Surface Science Division
Fachverband Oberflächenphysik (O)

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Overview of Invited Talks and Sessions

(lecture rooms TRE Phy, Phy C213, WIL A317, WIL B321, WIL B122, WIL C107, WIL C307 and CHE 184; poster P3 and P4)

Invited Talks

O 1.1	Mon	10:15–11:00	TRE Phy	**Chirality at surfaces from the single-molecule perspective** — •Rasmita Raval
O 9.1	Mon	14:00–14:45	TRE Phy	**Ultrafast nanooptical control** — •Walter Pfeiffer, Tobias Brixner, Martin Aeschlimann
O 24.1	Tue	10:15–11:00	TRE Phy	**Low Energy Electron Microscopy Studies of Thin Film Graphene Growth and Properties** — •Rudolf M. Tromp
O 33.1	Tue	14:00–14:45	TRE Phy	**Competition of magnetic excitations on a superconducting surface** — •Katharina J. Franke
O 34.1	Tue	14:45–15:30	TRE Phy	**A Bottom-up View of Sliding Friction: From Hopping Atoms to Superlubric Nanoparticles** — •Andre Schirmeisen
O 37.1	Wed	10:15–11:00	TRE Phy	**Writing nanostructures with a focused electron beam** — •Hubertus Marbach
O 61.1	Thu	10:15–11:00	TRE Phy	**Novel properties of topological insulator thin films of Bi2Te3 and Bi2Se3 prepared by molecular beam epitaxy** — •Qikun Xue
O 72.1	Thu	14:00–14:45	TRE Phy	**In-situ Study of Nanoparticle Shape Changes under Reaction Conditions** — •Andreas Stierle
O 94.1	Fri	10:15–11:00	TRE Phy	**Computational study of optical and structural properties of an organic dye sensitized solar cell** — •Ralph Gebauer, Filippo De Angelis
O 103.1	Fri	13:15–14:00	TRE Phy	**Beat the heat! First-principles based modeling of micro- and macroscopic heat dissipation in heterogeneous catalysis** — •Karsten Reuter

Invited Talks Focussed Session: Theory and computation of electronic structure: new frontiers (jointly with HL, DS)

O 2.1	Mon	11:15–11:45	TRE Phy	**Range separation: success, doubts and perspectives** — •Andreas Savin
O 26.1	Tue	11:15–11:45	TRE Phy	**Electronic and Optical Excitations in Magnetic Insulators** — •Claudia Rödl, Frank Fuchs, Friedhelm Bechstedt
O 48.1	Wed	15:00–15:30	TRE Phy	**Progress in diffusion quantum Monte Carlo calculations** — •Richard Needs
O 64.1	Thu	11:15–11:45	TRE Phy	**Electronic excitations in thin-film materials for solar cells: beyond standard density functional theory** — •Silvana Botti
O 87.1	Thu	17:15–17:45	TRE Phy	**Continuum mechanics for quantum many-body systems: the anti-adiabatic approximation** — •Giovanni Vignale, Xianlong Gao, Jianmin Tao, Stefano Pittalis, Ilya Tokatly
O 96.1	Fri	11:15–11:45	TRE Phy	**Tunable bandgaps and excitons in doped semiconducting carbon nanotubes made possible by acoustic plasmons** — •Catalin Spataru, Francois Leonard

Invited Talks Focussed Session: Transparent conductive oxides (jointly with HL, DS)

O 4.1	Mon	11:15–11:45	WIL A317	**Surface and Bulk Properties of Post-Transition Metal Oxide Semiconductors** — Philip D.C. King, Sepehr Vasheghani Farahani, Tim D. Veal, •Chris F. McConville
O 4.2	Mon	11:45–12:15	WIL A317	***Ab-initio* calculation of electronic and optical properties of transparent conductive oxides** — •André Schleife, Claudia Rödl, Frank Fuchs, Jürgen Furthmüller, Benjamin Höffling, Karsten Hannewald, Patrick Rinke, Joel Varley, Anderson Janotti, Chris G. Van de Walle, Friedhelm Bechstedt
O 4.3	Mon	12:15–12:45	WIL A317	**Bulk semiconducting oxides: crystal growth and physical properties** — •Roberto Fornari
O 30.1	Tue	11:15–11:45	WIL B122	**Experimental Electronic Structure of In_2O_3 and Ga_2O_3** — •Christoph Janowitz
O 30.2	Tue	11:45–12:15	WIL B122	**Transparent Electronics Using Oxide Materials** — •Marius Grundmann
O 30.3	Tue	12:15–12:45	WIL B122	**Optical properties of undoped and doped ZnO** — •Axel Hoffmann, Markus R. Wagner

Gaede Prize Talk

O 47.1	Wed	14:00–14:45	TRE Phy	**Spin-split metallic surface states on semimetals and topological insulators** — •Philip Hofmann

Invited talks of the joint symposium SYAP

See SYAP for the full program of the symposium.

SYAP 1.1	Mon	10:30–11:00	HSZ 01	**Observing Intra-atomic Electron Correlation by Tunnelling and Recollision** — •Paul Corkum
SYAP 1.2	Mon	11:00–11:30	HSZ 01	**Attosecond time-resolved molecular electron dynamics** — •Marc Vrakking
SYAP 1.3	Mon	11:30–12:00	HSZ 01	**Opportunities in Attosecond Science using Core Level Spectroscopy** — •Anders Nilsson
SYAP 1.4	Mon	12:00–12:30	HSZ 01	**Attosecond spectroscopy on solid surfaces** — •Reinhard Kienberger
SYAP 1.5	Mon	12:30–13:00	HSZ 01	**Condensed matter effects in attosecond physics** — •Pedro M. Echenique

Sessions

O 1.1–1.1	Mon	10:15–11:00	TRE Phy	**Invited Talk (Rasmita Raval)**
O 2.1–2.6	Mon	11:15–13:00	TRE Phy	**Focussed session: Theory and computation of electronic structure: new frontiers I (jointly with HL, DS)**
O 3.1–3.6	Mon	11:15–12:45	PHY C213	**Metal substrates: Adsorption of organic / bio molecules I**
O 4.1–4.4	Mon	11:15–13:00	WIL A317	**Focussed session: Transparent conductive oxides I (jointly with HL, DS)**
O 5.1–5.6	Mon	11:15–12:45	WIL B321	**Spin-Orbit Interaction at Surfaces I**
O 6.1–6.7	Mon	11:15–13:00	WIL B122	**Semiconductor substrates: Adsorption**
O 7.1–7.7	Mon	11:15–13:00	WIL C107	**Surface Dynamics I**
O 8.1–8.7	Mon	11:15–13:00	WIL C307	**Oxides and insulators: Adsorption I**
O 9.1–9.1	Mon	14:00–14:45	TRE Phy	**Invited Talk (Walter Pfeiffer)**
O 10.1–10.8	Mon	15:00–17:00	TRE Phy	**Metal substrates: Adsorption of organic / bio molecules II**
O 11.1–11.8	Mon	15:00–17:00	PHY C213	**Plasmonics and Nanooptics I**
O 12.1–12.8	Mon	15:00–17:00	WIL A317	**Metal substrates: Adsorption of O / H and inorganic molecules I**
O 13.1–13.8	Mon	15:00–17:00	WIL B321	**Solid / liquid interfaces I**
O 14.1–14.7	Mon	15:00–16:45	WIL B122	**Clean surfaces: Metals, semiconductors, oxides and insulators I**
O 15.1–15.8	Mon	15:00–17:00	WIL C107	**Nanostructures at surfaces: Dots, particles, clusters, arrays I**

O 16.1–16.8	Mon	15:00–17:00	WIL C307	**Scanning probe methods I**
O 17.1–17.8	Mon	17:15–19:15	TRE Phy	**Metal substrates: Adsorption of organic / bio molecules III**
O 18.1–18.8	Mon	17:15–19:15	PHY C213	**Plasmonics and Nanooptics II**
O 19.1–19.7	Mon	17:15–19:00	WIL A317	**Metal substrates: Adsorption of O / H and inorganic molecules II**
O 20.1–20.8	Mon	17:15–19:15	WIL B321	**Solid / liquid interfaces II**
O 21.1–21.5	Mon	17:15–18:30	WIL B122	**Clean surfaces: Metals, semiconductors, oxides and insulators II**
O 22.1–22.9	Mon	17:15–19:30	WIL C107	**Theoretical methods**
O 23.1–23.8	Mon	17:15–19:15	WIL C307	**Scanning probe methods II**
O 24.1–24.1	Tue	10:15–11:00	TRE Phy	**Invited Talk (Rudolf M. Tromp)**
O 25.1–25.4	Tue	11:00–13:00	GER 37	**[DS] Progress in Micro- and Nanopatterning: Techniques and Applications I (Focused Session, jointly with O - Organisers: Graaf, Hartmann)**
O 26.1–26.6	Tue	11:15–13:00	TRE Phy	**Focussed session: Theory and computation of electronic structure: new frontiers II (jointly with HL, DS)**
O 27.1–27.7	Tue	11:15–13:00	PHY C213	**Metal substrates: Adsorption of organic / bio molecules IV**
O 28.1–28.7	Tue	11:15–13:00	WIL A317	**Plasmonics and Nanooptics III**
O 29.1–29.7	Tue	11:15–13:00	WIL B321	**Graphene I**
O 30.1–30.5	Tue	11:15–13:15	WIL B122	**Focussed session: Transparent conductive oxides II (jointly with HL, DS)**
O 31.1–31.8	Tue	11:15–13:15	WIL C107	**Nanostructures at surfaces: Dots, particles, clusters, arrays II**
O 32.1–32.6	Tue	11:15–12:45	WIL C307	**Spin-Orbit Interaction at Surfaces II**
O 33.1–33.1	Tue	14:00–14:45	TRE Phy	**Invited Talk (Katharina J. Franke)**
O 34.1–34.1	Tue	14:45–15:30	TRE Phy	**Invited Talk (Andre Schirmeisen)**
O 35.1–35.20	Tue	18:30–22:00	P3	**Poster Session I (Scanning probe methods)**
O 36.1–36.128	Tue	18:30–22:00	P4	**Poster Session II (Metals; Nanostructures at surfaces; Surface or interface magnetism; Spin-Orbit Interaction at Surfaces; Electron and spin dynamics; Surface dynamics; Methods; Theory and computation of electronic structure)**
O 37.1–37.1	Wed	10:15–11:00	TRE Phy	**Invited Talk (Hubertus Marbach)**
O 38.1–38.8	Wed	11:00–13:00	GER 38	**[DS] Progress in Micro- and Nanopatterning: Techniques and Applications II (Focused Session, jointly with O - Organisers: Graaf, Hartmann)**
O 39.1–39.7	Wed	11:15–13:00	TRE Phy	**Focussed session: Theory and computation of electronic structure: new frontiers III (jointly with HL, DS)**
O 40.1–40.7	Wed	11:15–13:00	PHY C213	**Metal substrates: Adsorption of organic / bio molecules V**
O 41.1–41.7	Wed	11:15–13:00	WIL A317	**Plasmonics and Nanooptics IV**
O 42.1–42.6	Wed	11:15–12:45	WIL B321	**Graphene II**
O 43.1–43.4	Wed	11:15–12:15	WIL B122	**Surface Dynamics II**
O 44.1–44.8	Wed	11:15–13:15	WIL C107	**Nanostructures at surfaces: Dots, particles, clusters, arrays III**
O 45.1–45.7	Wed	11:15–13:00	WIL C307	**Oxides and insulators: Adsorption II**
O 46.1–46.9	Wed	11:15–13:30	CHE 184	**Surface magnetism I (jointly with MA)**
O 47.1–47.1	Wed	14:00–14:45	TRE Phy	**Gaede Prize talk (Philip Hofmann)**
O 48.1–48.7	Wed	15:00–17:00	TRE Phy	**Focussed session: Theory and computation of electronic structure: new frontiers IV (jointly with HL, DS)**
O 49.1–49.9	Wed	15:00–17:15	PHY C213	**Metal substrates: Adsorption of organic / bio molecules VI**
O 50.1–50.8	Wed	15:00–17:00	WIL A317	**Plasmonics and Nanooptics V**
O 51.1–51.9	Wed	15:00–17:15	WIL B321	**Graphene III**
O 52.1–52.9	Wed	15:00–17:15	WIL B122	**Nanostructures at surfaces: Wires, tubes**
O 53.1–53.7	Wed	15:00–16:45	WIL C107	**Solid / liquid interfaces III**
O 54.1–54.5	Wed	15:00–16:15	WIL C307	**Particles and clusters I**
O 55.1–55.7	Wed	15:00–16:45	CHE 184	**Surface magnetism II (jointly with MA)**
O 56.1–56.8	Wed	15:00–17:00	GER 38	**[DS] Progress in Micro- and Nanopatterning: Techniques and Applications III (Focused Session, jointly with O - Organisers: Graaf, Hartmann)**
O 57.1–57.2	Wed	16:30–17:00	WIL C307	**Nanotribology**
O 58.1–58.8	Wed	17:15–19:15	GER 38	**[DS] Plasmonics and Nanophotonics (jointly with HL and O)**

O 59.1–59.20	Wed	17:30–21:00	P3	**Poster Session III (Nanotribology; Polymeric biomolecular films; Organic electronics and photovoltaics, Covalent networks on surfaces; Phase transitions; Particles and clusters; Transparent conductive oxides)**
O 60.1–60.127	Wed	17:30–21:00	P4	**Poster Session IV (Solid/liquid interfaces; Semiconductors; Oxides and insulators; Graphene; Plasmonics and nanooptics; Electronic Structure; Surface chemical reactions; Heterogeneous catalysis)**
O 61.1–61.1	Thu	10:15–11:00	TRE Phy	**Invited Talk (Qikun Xue)**
O 62.1–62.6	Thu	10:15–11:45	GER 38	**[DS] Organic Electronics and Photovoltaics I (jointly with CPP, HL, and O)**
O 63.1–63.8	Thu	11:00–13:00	HSZ 103	**[MA] Surface magnetism III**
O 64.1–64.6	Thu	11:15–13:00	TRE Phy	**Focussed session: Theory and computation of electronic structure: new frontiers V (jointly with HL, DS)**
O 65.1–65.7	Thu	11:15–13:00	PHY C213	**Metal substrates: Adsorption of organic / bio molecules VII**
O 66.1–66.7	Thu	11:15–13:00	WIL A317	**Plasmonics and Nanooptics VI**
O 67.1–67.7	Thu	11:15–13:00	WIL B321	**Graphene IV**
O 68.1–68.7	Thu	11:15–13:00	WIL B122	**Polymeric biomolecular films**
O 69.1–69.8	Thu	11:15–13:15	WIL C107	**Electronic structure I**
O 70.1–70.5	Thu	11:15–13:45	WIL C307	**Gerhard Ertl Young Investigator Award**
O 71.1–71.4	Thu	12:00–13:00	GER 38	**[DS] Organic Electronics and Photovoltaics II (jointly with CPP, HL, and O)**
O 72.1–72.1	Thu	14:00–14:45	TRE Phy	**Invited Talk (Andreas Stierle)**
O 73.1–73.8	Thu	14:00–16:00	GER 38	**[DS] Organic Electronics and Photovoltaics III (jointly with CPP, HL, and O)**
O 74.1–74.6	Thu	15:00–16:30	TRE Phy	**Focussed session: Theory and computation of electronic structure: new frontiers VI (jointly with HL, DS)**
O 75.1–75.8	Thu	15:00–17:00	PHY C213	**Metal substrates: Adsorption of organic / bio molecules VIII**
O 76.1–76.5	Thu	15:00–16:15	WIL A317	**Plasmonics and Nanooptics VII**
O 77.1–77.8	Thu	15:00–17:00	WIL B321	**Graphene V**
O 78.1–78.5	Thu	15:00–16:15	WIL B122	**Surface chemical reactions**
O 79.1–79.8	Thu	15:00–17:00	WIL C107	**Electronic structure II**
O 80.1–80.8	Thu	15:00–17:00	WIL C307	**Epitaxy and growth: Metals and semiconductors I**
O 81.1–81.8	Thu	15:15–17:15	HSZ 103	**[MA] Surface magnetism IV**
O 82.1–82.7	Thu	15:15–17:00	HSZ 401	**[MA] Graphene (jointly with DY, DS, HL, O, TT)**
O 83.1–83.8	Thu	15:15–19:00	HSZ 403	**[MA] Focussed Session "X-ray absorption spectra - state of the art of theory and experiment" (jointly with DS, HL, MM, O)**
O 84.1–84.6	Thu	16:15–17:45	GER 38	**[DS] Organic Electronics and Photovoltaics IV (jointly with CPP, HL, and O)**
O 85.1–85.10	Thu	16:30–19:00	WIL A317	**Electron and spin dynamics I**
O 86.1–86.12	Thu	16:30–19:30	WIL B122	**Heterogeneous catalysis I**
O 87.1–87.7	Thu	17:15–19:15	TRE Phy	**Focussed session: Theory and computation of electronic structure: new frontiers VII (jointly with HL, DS)**
O 88.1–88.9	Thu	17:15–19:30	PHY C213	**Metal substrates: Adsorption of organic / bio molecules IX**
O 89.1–89.4	Thu	17:15–18:15	WIL B321	**Methods: other (experimental)**
O 90.1–90.9	Thu	17:15–19:30	WIL C107	**Electronic structure III**
O 91.1–91.9	Thu	17:15–19:30	WIL C307	**Epitaxy and growth: Oxides and insulators**
O 92	Thu	19:30–20:00	TRE Phy	**General Meeting of the Surface Science Division**
O 93	Thu	20:00–21:00	TRE Phy	**Post Deadline Session**
O 94.1–94.1	Fri	10:15–11:00	TRE Phy	**Invited Talk (Ralph Gebauer)**
O 95.1–95.1	Fri	10:15–10:45	HSZ 04	**[MA] Surface magnetism V**
O 96.1–96.5	Fri	11:15–12:45	TRE Phy	**Focussed session: Theory and computation of electronic structure: new frontiers VIII (jointly with HL, DS)**
O 97.1–97.7	Fri	11:15–13:00	PHY C213	**Heterogeneous catalysis II**
O 98.1–98.8	Fri	11:15–13:15	WIL A317	**Graphene VI**
O 99.1–99.7	Fri	11:15–13:00	WIL B321	**Electron and spin dynamics II**
O 100.1–100.5	Fri	11:15–12:30	WIL B122	**Organic electronics and photovoltaics**
O 101.1–101.7	Fri	11:15–13:00	WIL C107	**Particles and clusters II**
O 102.1–102.7	Fri	11:15–13:00	WIL C307	**Epitaxy and growth: Metals and semiconductors II**
O 103.1–103.1	Fri	13:15–14:00	TRE Phy	**Invited Talk (Karsten Reuter)**

Annual General Meeting of the Surface Science Division

Thursday 19:30–20:00 TRE Phy

- Report of the Chairman of the DPG Surface Science Division
- Miscellaneous

Post Deadline Session

Post deadline session on Thursday 20:00–21:00 in TRE Phy, followed by the Surface Science get-together.

O 1: Invited Talk (Rasmita Raval)

Time: Monday 10:15–11:00 Location: TRE Phy

Invited Talk O 1.1 Mon 10:15 TRE Phy

Chirality at surfaces from the single-molecule perspective — •Rasmita Raval — The Surface Science Research Centre and Department of Chemistry, University of Liverpool, UK

Chiral surfaces are of central importance in molecular recognition, sensors, asymmetric catalysis, and optoelectronics. The nanoscale details of how chiral phenomena are nucleated, controlled and propagated in molecular assemblies at metal surfaces have begun to emerge from scanning probe microscopy, a powerful range of surface science techniques and periodic density functional theory.

This talk will outline the mechanisms that underpin mirror-symmetry breaking during self-organisation and 2D crystallisation of molecules at surfaces, leading to sophisticated outcomes e.g. segregation of left-handed objects from right-handed objects, responsivity and self-adaptive behaviour. Ultimately, the chiral response of an entire molecular surface assembly can be traced back to single-molecule recognition events driven by attributes present within individual molecules, such as intrinsic chirality, skeletal distortions and the adsorption footprint placed onto the surface.

Turning to collective phenomena, we find that small population fluctuations of mirror-image molecules can lead to profound non-linearity in chiral behaviour. Further, it can shown that, even in the absence of any chiral bias, the influence of the surface is sufficient to scramble the chiral components of a monolayer and, thus, completely break organisational mirror symmetry. Finally, the progression from supramolecular to robust, covalent chiral superstructures will be demonstrated.

O 2: Focussed session: Theory and computation of electronic structure: new frontiers I (jointly with HL, DS)

Time: Monday 11:15–13:00 Location: TRE Phy

Topical Talk O 2.1 Mon 11:15 TRE Phy

Range separation: success, doubts and perspectives — •Andreas Savin — CNRS and UPMC Univ Paris 6, Laboratoire de Chimie Theorique, F-75252 Paris, France

The difficulty of finding simple approximations for density functionals can be alleviated by passing some of the exchange and correlation description to a wave function. A way to produce such hybrids is to consider that for short-range inter-electronic separations exchange and correlation effects are transferable and thus able to be captured by simple models.

Range-separated hybrids can be applied to different levels of density functional approximation (LDA, GGA, ...) and wave function approximation (single determinant, second order perturbation theory, RPA, coupled cluster, ...).

The methods do not bring significant improvement in most fields of application where density functional approximations have been successful. However, they improve accuracy when usual approximations fail, such as van der Waals interactions [1], or where self-interaction becomes an important issue. The computational effort is smaller than for the corresponding wave function method, mainly because smaller basis sets can be used.

Finally, some unexplored path / open questions will be discussed, such as the choice of the interaction operator, improving the density functional approximation, or the role of mixed "short-range/long-range terms".

[1] W. Zhu, et al, J. Chem. Phys., 132, 244108 (2010).

O 2.2 Mon 11:45 TRE Phy

Van der Waals interactions in semiconductor solids — •Guo-Xu Zhang, Alexandre Tkatchenko, Joachim Paier, Heiko Appel, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, Germany

The binding in semiconductor solids arises mainly from the covalent hybridization of atomic orbitals. Hence, it is typically assumed that van der Waals (vdW) interactions play a minor role for their cohesion. In order to probe this conventional wisdom we develop a method to calculate accurate long-range vdW coefficients for ions and atoms in crystals. We first assess the validity of the Clausius-Mossotti relation between the polarizability and dielectric function for bulk semiconductors by comparing periodic TDDFT calculations to direct extrapolation of the frequency-dependent TDDFT polarizability for finite clusters. We find a good agreement between these two approaches for computing vdW $C_6(V)$ coefficients for a broad variation in the unit cell volume V for diamond, Si, and Ge crystals. When using TDDFT@HSE with the Nanoquanta kernel, the volume-dependent dielectric constant of Si and Ge is in excellent agreement with experimental data. The crystal-field screening reduces the vdW coefficients by a factor of two compared to corresponding free-atom and effective hybridized $C_6[n(r)]$ values [1]. The use of accurate $C_6(V)$ coefficients in the PBE+vdW method [1] improves cohesive properties of Si and Ge in comparison to experimental data. [1] A. Tkatchenko and M. Scheffler, Phys. Rev. Lett., **102**, 073005 (2009).

O 2.3 Mon 12:00 TRE Phy

Van der Waals interactions in complex materials: Beyond the pairwise approximation — •Alexandre Tkatchenko[1], Robert A. DiStasio Jr.[2], Roberto Car[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Princeton University, NJ, USA

Despite the well-known fact that van der Waals (vdW) interactions are many-body in nature and the polarizability is a non-local function, popular vdW-DF [1] and DFT+vdW [2] methods are based on (semi)-local approximations for the polarizability and only model the pairwise part of vdW interactions. Here we show how to go beyond the pairwise (semi)-local approximation to vdW interactions by coupling the recently developed TS scheme [2] with the Fluctuating-Coupled-Dipole Model (CFDM) [3]. The TS scheme provides parameter-free input atomic polarizability distributions and the CFDM allows to model both polarizing and depolarizing local fields, and captures the many-body nature of vdW interactions. Results are presented for small and medium-size molecules, as well as solids. We find that the many-body screening plays a major role in modifying the polarizability of large systems. Our results for vdW coefficients in semiconductor clusters and solids are in excellent agreement with TDDFT calculations. [1] M. Dion *et al.*, Phys. Rev. Lett., **92**, 246401 (2004); [2] A. Tkatchenko and M. Scheffler, Phys. Rev. Lett., **102**, 073005 (2009); [3] M. W. Cole *et al.*, Mol. Simul. **35**, 849 (2009).

O 2.4 Mon 12:15 TRE Phy

The random phase approximation and beyond: an assessment for molecular binding energies and reaction barrier heights — •Xinguo Ren[1], Joachim Paier[2], Patrick Rinke[1], Andreas Grüneis[3], Georg Kresse[3], Gustavo E. Scuseria[4], and Matthias Scheffler[1] — [1]Fritz Haber Institute (Berlin) — [2]Humboldt University (Berlin) — [3]University of Vienna (Vienna) — [4]Rice University (Houston)

The random phase approximation (RPA) for the correlation energy has become a promising approach for describing electronic systems in various bonding situations. Recent efforts have focused mainly on correcting the general tendency of RPA to underestimate bond strengths e.g. by adding corrections from second-order screened exchange (SOSEX) [1,2] or single excitations (SE) [3]. In this work, we systematically assess the influence of SOSEX, SE and their combinations on the atomization energies of the G2-I molecular set, as well as the chemical reaction barrier heights of the HTBH38/04 and NHTBH38/04 benchmark sets [4]. We find that RPA+SOSEX+SE applied as a perturbation to the PBE exchange-correlation functional gives the most balanced description. However, for reaction barrier heights RPA based on PBE turns out to be better and is surprisingly accurate. The underlying mechanism governing the performance of RPA and its variants in different circumstances will be analysed. [1] A. Grüneis *et al.*, J. Chem. Phys. **131**, 154115 (2009). [2] J. Paier *et al.* J. Chem. Phys.

132, 094103 (2010). [3] X. Ren *et al.*, arXiv:cond-mat/1011.2724. [4] Y. Zhao *et al.* J. Phys. Chem. A **109**, 2012 (2005)

O 2.5 Mon 12:30 TRE Phy

Au$_N$ clusters (N=1-6) supported on MgO(100) surfaces: the effect of exact exchange and dispersion interactions on adhesion energies. — •Lauro Oliver Paz-Borbón[1], Giovanni Barcaro[2], Alessandro Fortunelli[2], Sergey Levchenko[1], and Matthias Scheffler[1] — [1]Fritz Haber Institut der Max Planck Gesellschaft, Berlin. — [2]Istituto per i Processi Chimico-Fisici del Consiglio Nazionale delle Ricerche, Pisa.

Understanding the interaction between a metal nanoparticle and an oxide surface is a prerequisite for further development of nanocatalysts displaying tailor-made properties. In this work, we study the interaction of an Au adatom and Au$_N$ clusters (N=2-6) supported on pristine and defected MgO(100) surfaces, using a DFT all-electron full-potential approach [1], under a hierarchy of exchange-correlation (XC) functional approximations: ranging from the generalized gradient approximation (PBE and RPBE) to hybrid functionals (PBE0, HSE06) and exact exchange (EX) plus correlation in the random phase approximation (EX-cRPA/cRPA+). Our results for the Au adatom at the oxygen site show that, by reducing the *self-interaction error* (SIE) through the inclusion of EX, smaller adhesion energies values are found when compared to those calculated using hybrid and semi-local functionals; concurrently, the diffusion energy barrier increases. Dispersion interactions [2] are found to play a crucial role in determining the energetics of Au$_N$ clusters. [1] Blum, V. *et al.*, *Computer Physics Communications* 2009, 2175, 180. [2] Tkatchenko, A., Scheffler, M., *Phys. Rev. Lett.* 2009, 102, 073005.

O 2.6 Mon 12:45 TRE Phy

One dimensional model systems in time-dependent density functional theory — •Nicole Helbig[1], Johanna I. Fuks[1], Ilya V. Tokatly[1,2], and Angel Rubio[1,3] — [1]ETSF Scientific Development Centre and Universidad del País Vasco, San Sebastián, Spain — [2]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

We present a local density approximation (LDA) for one-dimensional (1D) systems interacting via the soft-Coulomb interaction based on quantum Monte-Carlo calculations. Results for the ground-state energies and ionization potentials of finite 1D systems show excellent agreement with exact calculations, obtained by exploiting the mapping of an N-electron system in d dimensions, onto a single electron in $N \times d$ dimensions properly symmetrized by the Young diagrams. We conclude that 1D LDA is of the same quality as its three-dimensional (3D) counterpart, and we infer conclusions about 3D LDA. The linear and non-linear time-dependent responses of 1D model systems using LDA, exact exchange, and the exact solution are investigated and show very good agreement in both cases, except for the well known problem of missing double excitations. Consequently, the 3D LDA is expected to be of good quality beyond linear response. We employ the 1D LDA and exact exchange functionals to investigate the description of Rabi oscillations in time-dependent density functional theory and show that adiabatic approximations to the exchange-correlation potential lead to detuned Rabi oscillations.

O 3: Metal substrates: Adsorption of organic / bio molecules I

Time: Monday 11:15–12:45 Location: PHY C213

O 3.1 Mon 11:15 PHY C213

Electronic structure of a graphene quantum well system: highly ordered coronene and hexa-peri-hexabenzocoronene films on Ag(111) — •Michael Wiessner[1], Sofía Rodríguez[1], Johannes Ziroff[1], Sophia Huppmann[1], Frank Forster[1], Peter Puschnig[2], Achim Schöll[1], Lukas Dössel[3], Klaus Müllen[3], and Friedrich Reinert[1] — [1]Universität Würzburg, Experimentelle Physik VII, D-97074 Würzburg — [2]Chair of Atomistic Modelling and Design of Materials, University of Leoben, 8700 Leoben, Austria — [3]MPI für Polymerforschung, Ackermannweg 10, D-55128 Mainz

We present angular resolved photoemission measurements of highly ordered monolayer thin films of coronene and hexa-peri-hexabenzocoronene (HBC) on the single-crystalline Ag(111) surface. Coronene and HBC molecules can be viewed as finite pieces of a graphene layer containing 7 and 13 honeycomb rings, respectively, terminated by hydrogen atoms. Thus, the photoemission signal in these systems can be explained by the formation of quantum well states derived from graphene wave functions which are laterally confined by the spatial extension of the molecules. We also calculated the electronic structure of coronene/HBC by density functional theory (DFT) assuming a free molecule. The fourier-transformed molecular orbitals are shown to reproduce the angle dependent intensity distribution thereby providing a tool to identify different types of orbitals. In conclusion, the solid state derived quantum well states as well as the molecular based DFT orbitals are both applicable to explain the electronic structure of extended aromatic molecules.

O 3.2 Mon 11:30 PHY C213

Incorporation dynamics of molecular guests into 2D supramolecular host-systems at the liquid-solid interface — •Georg Eder[1], Stephan Kloft[1], Natalia Martsinovich[2], Wolfgang M. Heckl[3,4], and Markus Lackinger[1,3] — [1]LMU Munich, Germany — [2]University of Warwick, UK — [3]Deutsches Museum, Munich — [4]TUM School of Education, Munich

Self-assembly of threefold symmetric tricarboxylic acids at the liquid-solid interface can yield crystalline nanoporous monolayers. Prominent examples are 1,3,5-tricarboxylic acid (TMA) and 1,3,5-benzenetribenzoic acid (BTB), which both form hydrogen bonded porous structures at the nonanoic acid-graphite interface with pore sizes of ∼1.0 nm and ∼2.8 nm respectively. It has been shown - also for many other systems - that such nanoporous networks can be utilized as host-networks for the incorporation of molecular guests.

Up to now, predominantly the initial and final structures have been characterized by in-situ Scanning-Tunneling-Microscopy but very little is known about the dynamics. In order to gain a deeper understanding of the incorporation dynamics, we developed an injection system which allows us to simultaneously image the mononlayers with submolecular resolution while the guests are introduced to the liquid phase. Even with the modest time resolution of the STM, for coronene guests important differences were revealed for different solvents and different pore sizes. Supported by Molecular Mechanics Simulations, the nature of a comparatively long lived intermediate state could be identified.

O 3.3 Mon 11:45 PHY C213

Robust metal-organic networks with carbonitrile group functionalized polyphenyl backbones — •Matthias Marschall[1], Joachim Reichert[1], Florian Klappenberger[1], Willi Auwärter[1], Knud Seufert[1], Svetlana Klyatsakya[2], Mario Ruben[2,3], and Johannes V. Barth[1] — [1]Physik Department E20, TU München, James Frank Str., D-85748 Garching — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology, D-76021 Karlsruhe — [3]Université de Strasbourg, IPCMS, 22, Rue de Loess, F-67034 Strasbourg

During the last years metal directed assembly has been used to fabricate robust supramolecular nanostructures on metal surfaces. To determine the relevant interactions in the realized coordination networks scanning tunneling microscopy (STM) has been employed at low- and at room-temperature. Herein we report on structural changes in the 2D pattern formation on Cu(111) and Ag(111) induced by the position of functional carbonitrile groups in polyphenyl backbones. The observed structures range from highly ordered metal-organic honeycomb lattices to 2D random networks. A complex interplay of molecular interactions, substrate templating effects and molecular degrees of freedom steer the self assembling process in the observed structures and controls the coordination number of the metal coordination center.

O 3.4 Mon 12:00 PHY C213

Ab initio study of a mechanically gated molecule: From weak to strong correlation — Andreas Greuling[1], •Michael Rohlfing[1], Ruslan Temirov[2], Stefan Tautz[2], and Frithjof Anders[3] — [1]Fachbereich Physik,Universität Osnabrück, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, Germany, and JARA — [3]Fakultät für Physik, TU Dortmund, Otto-Hahn-Straße 4, Germany

The electronic spectrum of a chemically contacted molecule in the junction of a scanning tunneling microscope can be modified by tip retraction. We analyze this effect by a combination of density functional, many-body perturbation and numerical renormalization group theory, taking into account both the non-locality and the dynamics of electronic correlation. Our findings, in particular the evolution from a broad quasiparticle resonance below to a narrow Kondo resonance at the Fermi energy, correspond to the experimental observations.

O 3.5 Mon 12:15 PHY C213

Spectroscopy of STM-induced light emission from a molecular double decker on Ag(111) — •Natalia L. Schneider[1], Francesca Matino[1], Guillaume Schull[2], Sandro Gabutti[3], Marcel Mayor[3], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, 67034 Strasbourg, France — [3]Department of Chemistry, University of Basel, St. Johannsring 19,CH-4056 Basel, Switzerland

A low-temperature scanning tunneling microscope (STM) is used to investigate the electronic states and the STM-induced light emission from naphtalenediimide cyclophane molecules on Ag(111). The cyclophane consists of two parallel π-systems, one of which is adsorbed directly at the metal substrate while the other chromophore is hoped to be partially decoupled from the surface. This intra-molecular decoupling scheme complements previous approaches where molecular multilayers or dielectrics were used. Spectra of the light emission from a single cyclophane layer exhibit molecule-related features and provide information on the excitation processes involved.

O 3.6 Mon 12:30 PHY C213

Electronic Mapping of Molecular Orbitals at the Molecule-Metal Interface — Maria Christina Lennartz, •Vasile Caciuc, Nicolae Atodiresei, Silvia Karthäuser, and Stefan Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In the present contribution we report on a combined experimental and theoretical study aimed to investigate the electronic structure of an aromatic organic molecule like pyridine-2,5-dicarboxylic acid ($C_7H_4NO_4$) chemisorbed on the Cu(110) surface. From experimental point of view, the electronic structure of the molecule-Cu(110) was determined by performing scanning tunneling spectroscopy (STS) measurements which enabled us to map the molecular orbitals as a function of tip position. By comparing the experimental differential conductance curves with the calculated density of states for different conformers of this organic molecule on Cu(110), the character (σ or π) of the individual molecular orbitals probed in STS could be clearly identified.

[1] M. C. Lennartz, V. Caciuc, N. Atodiresei, S. Karthäuser, and S. Blügel, Phys. Rev. Lett. **105**, 066801 (2010).

O 4: Focussed session: Transparent conductive oxides I (jointly with HL, DS)

Time: Monday 11:15–13:00 Location: WIL A317

Topical Talk O 4.1 Mon 11:15 WIL A317

Surface and Bulk Properties of Post-Transition Metal Oxide Semiconductors — Philip D.C. King, Sepehr Vasheghani Farahani, Tim D. Veal, and •Chris F. McConville — Department of Physics, University of Warwick, Coventry, CV4 7AL UK

Oxide semiconductors have become of great interest lately with enormous opportunities for new uses that will potentially improve existing materials and device applications. The fact that some of these materials, such indium tin oxide, in a relatively low quality form, have seen significant industrial use as transparent conductors has perhaps contributed to the belated recognition of the possibilities as semiconductors in their purer form. Here, the surface and bulk electronic properties of epitaxially grown high-quality oxide semiconductors (In_2O_3, CdO, and ZnO) will be discussed. Optical, electronic and structural properties of these semiconducting oxide films will be presented. The valence band density of states and the surface electronic properties of these oxide semiconductors have been studied using high-resolution photoemission spectroscopy and compared with theoretical band structure calculations. A common property of these oxide semiconductors is found to be the presence of a surface electron accumulation layer, in marked contrast to the electron depletion generally observed at the surfaces of conventional semiconductors. Additionally, hydrogen is found to be a donor and any native defects have a propensity to be donors in already n-type material. The origin of these phenomena will be discussed in terms of the band structure and intrinsic properties of these materials.

Topical Talk O 4.2 Mon 11:45 WIL A317

***Ab-initio* calculation of electronic and optical properties of transparent conductive oxides** — •André Schleife[1,3], Claudia Rödl[1], Frank Fuchs[1], Jürgen Furthmüller[1], Benjamin Höffling[1], Karsten Hannewald[1], Patrick Rinke[2], Joel Varley[3], Anderson Janotti[3], Chris G. Van de Walle[3], and Friedhelm Bechstedt[1] — [1]IFTO and ETSF, FSU Jena, Germany — [2]FHI and ETSF, Berlin, Germany — [3]Materials Department, UC Santa Barbara, USA

Parameter-free calculations are a modern and sophisticated complement to advanced experimental techniques when exploring the properties of materials. Due to the rapidly increasing computing power they promise a deep understanding of the underlying physics also for more complex transparent conductive oxides.

We take the excitation aspect of photoemission processes into account by calculating the quasiparticle electronic structure using the modern HSE03+G_0W_0 framework. Solving a Bethe-Salpeter equation for the optical polarization function allows us to account for excitonic and local-field effects that govern the optical absorption.

After an introduction into these recent theoretical-spectroscopy techniques we apply them to ZnO, SnO_2, In_2O_3, and Ga_2O_3. We present results for the electronic band structure (including spin-orbit coupling), the band alignment, dielectric functions, exciton binding energies, and optical oscillator strengths. The influence of a degenerate electron gas, which occurs in these typically n-type materials, is investigated. Our findings are discussed with respect to available experimental results.

Topical Talk O 4.3 Mon 12:15 WIL A317

Bulk semiconducting oxides: crystal growth and physical properties — •Roberto Fornari — Leibniz Institute for Crystal Growth, IKZ, Max-Born-Str. 2, 12489 Berlin

Semiconducting oxides have attracted considerable interest in the last few years. In addition to the widely studied ZnO, much attention has recently been devoted to Ga2O3, In2O3 and SnO2. The epitaxial growth has already been achieved on different hetero-substrates; however due to the relatively poor crystallographic quality of the obtained layers it was not possible to get devices or even reliably measure their physical properties so far. It is thus urgent to provide homo-substrates which may allow the deposition of high-quality epilayers with low residual carrier density and fewer extended defects. IKZ has recently undertaken an effort to grow large single crystals of these oxide compounds. In this presentation the growth of transparent semiconducting Ga2O3 single crystals will be reviewed. Single crystals with diameter of 18 mm diameter and 50-60 mm length were grown along the b-axis from an Iridium crucible under a dynamic protective atmosphere. The transmission in IR-region was directly correlated with the free carrier concentration and was found to depend on the growth atmosphere and/or post growth annealing. Typical electrical properties at room temperature are: resistivity = 0.12 Ohmcm, electron concentration = 2-5E17 cm-3 and mobility = 110 cm2/Vs; these results seem to derive from a donor level with activation energy of about 32 meV. Results of thermodynamic calculations, dislocation density studies, ICP-OMS, DTA, EPR and High Resolution TEM are also presented.

O 4.4 Mon 12:45 WIL A317

The electronic properties of β -Ga_2O_3 — •Mansour Mohamed[1], Christoph Janowitz[1], Isaak Unger[1], Zbigniew Galazka[2], Justin R. Weber[3], and Recardo Manzke[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-

Born-Str. 2, 12489 Berlin, Germany — [3]Materials Department, University of California, Santa Barbara, California 93106-5050, USA

Ga_2O_3 belongs to the group of transparent conducting oxides (TCOs) with a wide band gap. It exhibits the largest band gap with E_g = 4.9 eV [1] and thus a unique transparency from the visible into the UV region. The n-type high-quality β -Ga_2O_3 single crystals were grown by the Czochralski method [2]. The crystals were characterized by different techniques (LEED, STM). The experimental valence band structure of β-Ga_2O_3 was determined by high-resolution angle-resolved photoelectron spectroscopy (ARPES) utilizing synchrotron radiation. The calculated band structure was determined using advanced density functional theory (DFT) calculations employing hybrid functionals and projector augmented wave (PAW) potentials. From theory, we obtained a direct band gap of 4.87 eV and a slightly smaller indirect band gap of 4.83 eV, with the valence-band maximum (VBM) located slightly away from the M symmetry point. The experimental band structure of β-Ga_2O_3 is compared and discussed with the theoretical calculations. The effect of changing the temperature from 300K to 20K on the experimental band structure β-Ga_2O_3 was studied.

O 5: Spin-Orbit Interaction at Surfaces I

Time: Monday 11:15–12:45 Location: WIL B321

O 5.1 Mon 11:15 WIL B321

Topologically trivial and non-trivial states at the surface of Bi_2Se_3 — •Hadj Mohamed Benia, Klaus Kern, and Christian R. Ast — Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany

Angle Resolved Photon Emission Spectroscopy (ARPES) measurements at the surface of Bi_2Se_3 single crystals show the existence of Rashba spin-split quantum-well states (QWS) together with the known topological surface state around the Γ point. Up to three QWS with different Rashba-splitting are observed between the Fermi level and the Dirac point. The origin of the QWS is traced back to a formation of a 2D electron gas at the crystal surface as a result to downward bending of the conduction band. A shift to higher binding energies of the QWS accompanied with a change in the Rashba splitting is observed as function of time and temperature. A triangular potential is used to model the band bending, fit the QWS levels, and extract the corresponding potential asymmetry at the surface for various measurement conditions.

O 5.2 Mon 11:30 WIL B321

Spin-resolved electronic structure of the surface Rashba-system Bi/Cu(111) — •Hendrik Bentmann[1], Takuya Kuzumaki[2], Gustav Bihlmayer[3], Kazuyuki Sakamoto[2], and Friedrich Reinert[1] — [1]Universität Würzburg, Experimentelle Physik VII, Am Hubland, D-97074 Würzburg, Germany — [2]Graduate School of Advanced Integration Science, Chiba University, Chiba 263-8522, Japan — [3]Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

Recently several surface adsorbate systems on metal and semiconductor substrates have been identified whose electronic structure is heavily influenced by the spin-orbit interaction. The spin orientation of the polarized electronic states in these systems can show quite unexpected effects including sign changes within a single band or even a complete rotation out of the plane [1,2]. Here we report spin- and angle-resolved photoemission experiments on the surface alloy Bi-Cu(111)$(\sqrt{3} \times \sqrt{3})R30°$. The results directly demonstrate that the Bi-induced surface state bands of sp_z orbital character are split in energy by the spin-orbit interaction. The spin orientation is found to be in accordance with the Rashba model within the probed energy window. Another surface state of p_xp_y character shows no spin polarization suggesting that this state consists of two unresolvable components of opposite spin orientation. First-principles calculations of the spin orientation vectors are in line with the experimental observations.

[1] H. Mirhosseini *et al.*, Phys. Rev. B **79**, 245428 (2009).

[2] K. Sakamoto *et al.*, Phys. Rev. Lett **103**, 156801 (2009).

O 5.3 Mon 11:45 WIL B321

Strong effect of substrate termination on Rashba spin-orbit splitting: Bi on $BaTiO_3(001)$ from first principles — •Samir Abdelouahed and Jürgen Henk — Max Planck Institute of Microstructure Physics, Halle, Germany

A sizable Rashba splitting of surface states requires a number of ingredients: a strong atomic spin-orbit coupling, a steep surface-potential barrier, and a large in-plane potential gradient. We demonstrate by first-principles calculations that a suitable substrate termination is another prerequisite.

Our calculations for a Bi adlayer on $BaTiO_3(001)$ show that the Rashba spin-orbit splitting in the Bi-6*p* states is strongly affected by the substrate termination. For the TiO_2 termination the absolute splitting is very large (about $0.23\,Å^{-1}$) and can be mildly affected by the orientation of the electric polarization in the ferroelectric substrate [1]. In striking contrast, the splitting becomes strongly reduced for the BaO termination (less than $0.07\,Å^{-1}$). Our findings are explained by the termination-dependent hybridization of the Bi surface states with electronic states in the substrate. It turns out that a strongly asymmetric charge density at the site of the heavy element (here: Bi) is a signature of a large Rashba splitting.

[1] H. Mirhosseini et al, Phys. Rev. B **81** (2010) 073406.

O 5.4 Mon 12:00 WIL B321

Local structure of the mixed surface alloy Bi_xPb_{1-x}/Ag(111) measured with scanning tunneling microscopy — •Fabian Zinser, Maximilian Assig, Klaus Kern, and Christian R. Ast — Max Planck Institute for Solid State Research, Stuttgart, Germany

The mixed surface alloy Bi_xPb_{1-x}/Ag(111) is part of a class of surface alloys that exhibit a 2D electronic structure with an extremely large spin-splitting [1]. In this surface alloy, changing the concentration ratio x allows the continuous tuning of the spin splitting as well as the band occupation [2]. With the ability of scanning tunneling microscopy (STM) to discern single bismuth and lead atoms from each other, new insight into the local structure of these systems is possible. Here we present our studies of the local structure for different compositions of the mixed surface alloy Bi_xPb_{1-x}/Ag(111).

