) were used to fabricate CB-STs. Second generation CB-STs were obtained at the solid-vacuum interface utilizing the Schiff-base reaction between 4,4'-dialdehyde-1,1':3',1''-terphenyl (TPDAL) and 1,3,5-tris(4-aminophenyl)benzene (TAPB) on Au(111). The CB-ST patterns persist at annealing temperatures as high as 500 K. Homotactic three-fold motifs, insufficient migration and irreversible covalent reaction are the main limitations for growing higher-generation STs. The present results provide new insights on the growth of STs on metal surfaces.

O 51.2 Tue 18:30 P1C
self-assembly of L-tryptophan on Cu(111) studied by LT-STM — QIANG XUE and YONGFENG WANG — Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, China.

The chiral nanoclusters and one-dimensional chains of L-tryptophan on Cu(111) were investigated by ultrahigh vacuum scanning tunneling microscopy at 4.4 K. Small isolated clusters and chains coexisted on Cu(111) when molecules were deposited onto the substrate at around 30 K with a coverage of 0.25 monolayer. Then almost all the molecules self-assembled into chiral hexamers after being annealed at room temperature. When increasing molecular coverage to the full layer, only chains were found on the surface. High resolution STM images revealed that chains were composed by neutral, zwitterionic and anionic molecules. Chiral hexamers were formed by anionic tryptophan molecules. The structure difference was attributed to the competition between intermolecular and molecule-substrate interactions.

O 51.3 Tue 18:30 P1C
robust Sierpiński triangle fractals on symmetry-mismatched Ag(100) — YAWEI WANG and YONGFENG WANG — Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, China.

Sierpiński triangle fractals were constructed on both Ag(111) and symmetry-mismatched fourfold Ag(100) surfaces through chemical reaction between H3PH molecules and Fe atoms under vacuum. Density functional theory calculations revealed that the fractals were stabilized by the strong coordination interaction between Fe and O atoms. In comparison, pure H3PH molecules formed fractals via moderately strong hydrogen bonds only on Ag(111), not on Ag(100).

O 51.4 Tue 18:30 P1C
charging single Co atoms on ultrathin NaCl films — CHENYANG YUAN and YONGFENG WANG — Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, China.

Single Co adatoms adsorbed on a double-layer NaCl film supported by Cu(111) were negatively charged after applying a positive voltage pulse to the sample in a scanning tunnelling microscope. Density functional calculations showed that the magnetic moment of Co changed from $3\mu_B$ to $2.2\mu_B$ after charge state manipulation.

O 51.5 Tue 18:30 P1C
Spin related transport of single molecule studied by LT-STM — YAJIE ZHANG and YONGFENG WANG — Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing, China

A revolution in electronics is with the contemporary evolution of the two novel disciplines of spintronics and molecular electronics. A fundamental link between these two fields can be established using organic magnetic materials. Using a low-temperature scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS), we are able to study the single molecules under ultrahigh vacuum conditions at 4.2 /0.4 K. In this talk, we measured the magnetic properties of

retinoic acid molecules, FePc and DyPc2 adsorbed on metal surface with corresponding spin carries of 2s, 3p, and 4f electrons. Unlike the pre-existing metal ion in FePc or DyPc2, retinoic acid molecules can be switched reversibly to a special state by placing the tip over the neck of the bulky heads at an appropriate sample voltage. The generation of a stable cationic radical makes the molecule have an unpaired electron. The dI/dV spectrum confirms the appearance of spin in switched states. In addition, we proposed that the two Pc ligands in the same double-decker DyPc2 molecules rotate by 45 degrees against each other, which can be directly deduced from the STM imaging.

O 51.6 Tue 18:30 P1C
Plasma Assisted Synthesis and Mechanism of Rare V2O5 Nanostructured Thin Films — MEGHA SINGH, PRABHAT KUMAR, and GADE B. REDDY — Thin Film Laboratory, Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016

Two rare nanostructures of V2O5 using facile plasma assisted sublimation process (PASP) have been synthesized. V2O5 nanoflakes and nanoplates assembled in microspheres (NPMs) were obtained on large area over nickel coated glass substrate. The temperature of growth is varied along with time duration of deposition in order to obtain the different kinds of nanostructure as well as to understand the role of Ni-seed layer playing in controlling the morphology of nanostructures.

