

O 35: Poster Session I (Metal, semiconductor and oxide substrates: structure and adsorbates; Graphene)

Time: Tuesday 18:15–21:45

Location: Poster B1

O 35.1 Tue 18:15 Poster B1

Electronic structure of Ag(100) revisited by STS — ●ROBIN OHMANN¹, CORMAC TOHER¹, JÖRG MEYER¹, ANJA NICKEL¹, FRANCESCA MORESCO¹, and GIANAURELIO CUNIBERTI^{1,2} — ¹Institute for Materials Science and Max Bergmann Center of Biomaterials, Technische Universität Dresden, 01062 Dresden, Germany — ²Division of IT Convergence Engineering, POSTECH, Pohang 790-784, Republic Korea

The Ag(100) surface is used for many surface science studies as a substrate. Therefore, a clear knowledge about its electronic properties is desirable. In contrast to previous results, we present an experimental study on Ag(100) revealing an electronic state, at which electrons behave like in a two-dimensional electron gas. Conductance maps taken with scanning tunneling spectroscopy (STS) show energy dependent standing wave patterns at step edges and defects, from which the dispersion relation is extracted. We find a parabolic behaviour with a state onset of 1.9 eV above the Fermi energy and an effective mass of 0.41 m_e . Scanning tunneling spectra reveal a clear feature at the relevant energy. Additionally, the lifetime, linewidth and coherence length have been measured as a function of energy. Theoretical calculations have been performed to elucidate the experimental findings.

O 35.2 Tue 18:15 Poster B1

Electron pair emission from surfaces upon He²⁺ impact — ●CHANG-HUI LI¹, CHRISTIAN TUSCHE¹, FRANK O. SCHUMANN¹, and JÜRGEN KIRSCHNER^{1,2} — ¹Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle — ²Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany

Using a two-electron coincidence spectrometer, we have studied the electron pair emission upon the impact of 10 eV normal incident He²⁺ ions on Ir(100) and Fe(100)-p(1×1)O surfaces. According to the commonly used two-step model [1], He²⁺ is firstly converted to He⁺ and then to He⁰. Two electrons are emitted incoherently by the two corresponding neutralization steps. As the ionization potentials of He²⁺ → He⁺ and He⁺ → He⁰ are 54.4 eV and 24.6 eV, respectively, a very unequal energy sharing is expected. In the two-electron coincidence spectra, the dominant events can be understood by the incoherent two-step mode, but we have found clear evidence that this approximation breaks down and the neutralization should be treated as a single process.

[1] P. A. Zeijlmans van Emmichoven, P. A. A. F. Wouters, and A. Niehaus, 1988 Surf. Sci. 195 115

O 35.3 Tue 18:15 Poster B1

A LEED investigation of the Au(111)-(1×1) surface — BIRGIT VOGT and ●JOCHEN VOGT — Chemisches Institut der Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Although the ground state of the clean Au(111) surface shows reconstruction [1], the latter can be lifted, e. g. electrochemically, by stress, or by the presence of surface imperfections. For the clean unreconstructed Au(111)-(1×1) surface, both a layer distance compression as well as an anomalous layer distance expansion have been proposed at the solid vacuum interface [2,3]. We have prepared and characterized clean Au(111) surfaces by means of LEED, STM, XPS, and AES. The softly-annealed surfaces exhibit bright LEED diffraction patterns of (1×1) symmetry over a large energy range up to 450 eV. The measured diffraction beam intensities as a function of electron energy were the basis of a surface structure analysis. The structural results for the Au(111)-(1×1) surface are discussed in the context of reported structure data in literature and possible sources of error.

[1] S. B. Darling et al., Langmuir 18 (2002), 7462

[2] G. M. McGuirk et al., 10th International Conference on the Structure of Surfaces, 2011

[3] L. Guan et al., Solid State Commun. 149 (2009), 1561

O 35.4 Tue 18:15 Poster B1

One-step or two-step core-resonant double photoemission from a Ag(100) surface — ●ZHENG WEI¹, FRANK O. SCHUMANN¹, CHANGHUI LI¹, LUCIE BEHNKE¹, GIANLUCA DI FILLIPPO², GIOVANNI STEFANI², and JÜRGEN KIRSCHNER^{1,3} — ¹Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany — ²CNISM and Dipar-

timento di Fisica, Università Roma Tre, I-00146 Rome, Italy — ³Martin-Luther Universität, 06120 Halle, Germany — ³Martin-Luther Universität, Halle, Germany

We studied core-resonant double photoemission (DPE) from a Ag(100) surface with coincidence electron spectroscopy, and mapped out the two-dimensional energy distribution of the DPE pairs. Our experiments demonstrate that the photo-excited Auger transitions involving the Ag $M_{4,5}$ core levels can be described by a simplified two-step picture, while the Auger transitions involving the Ag $N_{2,3}$ core levels can only be described by a one-step picture. Since the final states of both Auger transitions are the same, this variation is purely due to the different initial core-hole state with different lifetime. We experimentally extracted the intrinsic line shapes of the $M_{4,5}VV$ Auger spectra, and found out the spectral weight transfer of the 3F_4 component from the atomic- to the band-like region.

O 35.5 Tue 18:15 Poster B1

Pattern formation of Ni- and Fe-Tetramethyl-tetraazaannulene on Au(111) — ●THOMAS KNAAK¹, THIRUVANCHERIL G. GOPAKUMAR¹, BETTINA SCHWAGER², FELIX TUCZEK², and RICHARD BERNDT¹ — ¹Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel — ²Institut für Anorganische Chemie, Christian-Albrechts-Universität zu Kiel

Saddle shaped Ni- and Fe-tetramethyl-tetraazaannulene (TMTAA) on Au(111) were investigated using low-temperature STM. Surprisingly, we observed the formation of different patterns, depending on the central ion, Ni or Fe. While Ni-TMTAA aggregates at low coverages into chiral clusters, Fe-TMTAA molecules remain isolated from each other and arrange in a hexagonal array. Presumably, different degrees of bending of TMTAA due to Ni and Fe is the origin of the different aggregation behaviors. Financial support by the Deutsche Forschungsgemeinschaft via the SFB 677 is acknowledged.

O 35.6 Tue 18:15 Poster B1

Intramolecular resolved STM-data of Biphenyldithiol-molecules on Au(111) — ●MICHAEL LOCHNER, MICHAEL WAELSCH und RENE MATZDORF — Universität Kassel, Fachbereich Naturwissenschaften,

We have investigated submonolayers of the organic molecule Biphenyldithiol on an Au(111)-surface with STM-methods. The molecules are physisorbed on the surface. Three types of typical structures have been found, which are dependent on the local coverage. We show intramolecular resolved data of molecules in all three structures. Additionally, workfunction-maps were measured by lock-in-technique. In some cases they show even more details of the molecule structure than usual STM-topographies.

O 35.7 Tue 18:15 Poster B1

Final-State Diffraction Effects In Angle-Resolved Photoemission At An Organic-Metal Interface — ●BOCQUET F. C.^{1,2}, GIOVANELLI L.², AMSALEM P.³, PETACCIA L.⁴, TOPWAL D.⁴, GOROVKOV S.⁴, ABEL M.², KOCH N.³, PORTE L.², GOLDONI A.⁴, and THEM-LIN J.-M.² — ¹Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — ²Aix-Marseille Univ, IM2NP, 13397 Marseille, France — ³Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — ⁴Sincrotrone Trieste, 34149 Trieste, Italy

The growth of organic thin films on metallic substrates has become a field of growing interest for organic electronics as well as for fundamental surface science [1]. We show that angle-resolved photoemission performed using low-energy photons on an organic-metal interface allows to clearly distinguish genuine interface states from features of substrate photoelectrons diffracted by the molecular lattice [2]. As a model system, an ordered monolayer of Zn-phthalocyanine is used as a diffraction lattice to probe the electronic band structure of a Ag(110) substrate. Photoemission close to normal emission geometry reveals strongly dispersive features absent in the pristine substrate spectra. Density functional theory modelling helped identifying these as bulk sp direct transitions undergoing surface-umklapp processes. The present results establish the important role of final-state diffraction effects in photoemission experiments at organic-inorganic interfaces.

[1] Bartels, Nature Chemistry 2 87 (2010) [2] Bocquet et al. Phys.

Rev. B 84 241407(R) (2011)

O 35.8 Tue 18:15 Poster B1

Kinetic parameters of molecule dynamics and reactions determined with a scanning tunneling microscope at room temperature and above — ●MICHAEL STARK, STEFANIE DITZE, MARTIN DROST, FLORIAN BUCHNER, ELISABETH ZILLNER, MICHAEL RÖCKERT, HANS-PETER STEINRÜCK, and HUBERTUS MARBACH — LS. f. PC II and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058

The knowledge of kinetic parameters is generally important for a detailed understanding of chemical and physical processes, like the self-assembly of molecular building blocks into supramolecular structures. In this study we investigate the kinetics of surface diffusion and the self-metalation reaction of 2H-tetraphenylporphyrin (2HTPP) on Cu(111). The determination of the corresponding parameters and activation energies is thereby based on experimental data acquired with a scanning tunneling microscope (STM) at room temperature and above in ultra-high vacuum. One the one hand the focus of this study is on the “slow” unidirectional diffusion of 2HTPP along the close packed atomic rows of Cu(111) and on the rotation of the latter molecules on the same substrate. We also investigated the surface-mediated self-metalation reaction of 2HTPP with Cu atoms from the Cu(111) substrate. By counting individual molecules in the corresponding ST micrographs we are able to determine the rate constants of this reaction at different sample temperatures and thus to determine the activation energy for the metalation reaction based on these values.

This work has been funded by the DFG through SFB 583

O 35.9 Tue 18:15 Poster B1

Structural and electronic characterization of an adsorbed SMM building block: Cu₃-triplesalen on Au(111) — ●JUDITH NIEDENFÜHR¹, MANUEL STEINBRECHER¹, THORSTEN GLASER², and DANIEL WEGNER¹ — ¹Westfälische Wilhelms-Universität, Münster, Germany — ²Universität Bielefeld, Bielefeld, Germany

Single Molecule Magnets (SMMs) are potential candidates for the application in future technological devices for high-density memory storage and quantum computation. In an attempt to combine a high spin ground state and a large magnetic anisotropy in one molecule, triplesalen complexes are promising building blocks for a new generation of SMMs. For an efficient superexchange interaction, a delocalized aromatic π system in the center of the triplesalen complex is required. However, previous chemical analysis indicates that the central benzene ring inside this complex can change its configuration to cyclohexane, therefore causing a loss of aromaticity. This has a dramatic impact on the magnetic coupling and spin polarization of the triplesalen complex. Employing a combination of Scanning Tunneling Microscopy (STM) and Scanning Tunneling Spectroscopy (STS) we have investigated single Cu₃-triplesalen complexes adsorbed on a Au(111) surface. The relatively large molecules were deposited in situ using a pulse injection technique. A thorough structural and spectroscopic analysis allows us to discuss the electronic properties of the Cu₃-triplesalen complex, with a special focus on the state of the central carbon ring.

O 35.10 Tue 18:15 Poster B1

Single Component and Compound Monolayers of CuPc and PTCDA on a Ag(110) Surface — ●KATHRIN SCHÖNAUER^{1,2}, MARTIN WILLENBOCKEL^{1,2}, BENJAMIN STADTMÜLLER^{1,2}, CHRISTIAN KUMPF^{1,2}, SERGEY SOUBATCH^{1,2}, and STEFAN TAUTZ^{1,2} — ¹Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — ²JARA - Fundamentals of Future Information Technology, Germany

Organic semiconductors are of great interest for research due to their potential application in organic electronics. Organic layers of one component on top of a metal crystal have been studied for decades. Recently binary and multinary molecular films also have come into focus, e.g., for the application in organic p-n junctions and all-organic solar cells. Traditionally, (111) surfaces of Ag, Au and Cu single crystals were used for experimental studies. Here we report on the structure of ordered monolayers of CuPc and PTCDA on a Ag(110) surface, both single component and compound. Scanning Tunneling Microscopy and Low Energy Electron Diffraction were used.

O 35.11 Tue 18:15 Poster B1

Wave-function tuning in self-assembled monolayers — ●BERNHARD KRETZ, DAVID ALEXANDER EGGER, ELISABETH VERWÜSTER, and EGBERT ZOJER — Institute of Solid State Physics, Graz

University of Technology

The distribution of dipolar groups along phenylthiol-based self-assembled monolayers (SAMs) was shown to cause a modification of the electron wave-function and the vacuum level.[1] In particular the molecular orbitals, like the highest occupied molecular orbital (HOMO) and the lowest unoccupied orbital (LUMO), get shifted in energy and localized. In this work, we perform band structure calculations using density functional theory on phenylthiol-based SAMs where dipolar and non-conjugated groups are distributed along the SAMs. The results indicate that the localization can be supported by breaking the conjugation along the backbone. Analysing the influence of the dipolar and non-conjugated groups on the wave-function guides the way towards a toolbox for wave-function engineering.

[1] F. Rissner et al., J. Am. Chem. Soc. 2011, 133, 18634

O 35.12 Tue 18:15 Poster B1

Impact of disorder on the properties of self-assembled monolayers with embedded dipoles — ●IRIS HEHN¹, MANUEL VIEIDER¹, OTELLO MARIA ROSCIONI², LUCA MUCCIOLI², MARTIN STOLTERFOHT¹, MICHAEL ZHARNIKOV³, CLAUDIO ZANNONI², and EGBERT ZOJER¹ — ¹Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — ²Dipartimento di Chimica Industriale “Toso Montanari”, Università di Bologna, Viale del Risorgimento, 4, 40136 Bologna, Italy — ³Applied Physical Chemistry, Heidelberg University, Im Neuenheimer Feld 253, 69120, Heidelberg, Germany

In this work mid-chain ester functionalized alkanethiols adsorbed on a gold {111} substrate are studied using molecular dynamics simulations and density functional theory calculations. The lengths of the alkyl segments above and below the carboxylate dipolar groups as well as the molecular coverage are systematically varied to study the impact of those parameters on the order within the layers. The latter is quantified based on various structural parameters, like tilt-, azimuthal- and twist-angles. To assess the impact of disorder on the electronic properties of the monolayers, histograms of tilt angle and dipole orientation distributions have been calculated and the impact of coverage and molecular structure on charge and potential distributions within the SAMs were studied.

O 35.13 Tue 18:15 Poster B1

PTCDA on Cu(100) re-investigated by STM — ●STEFAN GÄRTNER, BENJAMIN FIEDLER, OLIVER BAUER, and MORITZ SOKOLOWSKI — Institut für Physikalische und Theoretische Chemie der Universität Bonn, Germany

Whether the adsorption of an organic adsorbate on a metal surface leads to ordered or disordered structures, possibly including molecular dissociation, depends on the interfacial chemistry. While PTCDA forms long-range ordered structures on all Au and Ag surfaces, different structure models [1,2] and even a molecular dissociation were discussed for PTCDA on Cu(100) on the basis of XPS data [1]. To clarify this we have performed so far missing STM investigations. Indeed, for Cu(100), we find that the preparation of long-range ordered structures requires elevated sample temperatures (400 K), pointing to a considerable corrugation of the surface bonding potential. However, from the STM images, we obtain no indications for dissociation. We put forward a structure model with an L-type arrangement of the molecules in the monolayer and the second layer in agreement with the proposed ($5\sqrt{2} \times 4\sqrt{2}$)R45° structure of ref. [1]. The lattice parameters of this model are in full agreement with our LEED results on this system. Supported by SFB 624.