[1] C. R. Ast *et al.*, Phys. Rev. B **75**, 201401(R) (2007)

[2] C. R. Ast *et al.*, Phys. Rev. B **77**, 081407(R) (2008)

O 5.5 Mon 12:15 WIL B321

Spin-resolved measurements of the Rashba-split surface state on Au(111) above the Fermi level — Sune N. P. Wissing[1], •Anna Zumbülte[1], Christian Eibl[1], Anke B. Schmidt[1], Jürgen Braun[2], and Markus Donath[1] — [1]Physikalisches Institut, Westfaelische Wilhelms-Universitaet, Wilhelm-Klemm-Str. 10, 48149 Muenster, Germany — [2]Dept. Chemie und Biochemie, LMU München, Germany

We report on the first spin-resolved measurement of an unoccupied Rashba-split surface state via inverse photoemission.

Since the discovery of the spin-orbit splitting on a Au(111) surface by LaShell *et al.* [1] in 1996, many different systems have been investigated for a better understanding of Rashba-type phenomena. Yet it was not possible to expand the present information by spin-resolved measurements above the Fermi level.

Spin and angle-resolved inverse photoemission is a powerful tool to determine the unoccupied electronic structure of solid surfaces and thin films. In order to demonstrate the potential of this method for investigating interesting Rashba phenomena, we present measurements of the prototype Rashba system: the Au(111) surface. We were able to confirm the Rashba splitting of the surface state as it continues above the Fermi level. Moreover, we investigated its behaviour when the surface state becomes degenerate with bulk states.

[1] S. LaShell *et al.*: Phys. Rev. Lett. **77**, 3419 (1996)

O 5.6 Mon 12:30 WIL B321

Anisotropic Scattering of Bi(111) Surface State Electrons at a Point Defect Visualized by Low Temperature Scanning Tunneling Microscopy and Spectroscopy — •Maren Cottin[1], Christian Bobisch[1], Johannes Schaffert[1], Andreas Sonntag[1], Giriraj Jnawali[1], Gustav Bihlmayer[2], and Rolf Möller[1] — [1]Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

The semimetal bismuth (Bi) has recently attracted a lot of attention due to its interesting transport properties. The metallic surface states which occur on various of its surfaces underlie a large spin orbit splitting. We use scanning tunneling microscopy to analyze the lateral variation in the local density of states in the vicinity of a point defect on a Bi(111)-surface. The observed pattern in the dI/dV-images visualizes the scattering of surface state electrons. At energies close to the Fermi level, the pattern is highly anisotropic and shows a threefold symmetry. Using the calculated Fermi surface of Bi(111) the scattering processes are ascribed to spin-conserving transitions between two spin orbit split surface states. The scattering pattern can be simulated by the superposition of three monochromatic waves where the phase with respect to the scattering center has a significant impact on the appearance and the symmetry of the pattern.

O 6: Semiconductor substrates: Adsorption

Time: Monday 11:15–13:00 Location: WIL B122

O 6.1 Mon 11:15 WIL B122

Silber-induzierte Vorstrukturierung vicinaler Si-Oberflächen für das Wachstum von Ge-Nanostrukturen — •Inga Heidmann[1], Moritz Speckmann[1], Thomas Schmidt[1], Miguel Angel Niño Orti[2], Tevfik Onur Menteş[2], Andrea Locatelli[2] und Jens Falta[1] — [1]Institut für Festkörperphysik, Universität Bremen, 28359 Bremen — [2]Sincrotrone Trieste, 34 149 Basovizza/Trieste, Italien

Der Einsatz von Adsorbaten ist ein vielversprechender Ansatz, das Wachstum von Ge-Nanostrukturen auf Si-Oberflächen durch Vorstrukturierung der Substratoberfläche und Modifikation des Wachstums selbst gezielt zu beeinflussen. Zu diesem Zweck kamen verschiedene oberflächensensitive Methoden wie hochauflösende niederenergetische Elektronenbeugung (SPA-LEED), niederenergetische Elektronenmikroskopie (LEEM) sowie Rasterelektronenmikroskopie (SEM) zur Anwendung. Während zur Vorstrukturierung bisher verstärkt Adsorbate aus den III. und V. Hauptgruppen untersucht wurden, wurde in diesem Fall das Adsorptionsverhalten von wenigen Monolagen Silber auf der Si(112)- sowie Si(113)-Oberfläche charakterisiert. Hierbei konnte jeweils eine Ausbildung von regelmäßigen Nanofacetten festgestellt werden. Zudem wurde der Einfluss der mit Silber vorstrukturierten Oberflächen auf das anschließende Ge-Wachstum analysiert, wobei anisotrope Inseln mit einer verstärkten Ausrichtung entlang der Facetten beobachtet werden konnten.

O 6.2 Mon 11:30 WIL B122

In situ surface analysis of Ge(100) for III-V heteroepitaxy — •Sebastian Brückner[1], Enrique Barrigón[2], Oliver Supplie[1], Johannes Luczak[1], Peter Kleinschmidt[1], Henning Döscher[1], Ignacio Rey-Stolle[2], Carlos Algora[2], and Thomas Hannappel[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Instituto de Energía Solar, Universidad Politécnica de Madrid, ETSI de Telecomunicación, Avda. Complutense s/n, 28040 Madrid, Spain

Ge(100) is the established substrate for current world record III-V triple junction solar cells. However, uncertainties still remain regarding the atomic surface structure of the Ge(100) substrates prior to the MOVPE III-V heteroepitaxy. Here, we have applied in situ reflectance anisotropy spectroscopy (RAS) to study the influence of different group V precursors and reactor background contaminations on Ge(100) surfaces, that affect the subsequent III-V layer growth. A contamination free MOVPE to UHV transfer system allowed us to analyse different Ge(100) surfaces with various UHV based surface sensitive techniques such as x-ray photo electron spectroscopy (XPS), low energy electron diffraction (LEED), and scanning tunneling microscopy (STM). In this way, we were able to correlate the results of these surface analysis with the characteristic in situ RA spectra of the different clean, As and P terminated Ge surfaces. For instance, XPS measurements confirmed oxide removal and the corresponding termination. On the other hand, LEED measurements showed the influence of group V precursors and background As pressure on the surface reconstruction.

O 6.3 Mon 11:45 WIL B122

Strukturelle Untersuchungen zur Ga-Adsorption auf Si(110) — •Torsten Wilkens, Thomas Schmidt und Jens Falta — Institut für Festkörperphysik, Universität Bremen, 28359 Bremen

Niederdimensionale Halbleiterstrukturen wie Quantendrähte versprechen vielfältige Anwendungsmöglichkeiten. Eine Methode der Herstellung solcher Nanostrukturen ist die Abscheidung sich selbstorganisierender Strukturen auf neuartigen Template-Substraten. In diesem Kontext wurde die Adsorption von Gallium auf der 16×2-rekonstruierten Si(110)-Oberfläche mit Hilfe von Rastertunnelmikroskopie (STM) und hochauflösender niederenergetischer Elektronenbeugung (HR-LEED) untersucht.

Als Ergebnis dieser Messungen werden erste Aufnahmen der Gaterminierten Si(110)-Oberfläche im Realraum präsentiert, welche eine $3\sqrt{3} \times \sqrt{3} - R54,7°$-Rekonstruktion zeigen mit in zwei Domänen ausgerichteten Streifen, deren mit HR-LEED bestimmten Orientierungen exakt senkrecht zu den Ausrichtungen der Streifen der darunter liegenden 16×2-Rekonstruktion sind, also in Richtung $\langle 1\bar{1}1 \rangle$ und $\langle \bar{1}11 \rangle$. Darüber hinaus belegen die STM-Messungen eine vollständige Bedeckung der Oberfläche unabhängig davon, ob zuvor unrekonstruierte Bereiche vorlagen oder nicht. Mit Hilfe hochauflösender STM-Aufnahmen lassen sich die Streifen der $3\sqrt{3} \times \sqrt{3} - R54,7°$-Rekonstruktion als Aneinanderreihung rechteckiger Einheiten sichtbar machen. Diese Rechtecke wiederum existieren in zwei unterschiedlichen Ausdehnungen, wobei der breitere der beiden Typen eine bevorzugte Anordnung in Ketten senkrecht zu den Streifen zeigt.

O 6.4 Mon 12:00 WIL B122

Adsorption dynamics of ethylene on Si(001) — •Marcus Lipponer[1], Nico Armbrust[1], Michael Dürr[1,2], and Ulrich Höfer[1] — [1]Philipps Universität, D-35037 Marburg — [2]Hochschule Esslingen, D-73728 Esslingen

The functionalization of semiconductor surfaces by means of organic molecules is of great interest due to possible applications in the field of nanoelectronics. However, only little information on the reaction dynamics of these systems is available. In this work, the adsorption dynamics of ethylene on Si(001) has been investigated. With ethylene being the most simple unsaturated organic molecule, the system serves as a model system for non-activated adsorption on semiconductor surfaces. In order to investigate its reaction dynamics, we employed a supersonic molecular beam which allows for the control of the kinetic energy of the impinging molecules. Additionally, surface temperature and the excitation of internal degrees of freedom were varied when measuring the sticking coefficients as a function of relative surface coverage by means of King and Wells techniques. With increasing kinetic energy of the impinging molecules, we find a decrease of the initial sticking coefficient as it is typical for non-activated reaction channels; with increasing surface temperature a decrease of the initial sticking coefficient is observed. Surprisingly, the maximum surface coverage also decreases with increasing surface temperature. The excitation of the internal degrees of freedom is shown to have a minor impact on the reactivity. The results are discussed in the context of a reaction channel via a mobile precursor.

O 6.5 Mon 12:15 WIL B122

Adsorption of small organic ring molecules on GaP(001)(2x4) — •Marcel Ewald[1,2], Johannes Falkenburg[1,2], Michael Kneissl[1], Norbert Esser[2], and Patrick Vogt[1] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin — [2]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Department Berlin, Albert-Einstein-Str. 9, 12489 Berlin

For the application of organic/semiconductor interfaces, in particular of III-V compounds, the interface atomic formation and structure are crucially important. We have investigated the binding configuration and binding structure of small organic ring molecules like cyclopentene, pyrridazine and pyrrole on the GaP(001)(2x4) surface reconstruction. The molecule terminated samples were analysed by low energy electron diffraction (LEED), Xray photoemission spectroscopy (XPS) and reflectance anisotropy spectroscopy (RAS) in a spectral range from 1.5eV to 8.5eV. We found, that the different molecules lead to different contributions within the optical anisotropy between 6-8eV resulting from the different electronic properties of the molecules. Numerical analysis of the C1s core level indicates different adsorption geometries of molecule and the GaP(001)(2x4) surface.

O 6.6 Mon 12:30 WIL B122

First-principles study of the organic/ZnO (000$\bar{1}$)-O interface: the role of van der Waals interactions — •Yong Xu, Patrick Rinke, Oliver Hofmann, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Hybrid inorganic/organic materials have opened up new opportunities for the development of optoelectronics, benefiting from the potential to combine the best features of two distinct material classes. The understanding of their interfacial properties is of critical importance to develop new basic concepts for optoelectronic devices or to optimize device designs. In this work, we studied the interface between the ZnO (000$\bar{1}$)-O surface and a prototypical organic acceptor 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ) by first-principles approaches implemented in the FHI-*aims* code, focusing on the effects of van der Waals (vdW) interactions. We applied and compared various methods to treat vdW interactions, including the non-local Langreth-Lundqvist exchange-correlation functional, exact-exchange plus correlation in the random phase approximation (RPA), and the $C_6[n]/R^6$ correction approach by Tkatchenko and Scheffler. While F4TCNQ binds strongly to the clean ZnO (0001)-Zn surface density-functional theory (DFT) with the PBE exchange-correlation funtional gives only weak physical adsorption on the ZnO (000$\bar{1}$)-O surface. VdW corrections pull the molecule closer to the surface and considerably enhance the binding energy, emphasizing the importance of vdW interactions for this material class.

O 6.7 Mon 12:45 WIL B122

Hydrogen Adsorption on polar ZnO(0001)-Zn - extending equilibrium surface phase diagrams to kinetically stabilised structures — •Mira Todorova[1], Markus Valtiner[2,3], and Jörg Neugebauer[1] — [1]Dept. for Computational Materials Design, Max-Planck-Insitut für Eisenforschung GmbH, Düsseldorf — [2]Dept. for Interface Chemistry and Surface Engineering, Max-Planck-Insitut für Eisenforschung GmbH, Düsseldorf — [3]Dept. for Chemical Engineering, University of California, Santa Barbara, CA 93106-5080, USA

Hydrogen adsorption on the Zn-terminated polar ZnO(0001) surface is studied by a combination of density-functional theory calculations and *atomistic thermodynamics*. Going beyond the thermodynamic limit and constructing meta-stable phase diagrams we extend the concept of equilibrium surface phase diagrams to include kinetically stabilised surface reconstructions. Using this approach we were able to identify new and hitherto not reported structures that become stable under non-equilibrium extreme H-rich conditions. Experimental situations that realise such conditions will be discussed.

M. Valtiner, M. Todorova, and J. Neugebauer, Phys. Rev. B **82**, 165418 (2010).

O 7: Surface Dynamics I

Time: Monday 11:15–13:00 Location: WIL C107

O 7.1 Mon 11:15 WIL C107

Observation of the Surface Segregation of Cu in Pd by Time-Dependend Positron-Annihilation-Induced Auger Electron Spectroscopy — •Christoph Hugenschmidt, Jakob Mayer, and Klaus Schreckenbach — FRM II und Lehrstuhl E21 Physik Department, Technische Universität München, 85747 Garching

Density functional theory calculations predict the surface segregation of Cu in the second atomic layer Pd which was not unambiguously confirmed experimentally so far. We report measurements on Pd surfaces covered with three and six monolayers of Cu using the element selective positron annihilation induced Auger electron spectroscopy (PAES) which is sensitive to the topmost atomic layer. Moreover, time resolved PAES, which was applied for the first time, enables the investigation of the dynamics of surface atoms and hence the observation of the segregation process. The time constant for segregation was experimentally determined to 1.38(0.21)h, and the final segregated configuration was found to be consistent with calculations. Within this work, we demonstrate that time dependent PAES is a novel element selective technique applicable for numerous systems for the investigation of e.g. heterogeneous catalysis, corrosion or surface alloying.

O 7.2 Mon 11:30 WIL C107

LEEM study of segregation and diffusion of impurities at Fe polycrystal surfaces — •Benjamin Borkenhagen[1], Thorsten Franz[2], Gerhard Lilienkamp[1], and Winfried Daum[1] — [1]IEPT, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — [2]ELMITEC GmbH, Albrecht-von-Grodeck-Str. 3, 38678 Clausthal-Zellerfeld

Surface properties of applied materials are frequently related to microstructural properties such as texture, grain boundaries and stacking faults in polycrystals. The application of methods providing information on surface crystallography and topography with sub-grain lateral resolution is a most promising route for the surface characterization of such materials. Recently we have demonstrated that low energy electron microscopy (LEEM) is well suited to image surfaces of crystallites and grain boundaries intersecting the surface of polycrystals. In this contribution we report on our application of LEEM to monitor segregation and diffusion processes at the surface of polycrystalline Fe samples. During thermal treatment of the Fe polycrystal, we observed formation of islands which consisted of bulk impurities segregated to the surfaces of the crystallites. Depending on temperature ramp and surface orientation of the crystallites, different shapes of these islands were observed. At elevated temperatures Ostwald ripening of the impurity islands occurred. Increasing the temperature even more caused dissolution of these islands via diffusion into the bulk of the polycrystal, mainly along grain boundaries. In the majority of these transformations the polycrystalline texture remained unaffected by segregation and diffusion processes, but we also observed grain boundary motion.

O 7.3 Mon 11:45 WIL C107

Ultrafast melting of a charge-density wave in the Mott insulator 1*T*-TaS$_2$ — •Stefan Hellmann, Christian Sohrt, Timm Rohwer, Matthias Kalläne, Michael Bauer, Lutz Kipp, and Kai Rossnagel — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel, Germany

Femtosecond time-resolved core-level photoemission spectroscopy with the free-electron laser FLASH as well as time- and angle-resolved photoemission spectroscopy with a higher-harmonics-generation source are used to measure the atomic-site and momentum specific charge-order dynamics of the charge-density wave in the Mott insulator 1*T*-TaS$_2$. After strong photoexcitation, melting of the charge-density wave and the accompanying periodic lattice disortion is observed on two timescales. The subsequent fast electron-phonon thermalization drives the system across a phase transition from a long-range charge ordered state to a quasi-equilibrium state with domain-like short-range charge and lattice order. The combination of the two complementary sources opens the way to study the nonequilibrium dynamics of condensed matter systems with full momentum, elemental, chemical, and atomic-site selectivity.

O 7.4 Mon 12:00 WIL C107

Waveguiding of hot surface state electrons by the Au(111) reconstruction — •Viktor Geringer[1,2], Dinesh Subramaniam[1,2], Florian Libisch[3], Marcus Liebmann[1,2], and Markus Morgenstern[1,2] — [1]II. Institute of Physics, RWTH Aachen University, Otto-Blumenthal-Str., 52074 Aachen, Germany — [2]JARA: Fundamentals of Future Information Technology — [3]Institute for Theoretical Physics, Vienna University of Technology, Wiedner Hauptstraße 8-10/136, A-1040 Vienna, Austria

Using scanning tunneling spectroscopy (STS) we perform a spatial and energy dependent study of the electronic scattering behavior on the Au(111) surface. In spite of the small surface reconstruction potential (35 meV), our measurements reveal a surprising effect of wave guiding. Electrons with energies up to twenty times larger than the corrugation of the potential follow the geometry of the reconstruction, observable through a strong anisotropy in the distribution of the wave vectors. In order to explain this behavior we calculated the square of the electronic wave function evidencing quantum-mechanical orthogonality as the origin of the waveguiding effect.

O 7.5 Mon 12:15 WIL C107

Kinetic energy distributions of vibrationally promoted electrons at metal surfaces: Comparison of different initial vibrational states — •Tim Schäfer[1], Jerry Larue[2], Daniel Matsiev[2], Luis Velarde[2], Daniel J. Auerbach[2], and Alec M. Wodtke[1] — [1]Georg-August Universität Göttingen, Institut für Physikalische Chemie, Tammannstr.6, 37077 Göttingen, Germany — [2]Department of Chemistry and Biochemistry, University of California, Santa Barbara, CA 93106-9510, USA

Kinetic energy distributions of exoelectrons produced by collisions of highly vibrationally excited NO molecules with a low work function Cs dosed Au surface were studied. The NO molecules were optically prepared in $X^2\Pi_{1/2}$ (v=16) and $X^2\Pi_{1/2}$ (v=22) using Stimulated Emission Pumping (SEP) and the electron energy distributions were measured with a home-built retarding field electron energy analyzer. The results obtained by these experiments indicate that many quanta, as high as Δv =17 for v=22, can be transferred to a single electron. The most probable transfer of vibrational quanta is Δv =11 for NO(v=16) and Δv = 12 for NO(v=22) and is in qualitatively good agreement with previous studies. In addition to the results obtained by the experiments with the SEP prepared molecules the study of vibrationally excited molecules produced by spontaneous emission (Franck-Condon pumping, FCP) supports the overall conclusion: The kinetic energy distribution of vibrationally promoted electrons strongly suggests a coupling of multiple vibrational quanta to a single electron and cannot be explained in a simple adiabatic picture.

O 7.6 Mon 12:30 WIL C107

Optimal control of open quantum systems applied on photochemistry on surfaces — Erik Asplund and •Thorsten Klüner — Carl von Ossietzky Universität Oldenburg, Germany

A quantum system in condensed phase, which undergoes strong dissipative processes, is an open quantum system. From the theoretical viewpoint it is important to model open quantum systems in a rigorous way. The description of open quantum systems can be realized within the “Surrogate Hamiltonian” approach, which is a non-Markovian approach. In the “Surrogate Hamiltonian” approach, a quantum system is separated into a primary system and a bath. Besides the traditional formulation of dissipative processes through the spectral density, the “Surrogate Hamiltonian” method enables a microscopic description of excitation and relaxation process for open quantum systems.

Light interacting with atoms and molecules is not only a source of information about the atoms and molecules studied, it can also initiate charge and energytransfer processes, i.e. manipulate the evolution of the molecules studied. A theoretical tool for the design of laser pulses to transfer an initial state to a final state is optimal control theory (OCT). Besides the traditionalfinal-time control algorithms, there exist methods to also handle time-dependent control targets. In this talk, OCT with time-dependent targets is combined with the “Surrogate Hamiltonian” method in order to gain control of dissipative quatum systems. Two model systems representing adsorbate-surface systems will be presented and the controllability of the systems will be discussed.

O 7.7 Mon 12:45 WIL C107

Rotational and constitutional dynamics of caged supramolecules — •Florian Klappenberger[1], Dirk Kühne[1], Wolfgang Krenner[1], Svetlana Klyatskaya[2], Mario Ruben[2], and Johannes V. Barth[1] — [1]Physik Department E20, TU München, Germany — [2]Institute of Nanotechnology, Forschungszentrum Karlsruhe, Karlsruhe, Germany

The confinement of guest species in nanoscale environments leads to dynamic phenomena. Notably the organization and rotational motions of individual molecules were controlled by carefully designed, fully supramolecular host architectures. Here we use an open 2D coordination network on a smooth metal surface to steer the self-assembly of discrete trimeric guest units, identified as noncovalently bound dynamers. Each caged chiral supramolecule performs concerted, chirality-preserving rotary motions within the template honeycomb pore, which are visualized and quantitatively analyzed using temperature-controlled scanning tunneling microscopy. Furthermore, with higher thermal energies, a constitutional system dynamics appears, which is revealed by monitoring repetitive switching events of the confined supramolecules chirality signature, reflecting decay and reassembly of caged units.

O 8: Oxides and insulators: Adsorption I

Time: Monday 11:15–13:00 Location: WIL C307

O 8.1 Mon 11:15 WIL C307

Ab initio calculations on the interaction of CO with C_{60} — •Jan Mitschker and Thorsten Klüner — Carl von Ossietzky Universität Oldenburg, PO Box 2503, 26111 Oldenburg, Germany

The outstanding properties of C_{60}-Fullerenes aroused high interest ever since this class of molecules has been discovered. In spite of the large number of atoms they are only composed of one element and are a new modification of carbon. They form *molecular* systems but are of well-defined shape and large size.

Our group is interested in elementary processes on surfaces, especially the dynamics of excited states. So far adsorption and photodesorption of small molecules on metal-oxide surfaces have been investigated. Photodesorption can be considered as a prototyp of non-adiabatic surface reactions.

In this study we use first-principle methods to characterize the interaction of CO with a *single* C_{60}-molecule. In contrast to metal-oxides C_{60} is a completely covalent system. Therefore, the interaction is very weak, making correlation methods and BSSE-correction necessary. Experimentally an adsorption energy of 8 kJ/mol has been estimated.[1] On MP2-level using a cc-pVTZ basis set an energy of 8.5 kJ/mol for the adsorption on top of a hexagon was found. Due to the large basis set (1860 basis functions) excited state calculations necessary for the theoretical modelling of photodesorption are very demanding. In order to encounter this challenge, we propose different computational strategies and report first results.

[1] M. Folman et al., *Langmuir* 13 (1997) 1118–1122.

O 8.2 Mon 11:30 WIL C307

DFT study of the Interaction of Hydrogen with $ZnO(10\bar{1}0)$ Surfaces — •Jakub Goclon and Bernd Meyer — Interdisciplinary Center for Molecular Materials ICMM and Computer-Chemistry-Center CCC, University of Erlangen-Nürnberg, Germany

Understanding the interaction of hydrogen with ZnO is of fundamental interest in view of its widespread use in heterogeneous catalysis for hydrogenation and dehydrogenation reactions. Using DFT calculations in combination with a thermodynamic analysis we have calculated the relative stability of various structural models of the mixed-terminated nonpolar $ZnO(10\bar{1}0)$ surface as a function of hydrogen and water chemical potentials. The coverage dependence of heterolytic hydrogen adsorption on O and Zn sites as well as surface hydroxylation via homolytic hydrogen and dissociative water adsorption were taken into account. From the adsorption energies a phase diagram of the lowest energy adsorbate structures in thermodynamic equilibrium with hydrogen and water reservoirs is constructed. It is found that at low hydrogen coverage only OH groups are formed, leading to a reduction of ZnO. However, as soon as a critical degree of reduction is reached, heterolytic hydrogen adsorption becomes more favorable, and at very hydrogen rich conditions a structure in which all surface O and Zn atoms are saturated with hydrogen is the most stable one. On the other hand, in water rich conditions a surface structure with a full zinc hydroxide layer is predicted to be the lowest energy structure.

O 8.3 Mon 11:45 WIL C307

Laser induced desorption of CO from rutile(110) — •Matthias Mehring and Thorsten Klüner — Theoretische Chemie, Carl von Ossietzky Universität Oldenburg, PO Box 2503, 26111 Oldenburg

Titania plays an important role in materials science. It serves as heterogenous catalyst, photocatalyst, white pigment or corrosion protective coating. Photodesorption can be described as a prototype of a huge group of non-adiabatic surface reactions like simple rotational and vibrational excitations of small molecules or photodiffusion. These reactions serve as a basis for photon driven molecular switches or molecular rotors. The present study provides an insight into the adsorption and desorption processes of carbon monoxide on a rutile surface. Using the embedded cluster approach, we employed a relaxed $Ti_9O_{18}Mg_7^{14+}$ cluster surrounded by 4421 point charges. Within this model we are able to calculate multi-dimensional PESs of both electronic ground state and necessary $5\sigma \rightarrow 2\pi^*$ electronically excited state(s) on MP2 and CASPT2 level, respectively. Quantum dynamical studies using the *ab initio* PES allow a detailed microscopic understanding of processes involved in the laserinduced desorption process. First 2D quantum dynamical studies regarding desorption coordinate Z and polar angle θ show interesting results with respect to the polar angle and the eigenstate of adsorbed CO molecule.

O 8.4 Mon 12:00 WIL C307

Silica-modified titania photocatalysts: a computational investigation — •Nicola Seriani[1], Carlos Pinilla[1], and Sandro Scandolo[1,2] — [1]The Abdus Salam International Centre for Theoretical Physics — [2]INFM-DEMOCRITOS National Simulation Center

Titanium dioxide is the catalyst of choice in solar-to-fuel applications. Silica can be used to enhance its catalytic activity, but its effect is not fully understood. Through a combination of classical and quantum simulations we build realistic models of titania/silica mixed oxides, interfaces and ultrathin films. The electronic structure of the oxide is heavily modified by the interaction with silica. Band bending is observed in a neighborhood of the interface, which might be responsible for the modified photocatalytic properties of titania-silica materials. This work is part of the FP7 project ADGLASS.

O 8.5 Mon 12:15 WIL C307

Interaction of H_2O and D_2O with NaCl(100) — •Stephan Härtel, Jochen Vogt, and Helmut Weiss — Chemisches Institut der Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

Interactions of water with the surfaces of solids play an important role in a variety of fields such as catalysis, corrosion, and atmospheric physics. Numerous studies have been carried out so far dealing with the adsorption of water on the NaCl(100) surface. However, the structure of the water molecules on this surface is still under discussion. There are evidences for a c(4×2) superstrucure as well as a (1×1) structure [1,2]. In the present work H_2O and D_2O were used as adsorptives on NaCl(100). In order to study the influence of water adsorption on the surface defect concentration, the latter was probed with CO_2 before and after the water experiments by means of Fourier transform infrared (FTIR) spectroscopy. The water-NaCl(100) adsorbate was prepared at crystal temperatures of 140 K. In low-energy electron diffraction (LEED) experiments the c(4×2) superstructure as well as the (1×1) structure could be observed. LEED I(V) curves in an energy range between 70 and 300 eV were recorded. First results of the LEED I(V) analysis will be presented. In additional experiments the adsorption of H_2O on a CO_2-precovered surface was examined. H_2O replaces the CO_2 quickly which indicates a growth of the H_2O mainly on the terraces.

[1] J. P. Toennies et al., J. Chem. Phys., **120**, 24 (2004)
[2] P. Cabrera-Sanfelix et al., J. Chem. Phys., **126**, 214707 (2007)

O 8.6 Mon 12:30 WIL C307

Sorption of Arsenic Complexes at FeOOH Surfaces from First Principles — •Katrin Otte, Wolfgang W. Schmahl, and Rossitza Pentcheva — Section Crystallography, Dept. of Earth and Environmental Sciences, University of Munich

Iron oxyhydroxides (FeOOH) possess high surface areas and are of relevance for various processes in nature and technology as cycling and retention of contaminants, e.g. for water treatment purposes. [1] Using density functional theory (DFT), we investigate the adsorption affinities of the FeOOH polymorphs goethite (α), akaganeite (β), and lepidocrocite (γ) to heavy metal complexes. The knowledge of the clean surfaces goethite(101), akaganeite(100), and lepidocrocite(010) is a starting point to address those. The GGA+U calculations reveal that the termination impacts the oxidation state of the topmost iron, providing a possibility to tune the catalytic activity. The energetics and bonding mechanisms of contaminants in different adsorption geometries on the surfaces are analyzed.

Funding by the BMBF programme Geotechnologies and Elitenetzwerk Bayern is acknowledged.

[1] R. M. Cornell and U. Schwertmann, The Iron Oxides (Wiley, Weinheim, 2001).

O 8.7 Mon 12:45 WIL C307

DFT studies of reaction mechanisms of methane combustion on PdO(100) — •Arezoo Dianat[1], Manfred Bobeth[2], and Lucio Colombi Ciacchi[1] — [1]Faculty of Production Engineering, University of Bremen, 28359 Bremen, Germany — [2]Institute for Materials Science, Dresden University of Technology, 01062 Dresden, Germany

Palladium oxides are renowned for their high activity in the catalytic combustion of methane. We have investigated the complex reaction mechanisms of methane combustion on the PdO(100) surface within the framework of density functional theory. From an analysis of the calculated driving forces and activation energies for the dissociative adsorption of methane and the successive dehydrogenation of adsorbed hydrocarbons, we conclude that the experimentally observed conversion rates at temperatures of about 600 K cannot be explained in terms of direct dehydrogenation processes.

Investigations of alternative reaction routes reveal that the reaction of oxygen molecules from the gas phase with hydrogen previously adsorbed on the catalyst surface can efficiently produce water. According to combined ab initio molecular dynamics and static total energy calculations, the combustion reaction proceeds through the spontaneous formation of H2O2 followed by its dissociation and water formation with an activation energy of about 0.7 eV. Following an analogous mechanism, oxygen molecules from the gas phase can also react with adsorbed CH3 groups to produce CH2O as an intermediate reaction product.

O 9: Invited Talk (Walter Pfeiffer)

Time: Monday 14:00–14:45 Location: TRE Phy

Invited Talk O 9.1 Mon 14:00 TRE Phy

Ultrafast nanooptical control — •Walter Pfeiffer[1], Tobias Brixner[2], and Martin Aeschlimann[3] — [1]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — [2]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg — [3]Fachbereich Physik and Research Center OPTIMAS, Technische Universität Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern

The most general investigation and exploitation of light-induced processes require simultaneous control over spatial and temporal properties of the electro-magnetic field on a femtosecond time- and nanometer length-scale. Based on the combination of polarization pulse shaping and time-resolved two-photon photoemission electron microscopy we demonstrate such control over nanoscale spatial and ultrafast temporal degrees of freedom of an electromagnetic excitation in the vicinity of a nanostructure. The present status of nanooptical control is reviewed, different control mechanisms are demonstrated, and the prospects of open-loop control of particular nanophotonic excitations are discussed. The flexible simultaneous control of temporal and spatial properties of nanophotonic excitations opens new possibilities to tailor and optimize the light-mater interaction in spectroscopic methods as well as in nanophotonic applications.

O 10: Metal substrates: Adsorption of organic / bio molecules II

Time: Monday 15:00–17:00 Location: TRE Phy

O 10.1 Mon 15:00 TRE Phy

Spin-sensitive tunneling through individual Terbium-Phthalocyanine Molecules by Spin-polarized Scanning Tunneling Microscopy — •Jörg Schwöbel[1], Yingshuang Fu[1], Andrew DiLullo[2], Jens Brede[1], Svetlana Klyatskaya[3], Mario Ruben[3,4], Germar Hoffmann[1], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, University of Hamburg, Germany — [2]Nanoscale & Quantum Phenomena Institute, Ohio University, USA — [3]Karlsruhe Institute of Technology, Institute of Nanotechnology, Germany — [4]Université de Strasbourg, IPCMS, France

Terbium-Phthalocyanine double-decker molecules (TbPc2) belong to the class of single-molecule magnets, which could serve as the smallest building blocks of future information technology devices such as for quantum computers and data storage. Because of its high blocking temperature (>10 K), TbPc2 attracted considerable interests in recent years [1].

Here, we locally address TbPc2 adsorbed on a ferromagnetic surface (Co nanoislands) with spin-polarized scanning tunneling microscopy. We detect a significant spin contrast by tunneling through TbPc2 molecules with intramolecular resolution. Thereby, the spin-polarization depends on the energy and the position within the molecule.

We present our experimental data and discuss the origin of the magnetic contrast observed.

[1] Ishikawa, N.; Sugita, M.; Ishikawa, T.; Koshihara, S.; Kaizu, Y.; J. Am. Chem. Soc., 2003, 125 (29), pp 8694-8695

O 10.2 Mon 15:15 TRE Phy

Low Temperature Scanning Tunneling Microscopy Study of Co-Phthalocyanine Molecules on Au (111) and Cu (111) — •Samuel Bouvron[1], Philipp Erler[1], Stefan Ambrus[2], Mikhail Fonin[1], Frank Matthes[3], and Claus Michael Schneider[3] — [1]Fachbereich Physik, Universität Konstanz — [2]Fachbereich Chemie, Universität Konstanz — [3]Institut für Festkörperforschung, Forschungzentrum Jülich

Metal-phthalocyanines are complexes of great technological and fundamental interest which are already extensively used as pigments and are possible candidats for future applications in molecular electronic devices. For a better understanding of the interaction between metal-phthalocyanines and surfaces, we investigated Co-phthalocyanine molecules (CoPc) on Au (111) and Cu (111) at a submonolayer coverage by means of low-temperature scanning tunneling microscopy (STM) and spectroscopy (STS). The adsorption behavior of CoPc on both substrates is studied, and a direct observation of the molecular orbitals is reported. STS measurements performed above the CoPc molecules on Cu (111) show a reproducible feature directly below E_F, whose origin is discussed. Furthermore the impact of an external magnetic field (up to 6 T) on the electronic density of states close to E_F is studied.

O 10.3 Mon 15:30 TRE Phy

2D-self-assembly of chiral buckybowls — •Quirin Stoeckl[1], Tobias Bauert[1], Davide Bandera[2], Manfred Parschau[1], Jay S. Siegel[2], and Karl-Heinz Ernst[1] — [1]Empa, Nanoscale Material Science, Dübendorf, Switzerland — [2]Organisch-chemisches Institut, Universität Zürich, Switzerland

So-called buckybowls, quasi-fragments of buckminsterfullerene, are promising candidates for suface modifications for organic photovoltaics and controlled carbon nanotube growth. Corannulene (COR, $C_{20}H_{10}$) is the simplest curved fragment with a central C_5 ring, surrounded by five aromatic C_6 rings. We investigated the self-assembly of the C_5-symmetric pentaphenyl-corannulene (Ph_5Cor), a chiral derivative with five phenyl groups at the rim, on Cu(111). Fivefold symmetry is incompatible with the translational order in all 17 2D plane groups, and this system is therefore of fundamental interest for 2D self-assembly. STM shows packing motifs in which the five substituents are interdigitated and are compatible with LEED results. Workfuntion change measurements via UPS reveal an unusual large interface dipole. We compare our findings with those obtained for other penta-substituted COR derivatives on Cu(111) and present preliminary results for thermally-induced dehydrogenation into polymeric structures.

O 10.4 Mon 15:45 TRE Phy

Negative differential resistance of C60 islands in scanning tunneling spectroscopy — •I-Po Hong, Yongfeng Wang, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel

Spectra of the differential conductance (dI/dV) of C_{60} layers on Cu(111) and on NaCl layers are investigated with a low temperature STM. In addition to various electronic states the spectra clearly show negative differential resistance (NDR). The presence of NDR depends on the thickness of the C_{60} layer. NaCl layers further modify the spectral structure. The experimental results are analysed using a double barrier model.

O 10.5 Mon 16:00 TRE Phy

Engineering Negative Differential Conductance in a single-$\mathbf{C_{60}}$ tunnel junction — •Benjamin W. Heinrich[1,2], Mircea V. Rastei[1], Deung-Jang Choi[1], Jean-Pierre Bucher[1], Thomas Frederiksen[3], and Laurent Limot[1] — [1]Institut de Physique et Chimie des Matériaux de Strasbourg, CNRS, Strasbourg, France — [2]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [3]Donostia International Physics Center, San Sebastián, Spain

Negative differential conductance (NDC) occurs when a voltage increase across an electronic device produces a decreasing current. The last two decades have seen a revived interest in this field following the observation of NDC at the atomic scale and in hybrid metal-organic junctions, which are potentially interesting for molecular electronics. The NDC characteristics in molecular systems are usually attributed to localized energy states, but can also result from inelastic or chemical processes.

Here we use a cryogenic STM to engineer an NDC with a single C_{60} molecule attached to the tip of the microscope. The original aspect of the observed NDC is that it results from electrons tunneling between the LUMO+1 of C_{60} and the dispersive Shockley surface states of Cu(111). The NDC intensity can then be tuned by varying the barrier thickness or by changing the C_{60} orientation up to complete extinction. In particular, this study underlines how the k-dependence of the tunneling process may be altered through the orientation of a molecular orbital: a single molecule acts as a k-filter for tunneling electrons.

O 10.6 Mon 16:15 TRE Phy

Scanning tunneling spectroscopy and microscopy of α-sexithiophene films on Au(100) — •Rene Hammer, Anke Höfer, Klaus Duncker, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Institute of Physics, Halle(Saale), Germany

The electronic and the structural properties of epitaxially grown ultrathin films of α-sexithiophene (6T) on Au(100) have been studied by scanning tunneling spectroscopy (STS) and microscopy (STM) at 80 K. The structure of the well-ordered first monolayer grown at 300 K and then cooled to 80 K is nearly identical to the structure reported at 300 K [1]. Subsequent growth proceeds layer-by-layer with flat-lying 6T molecules forming parallel molecular rows also in the second monolayer. Two rotational domains with an angle of 14° in between are found. The row direction in the second monolayer is parallel to the rows of the first layer underneath. STS spectra of the first and second 6T monolayer allow the determination of the lowest unoccupied molecular orbital (LUMO) at 1.2 eV, the LUMO+1 at 1.8 eV and the LUMO+2 at 2.4-2.5 eV with respect to the Fermi level. Additionally the second monolayer exhibits a strong STS feature at 2.15 eV. The highest occupied molecular orbital (HOMO) is found at -1.0 and -1.5 eV for the first and second monolayer, respectively. Mapping of the differential conductivity gives hints to the electron density within these orbitals which will be compared to calculated wavefunctions.

[1] A. Höfer, K. Duncker, M. Kiel, S. Wedekind, and W. Widdra, Phys. Rev. B (submitted)

O 10.7 Mon 16:30 TRE Phy

α-sexithiophene on silver: The influence of the surface miscut — •Thorsten Wagner, Daniel Roman Fritz, and Peter Zeppenfeld — Institute of Experimental Physics at the Johannes Kepler University Linz, Austria

The growth of α-sexithiophene (α-6T) on Ag(110) and Ag(441) was studied by means of scanning tunneling microscopy (STM) and photoelectron emission microscopy (PEEM). In contrast to (110) surfaces of other metals, α-6T molecules deposited on Ag(110) do not align exclusively along the close-packed atomic troughs but also perpendicular to them. The mixture of molecules arranged with their long axis parallel to the [001] and $[1\bar{1}0]$ directions lead to strained checkerboard pattern as described by Yokoyama.[1] Besides the checkerboard phase, a well ordered homochiral phase was found. STM images show that although the molecules in the second layer are exclusively aligned in the [001] direction their arrangement is strongly influenced by the perpendicular molecules of the first layer. By using a Ag(441) surface, the molecules of the first layer can be forced to align exclusively along the $[1\bar{1}0]$ direction. In this case, the molecules are parallel to the steps of the substrate. In addition, step bunching and faceting of the vicinal substrate surface was found upon adsorption of α-6T. For more than two monolayers of α-6T deposited on both, the Ag(110) and the Ag(441) surface, a 3D growth was observed by PEEM. The PEEM intensity curves recorded during film growth provide additional details on the complex growth of the molecules on both surfaces.

[1] T. Yokoyama, Applied Physics Letters **96**, 063101 (2010)

O 10.8 Mon 16:45 TRE Phy

Exciton dynamics at oligothiophene / Au(111) interfaces — •Erwan Varene, Isabel Martin, Christopher Bronner, Lea Bogner und Petra Tegeder — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany

Semiconducting materials based on organic molecules or polymers are promising candidates for applications in electronic devices such as organic photovoltaic cells. The electronic structure and carrier dynamics at interfaces between organic semiconductors and inorganic substrates are the most fundamental issues in order to understand the functionalities of organic films. Time-resolved two-photon photoemission (2PPE) spectroscopy is employed to determine the electronic structure, charge carrier dynamics and energetics at the sexithiophene (6T)/Au(111) interface. We found the HOMO and HOMO-1 to be located at -0.8 and -1.5 eV, respectively and two 6T-derived unoccupied states at 2.1 eV and 3.0 eV with respect to the Fermi level which we assign to the LUMO and LUMO +1. In addition an exciton state possessing a binding energy of 0.9 eV is observed. The timescale for the exciton breakup exhibits a strong 6T coverage dependency, i.e., the exciton lifetime increases with increasing coverage. For instance at a coverage 12 ML the decay times are around 700 fs for the fast component and ~ 5 ps for the slow component.

O 11: Plasmonics and Nanooptics I

Time: Monday 15:00–17:00 Location: PHY C213

O 11.1 Mon 15:00 PHY C213

Quasistatic plasmon resonances in the visible spectral range of arbitrary shaped nano-grooves — •Camille Maxime[1,2], Aude Barbara[1,2], and Pascal Quemerais[1,3] — [1]Institut Néel, CNRS-UJF, Grenoble, France — [2]IAPP, TU Dresden, Germany — [3]MPI-PKS, Dresden, Germany

As we previously reported, plasmonic resonances inside rectangular nano-grooves periodically made on a silver surface present a cross-over between two physical regimes [1]: an optical one for groove widths w larger than 10 nm, and a quasistatic one for lower values. In that case, the grooves resonate in the visible range even for grooves height h of only a few nanometers (5-15 nm). A very strong light absorption occurs at the resonance together with an electric field intensity enhancement (EFIE) of about 400. These results were obtained with a method only available for rectangular shapes. To generalize, we have implemented a surface integral method [2] and adapted it to periodic profiles to avoid surface boundaries problems. As an example, the behaviour of Gaussian shaped grooves was studied. It fully confirms the transition to a quasistatic regime as the groove width decreases leading to unusual EFIE (up to about 10000) and a very strong light absorption. These original results are fundamental to explain surface enhanced Raman scattering (SERS) experiments such as the historical ones of Albano et al.[3].

[1] J. Le Perchec et al., *Phys. Rev. Lett.* **100**, 066408 (2008)

[2] A.A. Maradudin et al., *Ann. Phys.* **203**, 255 (1990)

[3] E.V. Albano et al., *Phys. Rev. Lett.* **51**, 2314 (1983)

O 11.2 Mon 15:15 PHY C213

Coupled nanoantenna plasmon resonance spectra from two-photon laser excitation: longitudinal and transversal emission — •Matthias D. Wissert[1], Carola Moosmann[1], Konstantin S. Ilin[2], Michael Siegel[2], Uli Lemmer[1], and Hans-Jürgen Eisler[1] — [1]Light Technology Institute, DFG Heisenberg Group 'Nanoscale Science', Karlsruhe Institute of Technology, Germany — [2]Institute of Micro- and Nanoelectronic Systems, Karlsruhe Institute of Technology, Germany

We report on the plasmonic mode relaxation of coupled optical gold nanoantennas under two-photon laser excitation at 810 nm [1]. An oil immersion objective lens is used both for the excitation and detection channel. The plasmon emission intensity from single nanostructures is detected using a single-photon-counting avalanche photodiode, the response spectrum is observed with an EMCCD camera.

We show that the plasmon spectra are very similar to the well known scattering resonances [2] for such structures, albeit now obtained from single frequency excitation. We also show that not only the longitudinal, but also the transversal plasmon mode can be excited, using excitation light polarized exclusively along the long axis of the dipole antenna.

[1] M.D. Wissert, K.S. Ilin, M. Siegel, U. Lemmer, and H.-J. Eisler, Nano Letters **10**, 4161 (2010)

[2] M.D. Wissert, A.W. Schell, K.S. Ilin, M. Siegel, and H.-J. Eisler, Nanotechnology **20**, 425203 (2009)

O 11.3 Mon 15:30 PHY C213

Metallic nanorod arrays: negative refraction and optical properties explained by retarded dipolar interactions — •René Kullock[1], Stefan Grafström[1], Paul R. Evans[2], Robert J. Pollard[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, TU Dresden, 01062 Dresden, Germany — [2]Centre for Nanostructured Media, IRCEP, The Queen's University of Belfast, Belfast BT7 1NN, UK

Two-dimensional (2D) arrays of metallic nanorods arranged perpendicular to a substrate exhibit novel optical features: a short-axis resonance, and several long-axis surface plasmon resonances (LSPRs) which appear for excitation with p-polarized light at specific angles of incidence [1]. Especially the first LSPR mode is very sensitive to both geometry and environment. In order to make it accessible for different applications, a fundamental physical understanding is indispensable.

Here, we theoretically treat such a 2D nanorod array by applying the retarded dipolar interaction model (DIM). First, we nicely follow the LSPR changes when extending our calculations from the single nanorod to a 2D array of nanorods [2]. Then, using the DIM model we are able to explain how the LSPR depends on several physically relevant parameters, such as the nanorod length, diameter, neighboring distance, material, and surroundings. Furthermore, the DIM also delivers conditions under which negative and extraordinary positive refraction in such metallic nanorod arrays will occur.

[1] R. Kullock et al., *Opt. Express 16, 21671 (2008)*

[2] R. Kullock et al., *J. Opt. Soc. Am. B 27, 1819 (2010).*

O 11.4 Mon 15:45 PHY C213

Photoemission Microscopy on Surface Plasmon Polaritons in Ag Islands — Niemma Buckanie, Pierre Kirschbaum, Simon Sindermann, Michael Horn-von Hoegen, and •Frank Meyer zu Heringdorf — Universität Duisburg-Essen, Fakultät für Physik and Center for Nanointegration (CeNIDE), Lotharstrasse 1, 47057 Duisburg, Germany

The interaction of frequency doubled femtosecond laser pulses with Silver islands on Si in a photoemission electron microscope provides a fantastic toolbox to study the interaction of light with surface plasmon polaritons (SPP) in small Ag islands. In two photon photoemission microscopy (2PPE PEEM), SPPs are imaged as a time-integrated superposition of the electric field of the propagating SPP wave with the electric field of the exciting laser pulse that hits the surface under grazing incidence. A quantitative analysis of the experimentally observed moiré pattern allows studying of the SPP field strength and a determination of the propagation direction of the SPP. At the rear edge of the island the SPP wave can be converted back into light. The resulting superposition of the converted light with the incident laser pulse is manifested in an enhanced photoemission yield behind the island.