The morphological, structural, and vibrational properties of V2O5 nanostructured thin films are systematically investigated systematically as a function of time and deposition temperatures. Structural analysis carried out using the XRD shows the pure orthorhombic phase of V2O5 and revealed the dependence of crystallinity on the temperature and duration of growth. The Raman study of vanadium and oxygen atoms in nanostructured thin films (NTFs) is carried out by micro-Raman, which evidences the presence of single orthorhombic phase of V2O5 and accorded with XRD results. HRTEM analysis with SAED confirms that NFs and NPMs are polycrystalline in nature. The stoichiometry ratio obtained from XPS analysis is ~ 2.4 , shows the compositional purity and stoichiometric nature of V2O5 NTFs. Based on the observed results a three steps growth mechanism is proposed.

O 51.7 Tue 18:30 P1C
6-Mercaptopurine self-assembled monolayers on Au(100)-hex: revealing the fate of gold ad-atoms — KATHRIN MÜLLER¹, PILAR CARRO², FLAVIA LOBO MAZA³, CAROLINA VERICAT³, ROBERTO C. SALVAREZZA³, ULRICH STARKE¹, KLAUS KERN^{1,4}, and DORIS GRUMELLI³ — ¹Max Planck Institute for Solid State Research, Stuttgart, Germany — ²Área de Química Física, Departamento de Química, Universidad de La Laguna, Tenerife, Spain — ³Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas, UNLP- CONICET- La Plata, Argentina — ⁴Institut de Physique, Ecole Polytechnique Fédérale de Lausanne, Switzerland

Self-assembled monolayers (SAMs) can be used as inexpensive surface coatings for applications in sensors, surface protection and many more. Especially interesting is the interaction of the anchoring group (thiol, silane, phosphate) with the metallic substrate (e.g. gold, copper, silver), which determines the main properties of the SAMs. Here, we report on the adsorption of 6-mercaptopurine (6MP) on (100)-orientated reconstructed gold. The SAM was investigated with STM, LEED, XPS, electrochemical techniques and DFT calculations. We show that 6MP is unable to form vacancy islands in contrast to other thiol-gold SAMs, although its adsorption lifts the hex reconstruction. Thus, there is a large excess of gold adatoms in contact with the thiol molecules, which form disordered molecule-gold clusters. The remaining molecules arrange in two different well-ordered adatom-free domains. Our results show that the formation of ordered thiol-gold adatom complexes is not a general process and depends strongly on the thiol molecule.

O 51.8 Tue 18:30 P1C
New atomic models for Au-induced wire structures on Ge(001) surfaces at higher Au coverages — KAORI SEINO¹, SIMONE SANNA¹, WOLF GERO SCHMIDT¹, and FRIEDHELM BECHSTEDT² — ¹Lehrstuhl für Theoretische Physik, Universität Paderborn, Paderborn, Germany — ²Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Jena, Germany

One-dimensional (1D) electronic systems have been investigated extensively because of the interest both in fundamental physics and in nano or atomic scale devices. The atomic structure of Au-induced nanowires on Ge(001) substrates, which arguably belong to the most interesting quasi 1D systems, is still under discussion despite intensive research.

We have studied the structural, energetic and electronic properties of Au-induced nanowires on Ge(001) surfaces by means of density functional theory calculations [1,2]. We start the investigations from the original and a modified giant missing row structure, the Au-trimer stabilized Ge ridge model [3]. Three new structures for a higher Au coverage in the range between 1.25 monolayer (ML) and 1.75 ML are proposed. It is found that the new models are energetically more favorable than the models proposed previously. Moreover, they are able to explain several features of the experimental results.

[1] K. Seino and F. Bechstedt, Phys. Rev. B **93**, 125406 (2016).

[2] K. Seino and F. Bechstedt, J. Phys.: Condens. Matter **28**, 284005 (2016).

[3] S. Sauer *et al.*, Phys. Rev. B **81**, 075412 (2010).