[1] T. J. Schuerlein et al., JVSTA 12 (1994) 1992. [2] M. Andreasson et al. Synth. Met. 158 (2008) 45

O 35.14 Tue 18:15 Poster B1

Ordered structures of the acceptor molecule TNAP on Au(111) investigated by STM and LEED — ●QINMIN GUO, BENJAMIN FIEDLER, STEFAN GÄRTNER, and MORITZ SOKOLOWSKI — Institut für Physikalische und Theoretische Chemie der Universität Bonn

As a strong electron acceptor 11,11,12,12-tetracyanonaphtho-2,6-quinodimethane (TNAP) is attractive for synthesising molecular charge transfer compounds. As a preparatory step we have studied the rich phase diagram of TNAP on the Au(111) surface for varying coverages and temperatures using STM and LEED. We have found at least 4 different structures (α , β , γ , δ) depending on the coverage and post-annealing conditions. α is a 1-dimensional ordered linear struc-

ture, and β is the brickwall-like structure reported also in ref. [1]. By post-annealing at 400 K, β can be converted into γ with a T-shaped arrangement of the molecules. The structure δ is only obtained at low temperatures. We will discuss these intermolecular interactions relevant for the structures. In addition, we present first results on binary structures of TNAP with electron donating molecules both on Au(111) and thin epitaxial KCl films on Au(111). This work is supported by SFB 813.

O 35.15 Tue 18:15 Poster B1

Nanostructure formation of hexphenylnitril — ●JÖRG MEYER¹, ANJA NICKEL¹, ROBIN OHMANN¹, CORMAC TOHER¹, FRANCESCA MORESCO¹, and GIANAURELIO CUNIBERTI^{1,2} — ¹Institute for Materials Science and Max Bergmann Center of Biomaterials, Technische Universität Dresden, 01062 Dresden, Germany — ²Division of IT Convergence Engineering, POSTECH, Pohang 790-784, Republic Korea

We report the first STM and STS measurements of the asymmetric molecule hexphenylnitril on the Au(111) surface. This molecule consists of six phenyl rings connected via single bonds in the para position (forming a straight line). One side of the molecule is functionalized with a cyano group. At high surface coverages, the molecules exhibit a densely packed parallel structure. At lower surface coverage the molecules tend to adsorb on step edges and adatoms due to their high mobility on the Au(111) surface. Triplets of molecules have also been observed. This triplet structure also verifies the intended asymmetrical structure of the molecule, because bifunctionalized specimens are known to form extended networks with similar triplet structures. To clarify whether the molecules themselves form a self-stabilising nanostructure or just attach to an adatom, we varied the sample temperature during evaporation. With increasing substrate temperature the fraction of triplets among all adsorbates increased. Comparing this to the known increase in the density of adatoms on the Au(111) surface leads to the interpretation of three molecules gathering around single adatoms.

O 35.16 Tue 18:15 Poster B1

Self-assembled Monolayers of Paramagnetic Molecules on Gold revealed by Scanning Tunneling Microscopy — ●CHRISTIAN SALAZAR¹, DANNY BAUMANN¹, RONNY SCHLEGEL¹, TORBEN HÄNKE¹, JOCHEN LACH², BERTHOLD KERSTING², BERND BÜCHNER^{1,3}, and CHRISTIAN HESS¹ — ¹Institute for Solid State Research, IFW Dresden, Germany — ²Institute für Anorganische Chemie, Universität Leipzig, Germany — ³Department of Physics, TU Dresden, Germany

We have studied self-assembled monolayers of organic dinickel (II) complexes with an S=2 high paramagnetic state, anchored to a Au(111) surface via thiol groups using STM at room temperature. Our data clearly reveal the dense distribution of 2-4 nm sized objects on the Au surface, which evidences the growth of a closed molecular monolayer. The monolayers, however, do not show long-range order of the individual molecules.

O 35.17 Tue 18:15 Poster B1

STM investigation on the structure formation of the ionic liquid BMP-TFSA on different metal surfaces — ●DOROTHEA ALWAST^{1,2}, BENEDIKT UHL^{1,2}, FLORIAN BUCHNER^{1,2}, and R. JÜRGEN BEHM¹ — ¹Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany — ²Helmholtz-Institute Ulm (HIU) Electrochemical Energy Storage, D-89069 Ulm, Germany

The application of ionic liquids in electrolytes is a promising concept for the improvement of Li-Ion batteries. Therefore, a detailed knowledge of the behavior of ionic liquids on the electrode electrolyte interface is crucial for further development. As a model system, adlayers of 1-butyl-1-methylpyrrolidinium-bis(trifluoromethylsulfonyl)imide (BMP-TFSA) have been investigated by scanning tunneling microscopy (STM). Measurements were carried out under UHV conditions in the submonolayer and monolayer regime, with particular emphasis on the structure formation of the first adsorbate layer. On Ag(111), BMP-TFSA forms a 2D liquid at room temperature, whereas at 100 K an ordered structure is observed on this surface. High-resolution STM images have been acquired and the sub-molecular features will be discussed. Details on structure formation of BMP-TFSA on Ag(111) as well as a comparison to surface structures of BMP-TFSA on Au(111) and Cu(111) surfaces are presented.

O 35.18 Tue 18:15 Poster B1

Combined STM and XPS investigation on the Ethylene Carbonate | Cu(111) interface — ●HANIEH FARKHONDEH^{1,2}, FLO-

RIAN BUCHNER^{1,2}, BENEDIKT UHL^{1,2}, and ROLF-JÜRGEN BEHM^{1,2} — ¹Helmholtz-Institute Ulm (HIU) Electrochemical Energy Storage, D-89069 Ulm, Germany — ²Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

Ethylene Carbonate (EC) is an important component in Li-ion battery electrolyte. A molecular understanding of the solid electrolyte interphase (SEI) is crucial to improve the Li-ion battery performance. In this work, the behavior of the EC | Cu(111) interface, as a model system, was investigated at sub-monolayer and monolayer coverages. The adlayers were characterized with STM and XPS under UHV conditions at temperatures between \sim 100 K and room temperature. With XPS, the intact EC was observed in the multilayer, monolayer and sub-monolayer range around 100 K, where two peaks in the C1s and O1s core level region reflect its stoichiometry. STM data at 100 K show that the molecules aggregate in 2D ordered islands at mono- and sub-monolayer coverages. The contour of these domains strongly changes in time sequence of STM images, which means they are not stable, pointing to weak adsorbate-adsorbate interactions. At room temperature, only noisy features are observed, i.e., EC molecules move too rapidly to be imaged with STM. The co-deposition of Lithium will be conducted in forthcoming experiments.

O 35.19 Tue 18:15 Poster B1

Formation of NTCDA and CuPc (hetero-) organic phases on Ag (111) — ●SONJA SCHRÖDER, BENJAMIN STADTMÜLLER, CHRISTIAN WAGNER, MARTIN WILLENBOCKEL, CHRISTOPH KLEIMANN, SERGEY SUBACH, and CHRISTIAN KUMPF — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and Jülich-Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology

The future development of organic devices like solar cells, OLEDs or OFLETs is based on the understanding of the interactions at organic-metal and organic-organic interfaces. In particular, charge transfer and the bonding strength across the interface are important, which in turn depend on the structure and molecular orientation. PTCDA, NTCDA and CuPc are prototypical molecules which have been studied intensively in this context in the last years. Here we report on the adsorption of NTCDA on Ag (111) and on NTCDA-CuPc-heteroorganic films. We present a modified brick wall model for NTCDA on Ag (111) with the molecules oriented perpendicular to the [-1 1 0] direction. This model is based on scanning tunneling microscopy (STM) measurements, pair potential calculations, a LEED I-V analysis and angle resolved photoemission (ARPES) results. Furthermore, we have investigated mixed layers of CuPc and NTCDA at different coverages on the same surface. Three different phases could be identified by SPA-LEED: A NTCDA rich-, a "1:1"- and a CuPc rich phase. The NTCDA- and the CuPc rich phases are commensurate structures. ARPES studies were performed for investigating the electronic properties.

O 35.20 Tue 18:15 Poster B1

Adsorption geometry and chemical structure investigations of organic molecules with atomic force microscopy using functionalized tips — ●BRUNO SCHULER, LEO GROSS, FABIAN MOHN, NIKOLAJ MOLL, and GERHARD MEYER — IBM Research - Zurich, 8803 Rueschlikon, Switzerland

Atomic force microscopy (AFM) with functionalized tips has proven to achieve intra-molecular contrast due to Pauli repulsion [1]. Crucial factors affecting the image contrast are the tip termination, intramolecular chemical differences and adsorption geometry of the adsorbate. Here we present investigations on all of these three contrast decisive factors. Particularly, we investigated the contrast characteristics of several tip apices (Cl, Br, CO, NO, Xe, Kr) for scanning tunneling microscopy and AFM imaging and developed a new tip preparation method for halogens based on dissociation from molecule precursors [2]. Furthermore, using the high-resolution of the CO tip, we could distinguish bond-order differences in aromatically bonded hydrocarbon molecules [3].

References:

- [1] L. Gross, F. Mohn, N. Moll, P. Liljeroth, G. Meyer, *Science* 325, 1110 (2009)
- [2] F. Mohn, B. Schuler, L. Gross, G. Meyer, submitted
- [3] L. Gross, F. Mohn, N. Moll, B. Schuler, A. Criado, E. Guitián, D. Peña, A. Gourdon, G. Meyer, *Science* 337, 1326 (2012)

O 35.21 Tue 18:15 Poster B1

STM and X-ray spectroscopy study on the self-assembly and chemical behavior of orotic acid on close-packed coinage

metal surfaces — ●SYBILLE FISCHER, ANTHOULA C. PAPAGEORGIOU, JOACHIM REICHERT, KATHARINA DILLER, FRANCESCO ALLEGRETTI, FLORIAN KLAPPENBERGER, and JOHANNES V. BARTH — Physik Department E20, TU München, James-Franck-Straße, D-85748 Garching

Understanding the self-assembly of small biomolecules including the DNA/RNA bases and related molecules as well as their interaction with metal surfaces is an important step towards the creation of bio-functionalized interfaces. Orotic acid is an important molecule in the *de-novo* synthesis of pyrimidines which include the RNA bases uracil and cytosine. Here we report the results of a multitechnique study investigating the self-assembly and chemical behavior of orotic acid on the Ag(111) and Cu(111) surfaces by means of scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS) and near-edge X-ray absorption fine-structure (NEXAFS). While the molecules assemble in two room-temperature stable structures on the silver surface, we can only find a metastable structure on the copper surface. The XPS study as a function of temperature gives insight in the chemical transformations of the molecule's functional groups, which guide the self-assembly whereas NEXAFS allows us to conclude about the molecular orientation with respect to the surface. Our findings are discussed with reference to the physical and chemical behavior of the related molecule uracil on Ag and Cu.

O 35.22 Tue 18:15 Poster B1

Combined photoemission and STM study of the surface-assisted Ullmann coupling reaction — ●MIN CHEN¹, JIE XIAO², HANS-PETER STEINRÜCK², SHIYONG WANG³, WEIHUA WANG³, NIAN LIN³, and MICHAEL GOTTFRIED¹ — ¹Fachbereich Chemie, Philipps-Universität Marburg — ²Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg — ³Department of Physics, Hong Kong University of Science and Technology

The Ullmann reaction, a Cu catalyzed C-C coupling reaction for haloarenes has been used for surface-assisted synthesis two-dimensional covalent nanostructures. Generally, this reaction provides a versatile route to the formation of larger arenes and arene-based extended nanostructures, especially one-dimensional molecular wires and two-dimensional covalent organic networks. In this study, we provide evidence for the Ullmann reaction of 4,4'-Dibromo-p-terphenyl (DBTP) and 1,3,5-Tris(4-bromophenyl)benzene (TBB) on Cu(111) by using X-ray and ultraviolet photoelectron spectroscopy (XPS/UPS) as well as scanning tunneling microscopy (STM). Assisted by Cu atoms from substrate, the C-Br bonds break between 170 and 240 K, and neighboring molecules get linked through intermediate C-Cu-C bonds. Upon further increasing the temperature, the C-Cu-C bonds are transformed into C-C bonds, such that neighboring arene fragments are covalently coupled, while Cu is released from the bridge positions. STM gives insight into the reaction progress on the molecular level. Our results provide an example for a possible strategy towards the bottom-up construction of functional devices based on molecular building blocks.

O 35.23 Tue 18:15 Poster B1

A measurement of the hysteresis loop in force-spectroscopy curves using a tuning-fork atomic force microscope — ●MERLIN SCHMUCK, MANFRED LANGE, DENNIS VAN VOERDEN, and ROLF MÖLLER — Faculty of Physics, Center of Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

The Analysis of the frequency shift versus distance in noncontact atomic force microscopy (NC-AFM) allows to measure the force gradient between the oscillating tip and a surface (force-spectroscopy measurements). When nonconservative forces act between the tip apex and the surface the oscillation amplitude is damped. The dissipation is caused by bistabilities in the potential energy surface of the tip-sample system, and the process can often be understood as a hysteresis of forces between approach and retraction of the tip. We present the direct measurement of the whole hysteresis loop in force-spectroscopy curves at 77 K on the PTCDA/Ag/Si(111) sqrt(3) x sqrt(3) surface by means of a tuning-fork-based NC-AFM with an oscillation amplitude smaller than the distance range of the hysteresis loop. The hysteresis effect is caused by the making and breaking of a bond between PTCDA molecules on the surface and a PTCDA molecule at the tip. The corresponding energy loss was determined to 0.57 eV by evaluation of the force-distance curves upon approach and retraction. Furthermore, a second dissipation process was identified through the damping of the oscillation while the molecule on the tip is almost in contact with the surface. It reaches a maximum value of about 0.22 eV/cycle.

O 35.24 Tue 18:15 Poster B1

Dynamic studies of octaethylporphyrin Fe(III) chloride — ●DENNIS VAN VÖRDEN¹, MANFRED LANGE¹, MERLIN SCHMUCK¹, JOHANNES SCHAFFERT¹, ROBERTO ROBLES RODRÍGUEZ², and ROLF MÖLLER¹ — ¹Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany — ²CSIC-ICN, Universitat Autònoma de Barcelona 08193 Bellaterra, Barcelona. Spain.

The porphyrin molecule is an archetypal metallorganic complex, which is found in many biochemical molecules like chlorophyll, haemoglobin and cytochrome. Here we investigate submonolayer coverages of octaethylporphyrin Fe(III) chloride (Fe-OEP) on Cu(111) prepared *in-situ*-using a combined LT-scanning tunneling/atomic force microscope.

As a first step, the topography and the orientation of the Fe-OEP molecules is investigated. Two different appearances of the molecule (type A and B) can be found. Type A (unfilled) can be easily manipulated and is mainly found at step edges, while type B (filled) is found individually on the flat terrace.

The comparison of DFT-simulations and STM images reveals, that type A molecules can be identified as dechlorinated (Fe-OEP) while type B are intact octaethylporphyrin Fe(III) chloride molecules. This is further corroborated by the observation that type B molecules can be transformed to type A by an electric pulse which induces a dechlorination of the molecule.

The diffusion of the two types of molecules was studied by comparing different preparation, like evaporating the molecule to the surface at room temperature or direct to the cooled substrate.