O 11.5 Mon 16:00 PHY C213

Experimental observation of decoupled plasmon resonances in metallic nanoparticles — •Reto Giannini[1], Yasin Ekinci[1,2], and Jörg F. Löffler[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — [2]Laboratory for Micro and Nanotechnology, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland

The optical response of designed metallic nanostructures is of high interest due to its importance in sensing applications, nanoantennas and nanooptics. With the aim to analyze the optical response of metallic nanostructures in the visible wavelength range, we produced metallic nanoparticles with the simple geometry of cylinders standing on a glass substrate by e-beam lithography. Additionally, a measurement set-up was established that allows the directional excitation of nanoparticles in three dimensions. Based on the analysis of the nanocylinders, we show experimental evidence that the overall optical response of such a system is the superposition of individually tunable plasmon resonances, i.e. normal modes. In the case of the cylinder, three normal modes associated with the main axes and therefore excitable by a polarization along these axes have been observed. Finally, these results are compared with FEM-based simulations.

O 11.6 Mon 16:15 PHY C213

Modeling Metallic Nanostructures using a Discontinuous Galerkin Approach — •Jens Niegemann, Michael König, Christopher Prohm, Timo Köllner, and Kurt Busch — Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany

Over the past few years, the discontinuous Galerkin time-domain (DGTD) method has established itself as an extremely powerful and efficient numerical technique in the field of photonic. Due to its combination of an accurate spatial discretization with an explicit time-stepping scheme, the DGTD method is particularly well suited for studying ultra-short and/or plasmonic phenomena. Furthermore, the method is readily extended to also treat hydrodynamic equations, which allows us to also model the nonlocal and nonlinear properties of metallic nanostructures.

Here, we discuss our recent advances in using the DGTD method for the simulation of plasmonic devices. In particular, we present first results on a full hydrodynamical simulation of small metallic nanostructures.

O 11.7 Mon 16:30 PHY C213

Mode imaging and selection in strongly coupled nanoantennas — Jer-Shing Huang[1], •Johannes Kern[1], Peter Geisler[1], Pia Weinmann[2], Martin Kamp[2], Alfred Forchel[2], Paolo Biagioni[3], and Bert Hecht[1] — [1]Experimental Physics 5, University of Würzburg, Germany — [2]Technische Physik, University of Würzburg, Germany — [3]CNISM, Politecnico di Milano, Italy

Plasmonic nanostructures consisting of gold nano-wire pairs offer a large variety of different modes, depending on their geometric arrangement, for which the optical near-fields can be strongly confined in nanometerscale gaps. Of particular interest are modes which couple only weakly to the radiation field, e.g. due to a quadrupolar charge distribution. For such modes, simulations predict that the corresponding resonances should exhibit comparatively large quality factors due to the absence or the reduction of radiation damping.

In order to demonstrate a correspondence between simulations and experiments, we strive to fabricate gold nanostructures that are free of defects and exhibit ultra-smooth surfaces. To achieve this goal, we apply top-down nanofabrication methods, which rely on focused-ion-beam milling of large, but ultrathin single-crystalline gold flakes.

We will discuss simulations and experimental investigations of strongly-coupled optical antennas selectively excited to their antibonding resonance.

O 11.8 Mon 16:45 PHY C213

Size, gap, shape, and material dependence of third harmonic generation from bowtie nanoantenna arrays — •Mario Hentschel[1,2], Tobias Utikal[1,2], Markus Lippitz[1,2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, D-70569 Stuttgart, Germany — [2]Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany

We investigate third harmonic generation from gold bowtie nanoantenna arrays. We fabricated 9x11 arrays of 125x200 nanoantennas each, varying continuously the gap size as well as the bowtie size. Both structural parameters determine the resonance wavelength of these plasmonic dimers, leading to a wide range of resonance positions from 690 nm to 1020 nm. The linear transmittance spectra are measured by an FTIR microscope. 8 fs broadband laser pulses with a center wavelength of 820 nm are utilized to generate the third harmonic signal. We find that surprisingly the third harmonic signal does not scale with shrinking gap size as expected, but is rather a function of resonance energies in the hybridized plasmonic dimer. The third harmonic signal is strongest for maximum overlap of the extinction spectrum of the nanostructures and the laser spectrum, as well as when the plasmonic oscillator strength is largest. Furthermore we study variations of the nanoantenna system in order to gain further insight in the harmonic generation process. We are going to present resent results on the THG conversion efficiencies for different antenna designs, such as rod-, sphere-, and gap-antennas, as well as for different antenna materials.

O 12: Metal substrates: Adsorption of O / H and inorganic molecules I

Time: Monday 15:00–17:00 Location: WIL A317

O 12.1 Mon 15:00 WIL A317

Adsorption of atomic oxygen on PdAg/Pd(111) surface alloys and coadsorption of CO — •Arnold P. Farkas[1,2], Joachim Bansmann[1], Thomas Diemant[1], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — [2]Reaction Kinetics Research Group at the University of Szeged, Chemical Research Center of the Hungarian Academy of Sciences, H-6720 Szeged , Hungary

The interaction of dissociated oxygen with structurally well-defined PdAg/Pd(111) surface alloys and the coadsorption of CO was studied by high resolution electron energy loss spectroscopy (HREELS) and temperature-programmed desorption (TPD). After oxygen saturation of the non-modified Pd(111) surface at RT, we observed the formation of a prominent peak in the HREEL spectra at 60 meV corresponding to the perpendicular vibration of oxygen atoms adsorbed in threefold hollow sites. Deposition of small Ag amounts does not change the signal intensity of this peak; it decreases only above 20% Ag. Beyond this Ag content, the peak intensity steeply declines and disappears at around 55-60% Ag. CO coadsorption on the oxygen pre-covered surfaces at 120 K leads to the formation of additional features in HREELS. For a surface alloy with 29% Ag, three loss features due to CO adsorption in on-top, bridge, and threefold-hollow sites can be discriminated already after the lowest CO exposure. Annealing of the co-adsorbed layer to 200 K triggers a decrease of the oxygen concentration due to CO_2 formation. These findings are corroborated by TPD spectra of the CO desorption and CO_2 production.

O 12.2 Mon 15:15 WIL A317

Adsorption and reaction of sulfurdioxide on clean and oxygen precovered Pd(100) — •Karin Gotterbarm, Regine Streber, Christian Papp, Oliver Höfert, Michael Peter Andreas Lorenz, and Hans-Peter Steinrück — Lehrstuhl für physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91052 Erlangen

Sulfur and its oxides are well-known poisons in large scale applications of heterogeneously catalyzed reactions. We studied the adsorption and thermal evolution of SO_2 on a clean and oxygen precovered Pd(100) surface by in-situ high-resolution XPS applying synchrotron radiation at BESSY II, Berlin. Adsorption of SO_2 on the clean Pd(100) surface at 130 K leads to formation of two different SO_2 species: a highly populated upright standing SO_2 species and a small amount of flat lying SO_2. Upon annealing the sample standing SO_2 is transformed into lying SO_2, which is ultimately reduced to atomic sulfur. On the oxygen precovered surface a fraction of SO_2 reacts to SO_3 immediately upon adsorption, even at temperatures as low as 130 K. Heating of the resulting mixed adsorbate layers first results in the conversion of all remaining SO_2 species to SO_3 followed by subsequent oxidation to SO_4 above 300 K.

This work was supported by the BMBF under grant 05 ES3XBA/5 and by the Cluster of Excellence 'Engineering of Advanced Materials'.

O 12.3 Mon 15:30 WIL A317

Coadsorption of CO and hydrogen on submonolayer Pt/Ru(0001) films — •Heinrich Hartmann, Thomas Diemant, Joachim Bansmann, and R. Juergen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

Due to their high CO tolerance, bimetallic Pt-Ru catalysts are an attractive electrode material for the oxidation of H_2-rich fuel gases prepared by reforming of fossil fuels in low-temperature polymer electrolyte fuel cells. This makes the adsorption properties of PtRu systems an interesting topic for fundamental studies on model systems.

We have investigated the coadsorption of CO and hydrogen on submonolayer Pt films deposited on the Ru(0001) surface with TPD and IRAS under UHV conditions. Adsorption of either of the two molecules on the Pt covered parts of the bimetallic surface is weaker compared to adsorption on the remaining uncovered Ru parts. Coadsorption of hydrogen and CO leads to a displacement of hydrogen from the Ru areas to the energetically less favourable Pt islands. At the same time a further weakening of the hydrogen-Pt bond is observed, which is attributed to repulsive interactions between adsorbed hydrogen and CO molecules.

O 12.4 Mon 15:45 WIL A317

Non-adiabatic Effects during the Dissociative Adsorption of O2 at Ag(111)? A first-principles Divide & Conquer Study — •Itziar Goikoetxea^{1,2}, Juan Beltrán^{1}, Jörg Meyer^{1,3}, Maite Alducin^{2}, Iñaki Juaristi^{2}, and Karsten Reuter^{1,3} — ^{1}Fritz-Haber-Institut der Max-Planck- Gesellschaft, Berlin, Germany — ^{2}Centro de Fisica de Materiales, San Sebastian, Spain — ^{3}Technische Universität München, Germany

A predictive materials science modeling based on microscopic understanding requires a thorough knowledge of all underlying elementary processes at the atomic scale. The adsorption of individual oxygen molecules at metal surfaces is one example -crucially relevant not only but in particular in heterogeneous catalysis. Recent work on the dissociative adsorption of O2 at Al(111) has severely chal- lenged its prevalent understanding: A non-adiabatic transition of the molecular spin state favored by low density of states at the Fermi- level has been proposed to reconcile experimental observations with ab-initio theory [1]. Consequently, coinage metal surfaces might be fur- ther good candiates for such effects. With this motivation, we have used a first-principles based divide and conquer approach to study O2 on Ag(111). Experimental observables like e.g. (initial) sticking and scat- tering turn out to be semi-quantitatively reproduced with adiabatic dynamics already. Finally, the emerging picture for the interaction of oxygen molecules with this surface is compared to the low-dimensional model originally proposed by Kleyn et al. [2]. [1] J. Behler et al., Phys. Rev. Lett. 94, 036104 (2005). [2] A. W. Kleyn et al., Surf. Sci. 363, 29 (1996).

O 12.5 Mon 16:00 WIL A317

In-situ oxidation study of Pd(100) by surface x-ray diffraction — •Volkan Kilic^{1}, Natalia Martin^{2}, Miguel Mantilla^{3}, Dirk Franz^{1}, Edvin Lundgren^{2} und Andreas Stierle^{1} — ^{1}AG Grenzflächen, Universität Siegen, Germany — ^{2}Department of Synchrotron Radiation Research,Lund University,Sweden — ^{3}MPI für Metallforschung, Stuttgart, Germany

The oxidation of the Pd(100) surface at oxygen pressures in the 10^{-6} mbar to 10^{3} mbar range and temperatures up to 1000 K has been studied in-situ by surface x-ray diffraction (SXRD). The SXRD experiments were performed at the MPI beamline at the Angstrom Quelle Karsluhe (ANKA). We present the surface and crystal truncation rod (CTR) data from the $(\sqrt{5}X\sqrt{5})$ surface layer. We show that the transformation from the surface oxide to PdO bulk oxide can be observed in-situ under specific pressure and temperature conditions. We will compare our results with previously proposed structure models based on low energy electron diffraction (LEED) I(V) curves and density function theory calculations [1,2]. Finally, we will elucidate the question of commensurability of the surface oxide layer with respect to the Pd(100) substrate.

[1]P. Kostelnik, N. Seriani, G. Kresse, A. Mikkelsen, E. Lundgren, V. Blum, T. Sikola, P. Varga, M. Schmid, Surf. Sci. 601 (2007) 1574-1581

[2]M.Todorova, E. Lundgren, V. Blum, A. Mikkelsen, S. Gray, J. Gustafson, M. Borg, J. Rogal, K. Reuter, J. N. Andersen, M. Scheffler, Sur. Sci. 541 (2003) 101-112

O 12.6 Mon 16:15 WIL A317

Electron-Hole Pairs during Adsorption Dynamics of O_2 on Pd(100) – Exciting or not? — •Jörg Meyer^{1,2} and Karsten Reuter^{1,2} — ^{1}Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — ^{2}Technische Universität München, Germany

Diminishing resources have made energy research become more and more prominent over the recent years. Energy conversion and dissipation at interfaces are two examples about which microscopic knowledge is limited at best – despite their fundamental importance e.g. during catalytic reactions at surfaces. Theoretical first-principles based modeling can provide important insights on corresponding underlying elementary processes. Non-adiabatic excitations of electron-hole pairs during adsorption of molecules on metal surfaces fall into this category and have been controversially discussed only recently [1]. Therefore, we have investigated their importance for O_2-adsorption on Pd(100), a representative showcase for heterogeneous catalysis. Using our efficient implementation of a computationally appealing perturbative approach [2], we have obtained electron-hole pair spectra for several trajectories of different statistical relevance. Concomitant non-adiabatic energy losses do not exceed 4% of the available chemisorption energy, pointing towards other more dominant energy dissipation channels for this system. The role of the spin transition will be critically discussed.

[1] J. I. Juaristi et al., Phys. Rev. Lett. **100**, 116102 (2008); A. C. Luntz et al., *ibid.* **102**, 109601 (2009); J. I. Juaristi et al., *ibid.* **102**, 109602 (2009).

[2] M. Timmer and P. Kratzer, Phys. Rev. B **79**, 165407 (2009).

O 12.7 Mon 16:30 WIL A317

Surface oxidation of planar and stepped Pt(111) surfaces studied by DFT — •Jochen Bandlow, Payam Kaghazchi, and Timo Jacob — Abteilung Elektrochemie, Universität Ulm, Germany

The surface oxidation of Pt(111) plays an important role for a wide range of catalytic reactions in gas-phase surface science and electrochemistry. Despite the fact that many experimental studies are focused on single crystal systems with almost perfect surfaces, realistic catalysts always contain step edges, kinks, vacancies and other imperfections on the surface. Especially these lower-coordinated sites are believed to play a decisive role for surface reactions and the catalytic performance.

In the present work we investigated the adsorption of oxygen on perfect and stepped Pt(111) using density functional theory and the extended *ab initio* thermodynamics approach.[1] By comparing the (p,T) phase diagram for the system in contact with a gaseous O_2 atmosphere with the corresponding electrochemical (a,T,φ) phase diagram, characteristics of the surface morphology under specific conditions were evaluated. It turned out that the model of a pure and perfect Pt(111) surface, which is often used to study this reaction, is clearly incomplete.

[1] T. Jacob, *J. Electroanal. Chem.*, **607**, 158 (2007).

O 12.8 Mon 16:45 WIL A317

First-Principles Diffusion Barrier of O at Pd (100): A Benchmark beyond LDA/GGA — •Wei-Bing Zhang^{1,2}, Yongsheng Zhang^{1}, Jörg Meyer^{1,2}, and Karsten Reuter^{1,2} — ^{1}Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — ^{2}Technische Universität München

The diffusion of adsorbates at a solid surface is a core elementary process of critical relevance for many functionalities. The accurate determination of diffusion barriers is correspondingly an important aspect in first-principles kinetic modeling. At extended metal surfaces the state-of-the-art for this is still local (LDA) and semi-local (GGA) density-functional theory. Critically scrutinizing the reliability of such description for the diffusion of O atoms at Pd(100) we first use a cluster expansion approach to separate the overall diffusion barrier into the isolated-adatom limit and contributions arising from lateral interactions with other O adsorbates. Comparing LDA and GGA data suggests that the latter component is surprisingly well described already at this level of theory. However, comparison against experiment reveals a significant error for the barrier in the isolated O adatom limit. We therefore use an exchange-correlation correction approach based on finite cluster calculations [1] to assess the performance of higher level theory, including hybrid and RPA functionals. [1] Q.M. Hu, K. Reuter, and M. Scheffler, Phys. Rev. Lett. 98, 176103 (2007).

O 13: Solid / liquid interfaces I

Time: Monday 15:00–17:00 Location: WIL B321

O 13.1 Mon 15:00 WIL B321

On the Nature of the Pt(111)/H_2SO_4 Interface: A DFT Study

— •Aleix Comas-Vives, Jochen Bandlow, and Timo Jacob — Institut für Elektrochemie, Universität Ulm, Albert-Einstein-Allee 47, D-89069 Ulm, Deutschland

Anion adlayers such as SO_4^{2-} are influencing the adsorption and desorption processes on electrode surfaces, their properties, and the kinetics of electrochemical reactions.[1] Due to these effects (bi)sulfate-induced changes on the morphology of electrodes under electrochemical conditions have been investigated by surface-sensitive in situ and electrochemical techniques. However, the structure and composition of the adsorbed anion layer as well as the influence of possible co-adsorbates is still not completely understood. Motivated by our studies on the Au(111)/H_2SO_4 interface,[2,3] the aim of this work was to extend these investigations to Pt electrodes. Focusing on the well established $\sqrt{3} \times \sqrt{7}$ R19.1° adlayer periodicity, we performed DFT studies on sulfate/bisulfate co-adsorbed with different amounts of water and/or hydronium molecules. Besides structural and stability information, we used the charge density distribution of the most stable adlayers to propose distance tunneling spectroscopy profiles, providing the basis for upcoming experimental studies.

[1] O. M. Magnussen, *Chem. Rev.*, **102**, 679 (2002).
[2] S. Venkatachalam, T. Jacob, *Z. Phys. Chem.*, **221**, 1393 (2007).
[3] F. C. Simeone, D. M. Kolb, S. Venkatachalam, T. Jacob, *Angew. Chem. Int. Ed.*, **46**, 8903 (2007).

O 13.2 Mon 15:15 WIL B321

Static Dielectric Reponse of Water at Planar Interfaces

— •Douwe Jan Bonthuis, Stephan Gekle, and Roland Netz — TU München, Deutschland

The water structure close to an interface strongly influences the interaction between charged solutes. A key factor in these short-ranged interactions is the dielectric response function of the first few water layers, which differs appreciably from the bulk dielectric constant. From molecular dynamics simulations, we calculate the static dielectric tensor of water close to various surfaces, using two different methods: (1) relating the dielectric function to the fluctuations of the polarization density and (2) directly calculating the response to an external electric field. While the components of the tensor parallel to the surface closely follow the water density, the perpendicular component shows a highly non-trivial profile.

O 13.3 Mon 15:30 WIL B321

Ab-initio parameterisation of inter-atomic force fields for the description of solid-solid and liquid-solid interfaces

— •Carlos Pinilla[1], Nicola Seriani[1], and Sandro Scandolo[1,2] — [1]Abdus Salam International Centre for Theoretical Physics, Trieste, Italy — [2]Democritos Simulation Center, CNR-IOM, Istituto Officina dei Materiali, 34151, Trieste, Italy

We present a discussion on the generation of classical force field for the description of solid-solid and solid-liquid interfaces. We use the Tangney-Scandolo method [1] based on the use of forces, energies and stresses from ab-initio calculations for the generation of a potential able to provide a fully atomistic representation of the interface, by the inclusion of the most relevant two and three body interactions as well as polarisation. Hence, yielding a potential capable to describe correctly the structural properties of the interface within a wide range of pressures and temperatures. We discuss the application of this method to the generation of a force field for the a-SiO2/water interface and extend our study to the TiO2/a-SiO2 interface. Finally, we look into the generation of potentials that include ionic impurities. We compare our classical results to density functional calculations and show how our procedure leads to potentials that are greatly improved in comparison to the ones currently used to describe interfaces. This work is part of the FP7 project ADGLASS. [1] P. Tangney and S. Scandolo, J. Chem. Phys. 117, 8898 (2002)

O 13.4 Mon 15:45 WIL B321

Understanding the hydrophobic nature of nano-rugged solid surfaces at the molecular scale

— •Frédéric Leroy — Eduard-Zintl-Institut für Anorganische und Physikalische Chemie and Center for Smart Interfaces, TU-Darmstadt, Darmstadt, Germany

We aim to contribute to the understanding at a molecular level of the origin of the hydrophobic nature of surfaces exhibiting roughness at the nanometer scale. We present molecular dynamics calculations of the surface free energy of water in contact with graphite-based smooth and model surfaces whose roughness dimension stretches from a few Angstroms to a few nanometers.

Both Cassie and Wenzel wetting states are studied. All the rugged surfaces are observed to yield higher surface free energy than the perfectly smooth one.

The surface free energy of Cassie states is predicted from a Cassie-Baxter like equation. The origin of the hydrophobic nature of surfaces yielding Cassie states is therefore the reduction of the number of interactions between water and the solid surface having atomic defects.

On the contrary, Wenzel's theory fails to predict the variation of the solid-liquid surface free energy with respect to the roughness pattern. While graphite is found to be slightly hydrophilic, Wenzel states are dominated by an unfavorable effect arising from the hydrogen-bonding network perturbation that overcomes the favorable enthalpic effect induced by the surface roughness.

O 13.5 Mon 16:00 WIL B321

What fluorinated water-solid interfaces tell us about the origin of the hydrophobic gap.

— •Markus Mezger[1], Felix Sedlmeier[2], Dominik Horinek[2], and Harald Reichert[3] — [1]Max-Planck-Institut für Polymerforschung, Mainz — [2]Physik Department, TU München — [3]European Synchrotron Radiation Facility, Grenoble, France

The density deficit of water at hydrophobic interfaces, frequently called the hydrophobic gap, has been the subject of numerous experimental and theoretical studies. Recent experiments give values for the interfacial depletion that consistently correspond to less than a monolayer of water. However, its origin and the relation to the chemistry and molecular geometry of a particular hydrophobic coating or with macroscopic parameters such as the contact angle are still unclear. To elucidate how the underlying mechanisms affect the extent of the interfacial depletion we carried out a high-energy X-ray reflectivity study of water adjacent to a perfluorinated hydrophobic surface with a spatial resolution on the molecular scale. Comparison of experimental data and MD simulations on perflurinated and hydrocarbon water-solid interfaces revealed the influence of different contributions to the observed interfacial depletion.

Reference: M. Mezger et al., *J. Am. Chem. Soc.* **132**, 6735-6741 (2010).

O 13.6 Mon 16:15 WIL B321

Water lithography: a bottom-up solution

— Nicola Berger, •Masoud Amirkhani, Frank Zocholl, Mohamed Abdel Mohsen, and Othmar Marti — Institut für Experimentelle Physik Universität Ulm Albert-Einstein-Allee 11 89081 Ulm, Germany

Porous honeycomb-structured polymer films can be obtained by Breath Figure (BF) technique. Highly ordered honeycomb structures were readily formed by blowing airflow across the solution surface in a moist atmosphere (humidity 80%) after a 2 wt % polystyrene monocarboxy(PSC) terminated in toluene was drop-cast on a glass slide. The results show, solvent (toluene, chloroform and carbon disulfide) does not change bubble diameter and regularity of the pattern within an ordered area, whereas the size of the regular area is significantly larger for chloroform and carbon disulfide.

Silica particles were added to both solutions of PSC and polystyrene (PS) in order to find the effect of particles on the pattern formation.

Our study shows silica particles does not have any effect on the pattern formation of PSC solution. However, while linear PS cannot produce a regular pattern through BF technique, mixing of silica particles with PS solution can form a good pattern. The size of a bubble varies around 4% within a regular area, but it changes in the different area from 5 to 7 μm for PSC and from 6 to 9 μm for mixed particles and PS solution.

O 13.7 Mon 16:30 WIL B321

Light induced switching of surfaces: turning superhydrophobic into hydrophilic surfaces — •Jonas Groten and Jürgen Rühe — University of Freiburg - IMTEK, D-79110 Freiburg, Germany

We report on a method to generate a surface whose wettability can be switched between a superhydrophobic and hydrophilic state by simple, short UV irradiation. The system is based on a silicon surface with a nanoscale roughness (black silicon) to which a polymer monolayer is attached.The polymer contains a fluorinated azobenzene moiety. In these polymers the azobenzene moiety can be switched between the cis and trans states depending on the wavelength of the light used during illumination. In the described system the surface energy of the polymer coating is carefully adjusted to the energy value which separates distinct wetting regimes of the nanorough surface. This coupling of light induced switching to a wetting transition can cause large changes in the surface wetting behavior even when the surface energy is changed only in a rather small range. In one state the surface is superhydrophobic and has a critical tilt angle for roll off of only 3. Upon short illumination, however, the drop completely sticks to the surface and does not roll off upon tilting at any angle. Such strong changes in the wetting behavior offer an interesting potential for applications in microfluidic systems.

O 13.8 Mon 16:45 WIL B321

Probing the intrinsic switching kinetics of thermoresponsive polymer brushes at the water/substrate interface — Crispin Amiri Naini, Steffen Franzka, Sven Frost, Mathias Ulbricht, and •Nils Hartmann — Fakultät für Chemie, CeNIDE, NETZ, Universität Duisburg-Essen, Universitätsstr. 5, 45141 Essen

Stimuli-responsive polymers are widely used as actuators and sensors in a variety of applications including adaptive microoptics, microfluidic chips and smart membranes. A detailed knowledge of the intrinsic switching kinetics of such materials is of key importance. Here we demonstrate a stroboscopic photothermal laser manipulation technique, which allows for real-time observation of the switching behavior of poly-n-isopropylacrylamide brushes at the water/substrate interface. A modulated beam of a microfocused laser is used to intermittently heat the substrate surface and locally trigger swelling and deswelling of the thermoresponsive polymer film. Spatial variations of the swelling ratio are monitored using reflectometric interference video microscopy. This facilitates direct parallel measurement of the temperature-dependent switching kinetics of brush layers with thicknesses below one hundred nanometers. Response times range from the millisecond down to the microsecond range demonstrating the prospects of surface-grafted polymer films in fabrication of nanosized polymeric actuators and sensors with fast responsivities.

[1] M. Mathieu, A. Friebe, S. Franzka, M. Ulbricht, N. Hartmann, Langmuir 25 (2009) 12393.

O 14: Clean surfaces: Metals, semiconductors, oxides and insulators I

Time: Monday 15:00–16:45 Location: WIL B122

O 14.1 Mon 15:00 WIL B122

Change of the surface electronic structure of Au(111) by a monolayer MgO(001) film — •Yi Pan[1], Stefania Benedetti[2], Niklas Nilius[1], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany — [2]CNR, Istituto Nanoscienze, Centro S3, Via G. Campi 213/a, 41100 Modena, Italy

Monolayer films of MgO(001) have been prepared on an Au(111) surface and explored with scanning tunneling microscopy and spectroscopy. The symmetry mismatch between the hexagonal substrate and the squared over-layer results in the formation of a (6x1) superlattice, as revealed from the distinct stripe pattern observed in the STM. The presence of the oxide film modifies the potential situation at the interface, which induces a substantial up-shift of the Shockley-type surface band on Au(111). The resulting MgO/Au interface band is also characterized by a pseudo-gap at around 0.5 eV that opens at the position of the new Brillouin zone of the enlarged (6x1) cell. In addition, the oxide layer gives rise to a drastic decrease of the Au(111) work function, as deduced from the energy position of field-emission resonance on the bare and MgO-covered surface. The work function drop is explained by an interfacial charge transfer from the oxide film into the electro-negative gold surface.

O 14.2 Mon 15:15 WIL B122

Electronic structure and thermodynamics of oxygen vacancies on (100) and (111) surfaces of MgO. — •Sergey V. Levchenko, Norina Richter, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Polar metal oxide surfaces exhibit an increased sensitivity to the chemical environment due to major changes in surface stoichiometry driven by the requirement to compensate the surface charge. On top of such rearrangements, formation of surface point defects can greatly influence chemical properties of the surface. In this study, we employ density functional theory with HSE06 exchange-correlation functional with different values of the exchange screening parameter (including PBE as a limiting case) to calculate electronic structure and formation energies of neutral and charged O vacancies at the polar MgO(111) surface, which has been (and continues to be) a subject of extensive experimental and theoretical studies. The vacancies are calculated at the O-terminated octopolar reconstruction, which was predicted to be the most stable one for a wide range of O chemical potentials [1]. We use the *ab initio* atomistic thermodynamics approach [2] to estimate concentration, distribution, and charge states of the vacancies as a function of temperature, oxygen pressure, and electronic chemical potential. The properties of defects at the (111) surface are compared to the defects at the non-polar (100) termination.— [1] W. B. Zhang and B. Y. Tang, J. Phys. Chem. C 112 (2008) 3327; [2] K. Reuter and M. Scheffler, Phys. Rev. B 65, 035406 (2001); C. M. Weinert and M. Scheffler, Mat. Sci. Forum 10-12, 25 (1986)

O 14.3 Mon 15:30 WIL B122

NC-AFM Aufnahmen von reinem und wasserstoffterminierten Diamant C(100) — Markus Nimmrich[1], •Markus Kittelmann[1], Philipp Rahe[1], Andrew Mayne[2], Gerald Dujardin[2], Alexander von Schmidsfeld[3], Michael Reichling[3], Wolfgang Harneit[4] und Angelika Kühnle[1] — [1]Institut für Physikalische Chemie, Johannes Gutenberg-Universität Mainz, Germany — [2]Laboratoire de Photophysique Moléculaire, Université Paris-Sud, France — [3]Fachbereich Physik, Universität Osnabrück, Germany — [4]Institut für Experimentalphysik, Freie Universität Berlin, Germany

In diesem Beitrag stellen wir Ergebnisse unserer Untersuchung von hochreinem Typ IIa Diamant mit dem Nicht-Kontakt-Rasterkraftmikroskop (NC-AFM) vor. Wir präsentieren NC-AFM-Aufnahmen, die zum ersten Mal die einzelnen Wasserstoffatome der wasserstoffterminierten Diamant C (100) (2 x 1): H Oberfläche und die Kohlenstoffdimere auf der wasserstofffreien Diamant (100) (2 x 1) Oberfläche atomar aufgelöst zeigen.

Für die wasserstoffterminierte Oberfläche wird eine fast quadratische Elementarzelle abgebildet. Die beobachteten interatomaren Abstände sind in guter Übereinstimmung mit bereits publizierten Berechnungen der Diamant C (100) - (2 x 1): H Oberflächenstruktur.

Durch Entfernen des Wasserstoffs von der Diamantoberfläche wird die Probe nichtleitend. Wir stellen hochauflösende Aufnahmen vor, in denen die Kohlenstoffdimere einzeln dargestellt werden. Mit unseren Ergebnisse liefern wir einen experimentellen Nachweis für die (2 x 1)-Dimerrekonstruktion auf der nichtleitenden C (100) Oberfläche.

O 14.4 Mon 15:45 WIL B122

Construction of an Interatomic Potential for Zinc Oxide Surfaces by High-Dimensional Neural Networks — •Nongnuch Artrith, Tobias Morawietz, and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Zinc oxide (ZnO) is a technologically important material with many applications, e.g. in heterogeneous catalysis. For theoretical studies of the structural properties of ZnO surfaces, defects, and crystal structures it is necessary to simulate large systems over long time-scales with sufficient accuracy. Often, the required system size is not accessible by computationally rather demanding density-functional theory (DFT) calculations. Recently, artificial Neural Networks (NN) trained to first principles data have shown to provide accurate potential-energy surfaces (PESs) for condensed systems. We present the construction and analysis of a NN PES for ZnO. The structural and energetic properties of bulk ZnO and ZnO surfaces are investigated using this potential and compared to DFT calculations.

O 14.5 Mon 16:00 WIL B122

Electron localization in defective ceria films: An STM and DFT study — Jan Frederik Jerratsch[1], Xiang Shao[1], •Niklas Nilius[1], Hans-Joachim Freund[1], Cristina Popa[2], M. Veronica Ganduglia-Pirovano[2], and Joachim Sauer[2] — [1]Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany — [2]Humboldt-Universität zu Berlin, Unter den Linden 6, 10099 Berlin, Germany

Scanning tunnelling microscopy and density functional theory have been employed to identify the spatial correlation between an oxygen vacancy and the associated Ce3+ ion pair in a defective CeO2(111) film. The two Ce3+ ions can occupy different cationic shells around the vacancy (1st to 4th neighbour). The resulting variation in the chemical environment leads to a splitting of the filled Ce3+ f-levels, which is detected with STM spectroscopy. The position of the Ce3+ ion pair is also reflected in characteristic defect patterns observed in empty-state STM images, which result from the bright appearance of Ce4+ ions next to the defect while the Ce3+ remain dark. Both findings demonstrate that at least one extra electron localizes in a Ce ion that is not adjacent to the O vacancy.

O 14.6 Mon 16:15 WIL B122

Formation and coexistence of different surface structures on heavily reduced TiO2 (110) rutile surface: STM/STS study. — •Pavel Shukrynau, Marius Toader, Lars Smykalla, and Michael Hietschold — Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany

Cycles of Ar+ ion bombardment followed by specific temperature treatment leads to the formation and coexistence of two different phases onto single crystal TiO2 (110) rutile surface. One of the observed reconstructions is somehow similar to that cross-linked (1x2)-TiO2 structure, where the cross-link chains are perpendicular to the added rows of Ti2O3. In contrast, we observe cross-links that are rotated to 45° with respect to the <001> direction of the rows. This uncommon formation of the cross-link chains could be explained by the rearrangement of the top atoms at certain temperatures. STM topographs taken over the neighboring phase show bright rows, that run in <110> direction. Close inspection of the filled and empty images reveals zigzag arrangement of the bright protrusions within the particular line. Tunneling spectra acquired over various sites in the topographic image give the information about the bonding nature within the reconstruction. We propose the possible structural models of the coexisting phases and discuss their formation mechanisms on the base of atomically resolved STM images that were taken in both constant current and constant height modes.

O 14.7 Mon 16:30 WIL B122

Epitaxial films of praseodymia on Si(111): controlled modification from Pr_2O_3 to PrO_2 via plasma and thermal treatment — •Sarah Röhe[1], Andreas Schaefer[1], Volkmar Zielasek[1], Thomas Schroeder[2], and Marcus Bäumer[1] — [1]IAPC, Universität Bremen — [2]IHP, Frankfurt (Oder)

A cold RF oxygen plasma treatment is demonstrated as a successful route to prepare clean, well-ordered and stoichiometric PrO_2 layers on silicon which are very difficult to obtain by other techniques. As a starting point, cubic $PrO_{2-\Delta}$ films are obtained by growing hexagonal Pr_2O_3 on Si(111) by MBE and annealing these layers to 720 K in oxygen atmosphere. The subsequent plasma treatment is performed in a plasma cell directly attached to a UHV chamber so that samples can be transferred to XPS without breaking vacuum. The Pr 3d XP spectra show so far unobserved spectral characteristics presenting a fingerprint for PrO_2. The XPS data provide insight into the special role of praseodymia among the rare earth oxides. They also reveal that former XP studies of praseodymia suffered from significant reduction at the surface. Starting with PrO_2 films prepared by oxygen plasma, different oxidation states of praseodymia can be obtained by reducing the oxide in a controlled way via thermal treatment. Several temperature-programmed desorption peaks of O_2 are observed in the range from 300 to 900 K and indicate phase transitions. The different praseodymia phases are studied with respect to their activity towards CO oxidation at their surface under UHV conditions.

O 15: Nanostructures at surfaces: Dots, particles, clusters, arrays I

Time: Monday 15:00–17:00 Location: WIL C107

O 15.1 Mon 15:00 WIL C107

Formation of rare earth silicide clusters on Si(111)7x7 — •Martin Franz, Monir Rychetsky, Stephan Appelfeller, and Mario Dähne — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin, Germany

Magic clusters on surfaces are of high interest because of their fascinating quantum properties and their possible application in future nanodevices. Here, the formation process as well as the structural and electronic properties of dysprosium silicide clusters on the Si(111)7x7 surface were studied using scanning tunneling microscopy (STM). The dysprosium silicide clusters were grown by molecular beam epitaxy using the 7x7 reconstructed Si(111) surface as a template for cluster formation using submonolayer metal coverages and moderate annealing temperatures. It was found that the clusters grow self-organized preferentially on the faulted halves of the 7x7 unit cells, and a variety of cluster shapes could be observed. At appropriate growth conditions, the formation of magic clusters, which appear centered on the 7x7 half unit cells, could be achieved. This project was supported by the DFG through FOR 1282.

O 15.2 Mon 15:15 WIL C107

Tunable quantum dot arrays by self-assembled metal-organic networks — •Nenad Kepcija[1], Florian Klappenberger[1], Dirk Kühne[1], Wolfgang Krenner[1], Svetlana Klyatskaya[2], Andres Arnau[3], Javier Garcia de Abajo[4], Mario Ruben[2], and Johannes Barth[1] — [1]Physik Department E20, TU München, Germany — [2]Institute of Nanotechnology, Forschungszentrum Karlsruhe, Karlsruhe, Germany — [3]Centro de Fisica de Materiales CSIC-UPV/EHU, 20080 San Sebastian, Spain — [4]Instituto de Optica CSIC, Serrano 121, 28006 Madrid, Spain

The confinement of Ag(111) surface state electrons by self-assembled, nanoporous metal-organic networks is studied using low-temperature scanning tunneling microscopy/spectroscopy and electronic structure calculations. The honeycomb networks of Co ligands and dicarbonitrile-oligophenyl linkers induce surface resonance states confined in the cavities with a tunable energy level alignment. With the help of a boundary element method (BEM) based on Greens functions the electronic structure is analyzed and compared to different confinement situations. We find that electron scattering on the molecules is repulsive and stronger than on the weakly attractive Co and that the networks represent periodic arrays of coupled quantum dots featuring uniform electronic levels.

O 15.3 Mon 15:30 WIL C107

Comparing different molecular building blocks designed for covalent linking on noble metal surfaces — •Matthias Koch[1], Marie Gille[2], Stefan Hecht[2], and Leonhard Grill[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland — [2]Humboldt-Universität zu Berlin, Berlin, Deutschland

The self-organized formation of molecular nanostructures on surfaces is of high interest for potential applications in future nanotechnology. A key challenge in this field is the controlled variation of the intermolecular interaction with a particular focus on strong chemical bonds, which would ensure for high stability of the nanostructures. Moreover, it should allow the formation of extended conjugated electronic systems that are of interest for efficient charge transfer. The on-surface synthesis method [1] is very promising in this regard as it fulfills both requirements and allows to covalently bind individual molecular building blocks on a surface. It is realized by activating specific side groups, i.e. thermal dissociation of halogen substitutents. In this study, we have systemically compared the self-organization of various similar molecular building blocks on different noble metal surfaces by low temperature scanning tunneling microscopy (STM). The adsorption geometry and covalent connection of the poly-aromatic molecules turns out to depend strongly on the chemical structure of the molecules and their interaction with the metal surface. Moreover, the interaction of the molecules with the metallic surface was modified by tert-butyl-legs that lift the molecular core from the surface and compared with the same molecule without such groups. [1] L. Grill et al., Nature Nanotech., 2 687 (2007)

O 15.4 Mon 15:45 WIL C107

Self-assembly of Co rings on hexagonal boron nitride — •Fabian Donat Natterer, François Patthey, and Harald Brune — Institute of Condensed Matter Physics (ICMP), Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland

Upon deposition of minute amounts of cobalt on hexagonal (h) boron nitride at low temperature, we observe the formation of nanostructures lying like a necklace around the circular part of the (12 x 12) h-BN/Rh(111) moiré unit cell. These atomic chains, bent to a closed ring of 2 nm diameter, contain at least four and up to 10 equidistant Co atoms. Low temperature scanning tunnelling microscopy results indicate short range repulsion between the ring atoms. Interactions with the electric field of the tunnelling tip or gentle annealing either transform the ring into a compact Co cluster or completely remove it from the scanning region. Surprisingly, new atomic rings renucleate in different moiré cavities or are converted from existing Co clusters at elevated temperatures. At low Co coverage, the rings are several tens of (12 x 12) unit cells apart, implying large Co adatom diffusion rates, down to the lowest studied deposition temperatures of 8 K.

O 15.5 Mon 16:00 WIL C107

Growth of grooved Si and Ge/Si surfaces by selective adsorption of C_{60} — •Stefan Korte, Vasily Cherepanov, and Bert Voigtländer — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology

Ge/Si nanostructures can be grown using Bi as surfactant in order to suppress Si-Ge intermixing and to faciliate layer-by-layer growth. With an appropriate choice of growth conditions one can achieve a chemical selectivity for C_{60} adsorption on Bi terminated Si and Ge/Si surfaces. C_{60} molecules then adsorb only on the step edges of a Si(111) surface or onto the Ge area of Ge/Si heterostructures, respectively. During subsequent growth of Si and Ge C_{60} can be used to mask those parts of the surface and prevent growth of further Si and Ge layers. When Si or Ge is deposited onto the surface it grows layer-by-layer on the free Si terraces and not on the C_{60} covered areas.

This masking has been demonstrated for C_{60} covered Ge nanowires on Si and for C_{60} covered Si step edges. It enables us to grow Si and Ge thin films with parallel grooves by an appropriate sequence of MBE depositions. Surfaces with 3 nm deep and less than 10 nm wide trenches were fabricated.

O 15.6 Mon 16:15 WIL C107

Supported silver and copper clusters for photocatalysis — •Vladimir Popok, Ingo Barke, Antje Neubauer, Stefan Lochbrunner, and Karl-Heinz Meiwes-Broer — Institut für Physik, Universität Rostock, Universitätsplatz 3, 18051 Rostock, Germany

Nanometer-sized metal particles deposited onto surfaces are of significant interest for applications in catalysis. In the current study, nanoparticles of silver and copper in the size range from ca. 5 to 18 nm were formed using arc-discharge and magnetron sputtering cluster ion sources and deposited on silica glass substrates. The prepared cluster-assembled samples have been studied in order to increase the efficiency of existing catalytic schemes for hydrogen production, which is of high practical importance. In particular, Ir photosensitizers (PS) in combination with palladium, platinum or iron catalysts are known to be promising systems for reduction of aqueous protons to hydrogen. We deposited the PS on cluster-covered samples and studied their optical properties. It is found that in presence of metal clusters the ligand-centered optical transitions of the PS are significantly increased accompanied by a change of the photoluminescence. These findings indicate considerable effect of the metal nanoparticles on the electronic structure of the PS, a fact that might be of relevance for the improvement of photo-catalytic reactions.

O 15.7 Mon 16:30 WIL C107

CO induced unpinning of Pt clusters from the Ir(111)/graphene moiré — •Timm Gerber[1], Jan Knudsen[2], Patrick Stratmann[1], Elin Grånäs[2], Karina Schulte[3], Carsten Busse[1], Jesper Andersen[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Division of Synchrotron Radiation Research, Department of Physics, Lund University , Sweden — [3]MAX-Laboratory, Lund University, Sweden

The Stability of catalyst particles under reactive conditions is of crucial importance for their performance and durability. Here we investigated the adsorption of CO and its effect on the stability of Pt-cluster superlattices with a periodicity of 2.5 nm on a graphene layer on Ir(111).

XPS and TPD both suggest that CO adsorbs on-top and preferentially at cluster step edges, but also on cluster facets. Further, upon CO adsorption XPS signals a weakened binding of the Pt clusters to their graphene substrate: the C1s feature characteristic for cluster binding diminishes. For small clusters with an average size below 10 atoms this unpinning implies cluster diffusion and cluster coalescence, as observed dynamically through STM image sequences. Larger clusters with an average size around 20 atoms remain fixed upon room temperature CO adsorption.

To prevent cluster coalescence in the early stages of cluster growth and to obtain the most regular Pt-cluster superlattices the CO partial pressure during Pt deposition should be minimal. Otherwise adsorbed CO causes unpinning and subsequent coalescence of small intermediate clusters already during the growth process.

O 15.8 Mon 16:45 WIL C107

Frictional and electrical characterization of nanostructures induced by slow highly charged ion bombardment of HOPG surfaces — •Quan Shen[1], Robert Ritter[2], Gregor Kowarik[2], Friedrich Aumayr[2], and Christian Teichert[1] — [1]Institute of Physics, University of Leoben, A8700 Leoben, Austria — [2]Institute of Applied Physics, Vienna University of Technology, A1040 Vienna, Austria

Bombardment of a highly ordered pyrolitic graphite (HOPG) surface with slow, highly charged ions (Ar q+ and Xe q+) can be considered as a model system for surface layer modification. The topographic identification of the induced surface by atomic force microscopy (AFM) measurement in conventional tapping mode is difficult[1]. However, using Friction Force Microscopy, where the cantilever is scanned perpendicular to its long axis in contact mode, the ion impact locations (dots) can be revealed as zones of enhanced friction in both, topographic and friction images. For quantitative lateral force measurements, an improved wedge calibration method is employed[2]. The microscopic friction force coefficient of the ion impact locations on the surface has been determined as a function of ion charge state. The impact dot size detected by friction images clearly depend on the ion charge state. For electrical characterization of the ion bombarded surface, we employed conductive AFM, which clearly showed an increased conductivity at ion impact locations.

[1] R. Ritter, et al. , Nucl. Instrum. Meth. Phys. Res. B 268 (2010). [2] M. Varenberg, et al. , Rev. Sci. Instrum. 74 (2003).

O 16: Scanning probe methods I

Time: Monday 15:00–17:00 Location: WIL C307

O 16.1 Mon 15:00 WIL C307

Deconvolution of the local density of states from z-V spectroscopy and its application to Nb(110) — •Holger Pfeifer, Berndt Koslowski, and Paul Ziemann — Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm, Germany

In recent years, measurement of the differential conductivity at constant current (z-V spectroscopy) has been established as a powerful tool in scanning tunnelling spectroscopy in order to analyze the local density of states (LDOS) of a sample. However, in contrast to I-V spectroscopy [1], numerical methods are lacking to remove effects of the tunnelling barrier from the measurement and to deconvolve the LDOS of tip and sample. Here we introduce an adopted method from [1] to achieve a deconvolution of the LDOS from z-V measurements. We first demonstrate the deconvolution method using numerical data. Secondly, we apply this method to experimental data obtained on Nb(110) at low temperature and compare the results with the differential barrier height $\left(\frac{d^2I}{dV\,dz}/\frac{dI}{dV}\right)^2$ [2]. We show that the differential barrier is much more sensitive to changes in the DOS than the commonly used (integral) barrier height $\left(\frac{dI}{dz}/I\right)^2$.

[1] B. Koslowski, H. Pfeifer, P. Ziemann, PRB 80, 165419 (2009).