O 51.9 Tue 18:30 P1C

Continuously changing incommensurate adlayer: Coronene on Graphene — ●FALKO SOJKA, MATTHIAS MEISSNER, TOBIAS HUEMPFNER, LARS MATTHES, ROMAN FORKER, and TORSTEN FRITZ — Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

It has been reported previously that coronene (C₂₄H₁₂) grows on graphite in a commensurate manner [1]. However, by means of distortion-corrected low-energy electron diffraction (LEED) measurements we find that this is the case only under very special conditions. Rather, C₂₄H₁₂ grows preferably incommensurate on graphene as well as on graphite. Upon variation of temperature or coverage this well-defined structure changes continuously. On the basis of our experimental results we show how the lattice constant and the rotation angle of the layer are related. We further show that this type of incommensurate epitaxy is also accompanied by energy gain. Theoretical calculations are performed based on force-field calculations scaled by density functional theory (DFT) results as introduced recently [2]. The main claim here is to assume a flexible adlayer lattice instead of a rigid one. [1] M. Lackinger *et al.*, Anal. Bioanal. Chem. **374** (2002) 685. [2] M. Meissner *et al.*, ACS Nano **10** (2016) 6474-6483.

O 51.10 Tue 18:30 P1C

Epitaxy of Flexible 2D Crystals — ●MATTHIAS MEISSNER¹, FALKO SOJKA¹, LARS MATTHES¹, FRIEDHELM BECHSTEDT¹, XINLIANG FENG², KLAUS MÜLLEN², STEFAN C. B. MANNSFELD³, ROMAN FORKER¹, and TORSTEN FRITZ¹ — ¹Uni Jena Germany — ²MPI für Polymerforschung Mainz, Germany — ³cfaed, TU Dresden, Germany

The epitaxy of many organic films on inorganic substrates can be classified within the framework of rigid lattices which helps to understand the reproducible film orientations. For incommensurate systems, however, this classification fails as an explanation for an epitaxial alignment. Tiny shifts in atomic positions away from ideal lattice points, so-called static distortion waves (SDWs), had been proposed to be responsible for the orientational epitaxy in such cases. Using low-energy electron diffraction and scanning tunneling microscopy, we provide direct evidence for SDWs in the incommensurate monolayer of the molecule *hexa-peri-hexabenzocoronene* on graphite. They manifest as sub-Ångström molecular displacements away from an ideal, yet incommensurate lattice. By means of a density-functional-theory based gradient approach, we show that flexibility in the adsorbate layer is crucial to provide a total energy minimum for the observed domain orientation, constituting orientational epitaxy. While structural relaxation at an interface is a common assumption, the combination of the precise determination of the incommensurate epitaxial relation, the direct observation of SDWs in real space, and their identification as the sole source of epitaxial energy gain constitutes a comprehensive proof of this effect. [M. Meissner *et al.*: ACS Nano **10**, 6474-6483 (2016).]

O 51.11 Tue 18:30 P1C

Self-assembly of MoMo-Methyl molecules on Au surfaces — ●LU LYU¹, ZHENG WEI^{1,2}, JOBYNSON KOLLAMANA¹, MANUEL ZIMMER³, MARKUS GERHARDS³, BENJAMIN STADTMÜLLER¹, MIRKO CINCHETTI⁴, and MARTIN AESCHLIMANN¹ — ¹Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — ²College of Material Science and Engineering, Chongqing University, 400044 Chongqing, People's Republic of China — ³Department of Chem-

istry, University of Kaiserslautern, Erwin-Schrödinger-Straße 52, 67663 Kaiserslautern, Germany — ⁴Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund, Germany

We systematically investigated the self-assembly and ordering of MoMo-Methyl (3M) molecules on Au(111) and Au(788) surfaces with variable-temperature scanning tunneling microscopy (STM) at substrate temperature of 106 K. On Au(111), most of the molecules form two-dimensional ordered superstructures preserving the herringbone reconstruction of the substrate. In addition, one-dimensional zig-zag molecular chains were observed, in contrast to the straight chains that we previously studied for 3M grown on Cu(111). On the vicinal Au(788), two types of one-dimensional (1D) molecular chains were observed. On more narrow terraces, 2D-like molecular ribbons are formed. These differences indicate that the coordination of Au substrate atoms with 3M molecules can be ignored on Au(111) but not on Au(788).