O 35.25 Tue 18:15 Poster B1

Scanning Tunneling Microscopy Investigation of CU4Dinit on W(110) — ●DENNIS KLOCZAN¹, SANDRA DIEHL¹, TORSTEN METHFESSEL¹, JULIA KLANKE², EVA RENTSCHLER², and HANS-JOACHIM ELMERS¹ — ¹Institut für Physik, Johannes Gutenberg-Universität Mainz, D-55128 Mainz, Germany — ²Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg-Universität Mainz, D-55099 Mainz, Germany

Organic semiconductors are a class of π -conjugated molecules. Due to their property of charge separation by light induced electron transfer they have various applications in solar cells, sensors or switches.

In order to ensure a good adhesion on surfaces, the π -system of the molecule has to be planar. A promising molecule with an increased number of C-rings is Cu4Dinit (copper-tetraazaporphyrin with eight 4-tertbutylphenyl residues).

Using scanning tunneling microscopy (STM) we have imaged Cu4Dinit molecules on a W(110) surface with submolecular resolution at room-temperature. Scanning tunneling spectroscopy (STS) reveals the energetic position of molecular orbitals relative to the Fermi-level of the substrate.

O 35.26 Tue 18:15 Poster B1

Monitoring the ring closure on the ligand of an Fe-Porphyrin molecule — ●GELAVIZH AHMADI¹, VALENTIN MÜLLER¹, BENJAMIN W. HEINRICH¹, JOSÉ I. PASCUAL^{1,2}, and KATHARINA J. FRANKE¹ — ¹Institut für Experimentalphysik, Freie Universität Berlin, Germany — ²CIC nanoGUNE, 20018 Donostia-San Sebastián, Spain

We used Scanning Tunneling Microscopy (STM) and Spectroscopy (STS) at 4.5K to follow the stepwise transformation of Fe-Octaethylporphyrin (FeOEP) into Fe-Tetrabenzoporphyrin (FeTBP) on Au(111). The annealing to 470 K of submonolayer coverages of FeOEP on Au(111) activates an electrocyclic ring closure of the ethyl groups at the organic ligand. We can identify different intermediate species by STM topography as well as by STS measurements. To double check the proposed reaction scheme, we also produced Fe-TBP by an *in-situ* metalation of free-base TBP on Au(111). This allows for an unambiguous identification of our product.

O 35.27 Tue 18:15 Poster B1

Structural and Electronic Properties of Self-Assembled DCV5T-Me2 Molecules on Au(111): from Sub-Monolayer to Bilayer Coverage — ●ZECHAO YANG¹, MARTINA CORSO^{1,2}, CHRIS LOTZE¹, ELENA MENA-OSTERITZ³, PETER BÄUERLE³, KATHARINA J. FRANKE¹, and JOSE I. PASCUAL^{1,2} — ¹Institut für Experimentalphysik, Freie Universität Berlin, Germany — ²CIC nanoGune, 20018 Donostia-San Sebastián, Spain — ³Institute of Organic Chemistry II and Advanced Materials, University of Ulm, Germany

The functionality of organic electronic devices importantly depends on the structural and electronic properties of the metal-molecule interface.

Here, we investigate the structural and electronic properties of ultrathin films of substituted oligothiophene molecules on a gold surface using low temperature scanning tunneling microscopy and spectroscopy. The chosen molecule, dicyanovinyl-quinque thiophenes (DCV5T-Me2), is used in organic solar cells. DCV5T-Me2 molecules form either molecular chains, stabilized by intercalated Au atoms, or two-dimensional islands depending on the sub-monolayer coverage. The presence of Au atoms in the chains leads to local modification of their electronic structure: the LUMO of molecules in chains have a low energy unoccupied resonance downshifted due to coordination bonds. In fact, molecules at the chain end shows both the unperturbed state, at the free side, and the down shifted state, at the side in contact with Au atoms with no effect on the other side without coordination bonding. This behavior indicates that one can manipulate molecular orbital alignment within individual molecules by coordination bonding meditation.

O 35.28 Tue 18:15 Poster B1

Electrospray deposition of functionalized platform molecules on Au(111) — KRISTOF BUCHMANN¹, •NADINE HAUPTMANN¹, CHRISTIAN HAMANN¹, SANDRA ULRICH², FRANZISKA OTTE², RAINER HERGES², and RICHARD BERNDT¹ — ¹Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel — ²Otto-Diels-Institut für Organische Chemie, Christian-Albrechts-Universität zu Kiel

The electronic coupling to a metal substrate may affect the electronic and geometric structure of molecules. To preserve the intrinsic properties of molecules it is desirable to decouple the functional groups from the substrate. Partial decoupling can be achieved by supporting a molecule by a molecular platform, conceivably via a spacer group. Using low temperature scanning tunneling microscopy we investigate the triazatriangulenium (TATA) and the trioxotriangulenium (TOTA) platform molecule with various functional groups. The preparation of adlayers of these molecules by thermal sublimation is not feasible due to their thermal instability. We therefore use a home-built electrospray ionization setup for depositing the molecules onto Au(111) in ultra-high vacuum. The observed tunneling spectra are in good agreement with calculated spectra of the respective gas-phase molecules. This proves the electronic decoupling of the functional groups from the substrate. Financial support by the Deutsche Forschungsgemeinschaft via the SFB 677 is gratefully acknowledged.

O 35.29 Tue 18:15 Poster B1

Comparative study of periodic and non-periodic approaches: Organic π -systems on coinage metals. — •JAITA BANERJEE and REINHOLD FINK — Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Germany

We present a comparative study of metal-organic interface properties obtained from DFT calculations based on two different approaches: the periodic slab supercell technique and the cluster ansatz. Such interfaces of aromatic organic molecules with metal substrates form one of the important parts of organic optoelectronic devices. While it is well established that plane waves-pseudopotentials-periodic supercell approaches are reasonable methods to study the geometric and electronic structure of such interfaces, the cluster ansatz has not been much studied. We choose two different π -systems on silver and gold surfaces respectively. The strategy has been to obtain the structure and energetics of each system using the periodic supercell approach, then constructing the metallic clusters from the obtained periodic results. After optimizing the metal clusters, the molecule is placed on its surface and the respective adsorption energies and distances are computed. Our results indicate that while small clusters consisting of two metallic layers form unsuitable systems, clusters with 4 layers begin to show trends as obtained from the periodic calculations. The effect of van der Waals dispersion is also included. Our findings encourage possibilities of using the cluster ansatz to study molecule-metal interfaces since often the size of the organic molecule poses computational challenges in performing a full periodic calculation.

O 35.30 Tue 18:15 Poster B1

Site-specific geometric and electronic relaxation of cobalt-phthalocyanine on Cu(111) — •CHRISTOPH BÜRKER¹, ALEXANDER GERLACH¹, STEFFEN DUHM², TAKUYA HOSOKAI³, BLANKA DETLEFS⁴, SATOSHI KERA⁵, NOBUO UENO⁵, and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Universität Tübingen, DE — ²Institute of Functional Nano & Soft Materials, Soochow University, CN — ³Department of Materials Science and Technology, Iwate University, JP — ⁴European Synchrotron Radiation Facility, FR —

⁵Graduate School of Advanced Integration Science, Chiba University, JP

We present X-ray standing wave (XSW) and ultraviolet photoelectron spectroscopy (UPS) data of cobalt-phthalocyanine (CoPc) on Cu(111). The XSW technique yields a slightly distorted geometry of the molecule upon adsorption as the cobalt, carbon and nitrogen atoms show different bonding distances (2.50 Å, 2.55 Å, and 2.60 Å, respectively). The relatively strong, chemisorptive interaction between molecule and substrate is confirmed by angle-resolved UPS measurements, which show the appearance of interface states. Hence, these two techniques show a site-specific geometric and electronic relaxation of CoPc on Cu(111). Finally, we compare our data both with theoretical findings for the same system [1] and with ZnPc on Cu(111) [2].

[1] X. Chen and M. Alouani, *Phys. Rev. B* **82**, 094443 (2010)

[2] H. Yamane et al., *Phys. Rev. Lett.* **105**, 046103 (2010)

O 35.31 Tue 18:15 Poster B1

Influence of Bromine groups on the molecular arrangement and adsorption of CuTPPBr₈ on Au(111) — •LARS SMYKALLA¹, MICHAEL HIETSCHOLD¹, and HEINRICH LANG² — ¹Chemnitz University of Technology, Institute of Physics, D-09107 Chemnitz, Germany — ²Chemnitz University of Technology, Institute of Chemistry, D-09107 Chemnitz, Germany

The bromination of the molecule tetraphenyl-porphyrin leads to a very strong saddle-shape deformation of the macro-cycle and a change of the electronic states. We combine scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS), photoemission spectroscopy (PES) and density functional theory (DFT) to thoroughly investigate the molecular arrangement and electronic structure of copper-2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenylporphyrin (CuTPPBr₈) on the Au(111) surface. After slight annealing of the sample a well ordered adsorbate structure is observed. Thereby, the molecules are found to be rotated by 90° with respect to their neighbours in a checkerboard-like manner. Upon heating above 300°C the molecular arrangement transforms into a stripe-like structure with two different kinds of molecular appearances, which is due to the debromination of the molecules as could be confirmed by PES. Furthermore, we present a comparison of our results obtained from STS, PES and DFT for the electronic structure of CuTPPBr₈ adsorbed on Au(111) and discuss the interaction of the molecules with the substrate.

O 35.32 Tue 18:15 Poster B1

Bistable charge states in the acceptor-donor complex Tetracyanoethylene-Tetrathiafulvalene on Au(111) — •PAUL STOLL¹, JANINA LADENTIN¹, TOBIAS R. UMBACH¹, CHRISTIAN LOTZE¹, ISABEL FERNANDEZ TORRENTE¹, JOSÉ IGNACIO PASCUAL^{1,2}, and KATHARINA J. FRANKE¹ — ¹Institut für Experimentalphysik, Freie Universität Berlin — ²CIC nanoGUNE, Donostia-San Sebastián, Spain

The charge state of a molecule has a crucial influence on its physical and chemical properties. Using scanning tunneling microscopy and spectroscopy we investigate the charge-transfer complex consisting of Tetracyanoethylene (TCNE) and Tetrathiafulvalene (TTF) on a Au(111) surface. The two molecules self-assemble in highly ordered mixed islands. The TCNE molecules are found in two different charge states that are identified by the presence or absence of a Kondo resonance. We observe a current-induced bistability of the two states. The switching yield strongly depends on the bias voltage and varies by orders of magnitude.

O 35.33 Tue 18:15 Poster B1

Simulating Photoelectron Diffraction Measurements of Fe-Porphyrins on Ag(111) — •MICHAEL GREIF¹, TIBOR NAGY², MAKSYM SOLOVIOV², LUCA CASTIGLIONI¹, MARKUS MEUWLY², JÜRGEN OSTERWALDER¹, and MATTHIAS HENGESBERGER¹ — ¹Physik Institut, Universität Zürich, Winterthurerstrasse 190, 8052 Zürich, Schweiz — ²Department of Chemistry, University of Basel Klingelbergstrasse 80, 4056 Basel, Schweiz

Combining DFT- and force field calculation for iron-porphyrins on an Ag(111) surface not only yields parameters for the equilibrium structure of the molecules adsorbed on the surface, but also information about their dynamics. An experimental means enabling one to visualize structural dynamics are photoelectron diffraction measurements. In these experiments photoelectrons emitted from a molecular atom are coherently scattered by their neighboring atoms. Interference ef-

fects thus create a diffraction pattern in the photoelectron signal that is recorded by scanning the half sphere above the sample. From this pattern the structural parameters of the system can be found with a resolution on the sub Angstrom scale. An important analysis tool for those measurements are single scattering cluster (SSC) calculations, which can simulate the experimental outcome. Using Fe-porphyrin as an example we show how time resolved photoelectron diffraction may be used as tool to determine structural dynamics. By combining force-field computations and SSC calculations, it is possible to follow the molecular trajectories while the excited molecule crosses a conical intersection from the excited singlet state to the triplet ground state.

O 35.34 Tue 18:15 Poster B1

Low Temperature Scanning Tunneling Microscopy Study of Co-Phthalocyanine Molecules on Graphene/Ir (111) — ●SAMUEL BOUVRON, PHILIPP ERLER, STEFAN AMBRUS, ELIZABETA CAVAR, and MIKHAIL FONIN — Fachbereich Physik, Universität Konstanz

Because of its influence on the electronic and transport properties of a molecule, the interaction between a molecule and a substrate is of crucial importance for possible applications in molecular electronic devices. Furthermore, the adsorption behavior of molecules on surfaces is decisive in a bottom up approach to build molecular electronics. We have investigated the adsorption of cobalt phthalocyanine (CoPc) molecules on epitaxial graphene on Ir(111) by means of low-temperature scanning tunneling microscopy (STM). The small mismatch between graphene and the Ir(111) surface lattice results in a highly ordered hexagonal moiré superstructure with a periodicity of 2.5 nm, making graphene/Ir(111) an interesting template for molecular self-assembly. Here we present the analysis of the nucleation and the early stage growth of CoPc islands on graphene on Ir(111). We report on a subtle competition between intermolecular interactions and substrate-adsorbate interactions for different coverages of CoPc molecules, varying from a submonolayer to a multilayer. Depending on the coverage, we observed different growth modes. At a monolayer coverage, the CoPc molecules arrange in an oblique close-packed structure, whereas at lower coverage a moiré-supported network consisting of ring-like units of six CoPc molecules is observed.

O 35.35 Tue 18:15 Poster B1

Unraveling the adsorption geometry of a 2D metal-organic framework on Cu(111) — MANFRED MATENA¹, JONAS BJÖRK², KATHRIN MÜLLER³, JORGE LOBO-CHECA⁴, LUTZ H. GADE⁵, THOMAS A. JUNG¹, MATS PERSSON⁶, and ●MEIKE STÖHR³ — ¹University of Basel — ²University of Linköping — ³University of Groningen — ⁴DIPC, San Sebastian — ⁵University of Heidelberg — ⁶University of Liverpool

The interest in studying organic nanostructures on surfaces emerges from their prospective applications in nanoscale electronic or optoelectronic devices, in which the spatially addressable functional units are to be assembled on the molecular level. By making use of molecular recognition processes based on non-covalent interactions, well-ordered 1D and 2D molecular structures can be formed on surfaces. Especially, the understanding of the interplay of the underlying intermolecular and molecule substrate interactions are of great research interest since they are responsible for the structure formation and the resulting electronic properties. We report for the perylene derivative DPDI the formation of a nanoporous metal-organic framework (MOF) on Cu(111) upon annealing at 200°C. Scanning tunneling microscopy, low energy electron diffraction, photoemission spectroscopy and X-ray standing wave measurements as well as DFT calculations were carried out to obtain a thorough understanding of the involved interactions and observed (electronic) phenomena. By comparing these findings to similar metal-organic coordination networks common features and differences can be identified.

O 35.36 Tue 18:15 Poster B1

Temperature depending formation of ultrathin FeO(111) films on Ag(111) — ●SÖREN RICHARD LINDEMANN, DANIEL BRUNS, and JOACHIM WOLLSCHLÄGER — Universität Osnabrück, Fachbereich Physik, Barbarastr. 7, 49076 Osnabrück

Iron oxides are used in various applications in spintronic devices and heterogenous catalysis. Therefore, the preparation and characterisation of thin and ultrathin iron oxide films on different metal substrates stand in the focus of current research. In this study ultrathin iron oxide films were grown on Ag(111) by subsequent deposition of Fe films at room temperature, which is followed by annealing in 10^{-5} mbar

O₂ atmosphere at 150°C for 10 minutes to oxidize the submonolayer films. These films were post-deposition annealed at elevated temperatures in ULTRA HIGH VACUUM (UHV) to increase the order inside the film lattice. Structure, morphology and chemical composition of the films were investigated before and after this temperature treatment by SPOT PROFILE ANALYSIS LOW ENERGY ELECTRON DIFFRACTION (SPA-LEED) and AUGER ELECTRON SPECTROSCOPY (AES). Although the diffraction patterns suggest an increase of order at the surface due to annealing, a segregation of silver was observed via AES for temperatures above 300°C. For an annealing temperature of 400°C coexisting FeO(111) and Ag(111) domains at the surface were found with SPA-LEED.