[2] B. Koslowski et al. PRB 75, 035421 (2007).

O 16.2 Mon 15:15 WIL C307

Ultracompact nanopositioner for scanning probe microscopy — •Bert Voigtländer, Vasily Cherepanov, and Peter Coenen — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology

The coarse positioning unit consumes most space in a scanning probe microscope. Here we present a new type of ultra compact nano-drive which has diameter less than 2.5 mm and length smaller than 10 mm and can serve as an STM coarse positioning device. Alternating movements of springs move a tube which holds the STM tip or AFM sensor. Due to the operation principle we name it Koala-drive. The travel is limited only by the tube length used, which can be several cm long. The new operating principle provides a smooth travel and avoids shaking which is intrinsically present for nanopositioners based on inertial motion with saw tooth driving signals. No high slew rate of the driving electronics is required. Adding a piezo tube for xyz scanning integrates a complete STM inside a 4 mm outer diameter piezo tube. The use of the Koala-drive makes the scanning probe microscopy design ultra compact and leads accordingly to an high mechanical stability. The drive is UHV and magnetic field compatible. The smooth operation minimizes also the power dissipation which can be a problem of inertial drives when operated at cryogenic temperatures. Furthermore, we use the Koala-drive to design a multi tip STM where four independent STM units are integrated on a diameter of 50 mm. We present examples of the performance of STM's designed using the Koala-drive.

O 16.3 Mon 15:30 WIL C307

Imaging atomic-scale magnetic structures by means of lateral atom manipulation with an STM tip — •Boris Wolter[1], Yasuo Yoshida[1], André Kubetzka[1], Kirsten von Bergmann[1], Saw-Wai Hla[2], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, 20355 Hamburg — [2]Nanoscale & Quantum Phenomena Institute, Ohio University, Athens, Ohio 45701

While spin-polarized STM and lateral atom manipulation with an STM tip are known to be powerful experimental techniques that have been employed to great extent, there are not many studies regarding the combination of these two methods[1].

Stroscio *et al.* have shown the use of lateral atom manipulation for enhanced imaging of the Cu(111) surface[2]. We apply this approach to SP-STM as an innovative magnetic imaging technique, observing increased magnetic contrast and atomic resolution of the substrate at the same time. To improve our understanding of this process, we combine Monte Carlo simulations for a classical Heisenberg spin system and lateral atom manipulation[3] with a model for SP-STM imaging[4]. By evaluating and comparing the results, we expect to gain insight into the dynamics involved in the manipulation imaging with magnetic atoms.

1. D. Serrate *et al.*, Nature Nano. 5, 350-353 (2010)
2. J. Stroscio *et al.*, Science 8, 306, 5694, 242-247 (2004)
3. A. Kühnle *et al.*, Surf. Sci. 449, 15 (2001)
4. S. Heinze, Appl. Phys. A 85, 407-414 (2006)

O 16.4 Mon 15:45 WIL C307

Low noise transimpedance amplifyer for STM applications — •Wulf Wulfhekel and Roland Jehle — Physikalisches Institut, Karksruher Institut für Technologie, Wolfgang Gaede Str. 1, 76131 Karlsruhe

Transimpedance amplifiers, or short IV-converters, are used in scanning tunneling microscopes to amplify the small tunneling currents before processing in the feed back loop and thus largely determine the performance of the instrument. While modern operational amplifiers (OPAs) offer extremely low current input noises ($\approx$1 fA/$\sqrt{Hz}$), the feed back resistor in IV-converters limits their performance due to thermal or Johnson-Nyquist noise when operated at room temperature. At an amplification of 10^9V/A the latter corresponds to 4.2 fA/$\sqrt{Hz}$ setting the theoretical noise limit of IV-converters. We present a careful analysis of the different noise sources, i.e. noise of the feed back resistor as well as input current noise, shot noise of the input bias current and input voltage noise of the OPA and present a new approach to IV-converters that beats the noise limit given by the feedback resistor using a sophisticated feed back mechanism. Further, internal capacitances of the circuit are compensated to minimize gain peaking. Finally, we compare the performance (noise and band widths) of the home build IV-converter with commercial products.

O 16.5 Mon 16:00 WIL C307

Miniature active damping stage for Scanning Probe Applications in Ultra High Vacuum — •Maximilian Assig[1], Alexandra Ast[2], Andreas Koch[1], Wolfgang Stiepany[1], Carola Strasser[1], Klaus Kern[1], and Christian R. Ast[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart — [2]Institut für Technische und Numerische Mechanik der Universität Stuttgart

Scanning Probe experiments demand a low vibration level to keep the distance between tip and sample constant. Small changes in the spacing between probe and sample result in enormous variations of the measured signal no matter if it is the tunneling current in Scanning Tunneling Microscopy (STM) or atomic forces and phase shift in Atomic Force Microscopy (AFM) measurements. We present a six-degree of freedom active damping technique based on a Stewart platform (Hexapod) which is to operate in Ultra High Vacuum (UHV)[1]. We outline the main working principle and show the effect of the internal damping on Scanning Tunneling Microscopy measurements of a Si(111) 7x7 surface at Room Temperature.

[1] D. Stewart, Proc. Instn. Mech. Engrs, **180**, 371, 1965

O 16.6 Mon 16:15 WIL C307

Magnetic Exchange Force Spectroscopy on antiferromagnetic Fe/W(001) — •Rene Schmidt[1], Cesar Lazo[2], Alexander Schwarz[1], Stefan Heinze[2], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, University of Hamburg — [2]Institute of Theoretical Physics and Astrophysics, University of Kiel

With the invention of magnetic exchange force microscopy (MExFM)[1] a new powerful tool to investigate atomic scale magnetic structures on all kinds of surfaces became available. Recently, we were able to resolve the antiferromagnetic structure of the Fe monolayer on W(001)[2]. Here, we demonstrate that it is possible to directly measure the distance dependence of the magnetic exchange interaction across a vacuum gap by applying a spectroscopic mode, i.e. magnetic exchange force spectroscopy (MExFS). Experimentally acquired data are compared with first-principles calculations accounting for magnetically different tips composed of Cr, Fe or mixtures of both. While sign and magnitude of the magnetic exchange energy are well reproduced, the majority of tips exhibit a stronger distance dependence than predicted for simple pyramidal tips and a more sudden onset of the interaction. More complex tip models will be discussed, which can explain this behavior.

[1] U.Kaiser *et al.*, Nature **446**, 522 (2007)

[2] R. Schmidt *et al.*, Nano Lett. **9**, 200 (2009)

O 16.7 Mon 16:30 WIL C307

4-Tip LT-STM with High Resolution SEM — •Bastian Schnitzler[1], Frank Matthes[1], Daniel E. Bürgler[1], Claus M. Schneider[1], Bernd Günther[2], and Markus Maier[2] — [1]Peter Grünberg Institute (PGI-6), FZ Jülich — [2]Omicron Nanotechnology GmbH

A new type of in-situ 4-tip scanning tunneling microscope will be presented featuring low temperatures less than 5 K, four independent tips for scanning and conductance measurements as well as a high resolution scanning electron microscope (SEM) and a super conducting coil providing a magnetic field of 25 mT.

The LT-Nanoprobe system has been developed in a collaboration between Omicron and the Peter Grünberg Institute. It is designed to provide excellent STM-qualities in scanning and spectroscopy, while being compact to be cooled down to LHE temperature. Further applications regarding (4-Point) conductance measurements of nanostructures benefit of a SEM resolution down to 20 nm to locate and contact nanostructures like quantum wires and Nanotubes.

System design and features will be discussed and first measurements will be presented.

O 16.8 Mon 16:45 WIL C307

Low Temperature Scanning Tunneling Spectroscopy on high quality Nb(110) films — •Matthias Stocker, Holger Pfeifer, Berndt Koslowski, and Paul Ziemann — Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm, Germany

High quality Nb(110) films were prepared by evaporation onto (0001)oriented sapphire substrates at 850°C and analyzed in situ by Low Temperature Scanning Tunneling Spectroscopy (LT-STS). In this way, the superconducting gap in the quasi-particle density of states (DOS) of Nb(110) is investigated. The incomplete opening of this gap at 5.3 K can be attributed to the somewhat higher tip temperature of ~ 7K. Significant structures in the I-V data positioned symmetrically around zero energy and matching nicely known phonon energies of Nb indicate strong coupling behavior of this superconductor. These results suggest attempting an evaluation of the corresponding Eliashberg function, α^2 F(ω).

O 17: Metal substrates: Adsorption of organic / bio molecules III

Time: Monday 17:15–19:15 Location: TRE Phy

O 17.1 Mon 17:15 TRE Phy

Opto-electronically active block copolymers on metallic surfaces — •Cormac Toher, Jörg Meyer, Loka Mani, Anja Wadewitz, Francesca Moresco, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany.

Opto-electronically active organic polymer materials offer several advantages over traditional solid-state semiconductors in the fabrication of devices such as solar cells and light emitting diodes, including their low cost, low weight, and flexibility. Here, we present the results of ongoing combined theoretical and experimental analytical studies of a block copolymer consisting of a covalently bound polythiophene donor and fullerene acceptor, with the goal of developing a fundamental, systematic, atomistic-scale understanding of the origin of specific optoelectronic properties in order to facilitate the enhancement of the efficiency and functionality of these materials. The electronic structure and transport properties of both the full polymer chains and the individual components were investigated using ab initio density functional theory (DFT) and non-equilibrium Green's function calculations. The molecular components were then deposited on metallic surfaces for study using scanning tunnelling microscopy, in conjunction with DFT simulations of the density of states and investigations of the interaction with the substrate.

O 17.2 Mon 17:30 TRE Phy

Direct formation of a polyamide on Ag(111): Joint XPS and STM studies — •Martin Schmid[1], Christoph H. Schmitz[2], Julian Ikonomov[2], Hans-Peter Steinrück[1], J. Michael Gottfried[1], and Moritz Sokolowski[2] — [1]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg — [2]Institut für Physikalische und Theoretische Chemie, Universität Bonn

The polymer poly(p-phenylene terephthalamide) (PPTA) was synthesized on Ag(111) by co-adsorption of the reactive monomer compounds terephthaloyl chloride (TPC) and p-phenylenediamine (PPD) at 300 K. The resulting adsorbate phases were characterised by photoelectron spectroscopy (XPS) and scanning tunneling microscopy (STM). A detailed study of the chemical composition and morphology revealed a complex reaction mechanism, by which the formation of amide bonds leads to folded PPTA polymer chains. According to XPS, the chloride of the TPC precursor is not released as HCl as in the bulk reaction, but remains on the surface as chemisorbed Cl or AgCl. Further temperature-programmed XPS studies of pure TPC on Ag(111) reveal that the molecule decomposes already above 130 K, forming chemisorbed Cl (or AgCl) and a phenylene-dicarbonyl species, which is presumably stabilized by the substrate. The adsorbed chlorine partially desorbs above 800 K as molecular AgCl. Financial support by the Deutsche Forschungsgemeinschaft through SFB 624 and SFB 583 is gratefully acknowledged.

O 17.3 Mon 17:45 TRE Phy

Modeling of the adsorption of bis(terpyridine) molecules at the solid/liquid interface — •Daniela Künzel and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

Force field and DFT calculations have been quite successful in addressing properties of adsorbed organic molecules [1,2]. However, the calculations are typically performed at the solid/vacuum interface whereas the experiments are often done at the solid/liquid interface. This might be the reason for remaining discrepancies between experimental and theoretical results. Therefore, we attempt to implicitly include the effect of solvents into our force field calculations in order to obtain a better model of the experimental systems.

As a first step, we have determined average energies of solvated systems using molecular dynamics simulations. Calculations of solvent densities and solvation energies of small test molecules serve to validate the applicability of different force fields to the problem. Based on the knowledge gained from these validation steps, the solvation of BTP molecules and the adsorption of dissolved molecules on graphite is analyzed.

[1] C. Meier et al., Angew. Chem. Int. Ed., 2008, 47, 3821.

[2] D. Künzel, Th. Markert, A. Groß, and D. M. Benoit, Phys. Chem. Chem. Phys., 2009, 11, 8867.

O 17.4 Mon 18:00 TRE Phy

Scanning Tunneling Microscopy of Proteins in Ultrahigh Vacuum — •Stephan Rauschenbach[1], Nicha Thontasen[1], Deng Zhitao[1], Rinke Gordon[1], and Kern Klaus[1,2] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]Institut de Physique de la Matiere Condensee, Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland

Proteins are biosynthesized, self-assembled, functional polymers of unprecedented complexity and specify in their function. Since the shape which determines their behavior depends strongly on the environment they typically are investigated under physiological conditions. The functionalization of well defined surfaces with such molecules would be an important step towards using high performance vacuum based techniques, like scanning probe microscopes. Here we show the controlled deposition and in situ characterization of intact proteins on clean metal surfaces in ultrahigh vacuum by electrospray ion beam deposition (ES-IBD). We demonstrate that depending on the charge state, the protein can be deposited in a folded or unfolded state. For unfolded proteins, scanning tunneling microscopy reaches single amino acid level resolution.

O 17.5 Mon 18:15 TRE Phy

Dynamic Force Spectroscopy at a Single Molecule Junction — •Christian Lotze, Martina Corso, Gunnar Schulze, Katharina J. Franke, and Jose Ignacio Pascual — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

Recent Developments in Atomic Force Microscopy made it possible to probe not only electronic properties of single molecules and atoms on (conducting) surfaces but also acquiring information about forces in the pN regime simultaneously. Determination of the charged state of single metal atoms [1] or resolving the chemical structure of a molecule [2] are just some of the possibilities, opening a new field of scanning probe spectroscopy.

We utilize our tuning fork based LT STM/AFM in the well known qPlus design operated at 5K to do single molecule force spectroscopy combined with tunneling differential conductance measurements. With our STM tip we contact a functionalized polyarene molecule in one side and lift it up from the surface, while the other side remains attached to the substrate [3]. During lift up we observe sawtooth like features in the df spectra that allow us to determine potential barrier heights during the molecule pulling process.

[1] Leo Gross, *et al.*, Science **324**, 1428 (2009) [2] Leo Gross, *et al.*, Science **325**, 1110 (2009) [3] F. Pump, R. Temirov, O. Neucheva, S. Soubatch, S. Tautz, M. Rohlfing, G. Cuniberti, Appl. Phys. A **93**, 335 (2008)

O 17.6 Mon 18:30 TRE Phy

Modification of the electronic properties of Au/molecule/Pd junctions by adsorbed hydrogen: a DFT study — •Jan Kučera and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, D-89069 Ulm, Germany

Metal-molecule-metal contacts assembled from a Pd monolayer deposited on a Au-supported self-assembled monolayer (SAM) of 4-mercaptopyridine or 4-aminothiophenol were recently achieved by means of an electrochemical approach [1]. Subsequent photoelectron spectroscopy showed a strongly reduced Pd density of states (DOS) at the Fermi energy [2]. This phenomenon is still not fully comprehended, however, its understanding is crucial for the use of the sandwich design as a platform for future nanoelectronics.

Periodic density functional theory (DFT) calculation revealed that the dehydrogenation of the amino group and the subsequent strong bonding of the remaining nitrogen atom to the Pd layer could explain the observed modification of the DOS [3]. We have now extended this study in order to clarify the role of hydrogen atoms for the electronic properties of the Pd layers. In equilibrium, these layers should always show a considerable hydrogen coverage in an aqueous environment. Our calculations demonstrate that indeed the adsorbed hydrogen atoms significantly modify the electronic structure of the Pd layers.

[1] F. Eberle et. al., Angew. Chem. Int. Ed. 49, 341-345 (2010)

[2] H.-G. Boyen et. al., Nature Materials 5, 394 (2006)

[3] J. Kučera and A. Groß, Phys. Chem. Chem. Phys. 12, 4423 (2010)

O 17.7 Mon 18:45 TRE Phy

Interface properties of a biphenyl-based metal-molecule-metal junction — •Marc Saitner[1], Felix Eberle[2], Dieter M. Kolb[2], Johnny Baccus[1], Patrick Wagner[1,3], Marc D'Olieslaeger[1,3], and Hans-Gerd Boyen[1] — [1]Institute for Materials Research (IMO), Hasselt University, B-3590 Diepenbeek, Belgium — [2]Institute for Electrochemistry, Ulm University, D-89069 Ulm — [3]IMEC, Division IMOMEC, B-3590 Diepenbeek, Belgium

Here we report on the successful preparation of a metal/molecule/metal junction, in which a biphenyl (BP) self-assembled monolayer (SAM) on Au(111) is metalized by Pd using a recently developed electrochemical approach.[1] The junction is studied by cyclic voltametry (CV), in-situ scanning tunneling microscopy (STM) and ex-situ X-ray as well as ultraviolet photoelectron spectroscopy (XPS, UPS). A quantitative chemical analysis of the BP SAM points towards the formation of a densely packed molecular layer attached to the base electrode (Au single crystal) via Au-S bounds. The successful metallization of such SAMs with a Pd monolayer is demonstrated by means of angle-resolved XPS. Both metal-molecule interfaces in the junction can be studied in more detail using angle-resolved UPS thereby allowing to identify local-density of states effects [2,3] in the electronic structure of the involved metals.

[1] T. Baunach et al., Adv. Mater. 16, 2024 (2004)

[2] H.-G. Boyen et al., Nat. Mater. 5, 394 (2006)

[3] M. Manolova et al., Adv. Mater. 21, 320 (2009)

O 17.8 Mon 19:00 TRE Phy

STM investigation of the morphology of biphenylthiol self-assembled monolayers on Au(111) — •Heiko Muzik, Dan G. Matei, Laxman Kankate, Armin Gölzhäuser und Andrey Turchanin — Physik supramolekularer Systeme und Oberflächen, Universität Bielefeld

Self-assembled monolayers (SAMs) with an aromatic moiety directly attached to the sulfur head group are known to build highly corrugated surface morphologies on Au(111). A commonly observed pattern is the formation of islands with a gold step-edge height. The nature of this phenomenon has been rarely investigated, although it stands in contrast to the observation of so-called 'etch pits' in alkanethiol SAMs. In this contribution we present a scanning tunneling microscopy study of SAMs of 4'-nitro-1,1'-biphenyl-4-thiols and 1,1'-biphenyl-4-thiols on Au(111). We relate the different SAM morphologies to the molecular coverage, which was complementary determined by X-ray photoelectron spectroscopy. Based on these data we discuss why the classical picture of the molecule/substrate interface with the Au(111) binding sites has to be reviewed.

O 18: Plasmonics and Nanooptics II

Time: Monday 17:15–19:15 Location: PHY C213

O 18.1 Mon 17:15 PHY C213

Lithographically defined plasmonic waveguides on semiconductors for on-chip quantum optics applications — •Gregor Bracher, Konrad Schraml, Benedikt Mayer, Birgit Wiedemann, Simon Frédéric, Jonathan J. Finley, and Michael Kaniber — Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, D-85748 Garching, Germany

We present optical investigations on lithographically defined plasmonic waveguides (WG). The metallic WGs are fabricated on GaAs substrates by electron beam lithography and subsequent metallisation. Structural properties are probed by atomic force microscopy and scanning electron microscopy revealing a surface roughness below 3 nm. For the optical characterisation we use a two axis confocal micro-photoluminescence setup that enables us to excite and detect plasmons perpendicular and parallel to the sample surface. First measurements show that Au WGs with a thickness of 100 nm and width of 4 μm exhibit a propagation length of 15 μm at $\lambda = 820\ nm$. We clearly observe strong localisation of the excitation at the wire end and the expected polarisation dependence along the WG axis. Using the same technique we prove that plasmons can be excited in lithographically defined Au nanowires with a cross section down to 100x100 nm^2. The deterministic control of the position and shape of the plasmonic nanostructures by means of electron beam lithography combined with near surface self-assembled InGaAs/GaAs quantum dots promises efficient on-chip generation and guiding of single plasmons for future applications in nanoscale quantum optics.

O 18.2 Mon 17:30 PHY C213

Fabrication of high-quality large-area plasmonic oligomers — •Jun Zhao, Bettina Frank, and Harald Giessen — Universität Stuttgart

Plasmonic structures with a structure size of around $100nm$ are tremendously important for applications in the visible and near-IR range. Surface-enhanced Raman scattering substrates, localized surface plasmon resonance sensors, narrow resonances using plasmonic induced transparency, and local field concentration in oligomers to create hot spots are among those applications. Key issues in the design and manufacturing of such structures are small gaps in the range of sub-$20nm$, sharp edges, and narrow resonances. For applications, large fabrication areas in the range of cm^2 and low manufacturing costs are crucial. Here, we present a method that fulfils these requirements. Utilizing tilted-angle-rotation lithography with a polar and azimuthal rotation axis and shutter control together with monolayers of polystyrene spheres we create reproducibly homogeneous structures in $50nm$ to $200nm$ range with $10nm$ gaps over areas of cm^2. We fabricated triangular monomers, dimers, trimers, quadrumers, and pentamers, with open and closed gaps and with different size of nanospheres, and measured their transmittance spectra by FTIR microscopy. The spectra show well modulated resonances which depend sensitively on the incident polarization. We can attribute the various collective modes to the different features of the spectra and observe hybridization effects. This confirms the high quality of our fabrication method.

O 18.3 Mon 17:45 PHY C213

Plasmonic nanostructures for strong light confinement fabricated using soft-lithography and plasma etching techniques — •Manuel Gonçalves[1], Tobias Paust[1], Fabian Enderle[2], Stefan Wiedemann[2], Alfred Plettl[2], Paul Ziemann[2], and Othmar Marti[1] — [1]Ulm University - Inst. of Experimental Physics, Albert-Einstein-Allee 11, 89069 Ulm, Germany — [2]Ulm University - Inst. of Solid State Physics, Albert-Einstein-Allee 11, 89069 Ulm, Germany

Nanosphere lithography has been commonly used for fabrication of plasmonic nanostructures. Small triangular particles of less than 100 nm size, with sharp corners, can be obtained at low cost. These structures have been used for plasmonic based sensing applications.

We show how nanosphere lithography can be extended for fabrication of more complex structures as arrays of holes on corrugated dielectrica and arrays of metal-dielectric pillars, using in combination soft-lithography and reactive ion-etching techniques (ICP-RIE). Surface plasmon modes can be easily excited on metal coated periodic dielectric structures using light. On the other hand, geometrical singularities lead to strong localized surface plasmons. The fabricated structures can be used for plasmonic effects as enhanced optical transmission, light confinement and surface enhanced Raman spectroscopy, due to their geometrical and optical properties. Confocal microscopy and angle-resolved spectroscopy were used for study of far-field transmittance and reflectance. The near-fields were investigated by SNOM and confocal Raman microscopy. Simulations were carried out to obtain the near-fields and optical resonances.

O 18.4 Mon 18:00 PHY C213

Light Localization Effects in Commensurate Gratings — •Aude Barbara[1,2], Jerôme Le Perchec[3], Stéphane Collin[4], Camille Maxime[1,2], and Pascal Quémerais[1,5] — [1]Institut Néel, CNRS-UJF, Grenoble, France — [2]IAPP, TU Dresden, Germany — [3]CEA, Grenoble, France — [4]LPN, Marcoussis, France — [5]MPI-PKS, Dresden, Germany

We present a study in which infrared light localization phenomena are induced in commensurate gratings made of deep sub-wavelength metallic grooves. We combined the effects of light trapping within active sites (the deep cavities) with the properties of self-similar arrangements (commensurate gratings). We show that as the degree of commensuration tends to an irrational number new light localization states are produced. Interestingly, these have properties close to that reported for hot spots on disordered surfaces. In particular they present a very high sensitivity to the variation of the exciting field (wavelength and incident angle). We also experimentally demonstrated the existence of these new resonances and measured their dispersion diagrams. We observed selective light localization within the cavities, transition from localized to delocalized modes and modifications of the mode coupling with the incident light leading to the generation of black modes. The theoretical analyze is in full agreement with the experiments.

A. Barbara et al. *Opt. Exp.* **16**, 19127 (2008)
A. Barbara et al. *Opt. Exp.* **18**, 14913 (2010)

O 18.5 Mon 18:15 PHY C213

Parallel nanostructuring of fused silica exploiting local near fields — •Sören Maag, Rodica Morarescu, Frank Träger, and Frank Hubenthal — Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

In modern nanotechnology, there is an ongoing interest to decrease the dimensions of surface structures below the diffraction limit. Furthermore, parallel structuring of surfaces with light induced processes is of particular interest. Along these lines we are using nanosphere lithography to create highly ordered triangular gold nanoparticle arrays and exploit their localized optical near field to overcome locally the ablation threshold of fused silicia. Therefore, the nanoparticle arrays were irradiated with a single ultrashort laser pulse (35 fs), at a central wavelength of 790 nm. Depending on the polarization and the fluence of the laser light holes, grooves, or channels, with dimensions well below the diffraction limit have been created. For example, for a polarization along the bisector of the triangular nanoparticles, nanogrooves with a depth of 14 nm, a width at its waist of 45 nm, and a length of 290 nm have been generated, if fluences near the ablation threshold were applied. In contrast, tiny spherical nanoholes with diameters of only 23 nm can be achieved, for fluences significantly below the ablation threshold. The obtained structures can be explained by the enhanced electromagnetic near fields, which overcome locally the ablation threshold of fused silica in the vicinity of the irradiated nanoparticles.

O 18.6 Mon 18:30 PHY C213

Mapping infrared antenna resonances of particle arrays fabricated by nanosphere lithography — •Jens Richter[1], Andrea Hartung[1], Jón Mattis Hoffmann[1], Xinghui Yin[2], and Thomas Taubner[1,2] — [1]1st Institute of Physics, RWTH-Aachen University, Sommerfeldstrasse 14, 52074 Aachen, Germany — [2]Fraunhofer Institute for Laser Technology, Steinbachstr. 15, 52074 Aachen, Germany

Infrared vibrational spectroscopy is sensitive to characteristic molecule absorption bands, yielding a "fingerprint" spectrum of the molecules involved. The sensitivity of infrared spectroscopy has been increased by several orders of magnitude with optical antennas [1-3]. Arrays of hexagonal sorted triangular metallic infrared antennas created by Nanosphere lithography (NSL) have already been shown to exhibit IR resonances [4].

Our goal is the systematic variation of the NSL fabrication parameters in order to tune the antenna resonance over the whole mid-IR spectrum. We fabricate antenna arrays on different IR-transparent substrates and vary the particles lateral size and height. Using a Fourier-Transform-Infrared-Microscope (FTIR) we determine the plasmon resonance position of each sample. Applications of those structures to surface enhanced IR-Spectroscopy (SEIRA) will be discussed.

[1] R. Adato et al.; PNAS, 106, 19227 (2009)
[2] F. Neubrech et al.; PRL 101, 157403 (2008)
[3] R. Bukasov et al.; Analyt. Chem. 81, 4531 (2009)
[4] C. Haynes et al.; J. Phys. Chem. B, 105, 5599 (2001)

O 18.7 Mon 18:45 PHY C213

Plasmonic oligomers: the role of individual particles on collective behavior — •Mario Hentschel[1,2], Na Liu[3], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, D-70569 Stuttgart, Germany — [2]Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [3]Department of Chemistry, University of California, Berkeley, and Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

We theoretically and experimentally study the transition from isolated to collective modes in plasmonic oligomers which consist of a six-particle outer ring around a single center particle. The inter-particle gap distance plays a key role for the formation of collective modes. The plasmon hybridization method is applied to analyze the optical properties of plasmonic oligomers. The interference between a subradiant and a superradiant mode leads to a pronounced Fano resonance [1]. Furthermore we demonstrate the possibility to switch on and off the Fano resonance by the presence or absence of the central nanoparticle without breaking the system symmetry [2]. We also study the optical response upon modifications such as the introduction of defects by shifting the inner particle from the center position and the variation of the number of individual discs. The ability to observe and tune the collective resonances in metallic nanostructures will allow for the creation of a rich new set of artificial plasmonic molecules with a wide range of controlled optical properties. [1] B. Lukyanchuk et al., Nature Mat. 9, 707 (2010) [2] M. Hentschel et al., Nano Lett. 10, 2721 (2010)

O 18.8 Mon 19:00 PHY C213

Fabrication of nanocone arrays for high sensitivity biosensing — •Monika Fleischer, Christian Schäfer, Andreas Horrer, Katharina Broch, Dominik Gollmer, Frank Schreiber, and Dieter P. Kern — Institut für Angewandte Physik, Eberhard Karls Universität Tübingen, Auf der Morgenstelle 10, D- 72076 Tübingen

Plasmonic nanostructures, when resonantly interacting with an electromagnetic field, act as optical antennas focusing light to nanoscale volumes. Extremely high near-field enhancement is observed in the direct vicinity of the nanostructure surface, in particular at edges, corners, or tips. A process was developed for the fabrication of metallic nanocones with tip radii on the order of 10 nm. The cones are demonstrated to be efficiently excited by electric field components polarized parallel to the cone axis [1,2]. A narrow spot of high electric field strength is created near each cone apex due to the occurrence of localized surface plasmon resonances. Both serial and parallel methods for the fabrication of regular arrays of nanocones made from e.g. gold, silver, and copper are presented. Dense arrays of metal cones constitute a highly favorable system for high sensitivity sensing of biological or other organic molecules. For molecules located near a cone apex, strong Raman intensity enhancement is observed, similar to the effect of tip-enhanced Raman spectroscopy. This is demonstrated by the example of pentacene molecules [3] on gold cones.

[1] M. Fleischer et al., Nanotechnology 21, 065301 (2010)
[2] M. Fleischer et al., Appl. Phys. Lett. 93, 111114 (2008)
[3] A. Hinderhofer et al., J. Chem. Phys. 127, 194705 (2007)

O 19: Metal substrates: Adsorption of O / H and inorganic molecules II

Time: Monday 17:15–19:00 Location: WIL A317

O 19.1 Mon 17:15 WIL A317

Hydrogen adsorption on sulfur- and chlorine-precovered Pd(100) studied by ab initio molecular dynamics simulations — •Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm/Germany

The influence of coadsorbates on the adsorption properties of metal surfaces is of considerable technological and fundamental importance. For example, sulfur is well-known as a catalyst poison, i.e. its presence reduces the activity of catalysts. On the other hand, the electrochemical metal-liquid interface is typically characterized by halogen adsorption from the electrolyte. As a model system to understand the effect of such coadsorbates, the adsorption of hydrogen on sulfur- und chlorine-precovered Pd(100) has been studied by ab initio molecular dynamics simulations. The sticking probability has been determined as a function of the kinetic energy, the angle of incidence and the internal degrees of freedom of the impinging H_2 molecules. The results will also be compared to previous quantum dynamical studies on a fixed substrate [1]. It will be shown that sulfur and chlorine affect the adsorption properties of Pd(100) in a rather similar way, but there are also characteristic differences.
[1] A. Groß and M. Scheffler, Phys. Rev. B **61**, 8425 (2000).

O 19.2 Mon 17:30 WIL A317

The influence of monomer size on reaction kinetics and defect density for the synthesis of 2D Covalent Organic Frameworks: a combined Scanning-Tunneling-Microscopy and Density Functional Theory study — •Stefan Schlögl[1,2], Wolfgang M. Heckl[2,3], and Markus Lackinger[1,2] — [1]Geowissenschaftliches Institut & CeNS, LMU München — [2]Deutsches Museum, München — [3]School of Education, Department Physik, TU München

In order to tailor mechanical, chemical, and electronic properties of two-dimensional polymers, a bottom-up surface mediated fabrication process under controlled conditions is very promising. On one hand covalent intermolecular bonds give rise to the strength of 2D materials, on the other hand their irreversible character renders growth associated structural defects permanent. In order to control 'covalent self-assembly', a fundamental understanding of reaction kinetics and defect energetics is necessary.

In this contribution, we study and compare the surface mediated polymerization of 1,3,5-Triiodobenzene (TIB) and 1,3,5-Tris-(4-bromophenyl)benzene (TBPB). Deposition of the monomers onto dense packed metal surfaces under UHV conditions results in full dehalogenation and subsequent addition of the radicals into covalent aggregates. In this talk, we will address the fate of the split-off halogen atom, the topology of resulting covalent aggregates, the role of the organic backbone, and the influence of thermal after-treatments. The structures and energetics are analyzed and discussed by Scanning Tunneling Microscopy and Density Functional Theory calculations.

O 19.3 Mon 17:45 WIL A317

Interaction of H_2O molecules with Fe films investigated with metastable induced electron spectroscopy — •Kai Volgmann[1,2], Florian Voigts[2], and Wolfgang Maus-Friedrichs[2,3] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, 30167 Hannover — [2]Institut für Physik u. Phys. Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — [3]Clausthaler Zentrum für Materialtechnik, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld

The formation of an oxide layer on Fe films upon the interaction with H_2O molecules is relevant for both applications and in surface science. This work examines the interaction of H_2O molecules with Fe films grown on a tungsten substrate. X-ray Photoelectron Spectroscopy is used to determine the stoichiometry of the samples, while Ultraviolet Photoelectron Spectroscopy and Metastable Induced Electron Spectroscopy (MIES) are used to analyse their valence band region and to gain information about changes in the work function because of reactions on the surface. All measurements are done at room temperature. MIES is used as a very surface sensitive technique, especially towards hydroxide groups. Only after a high H_2O exposure, we observed the formation of OH groups. Our previous experiments reveal that a passivating oxide layer is formed during oxygen offer to a Fe surface [1]. A similar oxide layer growth may be observed during H_2O offer to iron. This oxide layer forms prior to the development of any observable OH groups. [1] *K. Volgmann, F. Voigts, W. Maus-Friedrichs*, Surface Science, **604** (2010), 906-913

O 19.4 Mon 18:00 WIL A317

Constructing the Wetting Layer of H_2O on Pt(111) — •Sebastian Standop[1], Georgia Lewes-Malandrakis[1], Markus Morgenstern[2], Thomas Michely[1], and Carsten Busse[1] — [1]II. Physikalisches Insitut, Universität zu Köln, Zülpicher Straße 77, D-50937 Köln — [2]II. Physikalisches Institut (IIB), RWTH Aachen, D-52056 Aachen

Adsorption of water molecules on Pt(111) leads to a number of complex superstructures in accordance with scattering experiments. A common and prominent feature of these layers are triangular shaped depressions. On the basis of density functional theory calculation these depressions were predicted to contain flat water molecule hexamers [1]. Through co-adsorption experiments with Xe and CO molecules and artificial manipulation using Scanning Tunneling Microscopy (STM) we directly show that the triangular depressions are indeed hexamers of flat lying water molecules rotated by about 30° with respect to the surrounding host structure of water molecules [2]. Under appropriate STM imaging conditions these hexamers act as nuclei for the growth of the $\sqrt{3} \times \sqrt{3}$ R30° water wetting layer, known to result from electron exposure in LEED experiments. Our observations explain how it is possible for the wetting layer to transform rapidly into this structure. Using graphene flakes grown by ethylene decomposition, we directly compare binding and structure of wetting layers on Pt(111) and on grapheme using thermal desorption spectroscopy and STM.
[1] S. Nie et al., PRL 105 (2010) 026102, [2] S. Standop et al., PRB 82 (2010) 161412(R)

O 19.5 Mon 18:15 WIL A317

Island growth of D_2O on Ag(111) at low temperatures — •Sarah-Charlotta Heidorn, Cord Bertram, and Karina Morgenstern — Institut für Festkörperphysik, Abteilung ATMOS, Leibniz Universität Hannover, Appelstr. 2, 30167 Hannover

Water is well-known to form hydrogen-bonded networks on metal surfaces, even at low temperatures. We investigate the growth mechanism of D_2O in the submonolayer range on Ag(111) with a low-temperature scanning tunneling microscope. Nucleation and island formation are studied during non-equilibrium growth processes for D_2O pressures between $1 \cdot 10^{-8}$ mbar and $1 \cdot 10^{-6}$ mbar and sample temperatures between 17 K and 130 K. The island shapes are analyzed in dependence of temperature and deposition flux. At low deposition rates and low temperature, amorphous, round-shaped islands are formed. At high deposition rates and low temperature, the generated patterns are fractal. At low deposition rates and high temperature, compact islands are grown. Details of the observed structures and mechanism underlying the island formation will be discussed in the presentation.

O 19.6 Mon 18:30 WIL A317

Influencing the bonding and assembly of a multiterminal molecule on a metal surface — •Maya Lukas[1,2], Kerrin Dössel[1,2], Alexandrina Schramm[1], Karin Fink[1,2], Olaf Fuhr[1,2], Christophe Stroh[1], Marcel Mayor[1,2,3], and Hilbert von Löhneysen[1,2,4] — [1]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, D-76021 Karlsruhe — [2]DFG Center of Functional Nanostructures (CFN), D-76049 Karlsruhe — [3]University of Basel, Department of Chemistry, CH-4056 Basel — [4]Karlsruhe Institute of Technology (KIT), Physics Institute and Institute for Solid State Physics, D-76049 Karlsruhe

The bond of a molecule to a metallic electrode is known to have a crucial influence on the molecular conductance. As electronic functionalities are integrated into molecules or several subunits are connected to a three-dimensional multiterminal molecule, it is not obvious that a "well-known" chemical linker group will lead to the bonding configuration known from simpler molecules.

We investigated a series of tripodal molecules on metal surfaces by STM. The chemical linker groups and the complex connecting the three wire-units are varied. We find that the position of molecules on the surface is governed by a subtle balance of intermolecular and molecule-surface interactions, partly in strong contrast to expectations. This emphasizes the need to characterize the nature of molecule-electrode contacts along with the investigation of the electronic conductance.

O 19.7 Mon 18:45 WIL A317

CuN structures on Cu(110) — •Mariella Denk, Richard Denk, Michael Hohage, Lidong Sun, and Peter Zeppenfeld — Institut für Experimentalphysik, Johannes Kepler Universität Linz, A-4040 Linz, Austria

Chemisorption of atomic nitrogen on Cu(110) leads, at a saturation coverage of 2/3, to the formation of a well ordered Cu(110)-(2x3)N reconstruction upon annealing at 650 K [1], [2].

An in-depth study concerning the formation of the nitrogen induced reconstruction has been performed to address open questions regarding the exact structure of the surface at the atomic scale. In case of an annealing temperature below 550 K, a precursory Cu-N phase which consists of elongated molecule-like structures, termed "CuN compounds", has been found on the surface by Scanning Tunneling Microscopy (STM). The CuN compounds are characterised by their high mobility on the surface and have been found to be stable up to at least 550 K. The compounds are expected to play a crucial role in the formation of the final (2x3)N phase, as the Cu coverage of the surface layer is increased to 4/3 compared to the pristine Cu(110) surface. A model structure for the CuN compounds has been derived on the basis of the STM images. The CuN compounds may consist of Cu_4N subunits, which appear as bright dots in the STM images.

[1] D. Heskett, A. Baddorf and E. W. Plummer, Surf. Sci., 195, p. 94 (1988)

[2] A. P. Baddorf and D. M. Zehner, Surf. Sci., 238, p. 255 (1990)

O 20: Solid / liquid interfaces II

Time: Monday 17:15–19:15 Location: WIL B321

O 20.1 Mon 17:15 WIL B321

dynamic electromechanical response during cyclic voltammetry: measurement strategies — •Qibo Deng[1,2], Maxim Smetanin[1,2], and Jörg Weissmüller[1,3] — [1]Institute of Materials Physics, Hamburg University of Technology, Hamburg, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Institute of Materials Mechanics, Helmholtz Zentrum Geesthacht, Geesthacht, Germany

We explore experimental strategies for measuring the impact of elastic strain on the electrode potential, E, of Au in weakly adsorbing aqueous electrolytes. More precisely, our experiment aims at measuring the potential-strain response dE/de|q at different states of the electrode. The symbols q and e denote superficial charge density and tangential (elastic) strain, respectively. Emphasis is on measuring the variation of response with E during cyclic voltammetry in extended potential intervals, including dominantly capacitive regions of the voltammogram as well as electrosorption processes. By means of validation, we explore three independent strategies for separating the cyclic variation of potential of current from the voltammogram proper. The results are in close quantitative agreement. We describe the setup and report results for 111-textured gold electrodes in aqueous H2SO4 and HClO4. We find that the response is generally negative-valued. Furthermore, the magnitude of response peaks at a potential which is close to the pzc and which is displaced relative to the potential of largest AC-capacitance.

O 20.2 Mon 17:30 WIL B321

Influence of the substrate on the chemical state of adsorbed organic molecules: A XPS-study — •Stephan Breuer[1], Thanh-hai Phan[1], Mayer Thomas[2], Broekmann Peter[3], and Wandelt Klaus[1,4,5] — [1]University of Bonn, Institute of Physical and Theoretical Chemistry, Wegelerstr. 12, D-53115 Bonn — [2]Technical University of Darmstadt, Department of Material Science — [3]Universtity of Berne, Department of Chemistry and Biochemistry — [4]University of Wroclaw, Institute of Experimental Physics, Poland — [5]University of Rome "Tor Vergata", Department of Physics, Italy

The template effect of an ordered surface and the self assembly of organic molecules due to their intermolecular interactions allow the formation of nano-structures in a bottom-up approach. We work in an aqueous solution which allows the deposition of thermolabile molecules. An electrochemical environment allows applying an electrical potential in order to change the redox state of organic adsorbates which in turn influences their intermolecular interactions. We have studied the adsorption of redox active organic molecules (e.g. viologens and porphyrins) on copper surfaces which are precovered with specifically adsorbed anions. The organic molecules are adsorbed as cationic moieties which bind electrostatically to the anion layer. Changes in the redox state influence their self-assembly behaviour. In this study we will show our characterization of the chemical and redox state of viologens on Cu(111) precovered with sulphide compared to former results on chloride precovered Cu(100) [1].

[1] St. Breuer et al., N. J. Phys, 10, 2008, 125033 (24pp.).

O 20.3 Mon 17:45 WIL B321

Dynamic Electromechanical Response during Cyclic Voltammetry: Interfacial Processes — •Maxim Smetanin[1], Qibo Deng[1], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics, Hamburg University of Technology, Hamburg, Germany — [2]Institute of Materials Mechanics, Helmholtz Zentrum Geesthacht, Geesthacht, Germany

An interest in the impact of elastic strain on the electrochemical behavior of metal electrodes was rapidly increasing over the past decade. Research scope in that context includes the impact of strain on the electrode potential at constant charge density as well as the repercussions of mechanical deformation for electrosorption phenomena and electrocatalytic reaction rates. Here, we show experimental data for the potential-dependence in typical potential regimes of cyclic voltammetry. The response of potential to the strain was measured using a lock-in technique. Aqueous H2SO4 and HClO4 electrolytes were used. We found that the electrode potential, E, linearly depends from the strain, at least within the potential range from -0.8 V up to 1.6 V vs Ag/AgCl - the range accessible in aqueous electrolytes. However, the amplitude of the potential-strain response depends significantly on E within the double layer - possibly due to the two factors specific ionic adsorption or double layer capacitance. According to our model the response parameter provides access for quantifying the amount of the charge transferee - the measure typically not accusable by over techniques.

O 20.4 Mon 18:00 WIL B321

Light-induced electron transfer and charge transport in mesoporous ZnO/D149 hybrid films — •Melanie Rudolph[1], Hidetoshi Miura[2], and Derck Schlettwein[1] — [1]Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de — [2]Chemicrea Co., Ltd., 2-1-6 Sengen, Tsukuba, Ibaraki 305-0047, Japan

Dye-sensitized solar cells (DSC) consist of a nanostructured semiconductor/dye hybrid layer as light absorbing and electron conducting phase, permeated by a liquid phase ensuring transfer of positive charges to a counter electrode. In this study, nanostructured ZnO was electrodeposited on fluorine-doped tin oxide (FTO) and loaded with the fully organic dye D149. The ZnO/D149 electrodes were analyzed in contact with a liquid iodide/triiodide electrolyte. Steady-state photocurrent and photovoltage measurements were performed to derive basic photovoltaic parameters like short-circuit photocurrent, open-circuit photovoltage and external quantum efficiency (IPCE). Open-circuit photovoltage decay measurements (OCVD) as well as intensity-modulated photovoltage spectroscopy (IMVS) were utilized to obtain information about the extent and mechanisms of recombination, i.e. unwanted back transfer of electrons from ZnO to D149 or to the liquid contact phase. Intensity-modulated photocurrent spectroscopy (IMPS) served to gain an insight into electron transport within the porous zinc oxide films. The interplay between light-induced charge transfer from D149 to ZnO, electron transport within the porous ZnO matrix and recombination of photoinjected electrons is discussed.

O 20.5 Mon 18:15 WIL B321

In situ Diffraction Studies of Homoepitaxial Growth of Cu(001) from Aqueous Electrolyte — •Frederik Golks[1,2], Yvonne Gründer[2], Jochim Stettner[2], Klaus Krug[2], Jörg Zegenhagen[1], and Olaf M. Magnussen[2] — [1]European Synchrotron Radiation Facility, Grenoble, France — [2]Universität Kiel, Institut für Experimentelle und Angewandte Physik, Kiel, Germany

Motivated by the pivotal role of copper electroplating in the production of interconnects for ULSI microelectronics, we have studied the homoepitaxial growth of Cu(001) in aqueous electrolytes containing 1 mM chloride and 1 or 5 mM Cu^{2+} by in-situ surface x-ray diffraction with high time resolution. Although diffusion-limited layer-by-layer growth is observed over a wide potential regime, a pronounced mutual interdependence of the interface structure and the growth behavior is found. Thus, the tendency towards surface roughening is increased in the presence of a complete c(2x2) Cl^- adlayer [1] while the ordering of the Cl^- adlayer is slowed down during Cu deposition. Furthermore, the presence of polyethylene glycol (PEG), a commonly used inhibitor in industry, results in significantly lower microscopic growth rates and an increased tendency towards 3D growth.

[1] Y. Gründer, D. Kaminski, F. Golks, K. Krug, J. Stettner, O. M. Magnussen, A. Franke, J. Stremme, E. Pehlke, Phys. Rev. B **81**, 17 (2010)

O 20.6 Mon 18:30 WIL B321

Electrochemical studies of excited charge carriers with thin platinum film electronic devices in sulfuric and hydrochloric solution — •Damian Bürstel, Michael Scheele, Andreas Barmscheid, Kevin Stella, and Detlef Diesing — Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany

Excited charge carriers induced by chemical processes like the adsorption or desorption of atomic hydrogen at metal surfaces have already been investigated under UHV conditions. These carriers can be detected by systems with an internal electric barrier, like MIM-(metal–insulator–metal), MIS- (metal–insulator–semiconductor) or MS- (metal–semiconductor) sensors. The internal barrier inside the sensors separates ground state carriers from excited carriers. It is an open question, whether electrochemical reactions on metal surfaces also evoke hot charge carriers. We study the electrochemical deposition of hydrogen (via H_{upd}) on platinum and the oxidation of platinum in sulfuric and hydrochloric solution. As sensors Pt–TaOx–Ta, Pt–SiOx–Si and Pt–Si-sensors were used with 10-30 nm thick Pt films. By electrochemical cyclovoltametry and simultaneous recording of the current at the tantalum or silicon back electrode it is possible to detect voids (down to a fraction of 10^{-3}) in the thin platinum film. 30 nm thick platinum films were found to cover the underlying layer completely. In this case the devices can be used to monitor deviations from the electronic equilibrium since excited carriers cause a device current through the internal barrier. Deviations from the electronic ground state were found in the case of the H_{upd} formation.