O 51.12 Tue 18:30 P1C

STM imaging and spectroscopy of diindeno-pyrene: theoretical modeling — ●SEDDIGHEH NIKIPAR¹, THOMAS LEHMANN¹, FRANK EISENHUT¹, DMITRY A. RYNDYK², FRANCESCA MORESCO¹, and GIANAURELIO CUNIBERTI¹ — ¹Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — ²Bremen Center for Computational Materials Science, Universität Bremen, Germany

One of the most promising experimental techniques to build new atomic scale materials is surface assisted synthesis in UHV condition. For its characterization and analysis, scanning tunnelling microscopy and spectroscopy are main tools. Recently our group observed the synthesis of diindeno-pyrene molecules by deposition of dibromo-diphenylpyrene on Au(111). Our current research focuses on exploring the structure and electronic properties of this new molecule on Au(111) by STM imaging and finite-voltage spectroscopy. To support the experimental results, we developed a computational method based on the CP2K computational package, by combining the density functional theory (DFT), first principle molecular dynamics, and electron transport approach starting from the Tersoff-Hamann approximation. We also used the Elastic scattering quantum chemistry approach (ESQC) for molecular transport to simulate the STM topography and dI/dV spectroscopy images. Using the localized/projected molecular orbital method, we analyze the molecular orbitals, energy alignment and electron density of states. The results of the theoretical modelling indicate good agreement with the experimental results.

O 51.13 Tue 18:30 P1C

Vibrational Eigenmodes of the Au-($\sqrt{3} \times \sqrt{3}$)/Si(111) surface reconstruction examined by Raman spectroscopy and first-principles calculations — ●BENEDIKT HALBIG¹, MARTIN LIEBHABER¹, UTZ BASS¹, JEAN GEURTS¹, EUGEN SPEISER², JOCHEN RÄTHEL², SANDHYA CHANDOLA², NORBERT ESSER², SERGEJ NEUFELD³, MARVIN KRENZ³, SIMONE SANNA³, and WOLF GERO SCHMIDT³ — ¹Uni. Würzburg, Exp. Physik III, Würzburg, Germany — ²Leibniz-Institut für Analytische Wissenschaften - ISAS e.V., Berlin, Germany — ³Uni. Paderborn, Dep. Physik, Paderborn, Germany

Submonolayer coverages of metal adatoms on semiconductor surfaces show particular reconstructions, e.g., (5×2) and ($\sqrt{3} \times \sqrt{3}$) for the Au/Si(111) system. Raman spectroscopy proves to be a sensitive probe analysing vibration eigenmodes of these material systems, as demonstrated for Au-(5×2)/Si(111) [1]. We report on the investigation of Au-($\sqrt{3} \times \sqrt{3}$)R30°/Si(111) by polarized *in situ* Raman spectroscopy in combination with first-principle calculations within Density Functional Theory. The Raman spectra, taken at 300 K and ≈ 20 K, reveal a main peak at 73 cm⁻¹ accompanied by adjacent peaks on the low-energy side, a singular peak at 30 cm⁻¹, and a group of three peaks around 115 cm⁻¹. Density Functional Theory Frozen-Phonon calculations were carried out for three structural models labeled twisted-trimer, conjugate honeycomb-chained-trimer and honeycomb-chained-trimer [2]. [1] M. Liebhaber *et al.*, PRB, accepted (2016). [2] J. Y. Lee *et al.*, JKPS, **55**, 6 (2009), and references therein.

O 51.14 Tue 18:30 P1C

Fabrication and investigation of near-surface spin centers in high-purity single crystal diamond — ●NICOLAS WÖHRL¹, REINHARD REMFORT¹, STEFAN BORGS DORF², TANMOY CHAKRABORTY³, ULRICH KÖHLER², DIETER SUTER³, and VOLKER BUCK¹ — ¹Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstraße

1, 47057 Duisburg, Germany — ²Experimentalphysik IV, AG Oberflächen, Ruhr-Universität Bochum, Germany — ³Experimentelle Physik IIIA, Technische Universität Dortmund, Germany

Photons from ideal single-photon sources exhibit quantum mechanical characteristics and therefore allow applications in novel fields including quantum cryptography and spintronics. One promising candidate for this task is the nitrogen-vacancy (NV) center in diamond. The main aim of this project is the fabrication and investigation of near-surface NV-centers in high-purity single-crystal diamond films. Preparation of these active elements is still challenging, especially when read-out is desired to be by optical as well as electronic means. In this work, pure single-crystal diamond films are homoepitaxially grown by microwave-plasma-assisted chemical vapor deposition, and the film quality is characterized. PL-measurements show, that the purity of these films surpasses the quality of commercially available electronic grade diamonds ($N < 5$ ppb) significantly. NV centers are created by ion implantation and their properties are investigated spectroscopically.