O 35.37 Tue 18:15 Poster B1

Segregation of Ag due to annealing of ultrathin Fe films on Ag(001) — ●CHRISTIAN OTTE, DANIEL BRUNS, STEFFEN JENTSCH, SÖREN LINDEMANN, and AND JOACHIM WOLLSCHLÄGER — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück

Thin Fe films are promising candidates for application in spintronic devices due to their electric and magnetic properties. In this work, ultrathin Fe films grown at room temperature on Ag(001) were post-deposition annealed in ULTRA HIGH VACUUM (UHV) at 250°C. This was monitored via X-RAY PHOTOELECTRON SPECTROSCOPY (XPS) and AUGER ELECTRON SPECTROSCOPY (AES). The surface structure and morphology was studied before and after annealing in UHV by SCANNING TUNNELING MICROSCOPY (STM) and SPOT PROFILE ANALYSIS LOW ENERGY ELECTRON DIFFRACTION (SPA-LEED). The as-deposited Fe forms column shaped islands. Annealing in UHV at 250°C leads to a strong change in surface structure and morphology accompanied by surface segregation of Ag. While SPA-LEED shows an additional $(\sqrt{2} \times \sqrt{2})R45^\circ$ superstructure after annealing, STM reveals large, flat Ag(001) terraces without any superstructures on them. Strongly three dimensional structures are likely to contain part of the deposited Fe. Nevertheless the XPS results suggest that most of the Fe has to be buried underneath the segregated Ag. This assumption is supported by energetic considerations comparing surface free energies of Fe(001) and Ag(001).

O 35.38 Tue 18:15 Poster B1

Epitaxial growth of Fe on Ag(001) revisited: Film stress measurements as a monitor of interface formation — ●KENIA N. FISCHER^{1,2}, DIRK SANDER¹, ANDRE A. PASA², and JÜRGEN KIRSCHNER¹ — ¹Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — ²LFFS, Universidade Federal de Santa Catarina, Florianópolis, Brazil

The growth of Fe on Ag(001) has created a lot of controversy regarding the growth mode in the first monolayers [1]. Early studies reported layer-by-layer growth up to 3 layers, whereas careful LEED studies [1] and EXAFS studies [2] ruled that out. Instead, surface alloying and a rough surface morphology were proposed for the first layers of Fe. Our measurements of Fe-induced film stress on Ag(001) show a non-monotonic change of stress in the first layers. A surprisingly large tensile stress of +7.3 GPa is observed for the first 0.5 ML Fe deposition, which is followed by a compressive stress of -0.73 GPa from 0.5 to 1.5 ML. Then a tensile stress sets in, which leads to an average film stress of +2 GPa in a 10 ML Fe film. The magnitude of stress and its change of sign come as a surprise. The epitaxial misfit of +0.8 % leads to a calculated misfit stress of +1.7 GPa, in contrast to our observations. The observed stress variations in the monolayer range cannot be ascribed to simple layer-by-layer growth of an epitaxially strained Fe film. Rather, intermixing and surface stress change of the substrate upon film deposition need to be considered [3]. [1] Li et al., Phys. Rev. B 42(1990)9195. [2] Hahlin et al, Phys. Rev. B 73(2006)134423. [3] Mahesh et al., Phys. Rev. B 68(2003)045416.

O 35.39 Tue 18:15 Poster B1

Thickness-dependent growth study of Bi on Au(111) — ●JEANNETTE KEMMER, JENS KÜGEL, PIN-JUI HSU, and MATTHIAS BODE — Institute of Experimental Physics II, University Würzburg, Am Hubland, 97074 Würzburg

We have performed a growth study of ultra-thin Bi films on a Au(111) substrate. Upon Bi growth at room temperature the film morphology was determined with a home-built low-temperature Scanning Tunneling Microscope (STM). Within the thickness range between submonolayer coverage up to 3 atomic layers (AL) topographic images show various surface reconstructions, including the so-called (6×6) -structure at 0.5 AL which has been reported previously [1] and resem-

bles the well-known Si(111)- 7×7 reconstruction. In addition, our data show extended areas with one-dimensional superstructures, which are preliminary assigned to $2\sqrt{3} \times 2\sqrt{3}$ R30°- and a larger $10\sqrt{3} \times 10\sqrt{3}$ R30°- unit cells.

[1] J.H. Jeon *et al.*, Surf. Sci. 603, 145 (2009).

O 35.40 Tue 18:15 Poster B1

Adsorbate-induced segregation: a quantitative first-principles study for C/Pt₂₅Rh₇₅(100) — ●TOBIAS C. KERSCHER¹, WOLFGANG LANDGRAF², DAVID REITH³, RAIMUND PODLOUCKY³, and STEFAN MÜLLER¹ — ¹TU Hamburg-Harburg — ²Universität Erlangen-Nürnberg — ³Universität Wien

For catalytic surfaces, such as Pt-Rh, it is essential to understand the change in the segregation profile due to the presence of adsorbates. Our prior first-principles studies of adsorbate-induced segregation in C/Pt₂₅Rh₇₅(100) have shown that, compared to the clean surface, a small amount of carbon impurities suffices to substantially decrease the Pt concentration in the top layer of the substrate. We corroborated this view at $T = 0$ K by DFT and the cluster expansion (CE).

Now, we have improved the CE to increase its accuracy for the complex interactions between several substrate and adsorbate layers. This enables us to quantitatively predict the T -dependent, layer-by-layer segregation profile of the substrate subject to C-contamination [1]. Our CE code UNCLE [2] uses a bisection of the simulation lattice into separate subsystems—already discussed during the last years—in combination with a new averaging procedure [3]. We discuss the coupling of the substrate and adsorbate layers in the CE, the $T = 0$ K stability diagram, and the T -dependent segregation profile for different C-contaminations. (Supported by DFG.)

[1] T. C. Kerscher *et al.*, Phys. Rev. B **86**, 195420 (2012)

[2] D. Lerch *et al.*, Modelling Simul. Mater. Sci. Eng. **17** (2009), 055003

[3] D. Reith *et al.*, Phys. Rev. B **86**, 020201(R) (2012)

O 35.41 Tue 18:15 Poster B1

Preparation of PtCu core-shell model catalyst electrodes — ●ALBERT K. ENGSTFELD, ANDREAS BENSCH, CHRISTOPH K. JUNG, REGINE WEISS, and R. JÜRGEN BEHM — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

Core shell particles consisting of a metal A rich shell and a bi- or multialloy core show a different catalytic activity compared to pure metal particles. An interesting example are Pt enclosed alloy particles containing Cu, Co and Pt, which have a much better activity towards the electrocatalytic oxygen reduction than pure Pt.

We will describe on the one hand the preparation of PtCu core on Ru(0001) and on the other hand the preparation of a Pt shell on these alloy surfaces, which reflects a model catalysts for core shell particles. The surfaces were investigated by scanning tunneling microscopy under ultra high vacuum conditions. The formation of PtCu monolayer alloys on Ru(0001), is found to be kinetically hindered, due to the strong binding of Pt to the Ru substrate. This limitation can be overcome, however, by careful selection of the experimental conditions (annealing time, deposition sequence ...).

Depositing Pt on Cu sub-monolayer films on Ru(0001), we find a strong tendency for a place exchange between Pt and the Cu upon room temperature deposition of Pt. This allows the fabrication of 2D PtCu model cores with at least 20 % Pt, which can be used as substrate for subsequent Pt deposition. We will discuss the homogeneity of the system after both preparation steps in view of potential use as model catalyst for further electrochemical/-catalytic investigations.

O 35.42 Tue 18:15 Poster B1

Improving the Quality of SiC Surfaces by Precise Definition of H₂-Etching Parameters — ●TOBIAS DENIG and ULRICH STARKE — Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart Germany

SiC is a material of great technical interest because it offers an attractive combination of chemical robustness and excellent thermal and electrical properties. However, in order to make use of these characteristics one needs a well-behaved, passivated surface. This has led to the prevalence of a H₂ etching step in SiC processing, as it simultaneously removes surface damage (e.g., polishing scratches), reduces the defect density, and leaves behind an "atomically-flat," H-terminated terraced surface. In the ideal limit, such steps should be one SiC bilayer (0,25 nm) thick. A common occurrence in such etching is for two or more steps to bunch, producing steps of one or several unit cell heights. The end result is a mixture of step heights, producing a sub-optimal sur-

face for further work. However, one unit cell height should be a natural step size due to the particular stacking order in SiC polytypes. Various etch parameters (gas flowrate, T, and p) can influence the amount of step bunching. We have performed parameterization studies aimed at limiting this process such that only steps of (single) unit cell height emerge. All samples used in these studies underwent a modified RCA clean prior to being etched. The results of varying the processing conditions as well as using Ar or H₂ as the cooling gas were examined using XPS, LEED, and AFM.

O 35.43 Tue 18:15 Poster B1

UV laser supported oxide removal from Si seed layers for thin-film Si solar cells — ●ROMAN BANSSEN, ROBERT HEIMBURGER, FRANZISKA SCHÜTTE, THOMAS TEUBNER, and TORSTEN BOECK — Leibniz Institute for Crystal Growth, 12489 Berlin, Germany

To achieve low temperature deposition of crystalline Si on glass for photovoltaic applications, a two-step process has been developed at Leibniz Institute for Crystal Growth. In the first step, amorphous Si films are crystallized at temperatures around 300°C by means of metal-induced crystallization. In the second step, they are used as templates for further Si deposition by steady-state solution growth. Between the two steps, during handling in high vacuum conditions, the templates form a thin layer of Si oxide. This is a major obstacle for the second step, as it hinders epitaxial growth. Conventionally, oxide desorption from Si is achieved by an annealing step above 800°C, a method which cannot be applied to glass substrates. We discuss several approaches involving in situ treatment of oxidized surfaces with UV laser irradiation in highly pure H₂ atmosphere. One approach is the removal of Si oxide by ablation. Another approach involves the lowering of the oxide desorption temperature during simultaneous UV laser irradiation below the ablation threshold.

O 35.44 Tue 18:15 Poster B1

And Now For Something Completely Different: Au Induced Faceting of Si(0 8 15) — ●CHRISTIAN WITT, MICHAEL HORN-VON HOEGEN, and FRANK-J. MEYER ZU HERINGDORF — Faculty for Physics and Center for Nanointegration CENIDE, University Duisburg-Essen Lotharstrasse 1, 47057 Duisburg

Au and Ag are known to induce faceting on many vicinal Si surfaces. Until now, studies have focused on the faceting kinetics in one dimensional systems, where a distinct step orientation of the vicinal substrate was transformed into a faceted surface with straight step edges and a zigzag cross section. Here, we show similar experiments on a surface that exhibits two faceting directions during deposition of Au at elevated temperatures. Si(0 8 15) is a vicinal Si(0 1 2) surface with a miscut of 1.51° towards (0 2 -1). We observed the faceting kinetics of this surface by low energy electron microscopy and low energy electron diffraction. During Au adsorption the surface initially forms one dimensional facets. This is followed by a second faceting transformation to form an Escher-like "checkered" pattern. After completed faceting we find three different types of facets with typical facet sizes of few hundred nm. The facets angles relative to the surface normal were determined by in-situ reciprocal space mapping and independently confirmed by ex-situ AFM measurements. The Au induced faceting transformation of the (0 8 15) face of Si produces two well-ordered facets while leaving the third facet a stepped area with characteristic convex and concave areas. [1] Phys. Rev. Lett. **86** (2001) 5088; [2] J. Phys.: Cond. Matter **18** (2006) 1; [3] Surf. Rev. & Lett. **5** (1998) 1164

O 35.45 Tue 18:15 Poster B1

Bi₂Se₃ films on Si(111): Growth optimization and in-situ SPA-LEED measurements — ●MICHAEL VYSHNEPOLSKY, CLAUDIUS KLEIN, ANJA HANISCH-BLICHARSKI, and MICHAEL HORN-VON HOEGEN — Fakultät für Physik und Center for Nanointegration CENIDE, Universität Duisburg-Essen, Lotharstr. 1, D-47057 Duisburg, Germany

Employing high resolution spot profile analysis low energy electron diffraction (SPA-LEED), atomic force microscopy (AFM) and x-ray diffraction (XRD) we studied the growth of Bi₂Se₃ on Si(111). The films were prepared by thermal co-deposition of Se and Bi with a flux ratio of 10:1 at temperatures between 200 and 250 °C. The strain relaxation during the growth of the first quintuple layers was measured in-situ during deposition by tracking the (01)-spot position with SPA-LEED. At a thickness of 6 nm the Bi₂Se₃ film exhibits a lateral lattice parameter of 4.02 Å. The decrease of the spot width of the (00)-spot reflects that the crystal quality improves by post-growth annealing up to temperatures of 350 °C. This is also confirmed in the AFM mea-

measurements, where remaining Se wires disappear with higher annealing temperature. XRD measurements of Bi₂Se₃ films with thickness of 70-80 nm verifies the high film quality and also confirms the vertical lattice parameter of 28.63 Å.

O 35.46 Tue 18:15 Poster B1

Cd-content analysis of capped and uncapped CdSe quantum dots on ZnSe by Raman spectroscopy — ●UTZ BASS, CONSTANTIN WEILER, JEAN GEURTS, ALEX FREY, SUDDHASATTA MAHA-PATRA, and KARL BRUNNER — Universität Würzburg, Physikalisches Institut, Am Hubland, 97074 Würzburg

Quantum Dots (QD) offer the intriguing opportunity to study fundamental low-dimensional physics and are simultaneously employed in optoelectronic applications. Wide band gap II-VI semiconductor QD are promising candidates to extend the applications to the visible energy regime. The self-assembly of the CdSe/ZnSe QD system is driven by the large lattice mismatch. The strain relaxation mechanism consists of dot formation together with intermixing of Cd and Zn. In this study we focus on the Cd-content analysis of CdSe QDs embedded in or on top of ZnSe. CdSe QD sample series with different nominal CdSe thickness values from various MBE growth procedures are investigated by Raman spectroscopy (RS), accompanied by photoluminescence (PL). Also for uncapped QDs with quenched PL, RS enables the Cd-concentration analysis and thus allows the in-situ study of QDs. The comparison of the capped and uncapped QD results shows that the overgrowth of the QDs with the capping ZnSe layer induces a considerable additional intermixing. This susceptibility for intermixing during overgrowth explains, why on overgrown QDs the observed Cd-content essentially only depends on the nominal CdSe-thickness, although AFM-studies of uncapped QDs showed clear morphology differences for the different growth procedures.