O 20.7 Mon 18:45 WIL B321

Dealloying studies of Cu3Pd single crystal surfaces — •Shilan Meimandi and Frank Uwe Renner — Max Planck Institute for Iron Research, Max Planck Strasse 1, 40237 Düsseldorf

Binary noble metal alloys serve as model cases for dealloying in the context of corrosion studies [1]. Dealloying is a common corrosion process during which the more active element of an alloy is selectively dissolved into the electrolyte. Several aspects of formation of porous surface during dealloying has not completely been understood. The nano-porous metals formed by dealloying methods have application potential in a variety of fields such as catalysts, actuators, and biomedical sensors. The Cu-Pd system is interesting as a model system for corrosion as well as a potential catalyst material. The initial dealloying and selective dissolution of single-crystals Cu3Pd (111) and Cu3Pd (100) in 0.1 M H2SO4 have been studied. With in-situ X-ray diffraction, we observed the epitaxial Pd layer peak by increasing the potential close to the critical potential. Also with Ex-Situ atomic force microscopy (AFM), the formation of nanoscale islands of Pd (5-25 nm) as nobler metal have been revealed. Our aim is to study the initial steps of dealloying of well-defined Cu-Pd surfaces on the atomic scale and to compare the results to the Cu-Au system [2]. [1] R.Newman, K.Sieradzki, Science 263 (1994), 1708. [2] Renner et al., Physical Review B 77 (2008), 235433

O 20.8 Mon 19:00 WIL B321

Stability and electrocatalytic activity of Pt nanoclusters supported on graphene monolayers on Ru(0001) — •Otavio B. Alves[1], Christoph Lorenz[1], Harry E. Hoster[1,2], and R. Jürgen Behm[1] — [1]Ulm University, Institute of Surface Chemistry and Catalysis, 89069 Ulm, Germany — [2]Present Address: Technische Universität München, Centre for Electromobility, 50 Nanyang Drive, Singapore 637553

We have investigated the electrochemical properties and the electrocatalytic activity of model electrodes consisting of nanosized Pt clusters (10 - 50 atoms) on a graphene monolayer film deposited on a Ru(0001) substrate. The graphene films are attractive supports since they provide a structurally well-defined nanostructured template for the formation of ordered arrays of metal nanoparticles or clusters [1]. Inasmuch as the graphene covered surface is electrochemically inert, these model systems allow us to determine the electrochemical characteristics and the electrocatalytic activity of the Pt clusters. Activity and stability of theses systems are measured in a wall-jet type flow cell located in an electrochemical pre-chamber attached to the main UHV system. Cluster arrays with different total Pt coverages and cluster size distributions, as determined by scanning tunnelling microscopy (STM), were investigated, concentrating on the O_2 reduction reaction as model reaction. The general electrochemical behaviour of the Pt cluster arrays will be discussed and compared to that of bulk Pt.

[1] A. T. N'Diaye *et al.*; Phys. Rev. Lett. 1997, 97, 215501.

O 21: Clean surfaces: Metals, semiconductors, oxides and insulators II

Time: Monday 17:15–18:30 Location: WIL B122

O 21.1 Mon 17:15 WIL B122

A combined Frequency Modulation Dynamic Force Microscopy (FM-DFM) and Scanning Tunneling Microscopy (STM) Study of a SiO_2/Ru(0001) Model System — •Christin Büchner, Leonid Lichtenstein, Lars Heinke, Markus Heyde, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Silica based support materials play an important role in catalysis. A stable and well characterized crystalline silica film can act as a model system for bulk silica and help us to understand silica's properties in detail. In order to examine catalytically relevant processes on such model surfaces, a thorough investigation of defect sites of any form is eminent. Recently, a double-layer silica film could be prepared on Ru(0001).[1] Here we used a combined frequency modulation dynamic force microscope (FM-DFM) and scanning tunneling microscope (STM) under low temperature and ultra-high vacuum conditions to unveil the thin film's structural and electronic surface properties. Atomically resolved images of the crystalline silica film grown on Ru(0001) are presented. Structural elements of the pristine film, as well as its defects, are highlighted. Based on atomic resolution FM-DFM and STM images a direct comparison with density functional theory calculation can be made. Theory as well as experiment favor a hexagonal honeycomb structure of the film. Spectroscopy measurements, i.e. scanning tunneling spectroscopy (STS) and Kelvin probe force microscopy (KPFM), provide first insights into electronic properties of the system. [1] Löffler et al., Phys. Rev. Lett. 105, 146194-1-4 (2010).

O 21.2 Mon 17:30 WIL B122

Imaging domain structures of ferroelectric and multiferroic surfaces by PEEM — •Anke Höfer, Klaus Duncker, Stefan Förster, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

$BiFeO_3$ is one of the very rare single-phase magnetoelectric multiferroics and shows ferroelectric and antiferromagnetic behavior at room temperature, whereas $BaTiO_3$ exhibits only a ferroelectric order. The surface domain structure of $BaTiO_3(001)$ and $BiFeO_3(001)$ has been studied by Laser-excited photoelectron emission microscopy (PEEM) under UHV conditions. The PEEM images of $BaTiO_3$ allow for discrimination of three domain types by their different photoemission yields. In wavelength dependent measurements the ferroelectric a and c domains exhibit approx. 100 meV different photoemission onsets. Based on the markedly high surface sensitivity of PEEM a specific ferroelectric surface domain structure on-top of a paraelectric bulk is observed in a temperature window up to 100 K above the bulk Curie temperature.

For the multiferroic $BiFeO_3(001)$ surface we demonstrate imaging of the ferroelectric and the antiferromagnetic domain structure by PEEM using threshold excitation with linearly and circularly polarized laser light. The specific polarization dependencies will be discussed.

O 21.3 Mon 17:45 WIL B122

Spin-orbit effects in two-electron emission from ferromagnets — •Franz Giebels[1,2], Herbert Gollisch[1], and Roland Feder[1,2] — [1]Theoretische Festkörperphysik,Universität Duisburg-Essen, 47048 Duisburg, Germany — [2]Max-Planck Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

The momentum-resolved detection of correlated electron pairs, which are ejected from ferromagnetic surfaces upon impact of spin-polarized low-energy electrons, yields information on exchange and correlation effects and on the spin-resolved electronic surface structure [1]. Furthermore, spin-orbit coupling (SOC) effects have been found experimentally [2]. We present a theoretical formalism for electron-induced electron pair emission from ferromagnetic surfaces, which is based on a Dirac equation with an effective magnetic field. Exchange interaction and SOC are thus incorporated simultaneously. The formalism has been implemented in a computer code. We present typical numerical results, which demonstrate the manifestation of SOC in pair emission energy and angular distributions. Depending on the relative orientations of the primary electron spin polarization, the reaction plane and the magnetization direction of the surface system, SOC effects may dominate over exchange effects or vice versa. In two-dimensional momentum distributions, SOC reduces the rotation symmetry of the exchange-correlation hole, e.g. for cubic (001) surfaces from four-fold to two-fold.

[1] F. Schumann et al., Phys. Rev. Lett. **104**, 087602 (2010)
[2] S. Samarin et al., Phys. Rev. Lett. **97**, 096402 (2006)

O 21.4 Mon 18:00 WIL B122

Photoemission induced gating of topological insulator — •A. A. Kordyuk[1,2], T. K. Kim[1], V. B. Zabolotnyy[1], D. V. Evtushinsky[1], M. Bauch[1], C. Hess[1], B. Büchner[1], H. Berger[3], and S. V. Borisenko[1] — [1]Institute for Solid State Research, IFW-Dresden, P.O.Box 270116, D-01171 Dresden, Germany — [2]Institute of Metal Physics of National Academy of Sciences of Ukraine, 03142 Kyiv, Ukraine — [3]Institute of Physics of Complex Matter, EPFL, 1015 Lausanne, Switzerland

The recently discovered topological insulators exhibit topologically protected metallic surface states which are interesting from the fundamental point of view and could be useful for various applications if an appropriate electronic gating can be realized. Our photoemission study of Cu intercalated Bi_2Se_3 shows that the surface states occupancy in this material can be tuned by changing the photon energy and understood as a photoemission induced gating effect. Our finding provides an effective tool to investigate the new physics coming from the topological surface states and suggests the intercalation as a recipe for synthesis of the material suitable for electronic applications.

O 21.5 Mon 18:15 WIL B122

Anomalous double layer step formation on Si(100) in hydrogen ambient — •Henning Döscher, Peter Kleinschmidt, Anja Dobrich, Sebastian Brückner, Oliver Supplie, Johannes Luczak, and Thomas Hannappel — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Generation of double layer steps on Si(100) is desirable for subsequent anti-phase domain-free heteroepitaxy of III-V semiconductors. In UHV established procedures exist for the formation of double layer steps at the clean Si(100) surface. In the (metal-organic) vapour phase epitaxy environment the situation is more complicated due to the presence of hydrogen in the process ambient. Both theory and experiment of the hydrogenated surfaces suggest that under equilibrium conditions no preference for double layer steps is to be expected. Previously, we have shown that annealing in hydrogen at near atmospheric pressure leads to termination of the surface by monohydride. Here, we show that a process using Si(100) with an intermediate offcut of 2° in <011> can lead to a double layer stepped surface. Our process consists of deoxidation, homoepitaxial growth employing silane, annealing and slow cooling to 500°C in hydrogen ambient. We observe the formation of double layer steps using Fourier-transform infrared spectroscopy, low-energy electron diffraction and scanning tunneling microscopy. In sharp contrast to established UHV results, the double layer steps are of the D_A type, where dimer rows of the reconstructed surface are parallel to the step edges.

O 22: Theoretical methods

Time: Monday 17:15–19:30 Location: WIL C107

O 22.1 Mon 17:15 WIL C107

High Temperature Thermal Conductivity from First Principles — •Christian Carbogno[1,2], Ramamurthy Ramprasad[1,3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin, Germany — [2]Materials Department, University of California Santa Barbara, USA — [3]Chemical, Materials & Biomolecular Engineering, University of Connecticut, Storrs, USA

In spite of significant research efforts, little is yet known about the atomistic details and mechanisms that underlie peculiarly low (or high) thermal conductivities, especially at elevated pressures and temperatures. Under such extreme conditions, systematic experimental measurements are hard to perform; conventional theoretical approaches typically fail to capture significant physical aspects of the problem, since these methods are either inherently limited to (a) low temperatures and/or (b) to perfect crystals. A recently developed *ab initio* simulation strategy [1] allows to overcome the latter limitation, but the assessment of the high temperature regime remains an unsolved challenge. Within this work, we present efficient strategies to overcome this serious restriction and show their applicability for zirconia based ceramics – a material typically used in high temperature applications, for instance in thermal barrier coatings [2].

[1] T. M. Gibbons, and S. K. Estreicher, *Phys. Rev. Lett.* **102**, 255502 (2009).

[2] D. R. Clarke, and C. G. Levi, *Annu. Rev. Mat. Res.* **33**, 383 (2003).

O 22.2 Mon 17:30 WIL C107

Representing Potential-Energy Landscapes by High-Dimensional Neural Networks — Nongnuch Artrith, Tobias Morawietz, and •Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, Germany

The construction of efficient interatomic potentials is a necessary condition for carrying out large scale molecular dynamics and Monte Carlo simulations. However, the identification of a suitable functional form to represent a given set of reference data from ab initio calculations with high accuracy is a formidable challenge.

Using several benchmark systems, we show that flexible artificial neural networks (NNs) are able to provide reliable high-dimensional potential-energy surfaces even if complex bonding situations are present. They can be applied to a wide range of systems from bulk metals and surfaces to small molecules. The scope and limitations of NN potentials are discussed, and the accuracy is compared with electronic structure calculations.

O 22.3 Mon 17:45 WIL C107

Stress formulation within the FLAPW method — •Aaron Klüppelberg, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Stress is an important quantity in characterizing the states of condensed matter. It can be modified by epitaxial growth relation or application of electric or magnetic fields. This makes the computation of the stress field particularly important for understanding the properties and functionality of ferroic and multiferroic oxides.

The full-potential linearized augmented plane wave (FLAPW) method is an all-electron electronic structure method based on the density functional theory (DFT) that is well suited to describe electronically and structurally complex materials. It is realized in the `FLEUR` code [1], where orbital-dependent functionals [2] are implemented to describe the exchange-correlation energy of oxides.

We present here a stress-strain formalism for elastic deformations using the frozen augmentation approximation. It takes into account the Pulay corrections to the Hellmann-Feynman stress that appear due to the use of an incomplete basis set (IBS). This procedure allows a simultaneous relaxation of lattice shape and atom positions. Furthermore, this formalism enables the application of pressure and shear making an investigation of phase transitions due to external mechanical impact accessible.

[1] www.flapw.de

[2] M. Betzinger, C. Friedrich, and S. Blügel, PRB **81**, 195117 (2010).

O 22.4 Mon 18:00 WIL C107

Massively Parallel Real-Space DFT Calculations — •Paul Baumeister[1], Daniel Wortmann[1], Tomoya Ono[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungzentrum Jülich and JARA, 52425 Jülich, Germany — [2]Dept. of Precision Engineering, Osaka University, Osaka, Japan

We present a new DFT tool developed in Jülich and Osaka that combines equidistant real-space grids and the Projector Augmented Wave (PAW) method. The code is explicitly designed for the structural relaxation of systems consisting of several thousands of atoms with very flexible boundary conditions. The specific advantage of our approach lies in the possibility to achieve a high degree of parallelization. The real-space treatment of wave functions, densities and potentials enables a simple and efficient parallelization with respect to communication and load balancing. Besides the parallel computation of k-points, we employ a domain decomposition to the real-space cell and a parallelization of eigenvalues (bands). Hence, we exploit the local character of the Kohn-Sham equation and approximate the kinetic energy operator by finite differences, avoiding Fourier transforms completely. The arising communication pattern suits perfectly the data network of IBMs BlueGene type massively parallel supercomputers. We will discuss the challenges of band parallelization, in which communication cannot be avoided as much as in k-points or even the real-space domain decomposition. Besides the demonstration of the efficiency of the parallelization, we will also report on the obtainable accuracy.

O 22.5 Mon 18:15 WIL C107

Tight-Binding Parameters from DFT Calculations: First Applications to Hydrocarbons — •Alexander Urban[1], Martin Reese[2,3], Matous Mrovec[2,3], Christian Elsässer[2,3], and Bernd Meyer[1] — [1]ICMM/CCC, University of Erlangen-Nürnberg, Germany — [2]Fraunhofer IWM, Freiburg, Germany — [3]IZBS, Karlruhe Institute of Technology, Germany

Tight-binding (TB) models for practical calculations are usually derived by fitting band structures and total energies to results of DFT calculations or experimental data. We have developed an alternative approach in which the TB parameters are determined directly from DFT data for arbitrary reference configurations without extensive fitting. Our method [1] is conceptually different from previous approaches [2] as it is based on a projection [3] of basis-set-converged wave functions from mixed-basis DFT computations onto a minimal basis of atomic orbitals. The radial shape of the atomic orbitals is optimized by minimizing the loss (spillage) in the projection procedure. The Slater-Koster tables are then calculated with the optimized minimal basis using the self-consistent DFT Hamiltonian. To demonstrate the quality of the derived TB models results for the electronic structures, total energies and forces for different carbon and hydrocarbon systems will be compared to DFT reference data.

[1] A. Urban, M. Reese, M. Mrovec, C. Elsässer, B. Meyer, submitted

[2] D. Porezag et al., *Phys. Rev. B* 51 (1995) 12947

[3] D. Sanchez-Portal et al., *Sol. State Comm.* 95 (1995) 685

O 22.6 Mon 18:30 WIL C107

Localized resolution of identity for efficient Hartree-Fock exchange, based on numeric atom-centered orbitals — •Jürgen Wieferink, Volker Blum, Xinguo Ren, Patrick Rinke, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Methods based on an exact exchange operator (EX) are increasingly popular, but are still restricted to analytical basis functions (e. g. Gaussians) for medium system sizes. We here introduce a localized resolution-of-identity approach for the two-electron Coulomb operator, based on expanding single-particle basis function products separately into auxiliary atom-centered basis sets that are restricted to two centers. Our approach produces accurate results for all-electron EX, can be applied both to analytical and numeric basis functions, requires only $\mathcal{O}(N^2)$ intermediate storage and retains a path towards $\mathcal{O}(N)$ EX for large systems. We demonstrate a total-energy accuracy of $< 1\,\mathrm{meV/atom}$ for systems including Alanine chains and the S22 benchmark molecule set [1], using the numeric atom-centered orbital based all-electron electronic structure code FHI-aims [2].

[1] P. Jurečka *et al.*, Phys. Chem. Chem. Phys. **8**, 1985 (2006).

[2] V. Blum *et al.*, Comput. Phys. Comm. **180**, 2175 (2009).

O 22.7 Mon 18:45 WIL C107

Accurate Calculation of the Single-Site Green Function in Relativistic Full-Potential Scattering — •Pascal Kordt, Rudolf Zeller, Phivos Mavropoulos, and Stefan Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Within the Korringa-Kohn-Rostoker (KKR) method the Green function for a single scattering centre can be calculated using the regular and irregular solutions of the corresponding angular Lippmann-Schwinger equation. We have developed a method for a relativistic treatment valid also for non-spherical potentials. It is based on an expansion in Chebyshev polynomials and their recursion relations. This allows us to rewrite the Lippmann-Schwinger integral equation into a system of algebraic linear equations. The computational effort for solving these equations is drastically reduced by dividing the radial integration into sub-intervals with a suitable matching technique. Compared to previous perturbation methods a much higher accuracy is achieved with modest increase in computational effort.

O 22.8 Mon 19:00 WIL C107

Wavefunction-based correlation method for metals: from bulk to surfaces and interfaces — •Elena Voloshina and Beate Paulus — Institut für Chemie und Biochemie, Freie Universität Berlin, 14195 Berlin, Germany

Theoretical determination of surface energies is a great challenge. While density functional theory (DFT) provides understanding of qualitative trends, absolute values depend strongly on the choice of the functional. An alternative approach with the advantage of the possibility of a systematical improvement are the wavefunction-based methods. One problem here is that a very accurate treatment, e.g. with the coupled-cluster method, scales very unfavorably with the number of electrons in the system. For this reason the method of increments was invented to calculate the correlation energy of bulk metals in terms of contributions from localized orbital groups [1,2]. This approach can be extended to system of low dimensionality, like surfaces. Furthermore, the method of increments is useful when considering surface adsorption phenomena, since DFT often fails to describe physisorption correctly. To demonstrate our approach we selected Mg(0001) surface, where the method of increments is used to calculate surface energy as well as Xe adatom interaction energy.

[1] E. Voloshina, N. Gaston, and B. Paulus, J. Chem. Phys. **126**, 13411(2007); [2] E. Voloshina and B. Paulus: Phys. Rev. B **75**, 245117 (2007); Chem. Modell. **6**, 162 (2009); Z. Phys. Chem. **224**, 369 (2010).

O 22.9 Mon 19:15 WIL C107

Exchange an Correlation effects in photoemission spec-

troscopy: from semiconductors to transition metal oxides — •Matteo Guzzo[1], Matteo Gatti[2], Francesco Sottile[1], Pina Romaniello[1], Fausto Sirotti[3], John Rehr[4], and Lucia Reining[1] — [1]LSI - ETSF, Ecole Polytechnique, Palaiseau, France — [2]ETSF, Universidad del Pais Vasco, San Sebastian, Spain — [3]Synchrotron Soleil, Gif-sur-Yvette, France — [4]University of Washington, Seattle WA, USA

As a prototype of strongly-correlated systems, NiO has been extensively studied, however the origin of its gap is still under debate. Many-Body Perturbation Theory (MBPT) (with the one-particle Green's function, *aka* the propagator of a particle, as key quantity) describes appropriately *ab-initio* photoemission gaps and spectra. GW approximation from MBPT includes dynamical correlation effects beyond H-F. The standard GW approach is not reliable on NiO since the Kohn-Sham band structure is too poor a starting point. COHSEX — a static approximation of GW — allows one to achieve full self-consistency, and to obtain a better starting point for the GW step. The COHSEX+GW result gives about 5 eV energy-gap, in good agreement with experiment and with other approaches beyond G_0W_0. An attempt to apply *vertex corrections* from TDDFT has shown no improvement in the spectrum. Here we focus on the effects of vertex corrections on quasiparticle energies and satellites and compare the cases of Si and NiO. The Cumulant Expansion approach is discussed as a possible alternative approach.

O 23: Scanning probe methods II

Time: Monday 17:15–19:15 Location: WIL C307

O 23.1 Mon 17:15 WIL C307

Simulation of a single molecule stretched within an nc-AFM junction — •Christian Wagner, Norman Fournier, Christian Weiss, Ruslan Temirov, and Frank Stefan Tautz — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and JARA-Fundamentals of Future Information Technology

The binding of organic molecules to metal surfaces is extensively studied both in experiment and theory. While techniques such as TDS are valuable tools to determine the binding energy of adsorbed molecules, it does not allow measuring the specific binding properties of individual functional groups or atoms. We approach this question by peeling single PTCDA molecules from a Ag(111) surface using a qPlus sensor. While previous studies already revealed that the molecule can be fully lifted when contacted by a STM tip [1], here, we go one step further and measure the potential energy profile during this pulling process. Due to its complexity, this experiment is very demanding concerning a modeling approach. On the one side, there is the (chemical) interaction between molecule and substrate. On the other side, the measured signal is a frequency shift obtained for an oscillation with a *finite* amplitude. We present a modeling approach that combines less demanding force-field calculations for the description of the molecule, and of its interaction with the substrate, while fully modeling the tip oscillation process. It shows that some of the key features found in the experiment can only be understood in the context of a finite amplitude.

[1] R. Temirov, A. Lassise, F. B. Anders, and F. S. Tautz, *Nanotechnology* **19** 065401 (2008)

O 23.2 Mon 17:30 WIL C307

A strange disturbance in the force — •Jay Weymouth, Thorsten Wutscher, Joachim Welker, Thomas Hofmann, and Franz Giessibl — Universität Regensburg, Regensburg, Germany.

Although atomic contrast with NC-AFM was first reported over fifteen years ago on Silicon [1], several interesting questions remain concerning simultaneous STM and NC-AFM. Arai and Tomitori previously showed that the force signal could be varied with applied bias voltage [2]. Sugimoto and coworkers have recently demonstrated that the distance at which one typically acquires STM data is approximately 4 Å further from the surface than the distance one acquires AFM data [3]. Both sets of experiments were made with a standard cantilever at amplitudes around 200 Å. We have performed similar experiments with smaller amplitudes (<5 Å). A smaller amplitude not only increases the signal to noise ratio, it also simplifies the physical interpretation of the observed frequency shift and makes the measurement more sensitive to short-range forces.

1. Giessibl, F.J., Science, 267, 68 (1995)
2. Arai, M. and Tomitori, M., Phys Rev Lett, 93, 256101 (2004)
3. Sugimoto, Y. et al, Phys Rev B, 81, 245322 (2010)

O 23.3 Mon 17:45 WIL C307

Simultaneous current and force microscopy on epitaxial graphene — •Thomas Hofmann, Markus Duschl, and Franz J. Giessibl — University of Regensburg, Faculty of Experimental and Applied Physics II - Physics, Universitätsstrasse 31, D-93053 Regensburg

Graphite has been investigated extensively with NC-AFM at low temperatures [1]. However, at room temperature atomic resolution could not be achieved. We speculate that the weakly bond layers of the graphite lead to large thermal oscillations normal to the surface. This prevents stable oscillation of the cantilever at room temperature. To circumvent this problem, single layer graphene on SiC [2] is used as sample system. We found that in contrast to the findings on graphite, stable imaging at room temperature and at small tip-sample distances is possible. In this talk we present constant height images which show atomic contrast in both the current and the Δf channel. In the current image both six-fold and three-fold symmetry are observed, attributed to the carbon rings and holes respectively. In both cases the Δf images only show the carbon rings. Consistent with the findings of Hembacher et al. [1], the carbon atoms can only be resolved at tip-sample distances, where the tip atom already feels repulsive forces.

[1] S. Hembacher and F.J. Giessibl and J. Mannhart, and C.F. Quate, Phys. Rev. Lett. 94, 056101 (2005)

[2] P. Lauffer, K. V. Emtsev, R. Graupner, Th. Seyller, and L. Ley, Phys. Rev. B 77, 155426 (2008)

O 23.4 Mon 18:00 WIL C307

Amplitude dependence of long- versus short-range forces on Si(111)7x7 — •Joachim Welker, Thomas Hofmann, and Franz J. Giessibl — Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany

Atomic force microscopy (AFM) senses the forces that act between a tip and a sample. The forces are composed of long- and short range interactions. Sugimoto et al. [1] recently demonstrated chemical identification of atoms by AFM using the short range forces. However, chemical identification was only possible here, because the atoms under investigation all were lying in the top surface layer, such that the long-range van der Waals (vdW) force was the same for all atoms. At step edges, the vdW forces vary strongly and we also expect that corner holes and dimer rows on Si(111) 7x7 lead to a spatial alteration in the vdW forces.

In NC-AFM, the sensitivity to forces of a different decay length can be tuned by the oscillation amplitude of the cantilever. Small amplitudes lead to a lower contribution of van-der-Waals forces to the experimental observable (frequency shift) than larger amplitudes. We performed measurements on Silicon(111)7x7 in constant height mode with oscillation amplitudes from picometer to nanometer range, investigating the contribution of the in-plane local spatial variation, e.g., the corner holes, to the long range van-der-Waals force.

[1] Y. Sugimoto, P. Pou, M. Abe, P. Jelinek, R. Perez, S. Morita, and O. Custance, Chemical identification of individual surface atoms by atomic force microscopy Nature, 446, 64 (2007)

O 23.5 Mon 18:15 WIL C307

Ac and dc Conductivity measurements vs. KPFM - a methodical study — •Anne-Dorothea Müller[1], Falk Müller[1], Stefanie Wengel[1], Kin Mun Wong[2], and Yong Lei[2] — [1]Anfatec Instruments AG, Melanchthonstr. 28, 08606 Oelsnitz, Germany — [2]Institute of Materials Physics & Center for Nanotechnology , University of Münster, 48149 Muenster, Germany

This contribution compares a large variety of electrical analysis methods in AFM, such as KPFM, dynamic EFM, CAFM, conductance microscopy and related spectroscopy. In order to push the limits of lateral resolution and to challenge the tip by means of geometry and electrical behavior at the same time, all investigations are carried out on metal nano-dot arrays on silicon with an almost one by one by one ratio of dot diameter, dot height and dot distance. Differences in achievable local resolution and dependencies on the tip geometry and conductance are explained and carefully discussed with the help of numerical simulations.

O 23.6 Mon 18:30 WIL C307

AFM an Nanodrähten: Oberflächenpotentiale und Dissipation aus abstandsabhängigen Resonanzkurven im intermittent-contact-Modus — •Moid Bhatti, Lars Ungewitter, Ivo Knittel und Uwe Hartmann — Fachrichtung Experimentalphysik, Universität des Saarlandes, 66123 Saarbrücken

Der intermittent-contact ist der am weitesten verbreitete Modus der Rasterkraftmikroskopie, insbesondere, weil er schonend mit Probe und Spitze umgeht. Wir haben abstandsabhängige Resonanzkurven im intermittent-contact-Regime aufgenommen und simuliert. Diese Kurvenscharen enthalten mehr Informationen als eine einzelne Kraft-Abstandskurve und erlaubten es, durch Vergleich mit Simulationen detaillierte Aussagen über das Spitze-Probe-Potential und Dissipation zu machen. Die Ergebnisse werden mit einer Analyse konventioneller Kraft-Abstandskurven verglichen.

Nanodrähte mit einer Federkonstanten um 1N/m und Resonanzfrequenzen von 10MHz bis 1GHz werden bereits als AFM-Spitzen mit hohem Aspektverhältnis verwendet und stellen wegen ihrer Resonanzfrequenzen im MHz-Bereich mögliche 'Nanocantilever' für Rasterkraftmikroskope mit hoher Datenrate dar. Die Wechselwirkung zwischen Nanodraht und AFM-Spitze wird für lithographisch hergestellte Silizum-Nanodrähte [1] (Länge 5000 nm, Durchmesser 150nm) und selbstorganisiert gewachsene Zinnoxid-Nanodrähte [2] (Länge 300nm , Durchmesser 20nm) untersucht.

[1] Shunfeng Li et al; Phys. Status Solidi C 7, 84 (2010). [2] S. Barth et al.; Nanotechnology 20, 115705 (2009).

O 23.7 Mon 18:45 WIL C307

Measuring forces in a single-molecule transport junction — •Norman Fournier, Christian Wagner, Christian Weiss, Ruslan Temirov, and Stefan Tautz — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich and JARA-Fundamentals of Future Information Technology

Understanding of the charge transport on a single-molecule level is vital for the future success of molecular electronics. At the present, however, this understanding is still hindered by the lack of data obtained under well-controlled experimental conditions. Recently we have shown that a low-temperature scanning tunneling microscope (STM) can be used to perform well-controlled and tunable single-molecule transport studies [1]. The high degree of structural control reached in our experiments allowed theoretical analysis of the junction on ab-initio level [2,3]. In this contribution we take further efforts towards even better experimental control over the molecular transport junction: contacting the molecule with the tip of the low-temperature AFM/STM, based on the q-Plus tuning fork design, we demonstrate that the forces acting in the junction can be measured simultaneously with the transport. The results of such measurements help us to gain further insights in the structure of a single-molecule junction and the process of the mechanical gating.

(1) R Temirov et al. Nanotechnology 2008, 19, 065401 (2) A. Greuling et al. submitted to Phys. Rev. Lett. (3) C. Toher, et al. submitted to Phys. Rev. B

O 23.8 Mon 19:00 WIL C307

Structure of the first water layer on Ru(0001) — •Sabine Maier[1,2], Ingeborg Stass[1], Peter J. Feibelman[3], and Miquel Salmeron[1] — [1]Lawrence Berkeley National Laboratory, Berkeley, CA, USA — [2]Friedrich-Alexander-Universität Erlangen, Erlangen — [3]Sandia National Laboratories, Albuquerque, NM, USA

The structure and chemistry of water at surfaces and interfaces, though fundamental to many areas of science and technology, is largely unknown. Low temperature scanning tunneling microscopy data in combination with DFT calculations can, however, reveal the molecular structure of monolayer thick water films. By these means, we have found that compact clusters of flat-lying H_2O molecules lie low on Ru(0001), and anchor the adsorbed layer to it. They alternate with clusters of molecules possessing a dangling H-bond, which bind weakly to the metal and, correspondingly, lie higher above the surface. Counter to conventional expectation, the high-lying molecular hexagons are rotated 30° relative to the principal axes of the metal crystal surface. This rotation leads to a bonding structure that significantly deviates from the conventional ice-like water model on hexagonal metals. Above 130K, we observed the formation of mixed water-hydroxyl structures following partial dissociation.

O 24: Invited Talk (Rudolf M. Tromp)

Time: Tuesday 10:15–11:00 Location: TRE Phy

Invited Talk O 24.1 Tue 10:15 TRE Phy

Low Energy Electron Microscopy Studies of Thin Film Graphene Growth and Properties — •Rudolf M. Tromp — IBM T.J. Watson Research Center, 1101 Kitchawan Road, Yorktown Heights, NY 10598, USA

We have used in-situ Low Energy Electron Microscopy (LEEM) and Photo Electron Emission Microscopy (PEEM) to study the growth and properties of thin graphene films on SiC as well as metallic substrates. These methods enable us to follow the growth at temperatures up to 1600 C, and in the presence of background gases up to 0.1 mTorr, in real time and with high spatial resolution, providing valuable insights into the growth processes. The intensity of the Low Energy Electron Diffraction (LEED) beams as a function of incident energy provides detailed atomic structure information, with a spatial resolution of just a few nanometers. The electronic structure can be accessed by energy and momentum resolved photo electron spectroscopy and microscopy, as well as spatially resolved Electron Energy Loss Spectroscopy. For instance, we find that the electronic structure of the first graphene layer depends sensitively on the electronic structure of the underlying substrate interface. Thus, LEEM/PEEM experiments give a comprehensive view of these thin films, including growth, morphology, atomic, as well as electronic structure. Combining LEEM with multiprobe Scanning Tunneling Microscopy has additionally allowed us to study electronic transport on the nanoscale, revealing the effect of defects such as atomic steps.

O 25: [DS] Progress in Micro- and Nanopatterning: Techniques and Applications I (Focused Session, jointly with O - Organisers: Graaf, Hartmann)

Time: Tuesday 11:00–13:00 Location: GER 37

Topical Talk O 25.1 Tue 11:00 GER 37

Microcontact chemistry: surface reactions in nanoscale confinement — •Bart Jan Ravoo — Organic Chemistry Institute, Westfälische Wilhelms-Universität Münster, Corrensstraße 40, 48149 Münster, Germany

Microcontact printing is an established method for the preparation of physical, chemical and biological patterns on solid surfaces. Typically, microcontact printing involves a microstructured elastomer stamp that delivers a molecular ink in the contact area between stamp and substrate. Recently, it has been shown that microcontact printing can also induce chemical reactions when an ink is printed on a substrate, even when the reaction partners are normally unreactive. Rapid and spatially controlled surface reactions induced by microcontact printing enable the molecular modification and patterning of a wide range of inorganic and organic substrates. This lecture will highlight our newest findings concerning the scope and kinetics of surface chemistry by microcontact printing as well as its application in bionanotechnology.

Literature: Ravoo, B.J. J. Mater. Chem. 2009, 18, 8902-8906. Wendeln, C. et al. Langmuir 2010, 26, 15966-15971 Kaufmann, T. et al. Adv. Mater. 2010, DOI: 10.1002/adma.201003564

Topical Talk O 25.2 Tue 11:30 GER 37
Electrochemical Microstructuring — Xinzhou Ma[1,2], Vadym Halka[1,2], and •Rolf Schuster[1,2] — [1]Physical Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Center for Functional Nanostructures, Karlsruhe, Germany

Small metallic structures of nanometer dimensions are mostly fabricated by lithographic methods, eventually followed by metal deposition under UHV conditions. Recently also electrochemical methods became very promising for microfabrication, because the number of steps involved in the fabrication process may be significantly reduced. However, often the application of conventional electrochemical methods is hampered by long range charging of the double layer and the weak spatial confinement of electrochemical reactions.

In this contribution we review recent methods by which the constraints of conventional electrochemical methods can be circumvented and which allow to structure surfaces on the micrometer to nanometer scale. These approaches are for example based on putting geometrical constraints, using small tools in combination with controlled nucleation or mechanical detachment of metal clusters from the tool or by locally charging the electrochemical double layer upon application of short potential pulses. Also first results on electron beam induced metal deposition from a thin electrolyte film will be presented.

Topical Talk O 25.3 Tue 12:00 GER 37
Electrochemical Oxidation and Anodization Lithography on Self-Assembled Monolayers — •Stephanie Hoeppener — Laboratory of Organic and Macromolecular Chemistry, Friedrich-Schiller-University Jena, Germany

The use of Scanning Probe Based lithography techniques dates back shortly after the introduction of SXM techniques. In particular bias mediated chemical oxidation processes can be used to induce changes in the substrate's properties, i.e., the conductivity, topography, etc.

Implementing the bias mediated electrochemical oxidation onto self-assembled monolayers was introduced as an alternative that permits the fabrication of surfaces bearing addressable chemically active functional groups. The research activities in this field will be highlighted.

In particular the fabrication of chemically heterogeneous nanostructures introduces the possibility for a site-selective fictionalization of nanostructures – a challenge which is difficult to establish by common photo- and electron lithographic structuring approaches. Besides of fundamental investigations of the electrochemical oxidation process, illustrative examples of the oxidation pattern modification will be presented with respect to nanofabrication approaches.

Topical Talk O 25.4 Tue 12:30 GER 37
Surface Structuring by Single Pulse Laser Interference: Principles and Applications — •Johannes Boneberg — University of Konstanz

A nanosecond laser pulse is split into several beams. These beams are then overlapped on the sample surface. The resulting interference pattern induces surface modifications. The physical mechanism which lead to surface modification are discussed for thin films and bulk materials. Periods achieved are below 200nm, while the structure sizes could be much smaller. Besides the direct application for the generation of nanostructures, the method can be used as well to generate laterally modified chemical surface structures. These can be utilized in different applications, like the lateral patterning by a sol-gel process.

O 26: Focussed session: Theory and computation of electronic structure: new frontiers II (jointly with HL, DS)

Time: Tuesday 11:15–13:00 Location: TRE Phy

Topical Talk O 26.1 Tue 11:15 TRE Phy
Electronic and Optical Excitations in Magnetic Insulators — •Claudia Rödl, Frank Fuchs, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

With the advent of electronic devices exploiting also the spin degree of freedom, magnetic materials attract more and more interest due to potential technological applications. However, describing the excitation properties of insulators with strongly localized and partially occupied d states by means of *ab-initio* methods remains a considerable challenge. Here, we focus on the antiferromagnetic transition-metal oxides (TMO) MnO, FeO, CoO, and NiO and ferromagnetic $CrBr_3$ as prototypical representatives for the class of magnetic insulators.

A perturbative treatment of Hedin's GW approximation based on (semi)local approaches to exchange and correlation in the subjacent density-functional calculation fails to reproduce the experimental photoemission spectra. Instead, we use the non-local HSE03 exchange-correlation functional to obtain a reasonable starting point for the GW calculation. The spin-polarized extension of the Bethe-Salpeter equation (BSE) is solved to calculate optical absorption spectra including excitonic and local-field effects. The spectra are analyzed in terms of dipole-allowed and dipole-forbidden transitions. For instance, it turns out that the main absorption peaks in the TMOs are due to d-d excitations which are dipole-forbidden at the Γ point. Further, the occurrence of spin-allowed and spin-forbidden Frenkel-like bound excitonic states within the fundamental band gap is investigated.

O 26.2 Tue 11:45 TRE Phy
LSDA+DMFT calculations of FeNi disordered alloys and Fe/Au(001) thin films — •Jan Minar, Jurgen Braun, Ara Cho, and Hubert Ebert — Dep. Chemie und Biochemie, LMU University of Munich, Germany

The combination of the local spin density approximation (LSDA) and the dynamical mean field theory (DMFT) provide a powerful tool to treat correlations beyond plain LSDA. The KKR or multiple scattering approach implemented on this basis allows among others to deal with alloy and surface systems as well as to study spectroscopic properties on equal footing [1].

Here, we present a LSDA+DMFT study of FeNi disordered alloys using the coherent potential approximation (CPA). In particular the influence of correlation effects on magnetic properties will be discussed. Special emphasis will be put on the additional information supplied by the spin-polarised relativistic mode allowing to deal with the spin-orbit coupling induced properties like orbital magnetic moments and dichroism. A detailed comparison to recent angle resolved photoemission with high resolution [3] allows for a discussion on the influence of correlations with the increasing Ni concentration. In the second part the results of fully self-consistent LSDA+DMFT calculations for the Fe/Au(001) system are presented. In particular the creation of quantum well states has been followed by angular resolved photoemission.

1. J. Minar et al., prb 72, 0415125 (2005), J. Sanchez-Barriga et al., prl 103, 267203 (2009) and Phys. Rev. B 82, 104414 (2010)

O 26.3 Tue 12:00 TRE Phy
Effective on-site Coulomb interaction in transition metals from constrained RPA — •Ersoy Sasioglu, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Effective on-site Coulomb interaction (Hubbard U) between localized d electrons in $3d$, $4d$, and $5d$ transition metals are calculated employing the recently developed constrained random-phase approximation (cRPA) within the full-potential linearized augmented plane-wave (FLAPW) method [1] using Wannier functions [2]. The obtained Hubbard U parameters lie between 1 and 5 eV and show a non-monotonic behavior across the transition-metal series. We find that the U depends on the crystal structure, spin polarization, d-electron number and filling of the d orbitals rather than d-character of the elements. For most of the isovalent transition metals, U assumes similar values. The obtained U parameters for the $3d$ series are in good agreement with previous studies as well as available experimental data. Using calculated U parameters we discuss the strength of the electronic correlations and instability of the paramagnetic state towards the ferromagnetic one for $3d$ transition metals. This work has been supported in part by DFG-FOR-1346.
[1] www.flapw.de

[2] F. Freimuth, Y. Mokrousov, D. Wortmann, S. Heinze, and S. Blügel, Phys. Rev. B. **78**, 035120 (2008).

O 26.4 Tue 12:15 TRE Phy

Ab-initio description of spin-dependent transport in disordered alloys — •Diemo Ködderitzsch, Stephan Lowitzer, and Hubert Ebert — Ludwig-Maximilians-Universität München, Department Chemie und Biochemie, Physikalische Chemie, Butenandtstraße 11, D-81377 München, Germany

Spin-orbit induced couplings are the source of many interesting physical phenomena like the anomalous- and spin-Hall-effects (AHE, SHE), which recently received a lot of attention due to their potential application in the field of spintronics. During the last years several theoretical works have dealt with the intrinsic AHE and SHE, based on the band structure of pure materials and only few of them use a parameter free *ab initio* approach.

We present a coherent *ab initio* description of both, the AHE and SHE, that is applicable to pure **and** disordered alloys by treating all sources, i.e. intrinsic as well as extrinisic contributions, on equal footing. We use an implementation of the Kubo-Středa equation employing the fully relativistic Korringa-Kohn-Rostoker (KKR) Green's function method in conjunction with the Coherent Potential Approximation (CPA) alloy theory. For discussing spin currents we employ our recently devised relativistic spin projection scheme [1] and a corresponding generalization of the Kubo-Středa equation. We illustrate the power and versatility of the approach by giving several examples.

[1] S. Lowitzer, D. Ködderitzsch and H. Ebert, Phys. Rev. B 82, 140402(R) (2010).

O 26.5 Tue 12:30 TRE Phy

Applying hybrid-functional and many-body methods to rare earths: a study of Cerium — •Marco Casadei[1], Xinguo Ren[1], Joachim Paier[2], Patrick Rinke[1], Angel Rubio[1,3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG (TH), Berlin, Germany — [2]Humboldt Universitaet (Institut fuer Chemie), Berlin, Germany — [3]UPV/EHV, San Sebastian (Fisica Materiales), Spain

The presence of localized, partially occupied f-electron states dictates many of the peculiar physical properties of rare-earth materials. In particular, the description of the iso-structural α-γ phase transition in Ce metal poses great challenges to density-functional theory (DFT) based approaches since local/semilocal (LDA/GGA) functionals completely fail to produce the phase transition. Here we address this problem by investigating bulk-like Ce clusters of increasing size using hybrid functionals, that incorporate a portion of exact-exchange, and full exact-exchange plus correlation at the level of the random phase approximation (EX+cRPA). In all clusters we find two stable configurations with different lattice constants and distinct electronic and magnetic properties, resembling the bulk situation. However, all hybrid functionals predict that the high volume phase (linked to the γ-Ce phase) is lower in energy at zero temperature, in contrast to experiment. Decreasing the amount of exact-exchange in the hybrid functional eventually restores the correct phase ordering, at the expense of introducing an adjustable parameter. We show that EX+cRPA – a physically meaningful screening of exact-exchange – achieves the same effect from first principles.

O 26.6 Tue 12:45 TRE Phy

Issues with J-dependence in the LSDA+U method for non-collinear magnets — •Eric Bousquet[1,2] and Nicola Spaldin[1] — [1]Department of Materials, ETH Zurich, Switzerland — [2]Physique Théorique des Matériaux, Université de Liège, B-4000 Sart Tilman, Belgium

We re-examine the commonly used density functional theory plus Hubbard U DFT+U method for the case of non-collinear magnets. While many studies neglect to explicitly include the exchange correction parameter J, or consider its exact value to be unimportant, here we show that in the case of non-collinear magnetism calculations the J parameter can strongly affect the magnetic ground state. We illustrate the drastic J-dependence of magnetic canting, magnetoelectric response and magnetocrystalline anisotropy by calculating trends in the magnetic lithium orthophosphate family LiMPO$_4$ (M = Fe and Ni) and difluorite family MF$_2$ (M = Mn, Fe, Co and Ni). These results can be readily understood by expanding the usual DFT+U equations within the spinor scheme. On the flip side, it is clear that non-collinear magnetic systems provide a challenging case for testing the correctness of new exchange correlation functionals within the density functional formalism.

O 27: Metal substrates: Adsorption of organic / bio molecules IV

Time: Tuesday 11:15–13:00 Location: PHY C213

O 27.1 Tue 11:15 PHY C213

Alkali-induced nanopatterning of Ag(110) surface mediated by molecular adsorbate — •Giuseppe Mercurio[1,2], Oliver Bauer[3], Martin Willenbockel[1,2], Benjamin Fiedler[3], Christian Weiss[1,2], Ruslan Temirov[1,2], Sergey Subach[1,2], Moritz Sokolowski[3], and Stefan Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology — [3]Institute for Physical and Theoretical Chemistry, University of Bonn

It is known for decades that alkali metals initiate the restructuring of fcc metal surfaces resulting in a composite patterned morphology. On the other hand, co-adsorbed metal atoms and organic molecules often form extended 2D networks due to the metal-molecular coordination reaction. Here we report on a new type of structural modification of the molecule-substrate interface, which is not only restricted to self-assembly of the adsorbed metal atoms and molecules, but it also involves significant morphological reorganization of the metallic surface. In the experiments, potassium atoms are deposited on a monolayer of the long-range ordered PTCDA/Ag(110) phase. Subsequent annealing forces potassium atoms to intercalate under the molecular layer partially unbinding PTCDA from the substrate. The complex interaction between potassium, PTCDA and substrate induces a significant silver mass-transfer and leads to the appearance of 1D stripe-structures of K atoms and PTCDA molecules on a nanopatterned silver surface. Structural and electronic properties of this pattern were studied by means of NIXSW, XPS, LEED and LT-STM.