O 51.15 Tue 18:30 P1C

Electron beam induced surface activation - a novel method to study and reduce proximity effects — ●CHRISTIAN PREISCHL, MARTIN DROST, FAN TU, and HUBERTUS MARBACH — Friedrich-Alexander Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058, Erlangen, Germany

We apply different focused electron beam-based nanolithographic techniques in an ultra-high vacuum (UHV) environment. Recently, we explored Electron Beam Induced Surface Activation (EBISA), in which a surface is first chemically activated by the highly focused electron beam. In a second step, the activated regions can be developed with certain precursor molecules, resulting in the catalytic decomposition and eventually autocatalytic growth of the latter [1]. Suitable substrates for EBISA are oxide surfaces, thin organic films or surface anchored metal-organic frameworks. EBISA does not only allow for the controlled fabrication of well-defined nanostructures but also enables detailed insights into electron back-scattering processes by exploring and visualizing the corresponding proximity effects. Along with the presentation of these results, we will also discuss strategies to reduce proximity effects in electron beam lithography.

[1] H. Marbach, Appl. Phys. A, 117 (2014), 987;

O 51.16 Tue 18:30 P1C

The influence of low energy electron irradiation on the work function of aromatic self-assembled monolayers investigated by Kelvin Probe Force Microscopy — ●PAUL PENNER¹, MARCIN KISIEL², SASCHA KOCH¹, THILO GLATZEL², ERNST MEIER², and ARMIN GÖLZHÄUSER¹ — ¹Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany — ²Department of Physics, University of Basel, 4056 Basel, Switzerland

Carbon Nano-Membranes (CNMs) are two-dimensional materials that are made by e.g. low-energy-electron irradiation induced cross-linking of Self-Assembled Monolayers (SAMs) of aromatic and organic molecules. The variation of different precursor molecules for the SAM and CNM formation allows not only to tune the properties of the final CNM but also to study the influence on the surface properties due to the specific SAM modification. Here we investigate the change in the work function of pristine SAMs and CNMs on a Au(111) substrate by means of Kelvin Probe Force Microscopy (KPFM) for different precursor molecules. The SAMs were partially cross-linked using a TEM-grid as a mask in order to compare the morphology and the work function of SAMs and CNMs simultaneously. Whereas no significant difference on the morphology due to the electron irradiation was observed, the analysis of the work function of pristine and cross-linked SAMs revealed a molecule dependent increase of the work function. On the one hand, this could be attributed to the modification of the dipole moment of the SAM and of the Au-S interface but also to the influence of different headgroups (H, NO₂, CN) on the other hand.

O 51.17 Tue 18:30 P1C

"Nunchakus" molecules on metallic surfaces investigated by scanning tunneling microscopy — ●LACHENG LIU^{1,2}, HONG-YING GAO^{1,2}, PHILIPP HELD³, ARMIDO STUDER³, and HARALD FUCHS^{1,2} — ¹Center for Nanotechnology, Heisenbergstr.11, 48149 Muenster, Germany — ²Physikalisches Institut, Westfaelische Wilhelms-Universitaet, Wilhelm-Klemm-Straße 10, 48149 Muenster, Germany — ³Organisch-Chemisches Institut und Center for Mutiscale Theory and Simulation, Westfaelische Wilhelms-Universitaet, Corrensstr.40, 48149 Muenster

Scanning tunneling microscopy (STM) is demonstrated to be a promising tool to investigate the molecular conformation on metallic surfaces with atomic precision. In this work, we studied the adsorption conformations and self-assembly structures of four different "nunchakus" shaped molecules: Bis(2-naphthyl) peroxide, 2-Naphthoic anhydride, Bis(2-naphthyl)ethanedione and trans-1,2-Bis(2-naphthyl)ethene. Different metal substrates Au(111), Ag(111) and Cu(111) were tested to reveal the interaction between organic molecules and metal surfaces. For these "nunchakus" shaped molecules, different adsorption conformations even on the same metallic surface were identified. The center to center distances of 2-Naphthyl groups in single molecules were measured, which are shorter than the ones in gas phase due to the specific interaction between O atoms and metallic surface atoms which leads to the tortuosity of the molecules.