O 35.47 Tue 18:15 Poster B1

Preparation of GaP/Si(111) quasi-substrates for III-V nanowire solar cells — ●WEIHONG ZHAO^{1,2}, AGNIESZKA PASZUK^{1,2}, MATTHIAS STEIDL^{1,2}, SEBASTIAN BRÜCKNER^{1,2}, ANJA DOBRICH², JOHANNES LUCZAK², PETER KLEINSCHMIDT^{1,3}, HENNING DÖSCHER^{1,2}, and THOMAS HANNAPPEL^{1,2,3} — ¹Technische Universität Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, D-98684 Ilmenau — ²Helmholtz-Zentrum Berlin, Institut für Solare Brennstoffe und Energiespeichermaterialien, D14109 Berlin — ³CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, D99099 Erfurt

Meeting the demands of high-quality-low-cost photovoltaics, III-V nanowires grown on Si(111) substrates present a promising new solar cell concept. GaP buffer layer can be grown almost lattice matched on Si(111) substrates. Successful nanowire growth requires atomically smooth/flat GaP(111)B surfaces. Therefore a suitable Si(111) surface preparation is crucial. We used a metal organic vapor phase epitaxy (MOVPE) reactor to prepare GaP/Si (111) quasi-substrates. A contamination-free transfer system enables us to assess the MOVPE prepared surfaces with numerous UHV based surface science tools. A dedicated wet-chemical pretreatment is crucial to obtain atomically flat Si(111) surfaces, and high temperature annealing removed all contamination. It is shown that our preparation in a hydrogen ambient results in a monohydride terminated (1x1)-reconstructed Si(111) surface. Since LEED can identify the different GaP(111)A and B surfaces we found that the Si surface termination influences the polarity of GaP films grown on Si(111) substrates.

O 35.48 Tue 18:15 Poster B1

Characterization of Carbon-Nitrogen-codoped TiO₂ with XPS - influence of annealing temperature — ●JULIAN FISCHER, CHRISTIAN GEBAUER, THOMAS DIEMANT, JOACHIM BANSMANN, and R. JÜRGEN BEHM — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

TiO₂ has been used for photo-electrochemical applications, e.g., in water splitting. However, the large band gap of the material limits its efficiency in the optical regime. Doping of TiO₂ with carbon and nitrogen is expected to reduce the band gap of the material by inducing defect states (acceptor and donor states) in the band gap and increase the electrical conductivity [1].

The samples used in this study were prepared via a sol-gel process [2] using urea (nitrogen donor source) and tetrabutyl titanate as a precursor. The materials were finally calcined in a temperature regime ranging from 175°C to 400°C (3h) and afterwards measured by XPS to characterize their chemical composition; special attention was paid to the inclusion of C and N species into the TiO₂ lattice. The doping

of the material can be traced back to two different species: (i) carbon doping is attributed to a C-O species and (ii) nitrogen doping to a Ti-O-N species.

[1] D. Chen et. al., Ind. Eng. Chem. Res. 2007, 46, 2741.

[2] H. Sun et. al., Ind. Eng. Chem. Res. 2006, 45, 4971.

O 35.49 Tue 18:15 Poster B1

XPS analysis of Carbon-Nitrogen codoped TiO₂ - influence of pH and codoped Boron — ●FABIAN ARGAST¹, CHRISTIAN GEBAUER¹, THOMAS DIEMANT¹, JOACHIM BANSMANN¹, MAXIMILIAN WASSNER², NICOLA HÜSING², and R. JÜRGEN BEHM¹ — ¹Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm — ²Paris-Lodron-University Salzburg, A-5020 Salzburg

TiO₂ has been used for photo-electrochemical applications, e.g., in water splitting. However, undesired recombination of photoexcited carriers and a high band gap of TiO₂ limit its practical application and efficiency. Doping of TiO₂ with boron, carbon and nitrogen is expected to reduce the band gap of the material by inducing defect states in the band gap and increase the photocatalytic activity for light absorption into the visible region [1].

The samples were prepared via a sol-gel process using tetrabutyl titanate as a precursor. In a first approach, tetrabutylammonium hydroxide or tetrabutylammonium nitrate were used as donor sources for C and N. Furthermore, the possible influence of different pH environments were investigated. Next, urea (N and C donor) as well as boric acid were used as co-dopands with the same precursor. The samples were calcined at a temperature regime ranging from 175°C to 400°C (3h) and afterwards measured by XPS to characterize their chemical composition, especially the inclusion of B, C and N species into the TiO₂ lattice.

[1] D. Chen et. al., Ind. Eng. Chem. Res. 2007, 46, 2741.

O 35.50 Tue 18:15 Poster B1

Density functional calculations for SrTiO₃(001) and Fe/SrTiO₃ — ●BRAHIM BELHADJI and ECKHARD PEHLKE — Institut für Theoretische Physik und Astrophysik, Universität Kiel

Magnetolectric coupling at, e.g., the interface of magnetic *d*-metals and BaTiO₃ [1] has attracted a lot of interest also in view of applications, like sensors. The magnetization of thin Fe-films on BaTiO₃ or SrTiO₃ has been shown to depend even qualitatively on the number of Fe-layers [2]. The comparison of *d*-metals on BaTiO₃ and SrTiO₃ will open up the opportunity to compare different contributions to the magnetolectric coupling mechanism at such interfaces. As a first step we have studied the clean (001) surface of SrTiO₃. The electronic structure is calculated using VASP code. We focus on the experimentally observed $\sqrt{5} \times \sqrt{5}$ reconstruction and compare the Sr-atom model proposed in [3] and the surface atomic geometry proposed in [4] (and two simple (1 × 1) surface terminations as a reference). Scanning tunneling microscopy images are simulated within the Tersoff-Hamann model for both surfaces and various voltages. Furthermore we report first calculations for a single up to few monolayers of Fe on the (001) surface of SrTiO₃ and compare to previous work [2]. This lays the basis for a future study of magnetolectric coupling mechanisms in case of thin *d*-metal films on these titanates.

[1] Chun-Gang Duan *et al.* PRL **97** (047201)(2006).

[2] M. Fechner *et al.* PRB **78**, 212406 (2008).

[3] T. Kubo *et al.* PRL **86**, 1801 (2001).

[4] D. M. Kienzle *et al.* PRL **106**, 176102 (2011).

O 35.51 Tue 18:15 Poster B1

Carbon monoxide on ZnO(10-10) Surface: An Infrared Reflection Absorption Spectroscopy study — ●MARIA BUCHHOLZ, ALEXEI NEFEDOV, and CHRISTOF WÖLL — Institute of Functional Interfaces, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

One of the most important oxides is zinc oxide (ZnO) according to its semiconducting and optical properties. Numerous IR investigations of oxide powders have been reported[1], but however, an unambiguous assignment of the features in the complex powder IR spectra recorded for molecules bound to the oxide powder particle is only possible on the basis of data recorded for well-defined reference systems, e.g. surfaces of single crystals.

The different surfaces of ZnO single crystals are used for investigations, both polar Zn- or O-terminated ZnO {0001} and mixed-terminated ZnO(10-10) surface, which is the dominating surface for ZnO powder particles and energetically most favorable. In this study we investigated adsorption of carbon monoxide on ZnO(10-10) surface,

which is model system for many reactions in catalysis. Our results give us the information about the orientation of CO on the surface, which is very important for the reaction mechanism[2].

M. Buchholz gratefully acknowledges the financial support from the Helmholtz Research School "Energy-Related Catalysis".

[1]H. Noei, C. Wöll, M. Muhler, Y. M. Wang, *Appl Catal a-Gen* 2011, 391, 31-35. [2]M. C. Xu, H. Noei, K. Fink, M. Muhler, Y. M. Wang, C. Wöll, *Angew Chem Int Edit* 2012, 51, 4731-4734.

O 35.52 Tue 18:15 Poster B1

The role of the anchoring ligand BINA to the binding of the N3 dye on TiO2 anatase (101) — ●C. DETTE¹, C. S. KLEY¹, S. JUNG¹, G. RINKE¹, J. CECHAL¹, S. RAUSCHENBACH¹, C. PATRICK³, F. GIUSTINO³, S. STEPANOW¹, and K. KERN^{1,2} — ¹Max Planck Institute for Solid State Research, Stuttgart, Germany — ²École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; — ³University of Oxford, Department of Materials, Oxford, United Kingdom

The rapid increase of power consumption demands new sustainable and low-cost energy sources like dye-sensitized solar cells (DSSCs) in which a layer of dyes is adsorbed on a mesoporous TiO₂ film. Even though a lot of work has been dedicated to DSSCs, the adsorption and electronic properties of a single dye molecule and the TiO₂ surface remain unclear. Since the adsorption of the dye molecules is determined by the anchoring ligand group, the adsorption geometry and electronic properties of these ligand groups are of crucial importance. Here, we study the properties of N3 dye anchoring ligand BINA (bi-isonicotinic acid) on the TiO₂ anatase (101) surface by means of scanning tunneling microscopy and spectroscopy methods in ultra high vacuum. We present different adsorption geometries consistent with first-principle density functional theory based calculations and the corresponding electronic properties. In addition, we discuss the influence of the different binding geometries of the ligand BINA to the N3 dye molecule which shows variable adsorption geometries in contrast to theoretical predictions suggesting only one specific thermodynamically stable N3 adsorption configuration.

O 35.53 Tue 18:15 Poster B1

Optical spectroscopy of PTCDA molecules on a KCl (100) surface in the limit of low coverages: site selection and diffusion — ALEXANDER PAULHEIM, MATHIAS MÜLLER, CHRISTIAN MARQUARDT, and ●MORITZ SOKOLOWSKI — Institute for Physical Chemistry, University of Bonn, Wegelerstraße 12, 53115 Bonn, Germany

We use optical spectroscopy as a tool to study aggregation and structural site transitions of molecules in the limit of isolated entities on a surface. For this purpose we performed optical spectroscopy on the model molecule perylene-3,4,9,10-tetracarboxyl acid dianhydride (PTCDA) for very low coverages (below 1% of a monolayer) on thin (100) oriented KCl films, epitaxially grown on a Ag(100) surface. The structural and optical properties were investigated by SPA-LEED and by fluorescence and FL excitation spectroscopy, respectively. Two different states of PTCDA molecules can be distinguished: an initial state which is observed directly after deposition onto the cold (20 K) sample, and a final state which is found after thermal annealing or intensive optical excitation. The spectrum of the final state is blue-shifted with respect to that of the initial state by 130 cm⁻¹ and exhibits a smaller FWHM due to reduced inhomogeneous site broadening. We explain this by a thermally or optically induced diffusion of the PTCDA molecules from initial terrace sites to energetically favored step edge sites as seen by Karacuban et al. [1] with STM. Polarization dependent spectroscopy reveals the same azimuthal orientation of the molecules on both adsorption sites.

[1] H. Karacuban et al., *Nanotechnology* 2011, 22, 295305.

O 35.54 Tue 18:15 Poster B1

DFT+D Van-der-Waals C₆ coefficients for ionic crystals — ●STEFFEN SEILER and BERND MEYER — Interdisziplinäres Zentrum für Molekulare Materialien und Computer-Chemie-Centrum, Universität Erlangen-Nürnberg

Previous studies have shown that Grimme's dispersion correction to DFT [1] leads to an overestimation of the binding energy of molecules on ionic surfaces. The reason is that in the Grimme D2 scheme no distinction is made between Van-der-Waals C₆ coefficients for neutral and charged species of the same element, although they clearly possess different polarizabilities. We propose a simple scheme for adjusting the C₆ coefficients of the cations in ionic crystals which is based on the static polarizability. Thin films are exposed to an external electric field and the film polarizability is determined by linear regression of

the induced dipole moment. The method has been applied to magnesium oxide and hydroxide and we obtained very similar C₆ values for the Mg cations as recently proposed by the Grimme group based on TDDFT calculations [2]. To demonstrate the impact of the modified Van-der-Waals correction, calculated binding curves for the interaction of different small molecules (CH₄, H₂O and SiMe(OH)₃) with magnesium oxide and hydroxide model clusters will be shown and the results will be compared to MP2 benchmark calculations.

[1] S. Grimme, *J. Comp. Chem.* **27**, 1787 (2006).

[2] S. Ehrlich et al., *Chem. Phys. Chem.* **12**, 3414 (2011).

O 35.55 Tue 18:15 Poster B1

Self-assembly of cobalt phthalocyanine molecules on ultrathin CoO(111) films on Ir(100) — ●TOBIAS SCHMITT, PASCAL FERSTL, LUTZ HAMMER, and M. ALEXANDER SCHNEIDER — LS f. Festkörperphysik, Uni. Erlangen, Germany

We investigated the adsorption of cobalt phthalocyanine (CoPc) molecules on a bilayer of CoO(111) on Ir(100)[1] by low-temperature scanning tunneling microscopy in UHV. CoPc molecules prefer to lie flat on that surface with the Co-Ion centered above oxygen atoms. The rotational orientation of the molecules is determined by the interaction of N-atoms of the macrocycle with the underlying Co-atoms and between π -electrons and the oxygen atoms of the substrate. This leads to adsorption geometries which are dominated by molecule-substrate interaction similar to those found on TiO₂[2]. At higher coverage (0,7ML) one-dimensional chains with a core-core distance of 1.3 nm are formed while the molecular adsorption site and orientation stay the same. This points to a short-ranged intermolecular interaction, that governs the self-assembly. Only at a coverage of \approx 1 ML the CoPcs rotate to decrease the C-N..H hydrogen bond length. We discuss these findings also in the light of the dense structures formed on metal surfaces [3].

[1] C. Tröppner, et al., *Phys. Rev. B*, in press

[2] Y. Wang, et al., *J. Phys. Chem. B* 2006, 110, 17960

[3] Y. Wang, et al., *J. Am. Chem. Soc.* 2009, 131, 10400

O 35.56 Tue 18:15 Poster B1

Interaction of N₂ with the NaCl(100) surface: a combined LEED and DFT-D study — ●JOCHEN VOGT — Chemisches Institut der Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

The NaCl(100) surface is one of the laboratory model systems to study the elementary processes of the heterogeneous chemistry of the earth's atmosphere [1], whose main constituent is N₂. Detailed experimental results on the adsorption geometry and the binding energy of the system N₂/NaCl(100) have been lacking so far. Low-energy electron diffraction experiments, using a microchannelplate-LEED optics and nanoampere beam currents, reveal a (1×1) symmetry of the first layer N₂ physisorbed on NaCl(100) at temperatures between 20 K and 45 K [2]. This contribution compares the results of a quantitative LEED structure analysis with the minimum energy structure predicted by dispersion-corrected DFT calculations. The experimental adsorption energy including lateral interactions, as determined experimentally within a Fowler-Guggenheim kinetic model of adsorption, are compared to the corresponding predictions from DFT-D. Differences between experiment and theory are discussed, along with possible sources of error.

[1] J. C. Hemminger, *Int. Rev. Phys. Chem.* 18 (1999), 387

[2] J. Vogt, *J. Chem. Phys.* 137 (2012), 174705

O 35.57 Tue 18:15 Poster B1

Adsorption of small molecules on ZnO surfaces — ●JAKUB GOCLON and BERND MEYER — Interdisziplinäres Zentrum für Molekulare Materialien und Computer-Chemie-Centrum, Universität Erlangen-Nürnberg

Despite much experimental effort the co-adsorption of H₂ and CO on ZnO surfaces, which is of considerable interest in the context of methanol synthesis from syngas, is not well understood. We performed DFT calculations on CO interaction with clean and partially hydrogenated flat ZnO(10 $\bar{1}$ 0) as well as stepped (10 $\bar{1}$ 1) and (20 $\bar{2}$ 1) surfaces, including both Zn and O terminations. For the thermodynamically most stable configurations we find a very good agreement for the characteristic Zn-H and O-H vibrational frequencies with the experimental IR signatures.