O 27.2 Tue 11:30 PHY C213

Adsorption of Tetrahydroxybenzene on Metal Surfaces — •Fabian Bebensee[1], Christian Bombis[1], Federico Masini[1], Svetlana Klyatskaya[2], Mario Ruben[2], Erik Laegsgaard[1], Flemming Besenbacher[1], and Trolle R. Linderoth[1] — [1]iNANO, Aarhus University, Aarhus, Denmark — [2]Karlsruhe Institute of Technology (KIT), Institut für Nanotechnologie, Karlsruhe, Germany

The synthesis of extended, well-ordered bi-dimensional molecular networks on surfaces has received a great deal of interest over the past years, fueled not least by potential applications such as functionalized surface coatings, sensors and molecular electronics. Here, we employ scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS) to study the adsorption of tetrahydroxybenzene (THB) on the Au(111) and Cu(111) surfaces. The molecule shows a complex adsorption behavior despite being structurally rather simple. Depending on post-deposition treatment, coverage and substrate, we find different adsorption structures: a hexagonal close-packed phase and a porous network structure exhibiting a high degree of order. The XPS results reveal that the transformation from the hexagonal close-packed phase to the porous network is linked to a chemical modification of THB, possibly involving dehydrogenation of the molecules. We tentatively propose that the porous network, which was observed solely on the Cu(111) surface, is a metal complexation structure involving native Cu released during post-deposition annealing.

O 27.3 Tue 11:45 PHY C213

Structure of self-assembled monolayers of 1,1'-biphenyl-4-thiols on Au(111): A combined STM, LEED and XPS study — •Dan G. Matei, Heiko Muzik, Andrey Turchanin, and Armin Gölzhäuser — Physik supramolekularer Systeme und Oberflächen, Universität Bielefeld

Self-assembled monolayers (SAMs) of aromatic molecules are in the focus of research due to their applications in nanotechnology ranging from the fabrication of biofunctional surfaces to the generation of freestanding graphene. However, important structural issues of aromatic SAMs on metal substrates are not yet well understood. In this contribution, we report on the structure of 1,1'-biphenyl-4-thiol (BPT) SAMs on Au(111) prepared from solvents and by vapour deposition in vacuum. We analyze molecular resolved scanning tunneling microscopy (STM) images of "as prepared" and annealed samples. Upon vacuum annealing regular molecular superstructures form on Au(111). Their unit cells were investigated by low-energy electron diffraction (LEED). X-ray photoelectron spectroscopy (XPS) was employed to study the chemical composition and effective thickness. We present a comprehensive analysis of these data.

O 27.4 Tue 12:00 PHY C213

Electronic many–body effects at metal–organic interfaces studied with PES, NEXAFS and Resonant Auger Raman Spectroscopy — •M. Häming[1], A. Schöll[1], E. Umbach[2], and F. Reinert[1] — [1]Universität Würzburg, Experimentelle Physik VII, D–97074 Würzburg, Germany — [2]Karlsruhe Institut für Technologie (KIT) D–76021 Karlsruhe, Germany

Electronic many–body and correlation effects have been studied intensively at transition metal compounds with localized d/f electrons. They are related to interesting material properties, e.g. Mott metal–insulator transitions, charge transfer satellites and superconductivity. Recent investigations of graphene,[1] C_{60},[2] and TTF–TCNQ[3] showed that many–body effects can also be important for organic thin films. We have investigated several organic thin films (PTCDA, PTCDI, BTCDA, BTCDI, SnPc) deposited on a Ag(111) surfaces with photoelectron spectroscopy, NEXAFS and resonant Auger Raman spectroscopy. Our data provide significant indications for electronic many–body effects involving substrate–adsorbate charge transfer, which can be understood by concepts developed for charge transfer compounds. These results give insight into new, interesting aspects of physics at metal–organic interfaces.

[1] I. Gierz *et al.*, Nano Letters **8**, 4603–4607 (2008)
[2] W. Yang *et al.*, Science **300**, 303–307 (2003)
[3] M. Sing *et al.*, Phys. Rev. B **68**, 125111 (2003)

O 27.5 Tue 12:15 PHY C213

Compensation of the odd-even effects in araliphatic monomolecular films by non-symmetric attachment of the aromatic part — John Dauselt[1], Jianli Zhao[2], Martin Kind[1], Robert Binder[1], Andreas Terfort[1], and •Michael Zharnikov[2] — [1]Institut für Anorganische und Analytische Chemie, Universität Frankfurt, Max-von-Laue-Straße 7, 60438 Frankfurt, Germany — [2]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

The integrity, chemical identity, packing density, and molecular orientation in SAMs formed by anthracene-substituted alkanethiols (Ant-n) with a variable number of methylene groups (n) in the aliphatic linker on Au(111) and Ag(111) substrates were studied by a combination of several complementary experimental techniques. The Ant-n molecules were found to form well-defined and highly ordered SAMs on these substrates, with very small inclination of the anthracene backbone. In addition, the Ant-n SAMs exhibited odd-even effects, i.e. dependence of the molecular orientation and packing density on the length of the aliphatic linker, with the parity of n being the decisive parameter. Whereas the direction (sign) of this odd-even behavior on gold and silver is the same as for SAMs of biphenyl- and terphenyl-substituted alkanethiolates and alkaneselenolates, the extent of the odd-even effects in the Ant-n films is noticeably smaller than in the latter systems. This behaviour can be explained by the additional rotational degree of freedom of the anthracene unit in the case of the Ant-n SAMs due to its non-symmetrical attachment to the adjacent alkyl linker.

O 27.6 Tue 12:30 PHY C213

4,4'-dithiodipyridine on Au(111): An STM and STS study — •Norbert Maurer, Anna Tschetschetkin, Berndt Koslowski, and Paul Ziemann — Institut für Festkörperphysik, Albert-Einstein-Allee 11, University of Ulm, D-89081 Ulm

Driven by the overwhelming possibilities of molecular electronics, systems of inorganic substrates covered with organic materials evolved to a widely investigated field. Promising candidates in this respect are thiols containing heterocyclic groups, e.g. the 4,4'-dithiodipyridine (PySSPy). We prepared PySSPy/Au(111) *in vacuo* at a reduced temperature and investigated the result by scanning tunneling microscopy and spectroscopy with emphasis on z-V spectroscopy. PySSPy forms islands on Au(111) exhibiting a $13\text{x}3\sqrt{3}$ superstructure where the substrate-induced enantiomeric-excess of the molecules plays an important role. In that structure the LUMO is found to be at 3.2 eV with a slight variation depending on the position/coordination of the PySSPy. By annealing the structure at room temperature, a chain growth can be observed. The LUMO is then found at ∼2.1 eV. We conclude that the PySSPy dissociates at RT on Au(111) and forms a thiolate.

O 27.7 Tue 12:45 PHY C213

STM-investigations on aza-BODIPYs at low temperatures — •Jörg Meyer, Anja Wadewitz, Cormac Toher, Loka Mani, Francesca Moresco, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany

Scanning Tunnelling Microscopy (STM) is a powerful experimental technique in surface science. It combines atomic resolution imaging with the opportunity to perform nanoscale manipulations. Additionally, STM enable the mapping of the density of states of materials. Here we report investigations on aza-BODIPY adsorbed on metal surfaces with a low-temperature STM/AFM-System. Aza-BODIPY (e.g. 1,3,5,7-tetraphenyl-8-azadipyromethene) are a class of organic fluorescent dyes characterised by the same molecular core region consisting of two pyrroles connected by a boronfluorine complex and a nitrogen atom. These molecules exhibit strong chemical stability and highly tuneable, sharp absorption wavelength. Aza-BODIPY has previously been used for immunostaining and photodynamic therapy during the last few years. Recently, electron donor materials for organic photovoltaics (OPVs) has emerged as another field of application, due to aza-BODIPYs strong infrared absorption. In this work we investigated single aza-BODIPY molecules adsorbed on Ag(110) and Au(111) by STM at 77 K and 5 K. We verified the adsorption configuration and geometry and found it to be in qualitative agreement with theoretical simulations. In addition we conducted spectroscopy measurements to determine the electronic structure of the molecule on the surface.

O 28: Plasmonics and Nanooptics III

Time: Tuesday 11:15–13:00 Location: WIL A317

O 28.1 Tue 11:15 WIL A317

Tip-enhanced Spectroscopic Mapping — •Dai Zhang, Xiao Wang, and Alfred J. Meixner — Inst. Phys. Theo. Chem.

When a sharp Au tip approaching very closely to the sample surface, the tip-sample system behaves as an optical antenna. It confines and enhances the excitation field to a small sub-diffraction volume in the gap between the tip-apex and the surface and retrieving emitted or scattered photons to the far field for detection.

In my talk, the influence of several parameters, such as the gap distance, the material properties of the tip and the substrate as well as the size of the tip, on the performance of the gap-mode near-field optical microscopy will be systematically discussed. Gap-mode near-field spectroscopic mapping technique has been recently developed in our lab. I will demonstrate the Raman and photoluminescence spectroscopic imaging of the chemical distribution in the polymer:fullerene organic solar cell blend film [1]. From the simultaneously recorded morphology and spectroscopic information, the interplay among the blend film morphology, the local donor and acceptor molecular distributions, and the photoluminescence quenching efficiency will be discussed. With the above demonstrations, we propose that the gap-mode near-field optical microscopy is a promising, high-resolution and multi-function characterization technique for material science [1,2].

References [1] X. Wang et al, Advanced Functional Materials 20, 492 (2010). [2] D. Zhang et al, Physical Revew Letters, 104, 056601 (2010).

O 28.2 Tue 11:30 WIL A317

Near-Field Imaging of Directive Optical Yagi-Uda Nanoan-

tennas — •Jens Dorfmüller[1], Daniel Drégely[1], Moritz Esslinger[2], Worawut Khunsin[2], Ralf Vogelgesang[2], Klaus Kern[2,3], and Harald Giessen[1] — [1]4. Physikalisches Institut und Research Center SCoPE, Pfaffenwaldring 57, Universität Stuttgart, 70569 Stuttgart, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [3]Institut de Physique de la Matière Condensée, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Apertureless Scanning Near-field Optical Microscopy (aSNOM) in a cross-polarization scheme allows us to map the E-fields of plasmonic nano-structures in real-space with a resolution far beyond the diffraction limit [1,2]. Maps of near-field amplitude and phase allow us to determine the excitation mode. Analyzing the amplitude at elements of optical nano-antennas allows us to measure the receptivity in dependence of antenna geometry as well as illumination conditions.

Here, we investigate the reception directionality of optical Yagi-Uda antennas. Depending on the illumination direction, the electromagnetic energy is either concentrated at the feed element or distributed over several antenna elements. Comparison with simulations shows a very good agreement.

[1] J. Dorfmüller, R. Vogelgesang, R. T. Weitz, C. Rockstuhl, C. Etrich, T. Pertsch, F. Lederer, K. Kern, *Nano Lett.* **9**, 2372 (2009).

[2] J. Dorfmüller, R. Vogelgesang, W. Khunsin, C. Rockstuhl, C. Etrich, K. Kern, *Nano Lett.* **10**, 3596 (2010).

O 28.3 Tue 11:45 WIL A317

Surface-Plasmon-Polariton interation with gratings — •Andreas Englisch, Stefan Griesing, Uwe Schmitt, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, Postfach 151150, D-66041,

Surface-Plasmon-Polaritons (SPP) couple with light through suitable periodical structures. In the case of SPP-excitation a typical decrease of the intensity in the diffracted orders can be observed. Two different kinds of gratings are investigated: periodically corrugated metal surfaces on the one hand and structured dielectric layers on flat metal surfaces on the other hand. The intensities of the diffracted orders as well as the near-field intensities are measured in dependence of the grating profile. The near-field is characterized with respect to the amplitude and the phase by the use of a phase-sensitive scanning near-field optical microscope (SNOM. Numerical modeling based on finite element simulations in Fourier space as well as in real space were performed and compared with the measurements.

O 28.4 Tue 12:00 WIL A317

Nonlocal, grating-coupled scattering-type near-field scanning optical microscopy of individual gold nano-particles — •Diyar Sadiq[1], Javid Shirdel[1], Jae Sung Lee[2], Namkyoo Park[2], and Christoph Lienau[1] — [1]Institut für Physik, Carl von Ossietzky Universität, 26111 Oldenburg, Germany — [2]Photonic Systems Laboratory, School of EECS, Seoul

Scattering-type near-field scanning optical microscopy (s-NSOM) is now routinely used for (sub-) 10-nm-resolution optical imaging of surfaces. The performance is, however, often limited by a rather substantial signal background resulting from a direct optical illumination of the scattering antenna. Various ideas for a nonlocal optical excitation have therefore been proposed, e.g., by grating-coupling of surface plasmon polaritons (SPP) onto adiabatic metallic tapers and three-dimensional focusing of SPP wavepackets towards the tip apex [1]. Recently, first line-scan images recorded by using such probes demonstrated 20 nm resolution and coupling of about 15% of the SPP intensity onto the tip apex [2]. Here, we use such a grating-coupled SPP microscope for the first time for s-NSOM imaging of single metallic nano-particles. We demonstrate sub-20-nm-resolution imaging of localized SPP fields and observe that more than 40% of the grating-coupled SPP field is localized at the taper apex. The results are supported with numerical simulation based on the finite-difference time-domain (FDTD) method. [1] C. Ropers et al. Nano Letters 7, 2784 (2007). [2] C. C. Neacsu et al, Nano Letters 10, 592 (2010).

O 28.5 Tue 12:15 WIL A317

Enhanced vibrational near-field spectroscopy of PMMA with infrared antennas — •Jón Mattis Hoffmann, Jens Richter, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University, Sommerfeldstraße 14, 52074 Aachen, Germany

Infrared spectroscopy allows for the investigation of chemical properties of a sample material by directly probing molecular vibrations. Combined with scattering-type near-field optical microscopy (s-SNOM), which relies on the scattering of light at a sharp metallic tip, it is possible to obtain such spectroscopic information in images with strongly subwavelength resolution [1]. For the probing of weakly absorbing samples, such as molecular vibrations in thin polymer layers [2], increased sensitivity of infrared near-field spectroscopy is needed. It has been shown that signals in near-field vibrational spectroscopy of thin films can be enhanced by reflecting substrates [3]. For even higher enhancement factors we investigate the possibility of using resonant substrates.

Here we employ triangular nanostructures fabricated by nanosphere lithography that exhibit strong resonances in the infrared region as substrate. We want to measure the resonant enhanced near-field spectra of a thin PMMA film on top of these infrared antennas.

[1] F. Keilmann et al. in Nano-Optics and Near-Field Optical Microscopy ed. by A. Zayats and D. Richards, 235 (ArtechHouse, 2009).

[2] T. Taubner et al., Applied Physics Letters 85, 5064 (2004).

[3] J. Aizpurua et al., Optics Express 16, 1529 (2008).

O 28.6 Tue 12:30 WIL A317

scattering near-field microscopy in the THz using a free-electron laser — •Hans-Georg von Ribbeck[1], Marc Tobias Wenzel[1], Rainer Jacob[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, TU Dresden, 01062 Dresden, Germany — [2]Institut für Ionenstrahlphysik und Materialforschung, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany

We present scattering-type scanning near-field optical micro spectroscopy (s SNOM) investigations successfully operated in the THz range with a wavelength independent spatial resolution of 90 nm. Our microscopy set-up bases on a true noncontact atomic force microscope (nc-AFM) combined with the free-electron laser (FEL) source at the Helmholtz-Zentrum Dresden-Rossendorf. This laser provides tunability from 30 to 250 μm. We were able to record, for the first time ever, s-SNOM signatures with a FEL at wavelengths ranging from 30 μm to 180 μm (10 to 1.67 THz). In addition to the near-field dependent optical signals we also demonstrate the imaging and spectroscopy capabilities of our THz-s-SNOM. Image scans were performed on a specially designed test structure consisting of a topography-free composite of a polymer/gold sample. On these samples a topography independent strong optical material contrast could be demonstrated at 150 μm wavelength. Furthermore we achieve a resolution of better than 90 nm on a Fischer-Pattern test structure, corresponding to an optical improvement of better than 1500 times the wavelength.

O 28.7 Tue 12:45 WIL A317

Background-Free Imaging with an Apertureless Scanning Nearfield Optical Microscope — •Moritz Esslinger[1], Jens Dorfmüller[1,2], Ralf Vogelgesang[1], Worawut Khunsin[1], and Klaus Kern[1,3] — [1]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany — [2]presently at 4. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany — [3]de Physique de la Matière Condensée, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

We present advances in experimental techniques of apertureless near-field optical microscopy (aSNOM). This technique achieves high spatial resolution by utilizing the field enhancement at the apex of sharp tips. Many conventional setups utilize p-polarized light in the illumination as well as in the detection path. The detected light of such a setup not only contains the optical near field signal, but is affected also by coupling effects between tip and sample.

By using p-polarized light for illumination and detecting the s-polarized component of the backscattered light we are able to measure the z-component of the electric field on the sample essentially without coupling effects. Here we outline how the proper choice of tip position, together with optimizing polarizer and analyzer angles of our cross-polarization scheme ensures plasmonic eigenmode mapping with a background of exactly zero. By comparison with simulation data not including the tip we show that the measurement has little to no influence on the eigenmodes.

O 29: Graphene I

Time: Tuesday 11:15–13:00 Location: WIL B321

O 29.1 Tue 11:15 WIL B321

Graphene Growth Kinetics on Ru(0001) as Function of the Termination of Graphene Islands — •Sebastian Daenhardt[1], Sebastian Guenther[2], Stefan Schmitt[3], and Joost Wintterlin[1] — [1]Department Chemie, LMU Muenchen — [2]Fachgebiet Phys. Chemie (Katalyse) , TU Muenchen — [3]SPECS GmbH, Voltastr. 5, 13355 Berlin

For a deeper understanding of the growth kinetics of graphene on metal surfaces it is important to monitor the growth of the islands in situ, at the high temperatures of the CVD process. Here we present the results of an in situ STM investigation of the growth of graphene on Ru(0001) during ethylene decomposition between 650 and 750°C. We have also monitored the removal of the graphene layer by oxidation in situ. We find that the graphene islands are all zig-zag terminated, but that there are still two different island terminations, which are rotated by an angle of 120°, that display different growth velocities. The two terminations also differ with respect to the binding to Ru steps. The slowly growing edges tend to bind to Ru steps during the growth, in contrast to the faster growing edges. The slowly growing edges can also etch into ascending steps, so that the graphene islands can grow on given terraces without crossing the steps. In all of these cases graphene grows in a "quantized" form, i.e., by addition of full unit cells of the moiré structure. The data demonstrate a massive restructuring of the Ru surface under the growth conditions, and they provide insight into the energetics of the graphene-Ru edges.

O 29.2 Tue 11:30 WIL B321

Graphene flakes growth study by ARPES — •Marin Petrović[1], Iva Šrut[1], Petar Pervan[1], Sven Runte[2], Carsten Busse[2], Thomas Michely[2], and Marko Kralj[1] — [1]Institut za fiziku, Zagreb, Croatia — [2]II. Physikalisches Institut, Köln, Germany

A well established route for the large-scale production of graphene is chemical vapor phase deposition (CVD) growth on various metal substrates [1]. However, in order to obtain highly oriented graphene covering the entire Ir(111) surface one needs to combine the temperature programmed growth (TPG) with CVD [2]. Moreover, by using just the TPG procedure, it is possible to grow graphene flakes of various average sizes, depending on the growth parameters used. The overall area of Ir(111) sample covered with flakes after each TPG cycle is always the same, regardless of the temperature [3]. Here we report a study of graphene flakes obtained by ethene decomposition on Ir(111) using the TPG procedure at various temperatures. As the decomposition temperature of the preadsorbed ethene increases, the average size of the flakes increases as well. Based on angle-resolved photoemission spectroscopy (ARPES), in particular the Dirac cone intensity analysis, we characterise graphene flakes on Ir(111) of varying sizes and compare these results with known STM and XPS data.

[1] X. Li et al., Science 324, 1312 (2009)
[2] R. von Gastel et al., Appl. Phys. Lett. 95, 121901 (2009)
[3] J. Coraux et al., New J. Phys. 11, 023006 (2009)

O 29.3 Tue 11:45 WIL B321

Growth of graphene on heteroepitaxial Ir(111)-films — •Patrick Zeller[1], Sebastian Dänhardt[1], Stefan Gsell[2], Matthias Schreck[2], and Joost Wintterlin[1] — [1]LMU München, Department Chemie — [2]Universität Augsburg, Institut für Physik

Monolayer graphene was epitaxially grown on thin iridium films by chemical vapor deposition (CVD) of ethylene. The films consist of a 150 nm thick (111)-oriented Ir layer on a Si(111) substrate with a 40 to 100 nm thick buffer layer of yttria-stabilized zirconia (YSZ) in between. The idea is to develop preparation techniques for epitaxial graphene without the need for bulk single crystals. The Ir films display a high crystalline quality with mosaic tilt and twist spreads lower than 0.2° [1]. The growth of graphene on these films was investigated by scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED). We find the same four rotational graphene domains that exist on bulk Ir(111) single crystals, with rotational angles of 0°, 13.9°, 19.1°, and 30° [2,3]. STM data of the 13.9° and the 19.1° phase are reported here for the first time. The quality of the graphene and the formation of the various domains can be controlled by the growth conditions. In summary we demonstrate that the quality of the epitaxial graphene on the Ir films is comparable to Ir(111) single crystals. The findings may open a new economic route for epitaxial graphene synthesis.

[1] Gsell, S., et al., Journal of Crystal Growth 2009, 311, 3731. [2] N'Diaye, A., et al. New Journal of Physics 2008, 10, 043033. [3] Loginova, E., et al. Physical Review B 2009, 80, 085430.

O 29.4 Tue 12:00 WIL B321

Long-Range Ordered Single Crystal Graphene on Heteroepitaxial Ni Thin Films Grown on MgO(111) — •Takayuki Iwasaki[1], Hye Jin Park[1], Mitsuharu Konuma[1], Dong Su Lee[1], Alexei Zakharov[2], Jurgen H. Smet[1], and Ulrich Starke[1] — [1]Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]Max Lab, Lund University, Box 118, Lund, S-22100, Sweden

The establishment of graphene-based electronics can be achieved when the size, crystal orientation and number of layers of graphene are controlled on a substrate. Growth of large area graphene has been reported on metal films [1] or foils [2]. The resulting graphene, however, is polycrystalline with rotational disorder and grain boundaries which can scatter carriers and thus impair the device properties. Here, we demonstrate the synthesis of large-size single crystal and uniform monolayer graphene on Ni(111) thin films that were heteroepitaxially grown on MgO substrates [3]. The Ni films have flat terraces and no large grain boundaries, and also the formation of twins is suppressed on the atomic scale. As confirmed by LEED and ARUPS measurements the Ni films as well as the synthesized graphene are single crystalline. The Ni films can be easily etched, so that the transfer of mm-scale single crystal graphene onto an insulating substrate could be achieved. Furthermore, we show the synthesis of twisted bilayer graphene by a combination of catalytic hydrocarbon reaction and carbon segregation. [1] K.S. Kim et al., Nature, 457, 706 (2009). [2] X. Li et al., Science, 324, 1312 (2009). [3] T. Iwasaki et al., Nano Lett., accepted for publication.

O 29.5 Tue 12:15 WIL B321

Direct graphene growth on insulators: The interaction with the substrate — •Olaf Seifarth, Gunther Lippert, Jaroslaw Dabrowski, and Grzegorz Lupina — IHP, Im Technologiepark 25, 15230 Frankfurt, Germany

Strong effort is devoted to grow graphene directly on insulators to create a technological step towards cost effective mass production of high-frequency transistors. We have shown recently, that direct graphene growth can be achieved on silicate substrates by solid carbon source deposition. Here, we present a systematic study on the interaction of the graphene with the insulator by means of Raman and photoelectron spectroscopy. We address temperature dependence, the correlation between graphene quality and the number of layers and unintentional background doping. Special notice is devoted to the agglomeration sites on the substrate.

O 29.6 Tue 12:30 WIL B321

Electrical conductivity of single functionalized graphene sheets measured by Kelvin probe force microscopy — Liang Yan[1], •Christian Punckt[2], Ilhan A. Aksay[2], Wolfgang Mertin[1], and Gerd Bacher[1] — [1]Werkstoffe der Elektrotechnik und CeNIDE, Universität Duisburg-Essen, Germany — [2]Dept. of Chem. and Biolog. Engineering, Princeton University, USA

Functionalized graphene can be produced in bulk amounts by the thermal exfoliation of graphite oxide resulting in a material exhibiting a large fraction of single functionalized graphene sheets (FGSs) which – in contrast to pristine (e.g. "Scotch Tape") graphene – contain a large amount of functional groups and lattice defects. The number density of functional groups and defects can be tuned either by modifying the exfoliation process or by subsequent thermal reduction or annealing. FGSs have been used in various applications ranging from polymer nanocomposites to supercapacitors and batteries. In these applications, both the intrinsic resistance of the FGSs as well as the electrical contact between adjacent sheets limit device performance. By measuring the conductivity of individual FGSs employing Kelvin probe force microscopy, we can eliminate the contribution of contact resistance, analyze the intrinsic sheet conductivity with spatial resolution, and correlate electronic and topographical features. Despite their large degree of lattice disorder and functionalization, we obtain conductivities on the order of 10^5 S/m for individual sheets. Results are put in perspective with emerging applications and competing materials.

O 29.7 Tue 12:45 WIL B321

Single and double layer graphenes as ultra-barriers for fluorescent polymer films — •Philipp Lange[1], Martin Dorn[1], Nikolai Severin[1], David A. Vanden Bout[2], and Jürgen P. Rabe[1] — [1]Humboldt-Universität zu Berlin, Department of Physics, Germany — [2]The University of Texas at Austin, Department of Biochemistry and Chemistry, USA

Graphene, with its combined high electrical conductivity, optical transparency and mechanical flexibility, offers great potential for electrodes in flexible organic optoelectronic devices. Since freely suspended graphene is also largely impermeable to gases, it could even serve as both transparent electrode and effective barrier to protect the device against the ubiquitous degradation by water and oxygen. However, in a working device graphene may be subject to structural degradation. Here we report on the chemical and structural stability of graphene *in-situ* on a conjugated polymer film. Fluorescence and scanning force microscopies were used to probe the degradation of the polymer protected from ambient by graphene. We detected individual permeable point defects in single layer graphene resulting from a rare event structural degradation. Double layer graphene in contrast is stable and protects the polymer most efficiently from degradation. We estimate an upper limit of the water and oxygen transmission rates through graphene in direct contact with the polymer film as low as 5x10^{-6} g m^{-2}day^{-1} and 6x10^{-3} cm^{3}m^{-2}day^{-1}, respectively, which is on the order of the technologically required transmission rates. This suggests that graphenes can function as both electrode and barrier layer in future devices.

O 30: Focussed session: Transparent conductive oxides II (jointly with HL, DS)

Time: Tuesday 11:15–13:15 Location: WIL B122

Topical Talk O 30.1 Tue 11:15 WIL B122

Experimental Electronic Structure of In_2O_3 and Ga_2O_3 — •Christoph Janowitz — Brandenburgische Technische Universität Cottbus — Humboldt Universität zu Berlin, Institut für Physik

Transparent conducting oxides (TCO's) pose a number of serious challenges. Besides the strive for high quality single crystals and thin films their application has to be preceded by a thorough understanding of their peculiar electronic structure. It is of fundamental interest to understand why materials transparent up to the UV spectral regime behave also as conductors. In this talk two binary oxides -In_2O_3 and Ga_2O_3 from the group of TCO's showing the smallest respectively largest optical gap- will be explored experimentally. The investigations on the electronic structure were performed on high quality n-type single crystals showing carrier densities of 10^{19} cm^{-3} (In_2O_3) and 10^{17} cm^{-3} (Ga_2O_3). Subjects addressed are the determination of the band structure along the high symmetry directions, effective masses and fundamental gap by angular resolved photoemission (ARPES). Also by resonant ARPES and a combination of X-ray photoemission and X-ray absorption complementary information on the orbital character of the valence- and conduction band regime and on the band gap are obtained. The observations are discussed by reference to calculations of the electronic structure and models for the conductivity mechanism.

Topical Talk O 30.2 Tue 11:45 WIL B122

Transparent Electronics Using Oxide Materials — •Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II

We discuss all-oxide transparent electronic devices, such as diodes, photodiodes, transistors and inverters, based on rectifying, transparent Schottky contacts from metal oxides, transparent semiconducting oxides and transparent substrates. In particular, MESFET devices are presented with crystalline and amorphous oxides as channel, exhibiting low operation voltage and voltage swing. Inverters built from such transistors exhibit high gain (>200). Directions of further research will be discussed.

Topical Talk O 30.3 Tue 12:15 WIL B122

Optical properties of undoped and doped ZnO — •Axel Hoffmann and Markus R. Wagner — Institut für Festkörperphysik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

A spectroscopic study of optical transitions and lattice dynamics of ZnO under the influence of external fields is reviewed. A comparative study of different ZnO single crystals and doped and undoped ZnO films reveals pronounced differences in the free and bound exciton luminescence which can be related to different impurity centers and strain levels. A correlation between the localization energies of excitons bound to the same chemical element in the neutral and ionized charge state is reported. The properties of the shallow impurity bound excitons are compared to defect related deeply bound excitons. The lattice dynamics of ZnO crystals are studied by Raman spectroscopy under the influence of external pressure. A variety of important material parameters is derived including high precision values of the hydrostatic pressure coefficients and Grüneisen parameters of all Raman active modes. For the Born transverse effective charge, an incorrect pressure dependence in the literature is discovered and revised. Raman measurements of ZnO single crystals under uniaxial pressure are reported. In combination with the hydrostatic pressure measurements on the same samples, the first experimental determination of the phonon deformation potentials of all Raman active modes in ZnO is achieved.

O 30.4 Tue 12:45 WIL B122

Thermodynamic stability, stoichiometry and electronic structure of bcc-In_2O_3 surfaces — •Peter Agoston and Karsten Albe — TU Darmstadt, Petersenstr. 32, 64287 Darmstadt

The thermodynamic stability of all experimentally observed low index surfaces of bcc-indium oxide (In_2O_3) have been investigated by means of density functional theory calculations. The effect of a changing environment has been studies as well as the influence of hydrogen and water. It is found that the (001) surfaces have the most complex behavior. For this surface additionally the effects due to dopants (Sn) as well as the in-plane lattice strain has been studied. Finally, scanning tunneling microscopy images are presented and discussed in the light of previous experiments.

O 30.5 Tue 13:00 WIL B122

Growth and characterization of In_2O_3 single crystals — •Valentina Scherer, Peter Hlawenka, Christoph Janowitz, Alica Krapf, Helmut Dwelk, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin

The scientific interest in transparent conducting oxides (TCOs) such as ZnO, Ga_2O_3, In_2O_3 and SnO_2 increases significantly. However, information on the electronic structure and the doping behaviour is very scarce. This is in part due to the challenging problem of growing high purity single crystals and substrates for homoepitaxy, which also limits the attainable progress in device production. High quality In_2O_3 single crystals were grown using the chemical vapor transport method (CVT). The crystals were of body centered cubic bixbyite-type structure with a lattice parameter $a = 10.12$. The temperature-dependent resistivity, Hall-constant, and mobility were measured and an electron density in the range of $\sim 10^{19} cm^{-3}$ was determined. The crystals were then investigated using high resolution photoemission and transport measurements. Emission from the valence band and the partially filled conduction band at the Γ-point yielded a direct band gap of ~ 3 eV. The weak conduction band emission near the Fermi edge enabled a Fermi-map and the determination of the Fermi surface. The obtained results are in good agreement with theoretical band structure calculations and with the previously experimental results of the thin films.

O 31: Nanostructures at surfaces: Dots, particles, clusters, arrays II

Time: Tuesday 11:15–13:15 Location: WIL C107

O 31.1 Tue 11:15 WIL C107

Electrochemical preparation of Co-Ag nanostructured materials for GMR applications — •José Manuel García — University of Barcelona, Barcelona, Spain

Although giant magnetoresistance (GMR) phenomenon was discovered in sputtered Fe/Cr multilayers, some years later other configurations (i.e. granular films or nanowires) as well as other systems (i.e. Co/Cu, CoFe/Ag) were found to exhibit this property. Among those systems the Co-Ag system seems to be a good candidate as magnetoresistive material, because sharp magnetic/non-magnetic interfaces are expected in view of the total immiscibility between the two metals shown by the phase diagram. On the other hand, electrodeposition is a technique that day by day is gaining positions among the mainly employed physical methods for the preparation of thin films. This is due to the fact that electrodeposition shows some advantages over the physical techniques: versatility, selectivity, higher deposition rates and higher thicknesses, among others.

This work focuses on the preparation of different kinds of Co-Ag nanostructured materials with giant magnetoresistance. Granular films, multilayers and nanowires were prepared taking profit of the versatility of electrodeposition. Co(Core)-Ag(Shell) nanoparticles were also prepared but by a chemical method. The interest was to compare the properties of the Co-Ag materials obtained under the different configurations. In all cases, the experimental conditions were optimized in order to obtain the highest magnetoresistance values as possible and trying to share light on the mechanism responsible of GMR.

O 31.2 Tue 11:30 WIL C107

F-center in a MgO-surface and MgO-bulk — •Daniel Berger and Paul-Gerhard Reinhard — Lehrstuhl für theoretische Physik II, Erlangen

A quantum-mechanical/molecular-mechanical (QM/MM) hierarchical model was applied to investigate electronic and optical properties of color centers in the insulating MgO material. F-centers situated directly at the surface as well as deeper inside had been studied and compared with previous results where available.

The color centers discussed here are oxygen vacancies filled by two electrons. The two electrons of such an F-center were treated quantum mechanically applying time-dependend DFT at the level of the local-density approximation. The DFT equations were solved in spacial grid representation. The hosting MgO lattice is described in the framework of the Gaussian Shell Model (GSM) at a classical level with appropriate ion-ion potentials within the lattice and pseudo-potentials for the interaction with the QM electrons. The dynamical polarization of the substrate ions is taken into account for the material in a vicinity of the defect, typically covering 2-4 shells of ions.

The density distribution of the defect electrons are in fair agreement with results from ab-initio calculations, while lattice relaxation is overestimated. Moreover, surface deformation through the color center shows a systematic dependency from the size of the active zone. The optical response shows marked resonance peaks whose properties change dramatically with the layer.

O 31.3 Tue 11:45 WIL C107

Catalytic Pt Nanoparticles on GaN Surfaces: In-situ Characterization of Nanoparticle-Support Interaction via High-pressure Synchrotron XPS — •Susanne Schaefer[1], Sonja Wyrzgol[2], Ian Sharp[1], Andreas Jentys[2], Detre Teschner[3], Axel Knop-Gericke[3], Johannes Lercher[2], and Martin Stutzmann[1] — [1]Walter Schottky Institut, Technische Universität München, Garching, Germany — [2]Catalysis Research Centre, Technische Universität München, Garching, Germany — [3]Fritz-Haber-Institut, Max-Planck-Gesellschaft, Berlin, Germany

Pt nanoparticles on GaN surfaces are investigated as a model system for the electronic control of catalytic reactions at the surface of a wide band gap semiconductor. In the synchrotron XPS study reported here, the electronic interaction of platinum nanoparticles with GaN surfaces was investigated with regard to semiconductor band bending as well as the chemical state of the nanoparticles due to charge transfer processes. Four nanoparticle geometries were tested on both, n-type and p-type GaN surfaces. All samples were measured at room temperature under vacuum and at 200°C, under oxygen, under hydrogen, under hydrogen/ethene (reaction gas, mixture 10:1), and in vacuum after gas exposure. Generally, the nanoparticles exhibited three Pt species, with varying relative intensities, depending on the nanoparticle geometry and substrate doping. From the presented results, we conclude a strong substrate-nanoparticle interaction, which depends on the GaN doping and band bending, as well as on the generation of electron-hole pairs under intense synchrotron illumination.

O 31.4 Tue 12:00 WIL C107

Dimensional Nanometrology with Grazing Incidence Small Angle X-ray Scattering (GISAXS) — •Jan Wernecke, Michael Krumrey, Levent Cibik, Stefanie Marggraf, and Peter Müller — Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, 10587 Berlin

Reliable methods for dimensional characterisation of structures in the nanometer range are now a necessity in many fields of industry and science, e.g. for next-generation EUV lithography, new photovoltaic devices or magnetic nanoparticles. The method we have chosen for measurements of statistically averaged structural properties of nanostructured surfaces is GISAXS. This is a versatile technique to probe statistic properties such as mean particle size, spacial distribution and roughness of nanostructured surfaces and nanoparticle assemblies on top of or buried in bulk material. The GISAXS experiments were performed at the Four-Crystal Monochromator (FCM) beamline in the laboratory of PTB at BESSY II using the SAXS setup of the Helmholtz-Zentrum Berlin (HZB). This presentation will give a short overview of the instrumentation and the capabilities of the laboratory to perform dimensional nanometrology with GISAXS and will show first experimental results. Gratings for EUV lithography have been investigated in terms of coating layer thickness, roughness, grating period and blaze angle. Furthermore, dimensional properties of Au nanoparticles on silicon substrate were determined. The obtained particle sizes were in good agreement with SAXS measurements of these particles in liquid suspension.

O 31.5 Tue 12:15 WIL C107

Röntgenbeugungsuntersuchung von Ir-Nanopartikeln auf einer Graphen/Ir(111) Oberfläche — •Dirk Franz[1], Stefan Schumacher[2], Miguel Mantilla[3], Carsten Busse[2], Thomas Michely[2] und Andreas Stierle[1] — [1]AG Grenzflächen, Universität Siegen, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Germany — [3]MPI für Metallforschung Stuttgart, Germany

Eine Graphen/Ir(111) Oberfläche kann als Templat für den Wachstumsprozess von Iridium-Nanopartikeln genutzt werden, um diese in einer geordneten, regelmäßigen Weise anzuordnen [1]. Mittels chemischer Gasphasenabscheidung wurde Graphen auf einer Iridium (111) Oberfläche unter Ultrahochvakuumbedingungen aufgewachsen und in eine mobile UHV-Kammer für Röntgenbeugungsuntersuchung und Oberflächenpräparation transferiert. Die Ausbildung von Ir Nanopartikeln wurde während des Aufdampfens von Iridium in-situ durch Oberflächen Röntgenbeugung und Röntgenreflektionsmessungen an der Angstrom Quelle Karlsruhe (ANKA) charakterisiert. Die Messungen erlauben direkte Rückschlüsse auf die Orientierung, Größe und Form der Nanopartikel.

[1]: A. T. N'Diaye, S. Bleikamp, P. J. Feibelman und T. Michely, Phys. Rev. Lett. **97**, 215501 (2006)

O 31.6 Tue 12:30 WIL C107

Fabrication of plasmonic nanostructures for efficiency enhancement of silicon solar cells — •Stefan Griesing, Andreas Englisch, Uwe Schmitt, and Uwe Hartmann — Inst. of Experimental Physiks, Saarland University, P.O. Box 151150, 66041 Saarbrücken

Plasmonic scatterers cause an increase of the light-conversion efficiency of silicon solar cells due to the extended light path. Especially nanostructures with a diameter of more than 100nm scatter a large fraction of the incoming irradiation in the wavelength regime of 550nm to 1050nm. A technical challenge is the fabrication of large homogeneous areas of plasmonic nanostructures with a narrow size distribution. We report an approach in which this is realized by sputtering or thermal evaporation of silver thin films (5- 20nm thickness) and subsequent vacuum annealing. SEM images show that size, shape and density of the particles are dependent on the annealing temperature and the mass thickness of the deposited layer. In addition, in-situ SEM measurements of the annealing process will be presented.

O 31.7 Tue 12:45 WIL C107

O2 and CO on noble metal clusters on C/W(110) templates — •Magdalena Bachmann, Norbert Memmel, and Erminald Bertel — Institute for Physical Chemistry, University of Innsbruck, Austria

Small noble-metal (especially Au) clusters on oxidic supports have gained a lot of attention in the last years due to their high activity and selectivity as catalysts for CO oxidation reaction. The importance of cluster-size effects and influence of the substrate material are still discussed controversially. We introduce two differently carburized W(110) surfaces (i.e. R(15x12)C/W(110) and R(15x3)C/W(110)) as templates for the growth of two different types of Au, Ag and Cu nanoclusters. Investigation of the adsorption properties of the reactants CO and O2 on these surfaces might yield illuminative results concerning the Au-catalyzed CO oxidation. In a first step towards this goal the influence of the reaction gases on the stability of the nano-clusters was investigated by scanning tunnelling microscopy. Differences and similarities concerning gas induced alterations on different types of clusters are discussed.

O 31.8 Tue 13:00 WIL C107

Physical and chemical properties of small supported coinage metal clusters — •Martin Amft[1], Natalia Skorodumova[1], Olle Eriksson[1], Sébastien Lebègue[2], and Biplab Sanyal[1] — [1]Department of Physics and Astronomy, Uppsala University, Box 516, S-751 20 Uppsala, Sweden — [2]Laboratoire de Cristallographie, Résonance Magnétique et Modélisations (CRM2, UMR CNRS 7036) Institut Jean Barriol, Nancy Université BP 239, Boulevard des Aiguillettes 54506 Vandoeuvre-lès-Nancy,France

We investigate, by means of ab-initio density functional theory calculations, the adsorption and catalytic activity of supported small coinage metal clusters.

Our focus lies on cluster-size effects, the influence of different support materials, e.g. metal oxides and graphene, mobility of the deposited clusters, and the co-adsorption of additional molecule species. In the case of adsorption on graphene, we especially account for van der Waals interactions by the vdW-DF and the PBE+D2 methods, and study the mobility and initial clustering processes of gold on this material.

In the case of metal oxide supports, we explain the experimentally found catalytic characteristics of Au_{1-4}/MgO(100) by studying their ability to (co-) adsorb CO and O_2 molecules and address the question whether the presence of H_2O influences the catalytic activity of small gold clusters on MgO towards CO oxidation.

O 32: Spin-Orbit Interaction at Surfaces II

Time: Tuesday 11:15–12:45 Location: WIL C307

O 32.1 Tue 11:15 WIL C307

Spin-orbit split occupied and unoccupied surface states of Bi alloys on Cu(111) and Ag(111) — •A. Akin Ünal[1], Christian Tusche[1], Francesco Bisio[2], Aimo Winkelmann[1], and Jürgen Kirschner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]CNR-SPIN, Corso Perrone 24, I-16152 Genova, Italy

We investigated the electronic band structure of Bi surface alloys on Cu(111) and Ag(111) surfaces by one- and two-photon photoemission experiments (1PPE and 2PPE) excited by the second and fourth harmonics of a mode-locked Ti:sapphire femtosecond oscillator with photon energies of 3.1 eV and 6.0 eV. Occupied and unoccupied states can be respectively probed by 1PPE and 2PPE, providing comprehensive information on the electronic band structures. The negative electronic dispersions and Rashba-splittings of the partially-filled sp_z and of the unoccupied p_xp_y surface states were measured using our momentum microscope, which directly maps the parallel momentum component k_x, k_y of the photoelectrons as a function of energy without the need for sample or detector rotation. 1PPE experiments show that in the $\sqrt{3}\times\sqrt{3}$-R30° Bi/Cu(111) system, the Fermi level is below the crossing point of the spin-split sp_z bands; however, in the case of Bi/Ag(111), the Fermi level lies above this crossing point. The 2PPE experiments, on the other hand, show the spin-splittings of the unoccupied p_xp_y states of both systems in the momentum space.

O 32.2 Tue 11:30 WIL C307

Spin-orbit interaction in magnetic quantum well states of Ni/W(110) — •Andreas Nuber[1], Hendrik Bentmann[1], and Friedrich Reinert[1,2] — [1]Experimentelle Physik VII, Universität Würzburg, Germany — [2]Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany

Nickel is a model system for ferromagnetism with an exchange splitting of the minority and majority bulk band structure of approximately 0.3 eV. Growing thin films of Nickel on a W(110) substrate results in the formation of quantum well states (QWS) within the film. Due to the non-perfect confinement, the wave function of the QWS extend into the first monolayers of the tungsten substrate leading to an interaction with the large potential gradient of the W atoms. We present a high resolution ARUPS study of the electronic structure of thin Nickel films on W(110) which is influenced by the spin-orbit interaction mediated by the substrate and the exchange interaction of Nickel.

O 32.3 Tue 11:45 WIL C307

The Rashba-Bychkov model in a simple *sp*-band tight binding framework — •Christian R. Ast, Isabella Gierz, and Klaus Kern — MPI für Festkörperforschung, Stuttgart

The Rashba-Bychkov model has been remarkably successful in describing the lifted spin-degeneracy of two-dimensional states at surfaces and interfaces. A more detailed description has been given by Petersen and Hedegård with a *p*-band tight-binding model accounting for the atomic spin-orbit coupling as well as an asymmetric orbital overlap resulting from the potential gradient perpendicular to the surface [1]. Here, we present an extension of this model by including other orbitals. In this way, contributions of the potential gradient originating from within an atom as well as from neighboring atoms become evident. The results will be applied to the model system graphene.

[1] L. Petersen and P. Hedegård, Surf. Sci. **459**, 49 (2000)

O 32.4 Tue 12:00 WIL C307

Visualizing spin-dependent scattering in strong spin-orbit systems — •Anna Strozecka[1], Asier Eiguren[2], and Jose Ignacio Pascual[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Dpto. Física de la Materia Condensada, Universidad del País Vasco, Bilbao, Spain

For surfaces which exhibit spin-orbit coupling, electrons originating from spin polarized surface bands are protected against backscattering by time reversal symmetry. Electron interference patterns observed in STM confirm the chiral spin texture of the surface Fermi contours of such materials and reveal the dominant role of spin in the scattering processes. Using a combined experimental and theoretical approach, we distinguish the role of spin in the electron scattering processes on Bi(110). By spectroscopic imaging of the local density of states in STM, we studied the energy dependence of the interference patterns formed around single adsorbates. Simulations based on Green‘s functions correctly reproduce the interference patterns, unveiling the role of spin in the interference process and allowing identification of the dominant scattering events.

O 32.5 Tue 12:15 WIL C307

Spin-resolved photoemission experiments of Rashba-split quantum-well electron states — •Sebastian Jakobs[1], Andreas Ruffing[1], Sabine Steil[1], Indranil Sarkar[1], Mirko Cinchetti[1], Stefan Mathias[1,2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]JILA and Department of Physics, University of Colorado, Boulder, CO 80309-0440, USA

The Rashba-Bychkov effect in a 2D electron gas, which originates from spin-orbit interaction and an asymmetric confinement of the electron gas, can produce spin-split energy bands in nonmagnetic materials without the need to apply any external magnetic field. The effect has been shown on various surfaces, and the resulting spin-split surface-state bands show a high spin polarization in the in-plane direction and perpendicular to the k-vector of the photoelectrons [1]. Recently, we reported on the observation of such a giant Rashba spin-orbit splitting of quantum-well state bands in the unoccupied electronic structure of a Bi monolayer on Cu(111) [2]. Due to an asymmetry in the alignment of the Bi-atoms in the incommensurate structure an additional out-of-plane spin component is to be expected. In this talk we will present first spin-dependent photoemission experiments on the one monolayer Bi/Cu(111) system, which confirm the expected out-of-plane spin component of the split quantum-well electron bands.