O 51.18 Tue 18:30 P1C

Highly ordered 3D nanostructure arrays with improved electrochemical performance for sodium-ion battery anodes — ●LIYING LIANG, YANG XU, CHENGLIANG WANG, MIN ZHOU, LIAOYONG WEN, HUAPING ZHAO, YAOGUO FANG, YAN MI, and YONG LEI — Institute for Physics and IMN MacroNano, Ilmenau University of Technology, Ilmenau 98693, Germany

Due to the lower cost and larger abundance of Na, Na-ion batteries have been a potential alternative to Li-ion batteries for energy storage devices. The development of electrode materials or structures with good electrochemical performance is currently key task in Na-ion batteries research. In this work, we presented a highly ordered 3D nanostructure array with large-scale high ordering, well vertical alignment, and large interval spacing, fabricated by a facile and cost-effective nanoimprinted AAO templating technique, might be successfully used as an electrode and showed an excellent electrochemical performance. This arrays conceptual design is universal to most of electrode materials. In return for this electrode design, high ion accessibility, fast electron transport, and strong electrode integrity are presented. Used as additive- and binder-free anode for Na-ion batteries, the electrochemical performances are greatly enhanced. This work may open up more applications of such highly ordered 3D nanostructure arrays in energy storage systems.

O 51.19 Tue 18:30 P1C

Tip-enhanced near-field optical microscopy on single-walled carbon nanotubes — ●SONJA TAUCHERT, XIAN SHI, NICOLAI F. HARTMANN, and ACHIM HARTSCHUH — Department Chemie and CeNS, LMU Munich, Germany

Tip-enhanced near-field optical microscopy (TENOM) [1] is a scanning probe technique with highest detection sensitivity. It is capable of providing a broad range of spectroscopic information on single objects and structured surfaces with nanometer spatial resolution. We utilized TENOM to investigate the photoluminescence (PL) of (6,5) SWCNT/PFO-BPy conjugates. PL images reveal the spatial homogeneity of both emission intensity and energy along individual nanotubes. The images provide detailed information on several key phenomena influencing the excited state properties of SWCNTs including the interaction with the environment, nanotube-nanotube coupling and defect density. Specifically, we focus on the photophysics of excitons at local dopant sites [2].

[1] Mauser, N. et al., Chem. Soc. Rev., Vol. 43, No. 4, 2014.

[2] Hartmann, N. et al., Nanoscale, Vol. 7, No. 48, 2015.

O 51.20 Tue 18:30 P1C

Analysis of molecular wire formation of cyano-functionalized porphyrins on Cu(111) by calculation of STM images — ●MARTIN GURRATH¹, WOLFGANG HIERINGER², MICHAEL LEPPER³, TOBIAS SCHMITT⁴, ALEXANDER SCHNEIDER⁴, HUBERTUS MARBACH³, and BERND MEYER¹ — ¹Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — ²Lehrstuhl für Theoretische Chemie, FAU Erlangen-Nürnberg — ³Lehrstuhl für Physikalische Chemie II, FAU Erlangen-Nürnberg — ⁴Lehrstuhl für Festkörperphysik, FAU Erlangen-Nürnberg

The structure of adsorbed cyano-functionalized free-base tetraphenyl porphyrins (2H-TCNPP) on Cu(111) and their appearance in scanning tunneling microscopy (STM) is investigated by density-functional theory (DFT) calculations. In experiment, a formation of one-dimensional 2H-TCNPP chains in which the molecules are strongly distorted along the chain axis is observed after annealing. The DFT calculations support that the molecular wire formation is triggered by Cu adatoms and they provide insights into the cause of the strong distortion of the

2H-TCNPP molecules.

O 51.21 Tue 18:30 P1C

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 performing molecular dynamics simulations with the generalized AMBER force field, we identified suitable structures and geometries and analyzed their behaviour and the reaction conditions.