The majority of catalysts are deactivated even by small amounts of sulfur-containing molecules that are present as impurities in the feed gas. Under reaction conditions those compounds are hydrogenated

to form H₂S, for which ZnO is a very efficient low-temperature adsorbent [1]. In the second part of this work, we examined different surface forms of H₂S on the ZnO(10 $\bar{1}$ 0) surface and determined the most stable configurations as function of the H₂S chemical potential [2]. In addition, results on sulfur incorporation into the ZnO surface will be shown.

[1] J.M. Davidson, C.H. Lawrie, K. Sohail, *Ind. Eng. Chem. Res.* **34**, 2981 (1995).

[2] J. Gocon, B. Meyer, submitted to PCCP.

O 35.58 Tue 18:15 Poster B1

Interaction of N₂O with TiO₂ and ZnO Surfaces Studied by IR Spectroscopy — ●MAX KAUER¹, HESHMAT NOEI², MARTIN MUHLER², KARINA MORGENSTERN¹, and YUEMIN WANG^{1,2} — ¹Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, D-44780 Bochum — ²Lehrstuhl für Technische Chemie, Ruhr-Universität Bochum, D-44780 Bochum

Metal oxides have recently attracted enormous attention because of their important applications in a variety of fields such as catalysis, chemical sensors, solar cells, and electronic devices. We investigated the adsorption of N₂O on rutile TiO₂(110) and ZnO(10-10) single crystal surfaces by UHV-FTIR spectroscopy. The high-quality IR data demonstrates that exposing both, TiO₂ and ZnO to N₂O at 120 K leads to molecular adsorption in a linear configuration. However, the binding energy of N₂O on ZnO(10-10) is much higher than that on TiO₂(110). It was found that N₂O is bound to surface Ti⁴⁺ ions on TiO₂(110) via its O-end, while it prefers to adsorb via its N-end at surface Zn²⁺ ions on ZnO(10-10). Our results reveal that the N₂O adsorption on oxide surfaces is structure-sensitive. The experimental data will be further discussed based on theoretical calculations.

O 35.59 Tue 18:15 Poster B1

Proton distribution and transfer at the titanate/water solid-liquid interface — ●CHRISTINA EBENSPEGER, CHRISTOF JÄGER, and BERND MEYER — Interdisziplinäres Zentrum für Molekulare Materialien und Computer-Chemie-Centrum, Universität Erlangen-Nürnberg

Layered sodium titanates show a rich structural behavior in aqueous environments. Sodium ions dissolve and the surfaces become protonated. In acid solution single titanate layers can detach and nanoscrolls are formed. To obtain a more detailed understanding of the surface protonation we performed DFT calculations and Car-Parinello molecular dynamics simulations for sodium titanate surfaces in contact with vacuum, a monolayer of water molecules and a liquid water reservoir. We find that the energetical hierarchy of preferred protonation sites and the proton distribution depend on the environment and change from vacuum to thin water films and the solid-liquid interface. A full explicit treatment of the liquid surrounding is thus mandatory for obtaining realistic surface structures. In the CPMD simulations we observe water-mediated transfers of surface protons between different adsorption sites. In rare cases spontaneous de-protonation events of the surface occur, which may explain the negative surface charge observed in experiments.

O 35.60 Tue 18:15 Poster B1

Investigation of the MgO adsorbate and the MgO/Fe on GaAs(001) surface by means of XPS and XPD — ●DOMINIQUE HANDSCHAK^{1,2}, TOBIAS LÜHR^{1,2}, FRANK SCHÖNBOHM^{1,2}, CHRISTOPH KEUTNER^{1,2}, ULF BERGES^{1,2}, and CARSTEN WESTPHAL^{1,2} — ¹Experimentelle Physik 1 - Technische Universität Dortmund, Otto-Hahn-Str. 4, D-44221 Dortmund, Germany — ²DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44221 Dortmund, Germany

We report on a combined high-resolution photoemission (XPS) and photoelectron diffraction (XPD) investigation of magnesium oxide on Fe. Magnesium oxide is an applicable insulator in magnetic tunnel junctions (MTJ) based on the tunnel magnetoresistance (TMR)[1]. TMR-components are also of interest in the research of magnetoresistive random access memories (MRAM) [2,3,4]. In this study we report on the crystalline properties of the MgO adsorbate and the MgO/Fe interface. The results of the diffraction patterns revealed an interface with oxidized iron layers and partially shifted magnesium layers in a halite structure.

[1] M. Julliere, *Physics Letters A* 54, 225 (1975) [2] M. Xue, et al., *Vacuum* 85 (2010) [3] S. Parkin et al., *Nature Materials* 3 (2004) [4] S. Tehrani et al., *Proceedings of the IEEE* 91, 703 (2003) [5] D. Handschak et al., *Phys. Rev. B* submitted (2012)

O 35.61 Tue 18:15 Poster B1

Thermal stability of thin HfO₂ films and structure determination of HfSi₂ islands on Si(110) surfaces. — ●FRANK SCHÖNBOHM^{1,2}, TOBIAS LÜHR¹, DOMINIQUE HANDSHAK¹, LOTHAR BROSDA¹, ULF BERGES^{1,2}, and CARSTEN WESTPHAL^{1,2} — ¹Fakultät Physik - Technische Universität Dortmund, Otto-Hahn-Str. 4, D 44221 Dortmund, Germany — ²DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D 44227 Dortmund, Germany

Thin SiO₂ gate dielectrics in MOSFETs lose their efficiency because of an increasing leakage current when their thickness is reduced below 2 nm. A possible way omitting this problem is substituting the SiO₂ gate dielectric by another material with a higher dielectric constant. Perspective replacement candidates among the so called *high-k* materials are the oxides of hafnium and zirconium. However, their thermal stability at elevated temperatures is important during the production process. Due to the recent interest in the Si(110) surface orientation we studied thin HfO₂ films on Si(110). Photoelectron spectra of Si 2p, Hf 4f, and O 2s signal as a function of annealing temperature were recorded in order to investigate the thermal stability of the system. The thin HfO₂ films are stable up to 730°C and form HfSi₂ under further annealing at 770°C. Further investigations showed that HfSi₂ is arranged in islands at the surface. The HfSi₂ islands were investigated by means of photoelectron diffraction (XPD) in order to examine their structure. We present the XPD diffraction pattern and the structure model of the HfSi₂ islands which was obtained by computer simulations.

O 35.62 Tue 18:15 Poster B1

Magnetic properties of ultrathin iron oxide films on MgO(001), grown in oxygen atmosphere — ●NICO PATHÉ¹, TOBIAS SCHEMME¹, TIMO KUSCHEL², and JOACHIM WOLLSCHLÄGER¹ — ¹Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück — ²Fakultät für Physik, Universität Bielefeld, Universitätsstrasse 25, 33615 Bielefeld

Due to its characteristics in GIANT MAGNETO RESISTANCE (GMR), iron oxides can be used in magnetoresistive memory devices. In this work, ultrathin iron oxide films were reactively grown on MgO(001) at 250°C. Therefore, the oxygen partial pressure was increased from 5 · 10⁻⁷ mbar to 5 · 10⁻⁴ mbar. Since this has a strong influence on the stoichiometry, the films were characterized by X-RAY PHOTOELECTRON SPECTROSCOPY (XPS). The surface structures were studied by LOW ENERGY ELECTRON DIFFRACTION (LEED) and the magnetic properties of the films were investigated via MAGNETO-OPTIC KERR EFFECT (MOKE). The XPS data shows that there's still elemental Fe at the surface after preparation in 5 · 10⁻⁷ mbar O₂. For oxygen partial pressures of 5 · 10⁻⁶ mbar and above only Fe²⁺ and Fe³⁺ ions can be found on the surface. Just between 5 · 10⁻⁶ mbar and 5 · 10⁻⁵ mbar Fe₃O₄ is formed at the surface. This is confirmed by LEED measurements, which show the expected ($\sqrt{2} \times \sqrt{2}$)R45° superstructure for these films. MOKE reveals, that the films grown at an oxygen partial pressure of 5 · 10⁻⁷ mbar and 5 · 10⁻⁵ mbar have a fourfold magnetic anisotropy. The easy axes are aligned in Fe₃O₄ [110] direction.

O 35.63 Tue 18:15 Poster B1

Epitaxial growth of NaCl on thin KCl(100) films on Ag(100) studied by SPA-LEED — ●CHRISTIAN MARQUARDT, ALEXANDER PAULHEIM, and MORITZ SOKOLOWSKI — Institute for Physical and Theoretical Chemistry, University of Bonn, Wegelerstraße 12, 53115 Bonn, Germany

Heteroepitaxy of insulators and ionic materials is of basic interest for understanding the interactions at the respective interfaces. So far the heteroepitaxy of alkali halides has been studied by various groups using single crystals and RHEED [1,2]. In the present work, we studied the epitaxy of NaCl on KCl by SPA-LEED. In order to avoid charging effects in the electron diffraction, we used thin films of KCl(100) epitaxially grown on a Ag(100) surface. For different growth temperatures we observed two different growth modes: At 300 K, we get highly disordered, but closed layers of NaCl. We observe a coherent transition between the lattices of KCl and NaCl and a relaxation of the NaCl lattice constant after few monolayers. At 500 K, we observe the formation of ordered NaCl islands with uncovered areas of the KCl and Ag surfaces in between. The quality of the NaCl films can also be characterized by optical spectra of isolated PTCDA molecules deposited on these. On NaCl structures grown at 500 K, the spectra are broadened, which we explain by a large diversity of adsorption sites related to structural defects of the NaCl films. Supported by SFB 624.

- [1] M. H. Yang, C. P. Flynn, Phys.Rev.Lett 62 (1989) 2476.
 [2] K. Saiki, Appl. Surf. Sci. 113 (1997) 9.

O 35.64 Tue 18:15 Poster B1

Investigation of the surface morphology of ultrathin hex-Pr₂O₃ on Si(111) — ●JARI RODEWALD¹, HENRIK WILKENS¹, SEBASTIAN GEVERS¹, MARVIN ZOELLNER², THOMAS SCHROEDER², and JOACHIM WOLLSCHLÄGER¹ — ¹Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49069 Osnabrück — ²IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

The surface morphology and chemical composition of hex-Pr₂O₃ grown by molecular beam epitaxy (MBE) on Si(111) is studied by SPOT PROFILE ANALYSIS LOW ENERGY ELECTRON DIFFRACTION (SPA-LEED) and AUGER ELECTRON SPECTROSCOPY (AES), respectively.

The samples were capped with an amorphous germanium layer, since hex-Pr₂O₃ is instable under ambient conditions. In a first step the removal of the capping layer is investigated. Perfect thermal removal was achieved for annealing at 500°C sample temperature in 10⁻⁶mbar oxygen atmosphere. X-RAY DIFFRACTION (XRD) reveals that the hexagonal structure of the entire praseodymia film is preserved during the removal process.

The Spot profile analysis resulted in a surface model consisting of single atomic step heights of the complete hex-Pr₂O₃ unit cell. Also, the grain size and terrace width are determined.

O 35.65 Tue 18:15 Poster B1

CoO(111) bilayer on Ir(100) revisited: An incommensurate Moiré overlayer with strong local binding — FLORIAN MITTENDORFER¹, ●JOSEF REDINGER¹, RAIMUND PODLOUCKY², MICHAEL WEINERT³, CARSTEN TRÖPPNER⁴, TOBIAS SCHMITT⁴, MARTINA REUSCHL⁴, LUTZ HAMMER⁴, and M. ALEXANDER SCHNEIDER⁴ — ¹Applied Physics, TU Vienna, Austria — ²Physical Chemistry, Vienna University, Austria — ³Dept. of Physics, University of Wisconsin-Milwaukee, USA — ⁴Solid State Physics, University Erlangen-Nuremberg, Germany

Although a CoO(111) bilayer on Ir(100) is a relaxed overlayer with a very strong structural response to the lateral modulation of the interface [1], it turns out to form an one-dimensional incommensurate Moiré structure [2] as revealed by large-scale, low-temperature STM topographies. Despite the non-commensurability of the film, the binding to the substrate is site specific, where the strong lateral modulation of the structural elements within the oxide film can be understood as a combination of the lateral variation in the Co-Ir binding potential and additional O-Ir binding. This is in agreement with recent DFT investigations of the complex magnetism in a CoO(111) bilayer on Ir(100) [3], which found energetic degeneracies with respect to registry shifts of the CoO(111) film along the [011] direction and predicted a registry shifted structure to be equally stable as the LEED structure in [1].

[1] C. Ebensperger et al., Phys. Rev. B 81, 235405 (2010)

[2] C. Tröppner et al., Phys. Rev. B, accepted (2012)

[3] F. Mittendorfer et al., Phys. Rev. Lett. 109, 015501 (2012)

O 35.66 Tue 18:15 Poster B1

Surface structure of crystalline Ce₇O₁₂ films on Si(111) studied by LEED and XPS — ●OLGA SCHUCKMANN¹, HENRIK WILKENS¹, ROBERT OELKE¹, MARVIN H. ZOELLNER², ANDREAS SCHAEFER³, THOMAS SCHROEDER², MARCUS BÄUMER³, and JOACHIM WOLLSCHLÄGER¹ — ¹Fachbereich Physik, Universität Osnabrück, Germany — ²IHP Frankfurt (Oder), Germany — ³Institute for Applied and Physical Chemistry, University of Bremen, Germany

Cerium oxide is a particularly interesting material for various applications in the field of catalysis due to its high oxygen mobility and storage capability. Hence, the knowledge of the surface structure and oxygen vacancy formation is necessary to understand the elementary catalytic processes as well as the ionic conductivity.

Stoichiometric and structural changes induced by reducing epitaxial cub-CeO₂(111) films grown on Si(111) was studied using low energy electron diffraction (LEED) and X-ray photoelectron spectroscopy (XPS). The composition was determined by means of factor analysis of the Ce 3d X-ray photoemission spectra. The results indicate that Ce⁴⁺ cations are reduced to Ce³⁺ by heating the cerium dioxide films in ultrahigh vacuum. At an annealing temperature of 1070 K a transition from a (1x1) CeO₂ surface to a ($\sqrt{7}\times\sqrt{7}$)R19.1° superstructure takes place. The analysis of the XP spectra reveals a ratio of 57% of Ce³⁺ and thus a stoichiometry of Ce₇O₁₂ for the reconstructed surface.

O 35.67 Tue 18:15 Poster B1

Surface investigation of ceria films on Si(111) after post deposition annealing — ●ROBERT OELKE¹, HENRIK WILKENS¹, OLGA SCHUCKMANN¹, REINHARD OLBRICH¹, MARVIN H. ZOELLNER², THOMAS SCHROEDER², MICHAEL REICHLING¹, and JOACHIM WOLLSCHLÄGER¹ — ¹Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany — ²IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

The surface morphology of 250 nm crystalline CeO₂(111) films grown on hex-Pr₂O₃/Si(111) annealed under UHV conditions was investigated with spot profile analysis low energy electron diffraction (SPA-LEED) and atomic force microscopy (AFM).

The two dimensional LEED pattern of the untreated sample exhibits triangular shaped reflexes due to surface facets, which is also confirmed by AFM measurements. Furthermore, the terrace width and single atomic step height are determined by an energy dependent analysis of the central diffraction spot profile.

Above an annealing temperature of 930 K the shape of the diffraction spots changes indicating that the surface facets vanish, which is also observed in the AFM images. Moreover, the AFM results show very large terraces.

Furthermore, several superstructures are observed at elevated temperatures indicating a periodic order of oxygen vacancies during reduction.