[1] J.H. Dil, J. Phys.: Condens. Matter 21, 403001 (2009)
[2] S. Mathias et al., Phys. Rev. Lett. 104, 066802 (2010)

O 32.6 Tue 12:30 WIL C307

Visualizing Electron Scattering near Step Edges in the Surface States of Bismuth (111) — •Christian Bobisch[1], Maren Cottin[1], Johannes Schaffert[1], Giriraj Jnawali[1], Gustav Bihlmayer[2], and Rolf Möller[1] — [1]Faculty of Physics, Center for Nanointegration Duisburg-Essen, University Duisburg-Essen, Lotharstr.1, 47048 Duisburg, Germany — [2]Institut für Festkörperforschung and Institute for Advanced Simulations, Forschungszentrum Jülich, 52425 Jülich, Germany

Recently, many studies focus on the group V element bismuth due to its rather unique physical properties. A thin and high quality epitaxial Bi(111) film of about 25 bilayers was grown on a Si(111)-7x7 substrate. Such a thin film can serve as a prototype system to study scattering in surface states with strong spin orbit splitting. We use a low temperature scanning tunneling microscope at cryogenic temperatures (80 K) to study the electronic surface structure in the vicinity of surface step edges, thus gaining insight into the electronic structure of the Bi film with high precision and lateral resolution. In dI/dV images of a surface area including surface steps, the scattering of propagating electrons is visualized by a wave like pattern. Moreover, the Fourier transform analysis of these dI/dV maps at various voltages, i.e. various energies, reveals the spectrum of scattering vectors of electrons impinging on the surface steps.

O 33: Invited Talk (Katharina J. Franke)

Time: Tuesday 14:00–14:45 Location: TRE Phy

Invited Talk O 33.1 Tue 14:00 TRE Phy

Competition of magnetic excitations on a superconducting surface — •Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin, Germany

On normal metal surfaces the magnetic moment of an atom or molecule can be screened by the itinerant electrons as described by the Kondo effect. On a superconductor, the opening of an energy gap at the Fermi level may lead to a significant reduction of the screening, leaving a net magnetic moment to interact with the Cooper pairs. As a result the pairing energy of the Cooper pairs is reduced and spin-polarized bound states appear in the vicinity of a magnetic impurity.

Using scanning tunneling spectroscopy we explore the different magnetic excitations of metal-phthalocyanine molecules on a superconducting Pb(111) surface. The delicate balance between Kondo screening and superconducting pairing leads to quantum ground states with different magnetic properties.

O 34: Invited Talk (Andre Schirmeisen)

Time: Tuesday 14:45–15:30 Location: TRE Phy

Invited Talk O 34.1 Tue 14:45 TRE Phy

A Bottom-up View of Sliding Friction: From Hopping Atoms to Superlubric Nanoparticles — •Andre Schirmeisen — Institute of Physics and Center for Nanotechnology (CeNTech), University of Muenster, Germany

Frictional motion plays a central role in diverse systems and phenomena that span vast ranges of scales, from the nanometer contacts in micromachines up to the geophysical scales of earthquakes. Despite the practical and fundamental importance of friction little progress has been made in finding an exact atomistic description. The advent of new experimental tools such as the friction force microscope enabled the investigation of frictional forces occurring on microscopic scales.

Our experiments show that at the molecular level friction is intimately connected to thermal activation of atomic jumps [1]. However, for slightly larger contact sizes, we found evidence for an inverse thermal activation effect, which is due to contact formation processes at the sliding interface [2]. Finally, by using the method of controlled nanoparticle manipulation, we reveal that metal particles can even coexist in two frictional states, exhibiting 'frictional duality': Some particles show linear scaling with contact area while others assume a state of virtually frictionless sliding [3]. This superlubricity phenomenon is based on the interlocking of interface atoms, exhibiting a characteristic sub-linear scaling of friction with contact area.

[1] Jansen et al., Phys. Rev. Lett. 104 (2010) 256101
[2] Barel et al., Phys. Rev. Lett. 104 (2010) 066104
[3] Dietzel et al., Phys. Rev. Lett. 101, 125505 (2008)

O 35: Poster Session I (Scanning probe methods)

Time: Tuesday 18:30–22:00 Location: P3

O 35.1 Tue 18:30 P3

Measurement of the interactions between two molecules with NC-AFM — •Martina Corso, Christian Lotze, and Jose Ignacio Pascual — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Non-contact atomic force microscopy (NC-AFM), operated in frequency modulation mode, has been recently the subject of extraordinary advances. One of its most striking achievement resides on its capability to resolve the chemical structure of molecules with unprecedented atomic resolution [1]. Such measurements are possible by detecting short-range bonding interactions between the foremost atom of a tip at the end of a cantilever and the atoms at the surface. In order to minimize contributions from van der Waals and electrostatic interactions, sharp STM tips are used. With our STM/AFM based in a qPlus sensor design operated at 5K we use CO modified STM tips to quantify the forces involved during imaging and manipulation of small (as CO) and large molecules (as DPBP) adsorbed on a Cu(111) surface. In particular we investigate with force spectroscopy site specific interactions between a CO-tip and C_2H_2 molecules. Short-range interaction force curves suggest that a local bond between two species might be formed. [1] L. Gross, F. Mohn, N. Moll, P. Liljeroth, G. Meyer, *Science* **325**, 1110 (2009).

O 35.2 Tue 18:30 P3

Electronic regulation in the etching process for STM-tips — •Volkmar Hess, Wolfgang Rosellen, and Mathias Getzlaff — Institute of Applied Physics,University Duesseldorf

The scanning tunneling microscope (STM) became one of the most important instruments for the surface science community because it enables the imaging with atomic resolution. The probe tip itself has crucial influence on the success of STM experiments. There are many routes to produce tips such as etching or cutting. In this contribution we report on the set up of an electronic circuit which should improve the quality and the reproducibility of etched tips. This should be archieved by immediate cut off the etching current after the tip dropped off. Former experiments showed a clear relation between cut-off time and tip radius. The functional properties of the electronic circuit were characterized by means of an analog-digital-converter. Furthermore, the influence of other parameters like etching potential and different etching solutions on the shape of tips were analyzed. Subsequently the tips were characterized with an optical microscope and a scanning electron microscope and compared to commercially offered tips.

O 35.3 Tue 18:30 P3

Developing a miniaturised device for in-situ STM tip cleaning using electron bombardment — •David Hellmann[1], Ludwig Worbes[1], and Achim Kittel[2] — [1]EHF, Fak. V, Physik, Carl von Ossietzky Universität Oldenburg — [2]Experimental Polymer Physics, Faculty of Mathematics and Physics, University of Freiburg, 79104 Freiburg

Most SPM techniques rely on the assumption that both sample and tip are free from adsorbates and other residues. Getting a clean sample surface can be readily accomplished by applying ion sputtering, whereas finding an adequate treatment for tips is much more complicated. In principle one wants to desorb any molecules which might interfere with the anticipated measurement. This must be achieved without reducing the sharpness or the general geometry of the tip. Several devices are described in the literature which employ accelerated electrons to do this [1]. When such a procedure is applied in a variable temperature SPM, one has to keep the duration of any treatment as short as possible to avoid thermal drifts. To achieve this, we constructed an electron source which can be put into the sample holder while the tip stays in place. In our case, a tiny thermocouple is incorporated at the foremost tipapex, designed to perform measurements of the heat flow between a cooled or heated sample and the tip [2]. By means of these tips a direct measurement of the tip temperature during electron sputtering is possible. Literature: [1] S. Ernst et al., Science and Technology of Advanced Materials 8 (2007) [2] U. F. Wischnath, J. Welker, M. Munzel, A. Kittel, Review of Scientific Instruments 79 (2008)

O 35.4 Tue 18:30 P3

A sub-Kelvin facility for cross-sectional scanning tunneling spectroscopy of metal-semiconductor heterostructures — •Peter Löptien, Focko Meier, Lihui Zhou, Jens Wiebe, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Germany

We investigate III-V semiconductors with magnetic dopants by spin-resolved scanning tunneling spectroscopy in order to achieve an atomic-scale understanding of magnetism in these systems [1, 2]. The method of choice for *ex-situ* grown heterostructures is cross-sectional scanning tunneling microscopy which enables to study their bulk properties by looking at nonpolar surfaces prepared by cleavage under ultra high vacuum conditions [3]. For these experiments we have planned and constructed a low-temperature scanning tunneling microscopy facility with the possibility to move the sample laterally. The main chamber being commercially available consists of a Joule-Thomson cryostat with a scanning tunneling microscope. It has a base temperature of less than 1 K using ^{4}He. There are two additional home built vacuum chambers for *in-situ* sample and tip preparation. These chambers include several electron beam evaporators, a customized sample heating manipulator, an electron beam heater and a sputter gun. The whole system is attached to a frame and supported by passive air damping legs. We will show first test measurements.

[1] F. Meier *et al.*, Science **320**, 82 (2008)
[2] A. A. Khajetoorians *et al.*, Nature **467**, 1084 (2010)
[3] M. Bertelli, P. Löptien *et al.*, Phys. Rev. B **80**, 115324 (2009)

O 35.5 Tue 18:30 P3

Design of a low-temperature scanning tunneling microscope with integrated lenses for in-situ optical access — •Jens Kügel, Paolo Sessi, and Matthias Bode — Institute of Experimental Physics II, University Würzburg, Am Hubland, 97074 Würzburg

While Scanning Tunneling Microscopy (STM) is a well-estabilished technique to gain information on surfaces topography and density of states on the atomic scale, its time resolution ist still rather limited. Under open loop conditions, values down to the nanoseconds regime have been recently reported [1]. This limitation can be overcome by laser spectroscopy which offers a time resolution down to a few attoseconds [2]. Here we present a low-temperature STM design able to combine these two experimental techniques. Besides standard STM features such as tip coarse movement and sample-nanopositioning, it includes lense holders for focused back and front side laser illumination. Potential measurement modes aimed, e.g., for the spatio-temporal investigation of excited molecular states, will be discussed.

[1] S. Loth *et al.*, Science 329, 5999 (2010)
[2] M. Schultze *et al.*, Science 328, 1658 (2010)

O 35.6 Tue 18:30 P3

Combined scanning tunneling and atomic force microscopy at low temperatures — •Tobias Herden[1], Markus Ternes[1], and Klaus Kern[1,2] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Institut de Physique des Nanostructures, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Quartz tuning forks have an interesting history in the evolution of scanning probe microscopy. Edwards et al. [1] were the first to use them with a tip glued to one prong as AFM sensor. In 1998 Giessibl [2] introduced a technique (qPlus) where the tuning fork is excited externally and a conducting tip is used allowing for simultaneous AFM and STM measurements. The capabilities of this design have been demonstrated by a broad variety of measurements: from quantitative forces measurements when an atom or molecule is moved over a surface [3] to sub-molecular resolution of pentacene by Gross et al. [4].

This type of sensor was implemented in a newly built STM head. It is designed to operate in UHV in a Joule-Thomson cryostat, at temperatures below 1 Kelvin and in magnetic fields up to 14 Tesla. The head was extensively tested at ambient conditions and in moderate vacuum and first measurements at low temperatures will be presented. The focus will be on the design, especially the mounting and contacting of the tuning fork.

[1] H. Edwards et. al, J. Appl. Phys. 82, 980 (1997) - [2] F. J. Giessibl, Appl. Phys. Lett. 73, 3956 (1998) - [3] M. Ternes et.al, Science 319, 1066 (2008) - [4] L. Gross et. al, Science 325, 1110 (2009)

O 35.7 Tue 18:30 P3

Development of a nanoscale scanning-probe magnetometer with single spin sensitivity — •Eike Oliver Schäfer-Nolte[1,2], Friedemann Reinhard[2], Markus Ternes[1], Fedor Jelezko[2], Jörg Wrachtrup[2], and Klaus Kern[1] — [1]Max-Planck Institut für Festkörperforschung, Stuttgart, Germany — [2]3. Physikalisches Institut, Universität Stuttgart, Germany

The detection of weak magnetic fields at small length scales is a long-standing challenge in physics. We report on our work constructing a scanning-probe magnetometer capable to measure small magnetic fields and single spins with sub-nanometer spatial resolution.

This experiment employs a nitrogen-vacancy (NV) center in diamond as an ultrasensitive magnetic field sensor. Its spin state can be monitored using optically detected magnetic resonance [1]. Attaching a nanodiamond containing this "probe spin" to the tip of an atomic force microscope (AFM) working in ultra-high vacuum at low temperature allows studies of magnetic fields at the atomic scale [2,3]. The details of the experimental setup are presented along with experimental data characterizing the individual components.

[1] F. Jelezko et al., phys. stat. sol. (a) 203, No 13 (2006)
[2] G. Balasubramanian et al., nature Vol 455 (2008)
[3] J.M. Taylor et al., nature physics Vol 4 (2008)

O 35.8 Tue 18:30 P3

Electromigration on Ag-nanowires studied down to the atomic scale — •Mark Kaspers, Alexander Bernhart, Christian Bobisch, and Rolf Möller — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

Energy dissipation due to electronic stressing can result in diffusion of material at surfaces. If the biased motion of atoms is induced by a current flow (wind force) or an applied electric field (direct force) this is referred to as electromigration. We present *in situ* measurements of electromigration, potentiometry and topography of monocrystalline Ag-nanowires grown on vicinal Si(001) substrates. We use an UHV multiprobe scanning tunneling microscope (STM) including different scanning probe techniques and a scanning electron microscope (SEM). Two STM-tips of the multiprobe system are used to contact the nanowire. The positioning of the tips is monitored by SEM. This setup allows to control and monitor electromigration processes on the nanowire's surface down to the atomic scale by video SEM and STM, thus revealing the evolution of the surface morphology, i.e. step edge diffusion, during electrical stressing [1].

[1] M.R. Kaspers et al., J. Phys.: Condens. Matter **21**, 265601 (2009)

O 35.9 Tue 18:30 P3

Probing the thermal near-field of thin Fe-Layers on Au(111) by NSThM

— •Ludwig Worbes[1], David Hellmann[1], and Achim Kittel[2] — [1]EHF, Fak. V, Physik, Carl von Ossietzky Universität Oldenburg, — [2]Experimental Polymer Physics, Faculty of Mathematics and Physics, University of Freiburg, 79104 Freiburg

The evaporation of a few monolayers of Fe on top of Au(111) surfaces is known to produce nano-meter sized Fe-islands which are found at specific locations of the herringbone surface-reconstruction.

We investigate the thermal near field of these surfaces by Near-field Scanning Thermal Microscopy (NSThM). The NSThM developed in our group is based on a STM, featuring a tunnelling probe with an integrated miniaturized thermocouple temperature sensor located about 500nm behind the tunnelling gap. Therefore, we can measure the temperature change of the tip due to heat flux between a heated or cooled sample and the probe at distances of a few nanometres, mediated by thermal near fields [1]. Thermal near-field (evanescent) modes, exponentially decaying with distance to the surface, surround every body with a finite temperature. They are generated by thermally fluctuating charges, analogously to the electromagnetic far field described by Stefan-Boltzman law.

In our experiments, we observe characteristic distributions of the heat flux by thermal near-fields. That is an enhanced heat transfer at the edges of the Fe-islands due to edge enhancement effects, already known in the realm of visible light optics.

[1] Achim Kittel et al., Appl. Phys. Lett. 93, 193109 (2008)

O 35.10 Tue 18:30 P3

A combined STM / FIM for tip specific tunnelling experiments

— •Ben Wortmann and Rolf Möller — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

We present details on a homebuilt, compact, low temperature scanning tunnelling microscope that allows insitu field ion microscopy of a cooled tunnelling tip inside the STM. Therefore a characterization of the tip is possible without transfer to a different position in the UHV system. This guarantees that the tip characterized by FIM is identical to the one used for the STM experiment. The geometry of the microscope resembles a cylinder with a height of only 13 cm and a diameter of 4 cm. Shutters at the bottom of the microscope can be opened to expose the tip to a channel plate or closed to assure even lower temperatures and minimal thermal drift while tunnelling. A combination of two piezo-electric accentuators is used to move a magnetically attached unit (*slider*) by a slip-stick motion. The tip is spot welded to the slider which can be easily exchanged in vacuum. The STM is screwed directly onto a commercially available continuous flow cryostat which allows cooling to about 5-7 K. Insulation from vibration is provided by a combination of springs and eddy current damping. Sister systems already show the performance of the STM setup[1]. The very compact design minimises helium consumption to about 1 liter/hour. [1] (H. Karacuban, M. Lange, J. Schaffert, O. Weingart, Th. Wagner and R. Möller, Surf. Sci. Lett., 603, Issue 5, L39 (2009).

O 35.11 Tue 18:30 P3

Nanoscale mapping of ion dynamics in solid electrolytes by time and space resolved electrostatic force spectroscopy

— •Marvin Stiefermann[1], Dirk Dietzel[1], Bernhard Roling[2], and Andre Schirmeisen[1] — [1]Institute of Physics and Center for Nanotechnology (CeNTech), University of Muenster, Germany — [2]Department of Chemistry, Philipps-University Marburg, Germany

For many technological applications, such as batteries or fuel cells, materials with good ionic transport parameters are of paramount importance. Recently, the search for improved ion conducting materials has lead to nanostructured materials, where the transport properties are often determined by interaction of different phases (e.g. crystalline and amorphous) and their interfaces. In this context an improved understanding of the local nanoscale transport properties is important to further optimize the performance of such ion-conducting materials. However, classical analysis techniques, such as conductivity spectroscopy, are not suitable to directly extract nanoscale information. In this contribution we will therefore demonstrate how ionic transport properties can be mapped by Atomic Force Microscopy based electrostatic force spectroscopy [1]. By systematic temperature dependent grid spectroscopy different ion relaxation channels can be identified and correlated with the structure of a Lithium ion conducting glass ceramics (LIC-GC by Ohara cooperation). Special attention is focused on the influence of grain boundaries, which are suspected to act as a bottleneck for the macroscopic ion conduction.

[1] Schirmeisen and Roling, Chemical Monthly 140, 1103 (2009)

O 35.12 Tue 18:30 P3

Nano scale mechanical characterization of surfaces

— •Alexander Malwin Jakob and S.G. Mayr — Leibniz-Institut fuer Oberflaechenmodifizierung, Translationszentrum fuer Regenerative Medizin und Fakultaet fuer Physik und Geowissenschaften der Universitaet Leipzig, 04318 Leipzig

With proceeding miniaturization in science and technology, mechanical properties at the nano scale have attracted increased interest during the past years. Although commercial nano indenters are widely available at this point, they usually probe the micro scale rather than measuring nano-mechanical properties. For real nanometer resolved mechanical characterization, atomic force microscope (AFM) based techniques like contact resonance force microscopy (CR-FM) are highly promising, as first proposed by Rabe and Arnold [1] as well as Yamanaka [2]. While our first setup employed a hardware realization of this technique [3], the present contribution deals with a purely software based implementation of CR-FM into a commercial AFM. Capabilities and limitations for exemplary surfaces are presented. The experimental studies are supplemented by finite element modeling of the cantilever-sample interaction.

This project is funded by the German BMBF, PTJ-BIO, Grant Number: 0313909.

[1] Rabe U., Arnold W., Appl. Phys. Lett. Vol.64, P1493-1495 (1994)
[2] Yamanaka K., Ogiso H., Kolosov O., Appl. Phys. Lett., Vol.64, P178-180 (1994)
[3] C. Vree, Dissertation, Göttingen (2009)

O 35.13 Tue 18:30 P3

Local surface spectroscopy with STHM junction

— •Georgy Kichin, Christian Weiss, Christian Wagner, Stefan Tautz, and Ruslan Temirov — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich and JARA-Fundamentals of Future Information Technology

Scanning tunneling hydrogen microscopy (STHM) is a new imaging regime in which a low temperature (5-10K) STM can be operated when $H_2(D_2)$ is adsorbed in the junction [1]. The imaging mechanism of the STHM has recently been identified: H_2 or D_2 confined between the tip and the surface plays a dual role of the sensor and transducer. The sensor samples interaction with the surface and translates this interaction into variations of the Pauli repulsion between the gas molecules and the tip. The transducer converts the changing Pauli repulsion into variations of the tip's density of states (DOS), which is finally recorded as laterally varying junction conductance [2,3]. In this contribution we study inelastic electron tunneling spectra of the STHM junction. The inelastic tunneling data suggest that the junction has a rich excitation spectrum. Moreover, characteristic energies of the observed excitations show a strong dependence on such parameters as the gas coverage, tip-surface distance and the local surface structure.

[1] R. Temirov et al. New J. Phys. 2008, 10, 053012 [2] C. Weiss et al. Phys. Rev. Lett. 2010, 105, 086103 [3] C. Weiss et al. J. Am. Chem. Soc. 2010, 132, 11865

O 35.14 Tue 18:30 P3

A low-noise STM equipped with a cryogenic transimpedance amplifier

— •Martin Kunz and Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, 98693 Ilmenau, Germany

We present the current status of a home-built scanning tunnelling microscope (STM) designed to be operated inside a helium cryostat at 4.2 K in an ultrahigh vacuum. The influence of electromagnetic interference on the tunnelling signal, which is a serious noise source in tunnelling experiments, is minimized by placing a transimpedance amplifier in close vicinity to the tunnelling probe. This custom-built amplifier has a bandwidth from DC to 100 kHz. It is thermally coupled to the cryostat and can be deployed at temperatures ranging from liquid helium to room temperature. In particular, at low temperatures the signal degradation due to Johnson noise is significantly smaller than in conventional STM setups that employ transimpedance amplifiers operated at room temperature. The microscope is primarily intended for spin-resolved spectroscopic investigations of electronic and vibrational excitations.

O 35.15 Tue 18:30 P3

Near-field heat transfer of alkanethiol on flat gold surfaces — •Christian Olling[1], Ludwig Worbes[1], David Hellmann[1], and Achim Kittel[1,2] — [1]Energy and Semiconductor Research Laboratory, Institute of Physics, University of Oldenburg, 26129 Oldenburg, Germany — [2]Experimental Polymer Physics, Faculty of Mathematics and Physics, University of Freiburg, 79104 Freiburg, Germany

In this contribution we discuss the heat transport through a molecular layer on a heated or cooled surface. As molecules we have chosen alkanethiol because it is well known that alkanethiols form self-organized monolayers on flat gold surfaces. The measurements are performed with a near-field scanning thermal microscope (NSThM) which was developed by our group. A coaxial micro thermocouple serves as tip of a commercial variable temperature UHV-STM is able to measure the heat flux through the molecular layer without any interfering heat conduction by a surrounding gas. Hence, the microscope can be operated in NSThM and STM mode at the same time. Changes in the heat transfer are investigated by retracting the tip from the surface and the heat transfer of the bare gold surface. Furthermore, surface roughness and morphology influence the heat transfer on the nanometer scale. This is investigated by scanning over the surface and mapping the heat transfer.

O 35.16 Tue 18:30 P3

Design of a low temperature four-tip Scanning Tunneling Microscope — •Hubertus Junker, Vasily Cherepanov, Peter Coenen, Helmut Stollwerk, and Bert Voigtländer — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology

The design of a low temperature ultra high vacuum (UHV) 4-tip Scanning Tunneling Microscope (STM) capable of charge and magneto transport measurements is presented. Four individual beetle-type STM units are stacked into each other in order to make the design as compact as possible. For the coarse approach of the tip towards the sample a new developed ultra compact nonpositioner which has a diameter of less than 3 mm is used. This multi tip STM is located inside the UHV part of a liquid Helium cryostat, which additionally hosts a 8 T superconducting magnet. In order to navigate the four tips a SEM is installed. The scanning areas on the sample overlap sufficiently in order to contact nanostructures with all four tips at the same time and execute transport measurements. To isolate the experiment from external vibrations, the chamber is located in a specially designed room. This room is sound protected and its 100 t concrete base plate rests on four air damping feet with a resonance frequency of 0.7 Hz. During tunneling, the experiment is controlled from the outside.

O 35.17 Tue 18:30 P3

Investigation of an operating resonant tunneling device by scanning tunneling spectroscopy — •Karen Teichmann[1], Martin Wenderoth[1], Rainer G. Ulbrich[1], Klaus Pierz[2], and Hans W. Schumacher[2] — [1]IV. Physikalisches Institut, Georg-August Universität Göttingen — [2]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig

A resonant tunneling diode structure in a three terminal setup was investigated by Cross-Sectional Scanning Tunneling Microscopy (STM) and Spectroscopy. We use a home built low temperature STM working under UHV conditions at 5 K, which allows applying a lateral voltage to the sample in addition to the usual tip-sample voltage. The diode structure was grown by molecular-beam epitaxy on a n$^+$-doped GaAs (100) substrate and consists of self-assembled InAs quantum dots embedded in AlAs barriers (4 nm) each followed by undoped GaAs prelayers (15 nm) [1]. The samples are cleaved in UHV to obtain a clean and atomically flat (110) surface perpendicular to the diode-structure. *I(V)* spectroscopy measurements were done with different applied lateral voltages. The shift of the valence band offset can clearly be seen. Differential conductivity peaks are visible to the left and right of the heterostructure and are explained by tip induced states. The shift of these states with lateral voltage can give insight in the tip induced band bending, which is known to be prominent on the GaAs (110) surface [2]. We acknowledge financial support by the DFG SPP 1285.

[1] I. Hapke-Wurst, *et al.*, App. Phys. Lett. **82**, 1209 (2003)
[2] R.M. Feenstra, *et al.*, J. Vac. Sci. Technol. B **5**, 923 (1987)

O 35.18 Tue 18:30 P3

Facts and artefacts in scattering scanning near-field optical microscopy. — •Anja Krysztofinski[1], Marc Tobias Wenzel[1], Rainer Jacob[2], Hans-Georg von Ribbeck[1], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, TU Dresden, 01062 Dresden, Germany — [2]Institut für Ionenstrahlphysik und Materialforschung, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), 01314 Dresden, Germany

Scattering scanning near-field optical microscopy (s-SNOM) is a versatile tool for optically probing nanoscale systems in the visible and infrared wavelength range. In our setup, we used a He-Ne Laser with a wavelength of 633 nm for measurements in the visible and a CO2-Laser of 10.6 μm in the infrared range. To avoid misinterpretation of s-SNOM measurements, it is important to consider several kinds of artefacts that can affect the optical signal. Here, we present and classify the main types of artefacts that occur in s-SNOM measurements. Furthermore, artefacts are first theoretically described and then experimentally demonstrated. We focus on effects such as background scattering, geometrical topography artefacts, and feedback controller-induced effects. In addition, we will also present results on polarization effects and most importantly, optical contrast reversal as occurring for small nanoparticles. An important benefit of our set-up is the possibility to essentially avoid all such artefacts in order to obtain completely artefact-free results. For this purpose, we use higher harmonic demodulation, heterodyne interferometry and phase-locked-loop-based true-non-contact measurements in our s-SNOM set-up.

O 35.19 Tue 18:30 P3

Preparation and characterization of metal coated STM tips — •Sergej Burbach, Martin Wenderoth, Bernhand Spicher, and Rainer G. Ulbrich — IV. Physikalisches Institut, Georg-August Univ. Göttingen, Germany

We present an in situ preparation technique to produce scanning tunnelling microscopy tips coated with different metals and with a high reproducibility. This approach allows to vary the workfunction of STM tips or to prepare probes suitable for spin polarized STM. Based on a movable UHV chamber working at a base pressure of $(1 \cdot 10^{-10}$ mbar) the prepared tips can be transferred directly into the STM without breaking the vacuum.

As a starting point we use electrochemically etched tungsten tips with a radius of a few nanometer. After heating and sputtering the tips in UHV, thin metal films (e.g. Fe, Ag) are deposited using an electron beam evaporator. Monolayer thickness control is implemented using a quartz balance. To control the different steps of the tip preparation (heating, sputtering, deposition) the set-up allows in situ characterization using field emission. A quick switching between preparation and characterization is possible and leads to a high yield of atomically resolving tips. The different steps of the preparation have been controlled by ex situ scanning electron microscopy. This project is supported by SPP 1285.

O 35.20 Tue 18:30 P3

Scanning Force Microscopy up to the Millimeter Scale — Alexander Förste[1,2], •Markus Moosmann[1,2], Manuel Rothenberger[1,2], Tobias Meier[1,2], Roland Gröger[1,2], Matthias Barczewski[1,2], Stefan Walheim[1,2], and Thomas Schimmel[1,2] — [1]Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT) Campus North — [2]Institute of Applied Physics and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT) Campus South

Using a novel Scanning Force Microscope (SFM) allowing the so far largest scan range achieved (800 μm x 800 μm), surface topography and properties as well as surface processes were studied in a wide range of length scales from the nanometer scale to the sub-millimeter scale. The resolution of single monolayer steps is demonstrated even at ultra-large scan ranges. As sample systems we investigated 1) structured ultrathin films made from self-assembled monolayers, 2) thin self-organized polymer blend films structured via phase separation and 3) strongly corrugated surfaces produced by embossing or UV lithography.

O 36: Poster Session II (Metals; Nanostructures at surfaces; Surface or interface magnetism; Spin-Orbit Interaction at Surfaces; Electron and spin dynamics; Surface dynamics; Methods; Theory and computation of electronic structure)

Time: Tuesday 18:30–22:00 Location: P4

O 36.1 Tue 18:30 P4

Electron pair emission from a Cu(111) surface — Rajendra S. Dhaka, •Frank O. Schumann, Grant A. van Riessen, Zheng Wei, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

We aim to explore the validity of an important assumption of the theoretical description of the (e,2e) process, namely an effective single electron description of the electronic properties of the sample. If affirmative the orbital character of the valence state can be identified and it would be of interest to find conditions where the emission is dominated by a particular valence state. In order to test the conjecture we selected a Cu(111) surface as sample which has a well-known electronic structure. We varied the primary energy in the range 19-65 eV. The sum energy spectra reveal features which can be directly related to the effective single particle band structure of the sample. This proves that for Cu an effective single particle picture is an adequate description within a (e,2e) experiment. The relative pair emission intensity from the surface state and 3*d* states is observed to vary dramatically with the primary energy. At low excitation energies the spectrum is dominated by the contribution from the Shockley surface state. We propose a simplified model based on the diffraction of pairs to explain this observation.

O 36.2 Tue 18:30 P4

Oxidation of Ruthenium Surfaces — •Marius Ernst[1,2], Thanh-Nam Nguyen[1], Sina Gusenleitner[1,2], Dirk Ehm[2], and Friedrich Reinert[1,3] — [1]University of Würzburg, Experimental Physics VII, Am Hubland, 97074 Würzburg, Germany — [2]Carl Zeiss SMT GmbH, Rudolf-Eber-Strasse 2, Oberkochen, Germany — [3]Karlsruhe Institute of Technology, Gemeinschafts Labor für Nano-Analytik, Germany

Multilayer mirrors for extreme ultraviolet (EUV) Lithography applications are threatened by various detoriation processes of the surface. During exposure, the dominating contamination processes are carbonization and oxidation due to adsorption of hydrocarbons and oxygen and their reaction with the mirror surface, reducing the mirror lifetime. One possibility to extent the lifetime is to coat the mirror with a dedicated capping material, such as Si, Ti, Mo, Pd, Ru, or their oxides. To study the influence of oxidative species (O2 and H2O), in this work Ru single crystals were used as model systems for real mirror capping layers. The (0001) surface of a Ru single crystal was exposed to oxidative environments with a total pressure ranging from 10 9 mbar to 10-4 mbar and analyzed with low energy electron diffraction (LEED), X-ray photoelectron spectroscopy (XPS) and ultra-violet photoelectron spectroscopy (UPS). Depending on pressure and exposure, different surface reconstructions could be found. At oxygen partial pressures higher than 10-4 mbar and sufficiently long oxygen exposure, bulk oxide formed, the thickness of which was analyzed with ellipsometry. The oxidation behaviour of single crystalline surfaces was compared with the oxidation of thin evaporated Ru layers.

O 36.3 Tue 18:30 P4

Scanning tunneling microscopy study of asymmetric Pd pincer complexes on a Cu(111) Surface — •Shih-Hsin Chang[1,4], Alessandro Scarfato[2,3], Christian Christian Kleeberg[3], Martin Bröring[3], Germar Hoffmann[1], and Roland Wiesendanger[1] — [1]Institute of Applied Physics and Microstructure Research Center Hamburg, University of Hamburg, Germany — [2]Dipartimento di Fisica E.R. Caianiello, Università degli Studi di Salerno, Italy — [3]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [4]Research Center for Applied Sciences, Academia Sinica, Taipei, Taiwan

The adsorption of asymmetric Pd pincer complexes on a Cu(111) surface was investigated by means of ultra-high vacuum scanning tunneling microscopy. The structural asymmetry is manifested in the observation of two chiral enantiomers. To enable an unambiguous identification of individual constituents, three closely related complexes with small modifications are investigated in parallel. Thereby, methyl substituents determine attractive molecule-molecule interaction. Depending on their distribution, dimerization and tetramerization can be observed.

O 36.4 Tue 18:30 P4

Self-Assembled Monolayers of Dimethyldiselenide on Au(111) — •Lydia El-Kareh, Axel Beimborn, Patrick Mehring, and Carsten Westphal — Experimentelle Physik I, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany

Self-assembled monolayers (SAMs) attract considerable attention due to their large potential in applications such as molecular electronics, tailoring of metallic surface properties and biological sensors. In recent years many studies of sulfur based SAMs have been performed. As the Se-Au bond is stronger than the S-Au bond selenium based SAMs are very interesting. In this study the structural formation of Dimethyldiselenide (DMDSe) monolayers on a Au(111) surface was investigated by scanning tunneling microscopy. SAMs were prepared by immersing the gold substrate in ethanolic solution of DMDSe. We report on the formation of a striped DMDSe phase at the surface and its thermal evolution upon heating. After annealing at 90°C the striped phase disappeared due to reorganization of molecules on the surface.

O 36.5 Tue 18:30 P4

Specific protein patterning in protein-repelling monomolecular matrix by UV promoted exchange reaction — •Jeyachandran Yekkoni[1], Andreas Terfort[2], and Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany. — [2]Institut für Anorganische und Analytische Chemie, Universität Frankfurt, Max-von-Laue-Straße 7, 60438 Frankfurt, Germany.

Oligo(ethylene glycol) (OEG) self assembled monolayers, well known for their protein resistance behaviour, could be used to produce protein patterns upon introduction of specific receptor groups by exchange reaction enabled by controlled degradation. We investigated the degradation of OEG monolayers using UV irradiation at 254, 312, and 366 nm to achieve well-controlled exchange reaction and protein patterning. OEG molecules with different lengths of the alkyl and OEG stems as well as with different tail groups (OCH3 or OH) were used to prepare monolayers on Au surface and biotinylated alkanethiol was used as a receptor for avidin or streptavidin. Experiments at zero dose showed that the OH terminated OEG monolayers with a sufficiently long alkyl linker and the EG chain (minimum 5 units) are stable towards non-specific receptor exchange reaction for at least 5 min. incubation. At 254 nm irradiation the degradation kinetics of the OEG chains was very fast that produced complete degradation (direct patterning) at dose below 8 J/cm2. However, 312 and 366 nm irradiation provided the possibility to control the degradation (defects formation) at low doses followed by direct patterning at doses greater than 103 J/cm2.

O 36.6 Tue 18:30 P4

Comparing CuPc and H_2Pc sub-monolayer films on Ag(111): A NIXSW and SPA-LEED study — •Ingo Kröger[1], Patrick Bayersdorfer[2], Benjamin Stadtmüller[1], Christoph Kleimann[1], Giuseppe Mercurio[1], Friedrich Reinert[2], and Christian Kumpf[1] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and JARA-Fundamentals of Future Information Technology — [2]Experimentelle Physik 7, Universität Würzburg, 97074 Würzburg

The sub-monolayer growth of metal-phthalocyanines (MePc) on the Ag(111) surface exhibits a rich phase diagram consisting of 2D gas-like phases, commensurate phases and - most interestingly - a continuous series of phases with point-on-line coincidence with the substrate [1,2]. The latter is caused by repulsive intermolecular interaction. In order to clarify the role of the central metal atom for this repulsion, we compare SPA-LEED and NIXSW data of the metal free H_2Pc/Ag(111) with CuPc/Ag(111). The similarity of the phase diagrams leads to the conclusion that in principle the intermolecular repulsion does not depend on the metal atom. For H_2Pc the adsorption heights show a significant bending of the nitrogen atoms toward the surface. This "N-down" configuration leads to a stronger and more localized bonding to the surface, and therefore stabilizes the commensurate phase in a wider coverage regime and at higher temperature compared to CuPc/Ag(111). [1] Kröger et al., New Journal of Physics 12, 083038 (2010) [2] Stadler et al., Nature Physics 5, 153 (2009)

O 36.7 Tue 18:30 P4

DFT studies on the adsorption of thiols at transition metal surfaces — •Porntip Seema, Jörg Behler, and Dominik Marx — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum

The interaction of sulfur-containing molecules with transition metal surfaces plays an important role for example in the poisoning of heterogeneous catalysts and the formation of self-assembled monolayers. A large number of theoretical and experimental studies has been carried out in recent years, but still several questions on the structures of these systems remain open. We present density-functional theory (DFT) calculations for the adsorption of several sulfur-containing species (e.g. S atoms, H_2S, CH_3SH) on Cu(111) and Ag(111) surfaces. Calculations have been carried out for a variety of adsorbate coverages, binding sites and surface models (slabs and clusters). We find that the order of the binding energies is $S > SH > SCH_3$, with an increased binding energy at surface defects. In general, the sulfur-metal interaction is stronger for Cu(111) than for Ag(111).

O 36.8 Tue 18:30 P4

Structural formation of thiophene-2-thiol on gold — Lydia El-Kareh[1], •Axel Beimborn[1], Patrick Mehring[1], Dominique Handschak[1], and Carsten Westphal[1,2] — [1]Experimentelle Physik 1 - TU Dortmund, Otto-Hahn-Str.4, D 44221 Dortmund, Germany — [2]DELTA -TU Dortmund, Maria-Goeppert-Mayer-Str. 2, D 44227 Dortmund, Germany

In recent years self assembled monolayers (SAMs) have been extensively studied because of their well-defined structures resulting from simple dipping preparation. An ideal system for the understanding of self-organisation processes are alcanethiols that were widely examined during the last decades. These molecules can be prepared with different head groups leading to different applications in molecular electronics, nanotechnology, bio-sensing, and corrosion inhibition. One possible head group is thiophene. The orientation of thiophene-2-thiol adsorbed on Au(111) has been investigated by scanning tunneling microscopy (STM). Thiophene-2-thiol molecules are found forming highly ordered adlayers. High-resolution STM reveals well ordered molecular stripes of different length. On the golf surface the stripes arrange displaced with respect to the substrate lattice forming a two-dimensional molecular network.

O 36.9 Tue 18:30 P4

Configurational and Electronic Switching of Single Azopyridine-Substituted Porphyrin Molecules — •Francesca Matino[1], Guillaume Schull[2], Umasish Jana[3], Felix Köhler[4], Rainer Herges[4], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Institut de Physique et Chimie des Matèriaux de Strasbourg, UMR 7504 (CNRS, Université de Strasbourg), 67034 Strasbourg, France — [3]Department of Chemistry, Jadavpur University, Kolkata-700032, India — [4]Institut für Organische Chemie, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Switching is an elementary step in many sophisticated functions, such as directed motion, pumping, information storage and processing, in the macroscopic world as well as at the molecular scale. For nanoscale applications of such functions, molecules have to be immobilized on solid supports in a well defined geometry and orientation, in order to achieve advanced and reproducible dynamic functions. Here we report on a new azopyridine functionalized porphyrin synthesized as a model switch for deposition on surfaces. The porphyrin platform provides bonding to the surface, some electronic decoupling and a defined orientation of the azopyridine unit. Two geometrically and electronically different states of single molecules on Au(111) were found and analyzed by Scanning Tunnelling Microscopy and Spectroscopy. Switching between two conformational states occurs upon tunneling of electrons through LUMO orbitals.

O 36.10 Tue 18:30 P4

Structural and electronic properties of thin organic heterointerfaces SnPc/PTCDA/Ag(111) — Mark Häming[1], •Christoph Sauer[1], Michael Greif[1], Achim Schöll[1], and Friedrich Reinert[1,2] — [1]Universität Würzburg, Experimentelle Physik VII, D-97074 Würzburg — [2]KIT, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe

Knowledge about the structural and electronic properties of organic heterointerfaces is of vital importance for electronic devices based on organic semiconductors. Yet information about these systems is still scarce due to difficulties in preparing well defined interfaces. With tin-phtalocyanine (SnPc) deposited on a Ag(111) surface precovered by perylene-tetracarboxylic acid dianhydride (PTCDA) we present a well suited model system to gain insight into such heterointerfaces. Photoelectron spectroscopy (XPS and UPS) as well as near edge X-ray absorption fine structure (NEXAFS) studies are applied in order to gain both structural and electronic information. Distinct features in core-level and valence spectra allow us to unambiguously distinguish between both molecules. We show clear evidence that SnPc forms a flat lying wetting layer on top of PTCDA with a mainly physisorptive character. Moreover a rigid level shift of all spectroscopic SnPc features with respect to the homomolecular SnPc films is observed, similar to what is known for Schottky contacts, which corresponds to a change in work function. We demonstrate that the built-in electric field at the interface can be explained by the formation of an interface dipole, which extends over several adsorbate monolayers.

O 36.11 Tue 18:30 P4

First STM measurements on a new class of nanowheels — •Anja Wadewitz[1], Jörg Meyer[1], Francesca Moresco[1], Gwénaël Rapenne[2], Henri-Pierre Jacquot[2], Christian Joachim[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany — [2]CEMES-CNRS, Toulouse, France

Manipulation of single molecules with a scanning tunneling microscope (STM) tip is a well established technique to study the adsorption of molecules and their mechanical properties on a surface. Recent progress in molecular manipulation has stimulated the design and synthesis of molecules that mimic macroscopic machinery, transposing mechanical functions to the scale of a single molecule. Here, we present the first low temperature STM measurements of a new class of nanowheels on Au(111). A nanowheel consists of two subphthalocyanine molecules connected by a carbon axis. The phthalocyanine fragments are nitrogen-tagged. Due to the tagging it should be possible to follow the rolling motion of the wheel just by imaging the molecule. A fast dissociation of the molecules with temperatures and light intensity is expected. Therefore, the evaporation temperature was kept as low as possible and after evaporation the sample was transferred immediately into the STM to minimize temperature and light effects. Nanowheels on Au(111) were imaged by STM, showing intact molecules as well as fragments. These first results show that the nanowheels can be deposited intact on a metal surface and that it is therefore possible to manipulate them with the STM tip.

O 36.12 Tue 18:30 P4

Electronic structure of novel air-stable n-type organic semiconductors: A comparison of different bay-substituted perylene-bisimide dyes — •Markus Scholz[1], Rüdiger Schmidt[2], Sebastian Fiedler[1], Achim Schöll[1], Frank Würthner[2], and Friedrich Reinert[1,3] — [1]Universität Würzburg, Experimentelle Physik VII, 97074 Würzburg — [2]Universitüt Würzburg, Institut für Organische Chemie, 97074 — [3]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie, 76021 Karlsruhe

The development of air stable n-conducting organic semiconductors are one of the current bottle necks in organic electronic. We present a comparative analysis of the electronic structure of various bay-substituted perylene bisimide (PBI) dyes, which have already demonstrated very high mobilities in thin film devices. The occupied and unoccupied valence levels were investigated by UPS and IPES, which allows determining the transport gap. Interestingly, the transport gap does not differ substantially between the different compounds. If the contact properties to a Ag(111) metal substrate are investigated, work function measurements reveal strong interface dipoles. In case of PBIs with fluoro alkyl chains the interface dipole is about 0.7 eV, which can be related to the C_4F_7-chains oriented out of the film surface. For Films of PBIs with isopropylphenyl-groups the magnitude and the direction of the interface dipole depend strongly on the film preparation and provide a possible route for a tailoring of the interfacial electronic structure.

O 36.13 Tue 18:30 P4

Surface-confined reaction of porphyrins with Cu atoms: An

X-ray photoelectron spectroscopy study — •Min Chen, Martin Schmid, Jie Xiao, Hans-Peter Steinrück, and J.Michael Gottfried — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Erlangen, Germany

Porphyrin derivatives are wide-spread in nature and of considerable technological importance as candidates for the construction of functional devices. Examples are the usage of metalloporphyrins and similar macrocycles as organic semiconductors or for the functionalization of surfaces in catalysis or sensor applications. As shown previously, free-base porphyrins readily form ordered monolayers on single-crystalline substrates and represent redox-active ligand precursors, which can oxidize and coordinate adsorbed metal atoms. In this study, we focus on the reactivity of various porphyrin derivatives towards adsorbed Cu atoms. As a first model system, we studied the reaction of tetrapyridylporphyrin (2HTPyP) with Cu atoms on Au(111). The co-adsorbed reactants form an intermediate at 300 K, which reacts further to Cu(II) tetrapyridylporphyrin at higher temperatures. If 2HTPyP is deposited on a Cu/Au(111) subsurface alloy, the metalation reaction leads to a segregation of Cu due to the strong Cu-porphyrin bond. Related experiments with tetraphenylporphyrin and phthalocyanine will be discussed. In addition, the above results for Cu atoms on Au(111) will be compared with reactions of porphyrins on Cu(111). Support by the Deutsche Forschungsgemeinschaft through SFB 583 and by the Alexander von Humboldt Foundation is acknowledged.

O 36.14 Tue 18:30 P4

Electrospray Ion Beam Deposition for Scanning Tunneling Microscopy Studies in Ultrahigh Vacuum — •Gordon Rinke[1], Stephan Rauschenbach[1], Nicha Thontasen[1], Zhitao Deng[1], Nicola Malinowski[1], and Klaus Kern[1,2] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Institut de Physique de la Matiere Condensee, Ecole Polytechnique Federale de Lausanne, 1015 Lausanne, Switzerland

The deposition of complex molecules in vacuum is an important technological step towards applications. In recent years, electrospray ion beam deposition (ES-IBD) was developed in our laboratory as a technique for the deposition of molecular layers of nonvolatile molecules on well defined surfaces in ultrahigh vacuum.[1,2] Thereby the key mechanism is the creation of molecular ions or clusters, which deposited on surfaces result in the growth of molecular nanostructures or films.