O 51.22 Tue 18:30 P1C

On-Surface Synthesis of Low-Dimensional Nanostructures from Haloarenes — ●QITANG FAN¹, TAO WANG², CICI WANG², JUNFA ZHU², MIN CHEN¹, CLAUDIO K. KRUG¹, MALTE ZUGERMEIER¹, JULIAN KUTTNER¹, GERHARD HILT¹, and J. MICHAEL GOTTFRIED¹ — ¹Fachbereich Chemie, Philipps-Universität Marburg, Germany — ²National Synchrotron Radiation Laboratory, University of Science and Technology of China

The fabrication of low-dimensional nanostructures via on-surface synthesis has attracted tremendous attention due to their potential applications in nano-scale electronics and devices. Robust zero-dimensional (0D) cycles and one-dimensional (1D) chains are fabricated on metal surfaces from 4,4'-dibromo-m-terphenyl (DBMTP) molecules. Hyperbenzene, a hexagon consisting of 18 phenyl rings, forms ordered arrays on Cu(111), Ag(111) and Au(111) with maximum yield under pseudo-high dilution conditions. Organometallic tetragons and hexagons with C-Cu-C bonds were obtained on Cu stripes (with width from 2.6 nm to 3.6 nm) of a Cu(110)-(2x1)O supergrating surface. Zigzag organometallic chains and the corresponding oligophenylene chains form from DBMTP on Cu(110), Cu(111), Ag(111) and Au(111) with different yields and length distributions. The comparison of the outcomes on different substrates may shed light on the control of the topologies of nanostructures.

O 51.23 Tue 18:30 P1C

Halogen bonding in molecular self-assemblies of functionalized triphenylamines on Au(111) and Ag(111) — ●SACHIN RAJ

MENON¹, CHRISTIAN STEINER¹, TIM SANDER¹, NATALIE HAMMER², MILAN KIVALA², and SABINE MAIER¹ — ¹Department of Physics, Friedrich-Alexander University Erlangen-Nürnberg, Erlangen, Germany — ²Chair of Organic Chemistry I, Department of Chemistry and Pharmacy, Friedrich-Alexander University Erlangen-Nürnberg, Erlangen, Germany

Halogen-substituted molecules are frequently used as precursors in the on-surface synthesis of carbon-based molecular architectures. It is therefore important to understand how they self-assemble on metal surfaces, because it might affect the structure of the covalent reaction products. Halogen bonds are comparatively weak and often compete with other interactions such as hydrogen bonds.

Herein, we report on the self-assembly of halogen-substituted, carbonyl-bridged triphenylamines on Au(111) and Ag(111) by high-resolution scanning tunneling microscopy at low temperatures. We studied the binding motifs of various triphenylamine networks that result from competing halogen bonding and hydrogen bonding interactions. In addition, we discuss the influence of the molecule-substrate interactions on the self-assembly as well as the strength of the sigma-hole bonding by comparing chlorine and iodine substituted moieties.

O 51.24 Tue 18:30 P1C

The electronic structure of the Si(553)-Au surface functionalized by small molecules — ●SVETLANA SUCHKOVA¹, EUGEN SPEISER¹, SANDHYA CHANDOLA¹, CONOR HOGAN², and FRIEDHELM BECHSTEDT³ — ¹Leibnitz-Institut fuer Analytische Wissenschaften - ISAS - e.V., Department Berlin, Schwarzschildstr. 8-10, 12489 Berlin, Germany — ²Universita di Roma "Tor Vergata", Via della Ricerca Scientifica 1, 00133 Roma, Italy — ³Friedrich-Schiller-University Jena, Institut fuer Festkoerpertheorie und optik, Helmholtzweg 3, 07743 Jena

We propose a method for surface modification and tuning the electronic structure of the stepped Si(553)-Au surface by site-specific adsorption of toluene-3,4-dithiol (TDT) molecules. We continue our research on the adsorption of the molecule using density functional theory (DFT) simulations. Hydrogen is used to passivate the step edge dangling bonds, and various orientations/adsorption geometries of TDT on terrace sites are analysed. In spite of expectations, that molecular thiol groups will interact with Au chains, it was shown that the most reactive surface adsorption sites are Si double bonds on the honeycomb chains. On the basis of the analysis of the electronic band structure it was shown that depending on the selective adsorption geometry, metallic or insulating phases of the surface are observed. Our approach offers microscopic manipulation and fine tuning of surface geometry and electronic properties, preparation of nanopatterned surface templates with controllable molecular adsorption sites, and suggests a switch of chemical reactivity on such surfaces