O 35.68 Tue 18:15 Poster B1

Oxidation of graphene on Rh(111) — ●KARIN GOTTERBARM, WEI ZHAO, OLIVER HÖFERT, CHRISTIAN PAPP, and HANS-PETER STEINRÜCK — Lehrstuhl für physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91052 Erlangen

We studied the oxidation of graphene sheets grown on a Rh(111) single crystal surface. The graphene was grown by chemical vapor deposition of propylene at 920 K. The growth process and oxidation were studied in-situ by fast XPS performed at the synchrotron facility BESSY II. The lattice mismatch of graphene on the Rh(111) surface induces corrugation of the graphene sheet leading to two separated signals in the C 1s region¹. These two signals become most pronounced for graphene layers with a low defect density. The oxidation of graphene was investigated depending on oxygen pressure, temperature and graphene layer quality. We found sigmoidal reaction kinetics indicating the following reaction mechanism: The oxidation starts at defect sites, inducing an induction period. With more free adsorption sites the reaction rate increases until most of the graphene is oxidised. The remaining carbon decays exponentially according to pseudo first order kinetics. The influence of the quality of the graphene layer on the reaction rate supports the assumption that oxidation starts at the defect sites.

1: A. B. Preobrajenski, May Ling Ng, A. S. Vinogradov, N. Märtenson, Phys. Rev. B 78, 2008, 073401.

O 35.69 Tue 18:15 Poster B1

Can graphene be turned into a topological insulator? — ●CAROLA STRASSER¹, BART LUDERBROOK², ANDREA DAMASCELLI², CHRISTIAN R. AST¹, and KLAUS KERN^{1,3} — ¹Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — ²Quantum Matter Institute, UBC, Vancouver, BC V6T 1Z4, Canada — ³Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

In 2005 Kane and Mele [1] claimed that graphene opens a band gap at very low temperatures due to spin orbit coupling (SOC) and becomes a quantum spin Hall insulator. Since the SOC is very weak in carbon atoms the size of the gap is very small and experimentally not observable. Recently Weeks et al. [2] showed theoretically that the intrinsic SOC can be enhanced by depositing small amounts of heavy adatoms on top of a graphene sheet. The electrons which hop on the adatoms and back to the graphene sheet induce higher SOC. Calculations showed that this gives rise to a band gap of $\Delta_{SOC}=25$ meV at the K-point which should be observable with spectroscopic methods.

We performed angular resolved photoemission spectroscopy measurements at very low temperatures on epitaxial graphene on SiC. To induce higher SOC we decorated the sample with small amounts of Thallium. We observed small doping effects due to electron transfer from the adatoms to the graphene sheet. The doping level is increasing with coverage until it saturates. The band shift and indications for a gap opening will be presented in detail.

[1] C. L. Kane et al., Phys. Rev. Lett. 95, 226801 (2005)

[2] C. Weeks et al., Phys. Rev. X 1, 021001 (2011)

O 35.70 Tue 18:15 Poster B1

High Temperature Angle-Resolved Photoemission from

Graphene — SØREN ULSTRUP¹, ●MARCO BIANCHI¹, RICHARD C. HATCH¹, DANDAN GUAN¹, ALESSANDRO BARALDI^{2,3}, DARIO ALFÈ⁴, and PHILIP HOFMANN¹ — ¹Dep. of Physics and Astronomy, iNano Centre, Aarhus University, Denmark — ²Dep. of Physics and CENMAT, University of Trieste, Italy — ³Lab. TASC INFN-CNR, AREA Science Park, Trieste, Italy — ⁴Dep. of Physics and Astronomy, TYC@UCL, University College London, United Kingdom

The temperature-dependent electronic structure and electron-phonon coupling of weakly doped supported graphene is studied by angle-resolved photoemission spectroscopy at temperatures up to 1300 K. The finding of an extremely weak electron-phonon coupling is accompanied by the observation of a complex and dramatic change in the graphene carrier density and type. Ab-initio molecular dynamics simulations show that these changes can be related to the temperature-dependent dynamic interaction with the Ir(111) substrate and are mainly caused by fluctuations in the graphene-substrate distance.

O 35.71 Tue 18:15 Poster B1

Defect creation in graphene by swift heavy ion irradiation — ●ALEXANDER LEVISH, OLIVER OCHEDOWSKI, HANNA BUKOWSKA, and MARIKA SCHLEBERGER — Universität Duisburg-Essen, Duisburg, Germany

Graphene, a single layer of carbon atoms arranged in a honeycomb lattice, is envisaged to play an important role in several future applications like semiconductor devices, solar cells, biosensors, fuel cells, etc. The irradiation of graphene with different kind of ions is still a new and promising way to alter the physical properties of graphene. In case of swift heavy ions (SHI) with kinetic energies in the MeV regime it has already been shown that SHI can be used to create closed bilayer edge structures on exfoliated single layer graphene sheets on a wide variety of substrates. Here, using Raman spectroscopy we will show that SHI can be used to create defects even in suspended graphene sheets. Moreover, atomic force microscopy is applied to study the formation of closed bilayer edge structures upon SHI irradiation. We demonstrate that this process is influenced by the crystalline quality of graphene as well as the orientation of the graphene lattice with respect to the ion trajectory.

O 35.72 Tue 18:15 Poster B1

Characterization of graphene on ferromagnetic materials — ●TORSTEN VELTUM, HENDRIK BETTERMANN, and MATHIAS GETZLAFF — Heinrich-Heine-Universität Düsseldorf

In the past few years graphene has gained the attention of scientists due to its unique mechanical and electrical properties. Perfect spin filtering has been predicted for interfaces between graphene and ferromagnetic materials. Iron nanoparticles have been shown to exhibit an in-plane magnetization aligned to that of a supporting thin film of a ferromagnetic material. In this study we want to discuss the properties of ferromagnetic surfaces regarding their suitability for graphene synthesis and their interaction with ferromagnetic nanoparticles.

Thin films of ferromagnetic materials like Ni, Co or Fe are prepared by electron beam evaporation on a W(110) crystal under ultra-high vacuum conditions. To achieve a structurally ordered monolayer graphene on the ferromagnetic substrate we use chemical vapor deposition with propylene. The structure of the thin film system is characterized in-situ by means of scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and Auger electron spectroscopy (AES). The well-characterized Fe nanoparticles are produced by a continuously working arc cluster ion source (ACIS), mass-selected by an electrostatic quadrupole ($\Delta m/m = 10\%$) and subsequently deposited on the single-layer graphene under softlanding conditions. The structural analysis of the nanoparticles is carried out by STM.

O 35.73 Tue 18:15 Poster B1

Hydrogenation of Graphene and Boron-doped Graphene — ●WEI ZHAO, KARIN GOTTERBARM, OLIVE HÖFERT, CHRISTOPH GLEICHWEIT, CHRISTIAN PAPP, and HANS-PETER STEINRÜCK — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

We studied the hydrogenation and dehydrogenation of pristine graphene and boron-doped graphene prepared on a Ni(111) surface. We used in-situ temperature programmed high-resolution XPS to study the degree of hydrogenation and the thermal stability of the resulting layer. B-doped graphene layers with differing boron contents of 0-5% were hydrogenated at 170 K by atomic hydrogen. Additionally

we also studied graphene layers intercalated with gold and still found hydrogenation. Hydrogenation at elevated exposures led to etching of the graphene layer by the atomic hydrogen. This process is hampered by boron doping. After gold intercalation we found that the etching is suppressed.

O 35.74 Tue 18:15 Poster B1

Coulomb- and phonon-induced inter-Landau-level carrier dynamics of graphene in a magnetic field — ●FLORIAN WENDLER, ANDREAS KNORR, and ERMIN MALIĆ — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany

Motivated by a recent experiment [1], we investigate the relaxation dynamics of Dirac electrons in graphene in the presence of a magnetic field. In the experiment, a pump-probe setup is used to measure the relaxation times of electrons in the energetically lowest Landau levels. Exploiting the optical selection rules emerging in a magnetic field as well as the graphene-specific non-equidistant Landau-level splitting, single Landau-level transitions can be selectively measured using circularly polarized light. Here, we apply a theoretical approach within the framework of the density matrix formalism [2], which allows us to microscopically track the equilibration of excited electrons in reciprocal space. We investigate the impact of Coulomb- and phonon-induced relaxation channels between the lowest Landau levels. We find a phonon-dominated picosecond decay time confirming the experimentally observed trend. Furthermore, we discuss the importance of disorder-assisted carrier-phonon scattering processes, which are known to be important for the relaxation dynamics close to the Dirac point [3].

[1] M. Mittendorf, S. Winnerl, and M. Helm (unpublished)

[2] E. Malić et al., Phys. Rev. B 84, 205406 (2011)

[3] J.C.W. Song et al., Phys. Rev. Lett. 109, 106602 (2012)

O 35.75 Tue 18:15 Poster B1

Excitonic oscillator strength of metallic and semiconducting carbon nanotubes — ●EIKE VERDENHALVEN and ERMIN MALIĆ — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany

The intrinsic oscillator strength of single-walled carbon nanotubes (CNTs) plays a crucial role for the optical assignment and the estimation of the abundance of a given nanotube species in a sample. In particular, pronounced absorption intensities do not necessarily correspond to a high abundance in the investigated sample. Based on a microscopic approach, we calculate excitonic absorption spectra for a variety of semiconducting and metallic CNTs allowing us to investigate the diameter and the chirality dependence of the oscillator strength for individual carbon nanotubes [1,2]. Our calculations reveal a pronounced chiral dependence, which strongly varies for different optical transitions and nanotube families. We find that semiconducting CNTs with large chiral angles (armchair-like) and large diameters show the most pronounced absorption intensities confirming the experimentally observed trend [3].

[1] Eike Verdenhalven and Ermin Malic, "Excitonic oscillator strength of metallic and semiconducting carbon nanotubes", submitted for publication (2012)

[2] Ermin Malic, Janina Maultzsch, Stephanie Reich, and Andreas Knorr, Phys. Rev. B 82, 035433 (2010)

[3] S. M. Bachilo et al., Science 298, 2361 (2002); Y. Miyauchi et al., Chem. Phys. Lett. 387, 198 (2004)

O 35.76 Tue 18:15 Poster B1

Work function study and surface photovoltage phenomena of graphene on SiC — ●SAMIR MAMMADOV¹, JÜRGEN RISTEIN¹, and THOMAS SEYLLER^{1,2} — ¹Lehrstuhl für Technische Physik Erwin-Rommel-Str. 1 91058 Erlangen — ²Technische Universität Chemnitz Institut für Physik * Technische Physik Reichenhainer Straße 70 09126 Chemnitz

Subject of this study is the investigation of the work function and band-bending of epitaxial graphene (EG) on SiC. Two types of samples were investigated: regular EG *lms and H-intercalated EG *lms, referred to as quasi-freestanding graphene (QFG). EG *lms were formed by thermal decomposition on the Si-face of 6H-SiC substrates and QFG samples were formed by subsequently intercalating EG samples by hydrogen. The work function and its dependence on the number of graphene layers was precisely determined for each type of sample by the Kelvin method. Additionally, laser induced surface photovoltage was measured in situ. The results are used to construct a full band

diagram for the graphene/SiC heterostructure.

O 35.77 Tue 18:15 Poster B1

Band renormalization, mini-cones and Fermi surface discontinuities in epitaxial graphene on SiC(0001) by Cu intercalation — ●STIVEN FORTI¹, KONSTANTIN V. EMTSEV¹, ALEXEI A. ZAKHAROV², CAMILLA COLETTI³, and ULRICH STARKE¹ — ¹Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany — ²MAX Lab, Lund University, Box 118, Lund, 22100, Sweden — ³Center for Nanotechnology Innovation @ NEST, Istituto Italiano di Tecnologia, Piazza San Silvestro 12, 56127 Pisa, Italy

The interaction of graphene with transition metals as well as the effects of a periodic perturbation on the graphene's band structure are fields of great interest. In this work we present photoemission spectroscopy (PES), low-energy electron diffraction (LEED) and microscopy (LEEM) to study the effects of an ordered layer of Cu atoms intercalated under epitaxial graphene (EG) on SiC(0001). By means of angle-resolved photoelectron spectroscopy (ARPES) measurements, we observed that the intercalated graphene is effectively decoupled from the substrate and the interfacial Cu layer imposes both a strong n-doping and a periodic potential, which deeply affect the graphene's band structure. The site-specific interaction between Cu and graphene, together with the chiral nature of the graphene's carriers, produce the development of minicones (mCs) located along the boundaries of the graphene's Brillouin zone. Mini band-gaps are observed at the mCs vertexes and the Fermi surface exhibits discontinuities caused by the emergence of new electronic states associated with the mCs.

O 35.78 Tue 18:15 Poster B1

Synthesis of epitaxial graphene on C-face SiC: influence of growth conditions — ●TIMO SCHUMANN¹, INNA SHTEINBUK^{1,2}, MYRIANO H. OLIVEIRA JR.¹, J. MARCELO J. LOPES¹, and HENNING RIECHERT¹ — ¹Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — ²City College of New York, New York, United States

Surface Si depletion of hexagonal SiC offers the possibility of producing high-quality graphene directly on an insulating substrate. However, while on the Si-face monolayer graphene can be prepared on a large area, on the C-face a precise control over the number of layers is hard to be achieved. Nevertheless, even films with many carbon layers behave like decoupled monolayer graphene sheets on C-face SiC, potentially offering higher electron mobilities than graphene layers on Si-face SiC. We investigated the influence of the growth conditions, *i.e.* temperature, growth time and environment (Argon, vacuum, enclosed space) on the growth of epitaxial graphene on C-face SiC. The quality of the resulting layers is investigated by means of atomic force microscopy, Raman spectroscopy and magnetotransport measurements. This work aims to offer a guideline for reproducible production of uniform and high-quality graphene sheets.

O 35.79 Tue 18:15 Poster B1

Optical properties of bilayer graphene — ●FARIS KADI and ERMIN MALIĆ — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany

We present a microscopic study of the optical properties of Bernal-stacked bilayer graphene. In particular, we show the excitonic absorption and conductance for all possible optical transitions. Our theoretical approach is based on the density matrix formalism in combination with tight-binding wave functions [1]. In contrast to the linear band structure of monolayer graphene, bilayered graphene exhibits four parabolic bands near the Dirac point. This results in bilayer-characteristic features in the absorption spectrum. We find that the low energy spectrum exhibits a pronounced peak, which is induced by interlayer transitions around the Dirac point. In the ultraviolet region, the spectrum exhibits two energetically close absorption peaks resulting from interband transitions at the saddle point of the Brillouin zone. We discuss the optical matrix element determining the strength of different optical transitions as well as the Coulomb interaction accounting for energy renormalization and formation of strongly bound electron-hole pairs.

[1] E. Malić, T. Winzer, E. Bobkin, and A. Knorr, *Phys. Rev. B* 84, 205406, (2011)

O 35.80 Tue 18:15 Poster B1

Atomistic simulations of defects in bilayer graphene — ●KONSTANTIN WEBER and BERND MEYER — Interdisziplinäres Zentrum für Molekulare Materialien und Computer-Chemie-Centrum,

Universität Erlangen-Nürnberg

Simple Lennard-Jones-based Van-der-Waals potentials are not capable to describe simultaneously the correct depth and corrugation of the interaction potential between two graphene sheets since they are too smooth and do not capture the short-ranged orbital overlap between graphene pi-electron systems. To cure this problem, Kolmogorov and Crespi [1] proposed a registry-dependent interlayer potential which we implemented into the LAMMPS software package in combination with the classical interatomic AIREBO potential [2] for the covalent carbon-carbon bonds. The improvements in the description of bilayer graphene with this new potential will be discussed and first results on the structure and energy of dislocations in bilayer graphene will be shown.

[1] A. Kolmogorov, V. Crespi, *Phys. Rev. B* 71, 235415 (2005).

[2] D.W. Brenner, et al., *J. Phys.: Condens. Matter* 14, 783 (2002).

O 35.81 Tue 18:15 Poster B1

Torque magnetometry on large-area graphene — ●MATTHIAS BLOCK¹, STEPHAN ALBERT¹, STEFANOS CHALKIDIS¹, FLORIAN SPECK², FELIX FROMM², THOMAS SEYLLER³, MARC WILDE¹, and DIRK GRUNDLER¹ — ¹Technische Universität München, Department Physik E10, James-Frank-Str. 1, 85747 Garching b. München — ²Universität Erlangen, Lehrstuhl für Technische Physik, Erwin-Rommel-Str. 1, 91058 Erlangen — ³Technische Universität Chemnitz, Institut für Physik, Technische Physik, Reichenhainer Str. 70, 09126 Chemnitz

Torque magnetometry performed at helium temperatures allows one to gain insight into the electronic properties of two-dimensional electron systems. Graphene with its unique electronic properties is in particular interesting. While much of fundamental knowledge about graphene was learned from small-sized exfoliated graphene, it is important for our technique to study large areas of graphene. We use graphene epitaxially grown on SiC as it offers similarly high electronic quality and is provided in wafer-scale sizes. For our experiment we use micromechanical cantilevers which are designed for sample sizes of 1.2 mm × 2 mm. We use SiC-graphene which has been characterized by Raman spectroscopy and atomic force microscopy to determine the amount of monolayer graphene. We report on our results of the magnetization measurements based on torque magnetometry. We acknowledge financial support by the DFG via project WI3320/1-1 in SPP 1459.

O 35.82 Tue 18:15 Poster B1

Downsizing graphene: routes towards epitaxial graphene nanoribbons (EGNR) on SiC — ●ALEXANDER STÖHR, STIVEN FORTI, and ULRICH STARKE — Max Planck Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany

In recent years, great efforts have been spent in trying to realize a facile and scalable technique to produce graphene-based nanostructures for logic electronics. In this work we illustrate different experimental approaches to achieve quasi-1D structures based on epitaxial graphene (EG) on SiC. We present our first results about vicinal 4H-SiC surfaces, the 6H-SiC(1109) facet and anisotropic etching of graphene by means of metallic nanoparticles. Vicinal SiC surfaces offer a promising template for producing 1D graphene nanostructures on a wafer size due to the self-ordering of narrow terraces. Narrow trenches can be patterned into graphene by self-organized catalytic etching with metallic nanoparticles. By combination with H-intercalation of the buffer layer free-standing structured monolayer graphene can be obtained. We show nanoparticles deposition in a monodispersed distribution and the catalytic propagation in preferential directions. The bottom-up approach for definition of graphene nanostructures is of crucial importance since it avoids possible contaminations typical of the ex-situ lithographical approach. Nevertheless, patterned graphene relaxes into basal plane terraces and facets (e.g. (1109)) when annealed at elevated temperatures. To understand the graphene growth mechanism on those facets we investigated the (1109)-surface of 6H-SiC itself.

O 35.83 Tue 18:15 Poster B1

Transfer of Ni grown graphene onto an insulating YSZ substrate — ●SAMUEL GRANDTHYLL¹, STEFAN GSELL², MICHAEL WEINL², MATTHIAS SCHRECK², STEFAN HÜFNER¹, FRANK MÜLLER¹, and KARIN JACOBS¹ — ¹Saarland University, Experimental Physics, 66041 Saarbrücken, Germany — ²Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Graphene has been grown epitaxially on several Ni(111)/YSZ/Si(111)

multilayer samples by chemical vapor deposition (CVD) of the precursor acetone [1]. The aim was to use the nickel film (thickness approximately 150 nm) as a catalyst for precursor fragmentation and graphene growth. Once the graphene film has formed, the thin metal film can be removed by etching in order to transfer graphene onto the underlying YSZ (Yttria-Stabilized Zirconium oxide) insulator.

During this synthesis route the samples were characterized in each step by several techniques, such as X-ray Photoelectron Spectroscopy (XPS), X-ray Photoelectron Diffraction (XPD), Low Energy Electron Diffraction (LEED), and Fermi Surface Mapping (FSM) by Angular Resolved Ultraviolet Photoelectron Spectroscopy. The results reveal that the transfer of ordered graphene layers is possible by this preparation mechanism.

References:

[1] J. Phys.: Condens. Matter 24 (2012) 314204

O 35.84 Tue 18:15 Poster B1

Electronic states of spatially coordinated graphene nanoribbons on Ag(775) — ●ALEXANDER TIMMER¹, NABI AGHDASSI¹, DINGYONG ZHONG¹, XINLIANG FENG², KLAUS MÜLLEN², HARRY MÖNIG¹, LIFENG CHI¹, HELMUT ZACHARIAS¹, and HARALD FUCHS¹ — ¹Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — ²Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

On-surface covalent coupling of specific organic primer molecules on vicinal metal surfaces under UHV conditions represents a reliable technique to prepare well-arranged molecular surface patterns [1]. Based on our previous work on Au(788) we created an array of precisely-aligned armchair graphene nanoribbons on Ag(775) [2]. The electronic properties of these GNRs are analyzed with angle-resolved ultraviolet photoemission spectroscopy (ARPES), angle-resolved inverse photoemission (KRIPES), and scanning tunneling microscopy (STM), which allows for the determination of the 7-aGNRs bandgap. This study is particularly focusing on the role of the metal-substrate interaction and possible doping effects [3]. The data for 7aGNRs on Ag(775) are compared to LDA and GW calculations conducted for isolated aGNRs and to a semiclassical model incorporating substrate polarization effects as well as to our previous study of 7aGNRs on Au(788) [4]. The results indicate that the chosen substrate plays a significant role for the electronic properties of the considered systems. [1] J. Cai et al., Nature 466, 470, [2] S. Linden et al., PRL 108, 216801, [3] D. Prezzi et al., Phys. Rev B 84, 041401(R), [4] L. Liang et al., Phys. Rev B 86, 195404

O 35.85 Tue 18:15 Poster B1

Graphene growth by Face-to-Face method and occurrence of step bunching process — ●PHILIPP ANSORG, THOMAS DRUGA, MARTIN WENDEROTH, and RAINER G. ULBRICH — Institute of semiconductor physics, Göttingen, Germany

Studying the outstanding properties of graphene requires a reliable production process. We have grown epitaxial graphene on n-doped 6H-SiC(0001) under UHV conditions and determined the influence of temperature on graphene growth. In addition an experimental arrangement after YU et al. [1], called *Face-to-Face* method, was used for the preparation of graphene. The quality of the sample surface was studied by Atomic Force Microscopy under ambient conditions. Domains of graphene up to $3 \times 30 \mu\text{m}^2$ are found. Besides determining optimal conditions for graphene growth we observed the mechanism of *step bunching*. The height of the final steps is equivalent to multiples of three times the height of a SiC-bilayer, pointing to a step bunching process of higher order. The width of the graphene domains corresponds to multiples of three times the width of substrate terraces first discovered by HUPALO et al. [2].

[1] X. Z. Yu, C. G. Hwang, C. M. Jozwiak, A. Köhl, A. K. Schmid and A. Lanzara, *Phys. Rev. B* 80 (2009), p. 041401

[2] M. Hupalo, E.H. Conrad and M. C. Tringides, *Journal of Electron Spectroscopy and Related Phenomena* 184 (2011), p. 100

O 35.86 Tue 18:15 Poster B1

Epitaxial growth of graphene on copper foil — ●CHRISTIAN RAIDEL¹, FELIX FROMM¹, ROLAND KOCH¹, JOHANNES JOBST², and THOMAS SEYLLER^{1,3} — ¹FAU Erlangen-Nürnberg, Technische Physik, Erlangen, Deutschland — ²FAU Erlangen-Nürnberg, Angewandte Physik, Erlangen, Deutschland — ³TU Chemnitz, Institut für Physik, Chemnitz, Deutschland

We investigated the growth of epitaxial graphene on commercial copper foil by atmospheric pressure chemical vapor deposition using methane

and pyridine as precursors. Pyridine was used to incorporate nitrogen as a dopant into graphene. For optimal growth conditions the copper foils were pretreated by electro-polishing and annealed at elevated temperatures for achieving low defect densities and large grains. The growth of the graphene layers was studied by x-ray photoelectron spectroscopy (XPS), while scanning electron microscopy (SEM) was used to determine structural details of the layers. In addition, Raman spectroscopy was employed to investigate the quality of the layers.

XPS measurements of the as-grown films revealed that the growth resulted in multi-layer graphene. Transfer of the graphene layers from the copper foil onto SiO₂ wafers was also studied. The XPS spectra remained basically unchanged. On the other hand, Raman spectroscopy indicates an increase in strain and defects after the transfer. Graphene layers grown with pyridine were transferred using a nitrogen-free resist. In that case, XPS showed the existence of nitrogen in the layer. The origin of the nitrogen content, however, cannot be absolutely pinpointed to the employed precursor, as will be discussed in the presentation.

O 35.87 Tue 18:15 Poster B1

Organic molecular self-assembly on epitaxial graphene — ●ALEXEI NEFEDOV¹, WENHUA ZHANG², MICHAEL NABOKA¹, HIKMET SEZEN¹, LIANG CAO², and CHRISTOF WOELL¹ — ¹Institute of Functional Interfaces, Karlsruhe Institute of Technology, Leopoldshafen, Germany — ²National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, PRC

The adsorption of organic molecules as pentacene (Pn) and terephthalic acid (TPA) on a single layer of graphene grown epitaxially on Ni(111) has been investigated by means of near-edge X-ray absorption fine structure (NEXAFS) spectroscopy and X-ray photoelectron spectroscopy (XPS) at room temperature. The assignment of the NEXAFS-resonances was aided by ab-initio calculations by StoBe package. For coverages up to a monolayer the molecular plane of TPA adopts a parallel orientation with regard to the epitaxial graphene (EG) layer. Deprotonation of TPA molecules at one monolayer coverage can be excluded. For TPA multilayers, the molecular plane is tilted on average by approximately 45° with respect to the sample surface. Pentacene molecules demonstrate a dependence of their orientation and electronic structure on the coverage. The observed effects will be discussed in detail during presentation.

O 35.88 Tue 18:15 Poster B1

Investigation of graphene contact resistivity on semi-insulating silicon carbide by Kelvin Probe Force Microscopy — ●FELIX LÜPKE, MARTIN WENDEROTH, THOMAS DRUGA, and RAINER G. ULBRICH — IV. Physikalisches Institut, Georg-August Universität Göttingen, Germany

We present first Kelvin Probe Force Microscopy (KPFM) and simulation of the lateral charge transport across few-layer graphene on the semi-insulating 6H-SiC(0001) surface. After preparation of the SiC crystal using common methods [1], atomically flat graphene layers of up to few hundred nm in lateral dimension were observed. Gold electrodes were prepared on top of the graphene layer by thermal evaporation through a shadow mask. For transport measurements a lateral voltage was applied across the sample at the gold electrodes in addition to the usual alternating tip-sample voltage used for KPFM [2]. The potential measured by KPFM is an overlay of the local work function of the sample and the voltage drop across the graphene layer. By subtracting measurements of reverse lateral bias the voltage drop was extracted. We find an ohmic behavior of the contacted graphene layer and a graphene sheet resistance of 1 kΩ/sq. By comparing the experimental transport measurements with a resistance network simulation the contact resistivity between graphene and a gold electrode can be determined to $< 1 \times 10^{-5} \Omega/\text{cm}^2$.

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O 35.89 Tue 18:15 Poster B1

Two-photon photoemission studies of graphene on Ir(111) — ●D. NOBIS¹, D. NIESNER¹, TH. FAUSTER¹, M. KRALJ², M. PETROVIĆ², P. C. YE³, S. Y. HONG³, W. JIN³, J. DADAP³, and R. M. OSGOOD³ — ¹Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — ²Institut za fiziku, Bijenička 46, HR-10000 Zagreb, Croatia — ³Columbia University, New York, NY 10027, USA

Graphene can be grown on Ir(111) with high quality by decomposi-

tion of hydrocarbons [1]. The band structure of this system has been studied with various techniques [2,3]. We have used two-photon photoemission (2PPE) to study the image-potential states of graphene on Ir(111). Using monochromatic 2PPE (photon energies 3.99 – 4.86 eV) and bichromatic 2PPE (pump pulse 4.77 eV, probe pulse 1.59 eV) we observe two $n = 1$ image-potential bands. The main peak agrees with previous data [3]. The weaker second band has a slightly larger binding energy and effective mass.

We discuss possible origins of the second band: (a) Splitting in odd and even bands with respect to the graphene layer [4]. (b) Umklapp bands or (c) localized states due to the moiré structure of graphene on Ir(111) [5].

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[4] Bose, S. *et al.*, New J. of Physics **12** (2010) 023028

[5] Armbrust, N. *et al.*, Phys. Rev. Lett. **108** (2012) 056801

O 35.90 Tue 18:15 Poster B1

Magnetism in graphene induced by the adsorption of atmospheric species — •NORA JENNY VOLLMEYERS¹, EVA RAULS¹, WOLF GERO SCHMIDT¹, UWE GERSTMANN¹, and FRANCESCO MAURI² — ¹Festkörpertheorie, Department für Naturwissenschaften, Universität Paderborn, Paderborn, Germany — ²Institut de Minéralogie et de Physique des Milieux Condensés, Université Pierre et Marie Curie, Paris, France

Besides its outstanding properties with respect to conductivity the two-dimensional material graphene has attracted a still increasing deal of interest due to an unconventional magnetism. Although, ideal graphene is nonmagnetic, already the presence of non-metallic defects induces magnetism in the material. Graphene has, thus, attracted great interest as a metal-free magnetic material. The defects can be

either introduced intentionally by irradiation or doping, however, in most cases they are unavoidable by-products of material growth, or simply by the exposure to air.

We use density functional theory and the Quantum Espresso package to investigate the influence of atmospheric species on monolayer graphene. Our main focus lies on the question, how the different atoms influence the electronic and magnetic properties of the substrate. We study the adsorption and substitutional incorporation of hydrogen, oxygen and nitrogen by analyzing the calculated total energies, magnetic moments and simulated spin-polarized STM images.

O 35.91 Tue 18:15 Poster B1

N-doped single-layer graphene by conversion of aromatic self-assembled monolayers — •OLIVER REIMER¹, NILS-EIKE WEBER¹, STEFAN WUNDRACK², RAINER STOSCH², and ANDREY TURCHANIN¹ — ¹Faculty of Physics, University of Bielefeld, 33615 Bielefeld, Germany — ²Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany

N-doped graphene sheets are promising for applications in transparent conductive coatings, supercapacitors or as catalysts for oxygen reduction. However, controllable fabrication of this material is not yet well established. Here, we present a molecular route to N-doped single-layer graphene based on electron-beam-induced crosslinking of N-containing aromatic self-assembled monolayers on copper foils and their subsequent temperature-induced conversion into graphene. We characterize this conversion as well as structural and chemical properties of the formed graphene sheets by complementary surface science techniques (X-ray photoelectron microscopy, low energy electron diffraction) and Raman spectroscopy. Functional properties of the formed single-layer graphene are tested by electrical measurements on oxidized silicon wafers.