Here we show that this technique has now matured into a ready tool for surface scientists to prepare a great variety of surface coatings with unprecedented control. By employing state of the art ion optics, ES-IBD offers mass-selection, deposition energy control and coverage monitoring as features that are intrinsic to the process. We demonstrate the versatility of the deposition method by showing surface coatings of highest quality from molecular magnets (Mn_{12}), proteins, host-guest compounds, dye molecules and membrane like layers.[2,3]

[1] Small 2 (2006), pg. 540
[2] ACS Nano 3 (2009), pg. 2901
[3] J. Phys. Chem. C 114 (2010), pg. 17768

O 36.15 Tue 18:30 P4

Substrate- and temperature-dependent adsorption studies of spiropyran molecules — •Alex Krüger[1], Marten Piantek[1], Ch. Felix Hermanns[1], Jorge Miguel[1], Matthias Bernien[1], Klaus Hermann[2], and Wolfgang Kuch[1] — [1]Freie Universität Berlin, Institut für Experimentalphysik — [2]Theory Department, Fritz-Haber- Institut der Max-Planck-Gesellschaft

The adsorption of trimethyl-6-nitrospiropyran, a photoswitch that can be optically switched between its spiropyran (SP) and merocyanine (MC) isomer forms, on Au(111) and Bi(110) single-crystal surfaces was studied as a function of coverage and substrate temperature by near-edge x-ray absorption fine structure (NEXAFS) and X-ray photoelectron spectroscopy (XPS). For one monolayer on Au(111) at 150 K and room temperature (RT), we find that the molecules are physisorbed in their SP conformation. After annealing the sample to 330 K, the angle dependence and intensity of the N π*-resonances changed, and a chemical shift of the N 1s XPS signal was observed and interpreted as a thermally induced ring-opening reaction of molecules from the SP into the MC form. On Bi(110) the adsorption behavior is similar but the nitro group experiences a chemical modification. Based on a peak assignment derived from DFT simulations of the NEXAFS spectra, this species is interpreted as the ring-opened MC conformer. The ability for conformational switching of the adsorbed molecules was studied by illuminating the sample with UV and visible light. The N K edge NEXAFS spectra showed a significant change after illumination with UV as well as with visible light.

O 36.16 Tue 18:30 P4

Cobalt phthalocyanine molecules adsorbed on Ag(111): Examination of interfacial interactions — •Martin Schmid, Andre Kaftan, Min Chen, Jie Xiao, Hans-Peter Steinrück, and J. Michael Gottfried — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II

The modification of interfacial properties by adsorbates is a fundamental aspect in catalysis and molecular electronics. As a model system for metal/organic interfaces, we studied the adsorption of Co(II)-phthalocyanine (CoPc) on Ag(111). In general, metallophthalocyanines form well ordered layers on metallic substrates. To obtain a deeper insight into the CoPc/Ag interaction, we examined submonolayers, monolayers, and multilayers of CoPc with photoelectron spectroscopy (XPS/UPS) and low-energy ion scattering (LEIS). Up to one monolayer, the adsorption of CoPc induces two new electronic states in the vicinity of the Fermi edge and a negative work-function shift. XPS shows a strong modification of the Co 2p3/2 and 2p1/2 core level states due to the CoPc-Ag(111) interaction. These levels exhibit a binding energy ~2 eV lower than in molecules without a direct contact to the metal interface. This finding can be interpreted by a charge transfer from the Ag(111) substrate into the molecules. Furthermore, the binding energy differences between the 2p1/2 and 2p3/2 levels are altered by the contact to the single crystal surface. This observation suggests a change in the electronic state of the central Co ion. Support by the DFG through SFB 583 is gratefully acknowledged.

O 36.17 Tue 18:30 P4

Spatially resolved electron-vibration coupling in an organic charge transfer salt on Au(111) — •Isabel Fernandez-Torrente, Katharina J. Franke, and Jose Ignacio Pascual — Institut für Experimentalphysik, Freie Universität Berlin

Understanding the process of vibrational excitations in molecules is a subject of fundamental importance in potential organic-based device application due to the crucial influence vibrations have in the electronic transport properties. We have measured the vibrational properties of the acceptor molecule TCNQ embedded in a self-assembled layer with TTF, a charge donor. We find that TCNQ hosts, upon charge transfer, an unpaired spin in its Lowest Unoccupied Molecular Orbital (LUMO). This state is demonstrated by the observation of a Kondo resonance. Besides Kondo, this spin is coupled to vibrational modes of the TCNQ that induce a splitting of the Kondo resonance in vibrational sidebands, each one consisting on a peak and a step. While the steps correspond to a pure inelastic process, the peaks have an elastic character (i.e. vibrations excited through the resonant Kondo channel), demonstrated by the quenching of intensity of the central Kondo peak with increasing number of excited vibrations. The vibrations are spatially localized in particular regions of the molecule. The analysis of the STS elastic peaks and STS maps taken on individual TCNQ molecules allow us to resolve with submolecular precision the strength of the electron-phonon coupling and its specific location.

O 36.18 Tue 18:30 P4

Local anchoring and functionalization of tetraphenylporphyrins on composite surfaces: A Scanning Tunneling Microscopy Study — •Michael Stark, Stefanie Glässel, Florian Buchner, Elisabeth Zillner, Michael Röckert, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058

The understanding of the adsorption behavior of large organic molecules on surfaces is a prerequisite to utilize their functional properties either in single molecule devices or in self-assembled supramolecular architectures.

Herein, we investigate to which extent composite surfaces can act as a template to engineer the adsorption of different tetraphenylporphyrins (TPP). In particular, we investigate the dynamics and assembly of different TPPs on Cu(111) covered with monoatomic thick Ni or oxygen islands via scanning tunneling microscopy (STM) in ultra-high vacuum (UHV), mainly at room temperature (RT). On Ni precovered Cu(111) we find, e.g., that TPP molecules are immobilized selectively on the Ni-islands at RT. Furthermore, we demonstrate the possibility of local anchoring and/or functionalization of the porphyrins on prestructured Cu(111) surfaces.

This work has been funded by the DFG through Sonderforschungsbereich 583.

O 36.19 Tue 18:30 P4

Tuning the energy level alignment at the SnPc/Ag(111) interface using an STM tip — •Marius Toader and Michael Hietschold — Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany

The tip influence on the energy level alignment at the SnPc/Ag(111) interface has been addressed via the Scanning Tunneling Spectroscopy (STS). A collective effect characteristic for both molecular conformations up and down is reported to shift the corresponding first filled (HOMO) and empty (LUMO) levels towards the Fermi energy via a tip-sample distance decrease. The importance of the tin ion coupling to the metal electrodes is emphasized for the newly reported cross-bending (cross-shifting) effect. The observation is proven to be driven by the bistable donor/acceptor character of the SnPc molecules. Distinct types of coupling to the metal surface have been found for the two molecular conformations. However, a similar adsorption geometry of the molecular plane is emphasized by the same energy position of the HOMO level. Moreover, the crucial importance of the HOMO-1 (found using DFT to show strong contribution from the Sn ion) for a conformational change is proven via a controllable and irreversible tip-induced single-molecule switching and nano-writing within densely packed molecular arrays.

O 36.20 Tue 18:30 P4

SnPc on Ag(111) investigated by STM — •Christoph Kleimann, Ingo Kröger, Christian Weiss, Christa Elsaesser, Benjamin Stadtmüller, and Christian Kumpf — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and JARA-Fundamentals of Future Information Technology

Tin(II)-phtalocyanine (SnPc) is a large, non-planar, organic molecule which shows a number of different structural phases when adsorbed on Ag(111). While at low coverages a gas-like phase was observed, larger coverages result in a series of ordered, incommensurate structures at room temperature, a behavior that indicates intermolecular repulsion. At low temperature the formation of commensurate SnPc islands was found within a certain range of coverage. These different phases have already been studied intensively in our group by SPA-LEED, XSW and other techniques [1]. Two different adsorption geometries have been identified using scanning tunneling microscopy (STM) in some of these structures: The central Sn atom can either be oriented towards (Sn down) or away from the surface (Sn up). Here we show STM measurements for different coverages at room temperature and low temperature. The results confirm and complement our previous findings and demonstrate that the fine interplay of molecule-molecule and molecule-substrate interactions is crucial for the structure formation in this system.

[1] Stadler et al, Nat.Phys. 5, pp 153-158 (2009)

O 36.21 Tue 18:30 P4

Multi-Technique Investigation of the Interface of Perfluoropentacene on Ag(111) — •Christian Schmidt, Manuel Marks, Jan Götzen, Christian H. Schwalb, Gerson Mette, Ulrich Höfer, and Gregor Witte — Fachbereich Physik und WZMW, Philipps-Universität Marburg, D-35032 Marburg

The performance of organic electronic devices is to a large extent determined by the interaction at the electrodes which affects the charge carrier injection and also the morphology of the organic semiconductor films. Since a common understanding of such interfaces properties is still lacking, a detailed characterization is required for every new available organic material. Here we have studied the structure and electron dynamics of the interface between Perfluoropentacene (PF-PEN) and a Ag(111) surface by combining STM, LEED, XPS, NEXAFS and 2PPE. While a recent study revealed the formation of a commensurate PF-PEN monolayer at 90 K [1], we observed reversible phase transition between this low temperature phase and a gas phase behavior at room temperature. While multilayer films can be selectively desorbed by gentle heating thus allowing the preparation of monolayer films the molecules reveal a cracking for temperatures above 400K. Further on 2PPE enables us to study the interface electron dynamics directly in the time domain. While no predominant contributions due to molecular states were observed in the time resolved 2PPE spectra, a series of surprisingly strongly bound image-potential related interface states occur that mainly determine the interfacial electron dynamics. [1] S.L. Wong et al. *J.Phys.Chem. C* **114**, 9356 (2010).

O 36.22 Tue 18:30 P4

Adsorption of metal-free phthalocyanine molecules on Pd(110) and Au/Pd(110) — •Daniel Dück[1], Tobias Pertram[1], and Klaus Wandelt[1,2,3] — [1]Institute of Physical and Theoretical Chemistry, University of Bonn, Germany — [2]Institute of Experimental Physics, University of Wrocaw, Poland — [3]Department of Physics, University of Rome Tor Vergata, Italy

The {110} surfaces of fcc metals show an intrinsic anisotropy due to the rectangular surface unit cell. This anisotropy is even more pronounced in case of the (1×2) missing row reconstruction. The clean Pd(110) surface does not show the tendency to reconstruct. But under the influence of hydrogen we find missing row reconstruction. After deposition of small amounts of Au (< 1 ML) on the unreconstructed Pd(110) surface pseudomorphic Au islands are observed, whereas in the case of higher Au amounts (> 2 ML) the resulting Au layer shows the characteristic (1×2) reconstruction, which still remains pseudomorphic to Pd(110) [2]. We have used these reconstructed surfaces as a substrate for the ordered ("templated") deposition of phthalocyanine molecules.

Phthalocyanines have attracted considerable attention owing to their promising application in optical and electronic devices. Especially the adsorption behaviour and film growth have been investigated.

STM investigations under UHV reveal a specific adsorption behaviour of the metal-free phthalocyanine molecules, which are oriented along rows of the reconstructed surfaces, and detailed structure models are discussed.

O 36.23 Tue 18:30 P4

Two photon photo-emission study of doped and undoped Pentacene thin films on Cu(111) — •Martin Laux, Indranil Sarkar, Andreas Ruffing, and Martin Aeschlimann — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern

Organic-metal interfaces plays a very important role in the performance of opto-electronic devices based on organic semiconductors, as the interface strongly affects the carrier injection in these devices. So, it is of utmost importance to understand the energy level alignment and corresponding energetics at organo-metallic interfaces [1]. Among various organic semiconductors, Pentacene ($C_{22}H_{14}$) forms a very important organic compound for organic devices due its intrinsically high carrier mobility and controllable electronic properties by doping [2]. Here we report, one-photon photoemission (1PPE) and two-photon photoemission (2PPE) measurements on pentacene thin films on Cu(111). Our results show presence of highly dispersive HOMO band, with effective mass of $0.35\,m_e$. For very low thickness of pentacene an unoccupied interface state appears. We also present time resolved 2PPE measurements on Cs doped pentacene thin films. Our results, indicate strong Cs induced modification of surface, bringing out the possibility of tuning the organic metal interface state using dopants.

[1] T. S. Kuhlman et. al. J. Am. Chem. Soc. 132, 3431 (2010)
[2] A. Scheybal et. al. Phys. Rev. B 79, 115406 (2009).

O 36.24 Tue 18:30 P4

Infrared Reflection Absorption Spectroscopy (IRRAS) of Ethene (C_2H_4) Chemisorbed on the Bare and Roughened Cu(110) and Cu(111) Surfaces — •Jan Pischel, Olaf Skibbe, and Annemarie Pucci — Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, D-69120 Heidelberg

As a model for an organic-metal interface, the chemisorption systems C_2H_4/Cu(111) and C_2H_4/Cu(110) have attracted attention because of their remarkable absorption properties in infrared (IR) spectroscopy [1-4]. Not only were two gas phase Raman active modes observed that are expected to be IR forbidden by the Raman-IR exclusion principle for centrosymmetric molecules, but also the only IR active mode allowed by the metal surface selection rule seemed to disappear at higher coverages on Cu(110). No final conclusion concerning these findings has been drawn so far. This brought us to reinvestigate the system C_2H_4/Cu(110) by means of IRRAS. Additionally the influence of small amounts of cold-evaporated copper in the submonolayer region has been studied. The results are compared to those of ethene adsorbed on Cu(111) [4]: While the spectra obtained on the bare surfaces are found to differ strongly, the absorption properties become similar with increasing surface roughness.

[1] C. J. Jenks et al. Surf. Sci. Lett., 277:L89-L94, 1992.
[2] J. Kubota et al. Phys. Chem., 98:7653-7656, 1994.
[3] R. Raval. Surf. Sci., 331-333:1-10, 1995.

[4] O. Skibbe et al. J. Chem. Phys., 128:194703-1 - 194703-6, 2008.

O 36.25 Tue 18:30 P4

Ballistic hole transport through PTCDA molecules — •Alexander Bernhart, Mark Kaspers, Christian Bobisch, and Rolf Möller — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

Ballistic Electron Emission Microscopy (BEEM) not only represents an ideal technique to study the electronic transmission at the Schottky-interface between a metal and a semiconductor, but moreover it offers capabilities to analyze the ballistic transport through adsorbates on top of a metal. By using a 6 nm Bi film on a p-doped Si(001) substrate it is possible to analyze the ballistic transport of holes through the occupied states of organic adsorbates. For the perylene derivate PTCDA the ballistic current varies between alternating rows of molecules. The comparison to the bare Bi surface reveals that the total BEEM current is reduced by the molecular layer.

O 36.26 Tue 18:30 P4

Monolayer formation and electronic structure of tetracyanoethylene on Ag(111) and Ag(100) studied by scanning tunneling microscopy — •Hasmik Harutyunyan, Tatjana Walth, Tobias Allmers, and Daniel Wegner — Physikalisches Institut and CeNTech, WWU Münster, Germany

Tetracyanoethylene [TCNE, $(CN)_2C{=}C(CN)_2$] is a very strong π-electron acceptor that easily forms metal-organic charge-transfer complexes. Particular interest exists for TCNE-based complexes involving transition-metal atoms because they are promising candidates for molecular magnets [1]. Recent studies showed that TCNE adsorbs quite differently on various noble metal surfaces due to a varying ratio of molecule-molecule vs. molecule-substrate interaction [2]. Here we present new results of the growth of TCNE on Ag(100) and Ag(111) studied by low-temperature STM and STS. We show that, different from previous results, TCNE can form closed-packed monolayer patterns on both surfaces. In case of Ag(100), we find local order in shifted rows that form zig-zag patterns with $(3 \times 5n)$ unit cells $(n = 1 \ldots 4)$. On Ag(111), TCNE forms an ordered porous network with a $(\sqrt{67} \times \sqrt{67}){-}\mathrm{R}12.1^\circ$ unit cell containing six molecules. The arrangement of the molecules leads to chirality. STS reveals molecular orbitals as well as vibrations whose dependence on molecule-molecule and molecule-substrate interaction will be discussed.

[1] D. Wegner et al., PRL 103, 087205 (2009).

[2] D. Wegner et al., Nano Lett. 8, 131 (2008).

O 36.27 Tue 18:30 P4

Investigations of Aza-Bodipy adsorbed on metallic surfaces — •Loka Mani, Cormac Toher, Jörg Meyer, Anja Wadewitz, Francesca Moresco, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany.

Bodipy dyes (difluoroboradiaza-s-indacene) are notable for their high quantum yield, intense fluorescence, strong chemical stability and highly tuneable, sharp absorption wavelength with uniquely small Stokes shift. Aza-Bodipy dyes, resulting from the replacement of the methene carbon atom in the bodipy core with a nitrogen atom, additionally show sizable red-shift of the absorption wavelengths. Electron donor materials for organic photovoltaics has recently emerged as promising application of Aza-Bodipy, due to its strong infra-red absorption. Here we present the results of a combined theoretical and experimental investigation of the adsorption characteristics, electronic structure and bonding geometry of single Aza-Bodipy molecules on Au(111) and Ag(110) surfaces. Density functional theory calculations of the density of states (DOS) and adsorption geometry were found to be in qualitative agreement with local DOS and scanning tunneling spectroscopy measurements with a low-temperature scanning tunneling microscope (STM). The strength of the bonding interaction to the substrate was also calculated, and the mobility of the molecule on the surface was investigated by calculating the energy barrier for translations and rotations which were compared with data obtained from STM manipulations.

O 36.28 Tue 18:30 P4

Site-specific polarization screening in organic thin films: Tetracene on Ag(111) — Tomoki Sueyoshi[1,2], Christian Weiss[1], Axel Delhey[1], Markus Eschbach[1], •Sergey Subach[1], and Stefan Tautz[1] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and JARA-Fundamentals of Future Information Technology — [2]Graduate School of Advanced Integration Science, Chiba University Yayoi-cho, Inage-ku, Chiba 263-8522, Japan

Organic semiconductors attract considerable attention due to their relevance for electronic devices. The electronic properties of molecules on metals have been studied in particular. For example, it has been shown that the chemical bonding to a metal surface may change both the electronic levels and geometric structure of organic molecules profoundly. Upon charge transport, the electronic states of a molecular material may also be influenced by polarization screening, i.e., the stabilization of a locally injected charge through the polarization of the surrounding molecular environment. Another aspect we report on, namely, the site specificity of the polarization energy in complex unit cells and at surfaces of organic materials can thus have a significant influence on transport properties. Scanning tunneling spectroscopy and ultraviolet photoelectron spectroscopy of tetracene films reveal strong energy level shifts by up to 1 eV from molecule to molecule. This effect can be traced back to the site specificity of polarization energy caused by a combination of different molecular environments, the intrinsic anisotropy of molecular polarizability, and the influence of the substrate.

O 36.29 Tue 18:30 P4

Long range odered monolayers and lifting of the Au(111) reconstruction by sulfur containing organic donor molecules — •Benjamin Fiedler[1], Elena Rojo-Wiechel[1], Johann Classen[1], Julia Simon[2], Johannes Beck[2], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn — [2]Insititut für Anorganische Chemie der Universität Bonn

We have studied the adsorption and monolayer formation on Au(111) of the well-known donor molecule TTT (Tetrathiotetracene) and the novel donor molecules TBTA (Tetrabenzothianthrene) by high resolution LEED. TTT forms a commensurate monolayer, whereas the submonolayer is disordered, which we interpret to be related to repulsive intermolecular interactions. Interestingly, the $(\sqrt{3}\ \mathrm{x}\ 22)$ herringbone reconstruction of the Au(111) surface is lifted already for small coverages. Quite differently the reconstruction is preserved for adsorption of TBTA, which also forms a highly ordered monolayer, which is incommensurate. With respekt to the molecule in the bulk, the surface bonded molcule is planarized. We discuss these findings in the relation to the electron donating character of the molecules and the chemical bonding to the surface.

This work was supported by the DFG under SFB 813.

O 36.30 Tue 18:30 P4

Investigation of Interface Dipole Formation of Dithiocarbamate Molecules on Gold by Density Functional Theory and Photoelectron Spectroscopy — •Tobias Schäfer[1], Philip Schulz[1], Dominik Meyer[1], Riccardo Mazzarello[2], and Matthias Wuttig[1] — [1]I. Physikalisches Institut (IA), RWTH Aachen University — [2]Institut für Theoretische Physik C, RWTH Aachen University

One of the main challenges in constructing organic optoelectronic devices is to control the charge carrier injection between the active organic material and metal contact electrodes. The insertion of a self assembled monolayer (SAM) between the organic/inorganic interface depicts an advantageous way to align the metal work function to the frontier molecular orbitals of adjacent organic species.

In this study Dithiocarbamate terminated molecules (DTC) on gold have been investigated as a potential SAM building block. Photoelectron Spectroscopy reveals a strong lowering of the metal work function upon adsorption of DTC molecules. Hence, calculations employing density functional theory (DFT) have been conducted in order to correlate this effect to the formation of a layer of permanent as well as induced dipoles.

O 36.31 Tue 18:30 P4

Stability and Structure of Benzenethiol, Pentafluorobenzenethiol and mixed SAMs on Pd(111) prepared by immersion — •Heiko Heim, Christian Schmidt, and Gregor Witte — AG Molekulare Festkörperphysik, Philipps-Universität Marburg, D-35032 Marburg

Self assembled monolayers of (partly) fluorinated aromatic organothiols have been successfully employed to modify metal-organic interfaces such as gold electrodes in order to improve the properties of organic electronic devices [1,2]. Recent studies have further shown that apart from gold also palladium constitutes a promising electrode material for such devices [3,4]. However, compared to the case of gold the thiol/palladium interface is by far less extensive investigated. In this study we have characterized the structure and thermal stability of benzenethiol- (BT) and pentafluorobenzenethiol-SAMs (PFBT) on Pd(111) by means of XPS, NEXAFS and TDS. Moreover, since perfluorination causes an inversion of the quadrupole moment of the phenyl rings which may lead to an additional stabilization between fluorinated and non-fluorinated molecules also SAMs of different stoichiometric mixtures of BT and PFBT have been studied.

[1] D.J. Gundlach et al., *Nature Materials*, **7**, 216 (2008)
[2] N. V. Venkataraman et al., *J. Phys. Chem.*, **113**, 5620 (2009)
[3] J. Love et al., *J. A. Chem. Soc.*, **105**, 1171 (2005)
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O 36.32 Tue 18:30 P4

Shape and dynamics of 2D hierarchic bicomponent networks — •Wolfgang Krenner[1], Florian Klappenberger[1], Younes Makoudi[1], Nenad Kepcija[1], Dirk Kühne[1], Svetlana Klyatskaya[2], Mario Ruben[2,3], and Johannes V Barth[1] — [1]Physik Department E20, TU München, München, Germany — [2]Insitute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]IPCMS-CNRS UMR 7504, Université de Strasbourg, Strasbourg, France

Towards the construction of molecular networks driven by hierarchic principles, the combination of tailored molecular building blocks has proven to be an essential tool. We present an UHV, low-temperature scanning tunneling microscopy study employing a hierarchic growth scenario to realize bicomponent, self-assembled molecular networks. The molecular templates constructed in this fashion display two types of bonding schemes.

The two building blocks, namely dicarbonitrile sexiphenyl and N,N' diphenyl oxalic amide, arrange in a variety of molecular networks. By tuning the stochiometry, the formation of a predominant type of the long range networks found on the Ag(111) surface, can be steered. With this approach it is possible to construct open-porous networks with variable pore size and geometry.

Moreover, thermally induced molecular motion is found to occur in the networks with the largest pore size. A migration of sexiphenyl, acting as weaker bound spacers in these networks, along the chain direction of the bi-molecular template is encountered.

O 36.33 Tue 18:30 P4

Structural transformation of the PTCDA/Ag(110) interface induced by potassium adsorption — •Martin Willenbockel[1], Giuseppe Mercurio[1], Oliver Bauer[2], Benjamin Fiedler[2], Christian Weiss[1], Ruslan Temirov[1], Sergey Subach[1], Moritz Sokolowski[2], and Stefan Tautz[1] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and JARA - Fundamentals of Future Information Technology — [2]Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn, Germany

Using X-ray photoemission spectroscopy, scanning tunneling microscopy and low energy electron diffraction, the transformation of PTCDA/Ag(110) after deposition of potassium and subsequent annealing is studied. The initially planar molecule/metal interface undergoes significant structural modification: upon annealing, potassium atoms intercalate under the molecular layer partially unbinding PTCDA molecules from silver. This induces significant reorganization of the top-most silver layer resulting in the formation of silver terrace trains with K+PTCDA chains on top.

O 36.34 Tue 18:30 P4

Bisterpyridine adlayers on metal surfaces as 2D model systems - A STM study — •Thomas Waldmann[1], Harry E. Hoster[1,2], and R. Jürgen Behm[1] — [1]Ulm University, Institute of Surface Chemistry and Catalysis, 89069 Ulm, Germany — [2]Current address: Technische Universität München, Centre for Electromobility, 50 Nanyang Drive, Singapore 637553

Adlayers of the bisterpyridine derivative 2,4'-BTP on Au(111), Ag(111) and Ag(100) are used as two-dimensional (2D) model systems for studying self-assembly and for direct observation of (reaction)dynamics by scanning tunneling microscopy (STM). (i) At low coverages, we find a preference for a step-crossing behavior of 2,4'-BTP that can be explained by the intramolecular building blocks of the adsorbate. The self-organization on terraces is influenced by (N...metal)-type molecule-substrate interactions, producing 12 preferred azimuthal orientations of the adsorbates with respect to the close packed surface directions in both, ordered and disordered areas [1]. (ii) Domains of freely rotating molecules, which are stabilized significantly by rotational entropy resulting from the large moment of inertia of 2,4'-BTP [2] exist in a dynamic equilibrium with non-rotating molecules at 300 K. We compare the stabilization by rotational entropy with that for other typical small and large adsorbates. (iii) Ordered monolayers of 2,4'-BTP on Ag(111) are used as a model system for direct STM observation of the reaction between the adlayer and oxygen to a N-oxide network.

[1] T.Waldmann et al., ChemPhysChem 11, 1513 (2010).
[2] M.Roos et al., PCCP 12, 812 (2010).

O 36.35 Tue 18:30 P4

Intermolecular vs. molecule-substrate interactions - a STM study — •Michael Roos[1], Daniela Künzel[2], Harry E. Hoster[1,3], Axel Gross[2], and R. Jürgen Behm[1] — [1]Ulm University, Institute of Surface Chemistry and Catalysis, 89069 Ulm, Germany — [2]Ulm University, Institute of Theoretical Chemistry, 89069 Ulm, Germany — [3]Current address: Technische Universität München, Centre for Electromobility, 50 Nanyang Drive, Singapore 637553

The formation of 2D molecular networks is governed by a competition between intermolecular interactions and the lateral variation in molecule-substrate interactions. In this contribution we study the effect of varying the location of the heteroatoms (N atoms) in planar organic adsorbates by using two Bis(terpyridine) derivatives (BTP) as model systems. On smooth surfaces the resulting structures are dominated by weak C-H$\cdots$N-type hydrogen bonds. We will compare the ordering behavior with the network formation on graphene monolayers supported by Ru(0001). The moiré pattern of these surfaces has a periodicity of 3 nm, i.e., in the order of the BTP dimensions. Submolecularly resolved STM images show that the BTP molecules are confined to the valleys of the graphene ripple structure. We will discuss the template effect quantitatively by means of force field calculations and supporting thermal desorption experiments.

O 36.36 Tue 18:30 P4

Interactions of the biomolecules L-cysteine and adenine with metals investigated by STM — •Sybille Fischer, Anthoula Papageorgiou, Matthias Marschall, Joachim Reichert, and Johannes V. Barth — Physik Department E20, TU München, James-Franck-Straße, D-85748 Garching

Understanding the interactions between biomolecules like amino acids and nucleobases as building blocks of the DNA and metal binding sites of proteins are important for the comprehension of many neurodegenerative diseases. Metal-organic coordination networks can act as model systems to investigate these interactions and represent at the same time robust, room temperature stable bio-interfaces which might be useful for enantio-selective catalysis. Here we present a scanning tunneling microscopy (STM) study of L-cysteine and adenine with and without metal adatoms on noble metal surfaces to visualize the self-assembly of these molecules at varying temperatures.

O 36.37 Tue 18:30 P4

Self-Assembly of Individually Addressable Complexes of C60 and Phthalocyanines on a Metal Surface: Structural and Electronic Investigations — Tomas Samuely[1], Shi-Xia Liu[2], Marco Haas[2], Silvio Decurtins[2], Thomas Jung[3], and •Meike Stöhr[4] — [1]University of Basel, Switzerland — [2]University of Bern, Switzerland — [3]Paul-Scherrer-Institute, Switzerland — [4]University of Groningen, Netherlands

A complex phase behavior was found for a specific phthalocyanine (Pc) derivative adsorbed on either Au(111) or Ag(111). The Pc molecule is symmetrically substituted with eight peripheral di-(tert-butyl)phenoxy (DTPO) groups. The pronounced ability of the DTPO groups to rotate, allows the molecule to adopt different conformations and hence to arrange itself in different ordered patterns. In particular, when all DTPO substituents are arranged above the plane of the Pc core (a bowl-like structure is formed), the interaction of the Pc core with the metal substrate is enabled. Moreover, for such an assembly the hosting properties for the adsorption of C60 were investigated. The C60 molecules adsorb at two clearly distinguishable positions on the predeposited Pc layer: they are in contact either with the metal substrate in between two adjacent Pc molecules or with the Pc core. For the latter case, the C60 is located directly above the pi-conjugated Pc core. Hence, the presented system combines the three following features: (i) the direct electronic interaction between donor and acceptor moieties,

(ii) the formation by self-assembly, and (iii) thermal stability. Thereby, the direct investigation of a single donor-acceptor complex is enabled.

O 36.38 Tue 18:30 P4

A local structure determination of Uracil on Cu(110) by energy scanned photoelectron diffraction — David Duncan[1], •Werner Unterberger[2], Tsenolo Lerotholi[1], Dagmar Kreikemeyer-Lorenzo[2], and Phil Woodruff[1] — [1]University of Warwick — [2]Frtiz-Haber-Institut

While there is growing interest in investigations of biologically-related molecules on surfaces, very few such studies involve quantitative determination of the local adsorption geometries. The technique of photoelectron diffraction (PhD) is particularly well-suited to this problem because it allows one to determine the local adsorption site of the molecule's atoms. Here we report the results of a new study, namely of the nucleobase molecule uracil (a six-membered ring comprising CH.CH.CO.NH.CO.NH) on Cu(110). The results for uracil, as one might expect, are closely similar to those reported previously for thymine [1]. Analysis of the O 1s and N 1s PhD spectra shows that the molecular plane is essentially perpendicular to the surface, and the molecule bonds to the surface through the two O atoms and the deprotonated N atom that lies between them. All three of these bonding atoms occupy near-atop sites on the Cu(110) surface, with the molecular plane twisted 11+-5° off of the <1-10> plane.

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O 36.39 Tue 18:30 P4

New ordered structures of ω-(4'-methyl-biphenyl-4-yl)alkanethiols Bp4 evaporated under UHV conditions on Au(111) surfaces — •Mirko Müller[1,2] and Gerhard Pirug[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology

Depending on the evaporation conditions we observed under UHV two new structures for ω-(4'-methyl-biphenyl-4-yl)alkanethiols (Bp4) molecules adsorbed on Au(111) surfaces using a Micro-Channel-Plate (MCP)-LEED system. The resulting patterns could be identified assuming a $\begin{pmatrix} 1 & 2 \\ 12 & 1 \end{pmatrix}$ $((\sqrt{3}$ x $\sqrt{133})\angle$ 85.7°) and a $\begin{pmatrix} 14 & 7 \\ 0 & 7 \end{pmatrix}$ $((7\sqrt{3}$ x 7$)\angle$ 90°) unit cell. Possible surface structures will be discussed on the basis of a detailed interpretation of these LEED patterns. Apart from the corresponding sharp spots of the $(\sqrt{3}$ x $\sqrt{133})\angle$ 85.7° structure the first pattern contains streaks lining up at positions which would be expected for additional spots from a $\begin{pmatrix} 2 & 4 \\ 12 & 1 \end{pmatrix}$ $((2\sqrt{3}$ x $\sqrt{133})\angle$ 85.7°) structure. These streaks result from characteristic domain shapes und boundaries. Missing spots in the $(7\sqrt{3}$ x 7$)\angle$ 90° pattern can be explained by a pgg symmetry group with two perpendicular glide mirror planes. Consequences on the packing within such selfassembled layer of Bp4 molecules will be discussed.

O 36.40 Tue 18:30 P4

Surface-enhanced and tip-enhanced Raman spectroscopy of biological molecules on nanostructured metallic surfaces — •Laura E. Hennemann[1], Andreas Kolloch[2], Josip Mihaljevic[1], Kai Braun[1], Alfred J. Meixner[1], and Dai Zhang[1] — [1]Institute of Physical and Theoretical Chemistry, University of Tübingen, Auf der Morgenstelle 8, 72076 Tübingen, Germany — [2]Department of Physics, University of Konstanz, Universitätsstrasse 10, 78457 Konstanz, Germany

We use a custom built apertureless scanning near-field optical microscope (SNOM) to investigate several kinds of biological molecules. The setup is an extended parabolic mirror based confocal microscope working with higher order laser modes in order to tune the polarization of the light in its focus. We detected the presence of a (sub)monolayer of biological molecules ranging from DNA bases to double stranded DNA by collecting their unique Raman fingerprint spectrum.

In order to detect such small amounts of molecules, we performed surface-enhanced Raman scattering (SERS) or tip-enhanced Raman scattering (TERS). For SERS, either the irregular rough edges of evaporated noble metal grids or regular arrays of gold nano triangles served as enhancing substrates. We compared the plasmonic properties of gold triangles of different aspect ratios and on different substrates to optimize the electromagnetic enhancement for the 632.8 nm laser excitation. The obtained optical patterns were compared to those computed in simulations.

In the case of TERS, an electrochemically etched sharp gold tip (approx. 20 nm tip apex diameter) was approached to the surface, thus acting simultaneously as a scanning probe microscopy tip for topographic measurements and as a near-field antenna collecting optical information. We collected TERS spectra of single calf thymus DNA molecules immobilized on smooth Au (111) surfaces. Strongly enhanced spectra were obtained both in the SERS and in the TERS measurements.

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O 36.41 Tue 18:30 P4

Structures of metal electrodes at the solid-liquid interface studied by density functional theory — •Xiaohang Lin and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

Recently, the operation of an electrochemical atomic-scale quantum conductance switch has been demonstrated, which is controlled by an external electrochemical voltage applied to an independent third gate electrode [1]. However, the microscopic processes underlying this atomic switch are still unclear. Using density functional theory (DFT) calculations, we have addressed the structure of Ag and Pb metal surfaces which are both used as electrode materials for the switch. We have considered the presence of water layers and the self-diffusion on flat and stepped metal surfaces in order to contribute to the understanding of electrodeposition. We find that the substantial difference in the lattice constants between Ag and Pb leads to significant changes, as far as the stable water structure at the metal-water interface is concerned. With respect to the metal diffusion, the DFT results indicate that exchange processes can have considerably lower barriers than hopping processes.

[1] F.-Q. Xie *et al.*, Phys. Rev. Lett. **93**, 128303 (2004).

O 36.42 Tue 18:30 P4

Surface Structure and Morphology of Cu–free and Cu–covered Au(1 0 0) and Au(1 1 1) Electrodes in Alkaline Solution — •Christian Schlaup[1], Daniel Friebel[2], and Klaus Wandelt[3] — [1]Technical University of Denmark, Department of Physics, Fysikvey, DK–2800 Kongens Lyngby, Denmark — [2]Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, 2575 Sand Hill Rd, Menlo Park, CA 94025, USA — [3]University of Bonn, Institute for Physical und Theoretical Chemistry, Wegelerstr. 12, D–53115 Bonn, Germany

For both Cu–free Au-electrodes three different phases were observed as a function of the applied electrode potential. While at low potentials the onset of surface reconstruction points towards an apparently adsorbate free surface and, thus, a weak interaction with species from the electrolyte, a Au–hydroxide and a Au–oxide phase are formed subsequently during potential increase.

A similar phase behavior was also found for Cu–covered Au–electrodes, while at low potentials an apparently adsorbate free Cu layer is observed, a Cu–hydroxide coadsorbate phase and a Cu–oxide phase are formed under increased potential conditions. In addition the apparently adsorbate free Cu–film tends to form a Cu–Au alloy phase while keeping the electrode for a sufficient long time at low potential conditions.

O 36.43 Tue 18:30 P4

Equilibrium Step Fluctuations on Stepped Au(001) in Electrolyte — •Mohammad Alshakran[1], Guillermo Beltramo[1], Harald Ibach[2], and Margret Giesen[1] — [1]Institut für Complexe Systeme Biomechanik ICS-7, Forschungszentrum Jülich GmbH — [2]Peter Grünberg Institut PGI-3 , Forschungszentrum Jülich GmbH

Equilibrium step fluctuations on stepped Au(001) with Miller indices (1 1 17) and (1 1 29) in electrolyte were studied by electrochemical scanning tunneling microscopy. Measuring the step-step correlation function we determine the time dependence of the fluctuations. From the time dependence one can deduce the dominant mass transport involved in the fluctuations as a function of the electrode potential. For both samples we find an exponent close to 1/4. Unexpectedly, the fluctuations depend also on the step-step distance with an exponent

3/2. The strong dependence on the step-step distance indicates a mass transport mechanism not considered yet theoretically. We furthermore obtained kink energies as a function of electrode potential. From that potential dependence we obtain a kink dipole moment in the order of 2.2 +/- 0.6 e pm.

O 36.44 Tue 18:30 P4

AIMD simulations of adsorption processes of water on metal surfaces — •Anja Kobel and Axel Gross — Institute for Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

Studying surface adsorption processes, ab initio molecular dynamics (AIMD) simulations have proven a useful tool for obtaining statistically meaningful results with respect to kinetic quantities such as sticking coefficients. There have been various investigations considering surface adsorption of diatomic molecules, hydrogen in particular, employing AIMD [1]. We focus in our study on the quantitative modelling of the interaction of water on a platinum(111) surface, evaluating an ensemble of AIMD trajectories. This will provide insight into reaction probabilities and distributions of molecules beyond diatomics and give important trend understanding for more complex molecules. Besides the adsorption of single molecules on clean metal surfaces, we also consider the adsorption of water molecules on water-precovered metal surfaces in order to address the first steps of the formation of a water layer on a metal surface.

[1] A. Groß, ChemPhysChem **11**, 1374 (2010).

O 36.45 Tue 18:30 P4

Laterally resolved dependence of the surface-state band edge on Ag islands on Nb (110) — •Tihomir Tomanic[1], Christoph Sürgers[1], Dominik Stöffler[1], and Hilbert v. Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe — [2]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe

We investigate the growth of Ag on Nb (110) by in-situ STM at low temperatures ($T_{\mathrm{min}} = 3$ K). The surface of a Nb (110)-oriented single crystal is prepared by repeated cycles of flashing up to 2300 °C and subsequent Ar$^+$ sputtering. At a substrate temperature $T_S = 573$ K, evaporation of nominal 5 nm Ag on Nb (110) leads to the formation of large, flat, and well separated islands. On top of these islands the band edge of electronic surface state in the Γ-L bandgap is resolved by local tunnelling spectroscopy. This state is shifted by 70 - 100 meV towards the unoccupied band - when compared to homoepitaxially grown Ag on Ag (111) - due to large tensile strains originating from the difference in thermal expansion of Ag and Nb between 573 and 3 K. This allows a laterally resolved investigation of the strain distribution in these Ag islands on the nanometer scale.

Work supported by the Kompetenznetz Funktionale Nanostrukturen der Baden-Württemberg Stiftung and by the DFG Center for Functional Nanostructures.

O 36.46 Tue 18:30 P4

Structural Phases and Magnetism of the Co Monolayer on W(001) — •Arne Köhler, René Schmidt, Alexander Schwarz, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Jungiusstraße 11, 20355 Hamburg

Theory predicts an antiferromagnetic ground state for a monolayer (ML) of Fe or Co grown pseudomorphically on W(001) [1]. Spin-polarized scanning tunnneling microscopy (SP-STM) could detect the characteristic c(2×2) checkerboard pattern for the Fe ML [2], but not for the Co ML. An alternative approach to map spin-structures with atomic resolution is magnetic exchange force microscopy (MExFM) [3], a novel atomic force microscopy (AFM) based technique, which has been successfully applied to the Fe ML on W(001) [4].

With STM we could detect three phases in the Co ML: a pseudomorphic p(1×1) phase, a reconstructed (2×1) phase and a third unidentified phase. Temperature dependent measurements indicate that the (2×1) phase is more densely packed than the p(1×1) phase. Employing AFM the p(1×1) phase could be also imaged with atomic resolution. Moreover, AFM data revealed the arrangement of atoms within the (2×1) phase, because the positions of atoms are not masked by peculiarities in the local density of states like with STM. First MExFM experiments have been performed as well.

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[4] R. Schmidt *et al.*, Nano Lett. **9**, 200 (2009).

O 36.47 Tue 18:30 P4

Role of closed compact island during submonolayer pulsed deposition — Martin Mašín and •Miroslav Kotrla — Institute of Physics, ASCR, Na Slovance 2, Prague, Czech Republic

We study temperature dependence of island densities during Pulsed Laser Deposition (PLD) in submonolayer regime. We employ full diffusion kinetic Monte Carlo simulation. Attachment of monomers to islands is irreversible at low temperatures while it becomes reversible at higher temperatures. Our model allows us to study processes on different time scales with parameters for typical PLD experiments: fast deposition (on scale order of 10^{-5} s), and relaxation between pulses (on scale of order of 0.1 s).

In this contribution, we further explore recently observed anomalous behavior of temperature dependence of island density [EPL 90 (2010) 18006] which is due to interplay between the cluster decay time and the interval between pulses. The anomalous behavior is caused by the temperature limited stability of *closed–compact* clusters. We investigate temperature dependent distribution of the closed–compact island for different material and deposition parameters. In particular, we study the dependence on range and strength of the binding interaction (we include interactions to second and third neighbors) and on frequency of pulses. We compare island density of small islands for two modes: PLD and continuous Molecular Beam Epitaxy (MBE) growth. Furthermore, by varying interactions energies, diffusion barrier and parameters of deposition, we compare results of simulations with the PLD experiment for Fe/Mo system.

O 36.48 Tue 18:30 P4

Rational design of two-dimensional metal-organic frameworks for functional catalysis — •Christopher Kley[1], Jan Cechal[1], Takashi Kumagai[1], Frank Schramm[2], Sebastian Stepanow[1], Mario Ruben[2], and Klaus Kern[1,3] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [3]École Polytechnique Fédérale de Lausanne, Institut de Physique de la Matière Condensée, 1015 Lausanne, Switzerland

The prospect of tailored metal-organic frameworks (MOF) by rational design makes them attractive candidates for functional structures. Here, we perform surface-confined bimetallic coordination with organic ligands to build-up two-dimensional MOFs with metal rich nanopores for heterogenous catalysts. We study the self-assembly and metal coordination of a rod-like organic ligand with transition metal atoms on Cu and Ag surfaces. The ligand comprises carboxylic and alkynyl functionalities for the selective binding of metal centers. By means of variable temperature scanning tunneling microscopy we observed substrate induced conformational changes of the organic molecule with strong molecular relaxations on the Cu(100) surface. Regular and open metal-coordination networks have been obtained with Fe centers coordinating preferably to the carboxylate oxygen atoms, while Ni atoms tend to bind to the alkynyl groups. This allows for the rational design of bimetallic coordination networks comprising different metal atoms for the structural and catalytic properties at surfaces.

O 36.49 Tue 18:30 P4

Epitaxial growth of hexagonal boron nitride monolayers by a three-step boration-oxidation-nitration process — •Frank Müller[1], Stefan Hüfner[1], Samuel Grandthyll[1], Hermann Sachdev[2], Stefan Gsell[3], and Matthias Schreck[3] — [1]Department of Experimental Physics, Saarland University, D-66041 Saarbrücken, Germany — [2]Inorganic Chemistry, Saarland University, D-66041 Saarbrücken, Germany — [3]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

The formation of well-ordered monolayers of hexagonal boron nitride on the surface of a Rh/YSZ/Si(111) multilayer substrate via a three-step boration-oxidation-nitration process was investigated by X-ray photoelectron spectroscopy (XPS), X-ray photoelectron diffraction (XPD) and low-energy electron diffraction (LEED). The chemical vapor deposition (CVD) of trimethylborate (BOCH3)3 results in a selective decomposition of the precursor leading to a dilute distribution of boron within the interstitials of the Rh lattice. After oxidation, the layer of a boron oxygen species of about 1 nm thickness can be transformed into a hexagonal monolayer of BN by annealing in an appropriate NH3 atmosphere. The results of the present study clearly show that the formation of BN monolayers is also possible when boron and nitrogen are provided successively from separate sources. This procedure represents an alternative routine for the preparation of well-ordered BN monolayers, which benefits from a strong reduction of hazardous potential and economic costs compared to the use of borazine as the current standard precursor. Phys. Rev. B 82, 075405 (2010)

O 36.50 Tue 18:30 P4

Epitaxial growth of hexagonal boron nitride on Ag(111) — •Frank Müller[1], Stefan Hüfner[1], Hermann Sachdev[2], Robert Laskowski[3], Peter Blaha[3], and Karlheinz Schwarz[3] — [1]Department of Experimental Physics, Saarland University, D-66041 Saarbrücken, Germany — [2]Inorganic Chemistry, Saarland University, 66041 Saarbrücken, Germany — [3]Institute of Materials Chemistry, Vienna University of Technology, A-1060 Vienna, Austria

The epitaxial growth of hexagonal boron nitride on a Ag(111) surface by chemical vapor deposition of borazine (HBNH)3 and trichlorborazine (ClBNH)3 is investigated by X-ray photoelectron spectroscopy (XPS) and low-energy electron diffraction (LEED). In contrast to other transition-metal surfaces of hexagonal symmetry, such as Ni(111), Rh(111), or Ru(0001), the hexagonal BN layers form domains of arbitrary orientation, independent on the precursor. This indicates that - with respect to the Ag(111) lattice - there is no preferred direction for the growth of BN. These results are in accordance with recent ab initio calculations that predict vanishing or at least very weak bonding energies for BN on (111) surfaces of noble metals. Phys. Rev. B 82, 113406 (2010)

O 36.51 Tue 18:30 P4

Surface Phases and Structure Determination of Thin Gold Films Grown on a Re($10\bar{1}0$) Surface — •Lyria Messahel, Christian Pauls, and Klaus Christmann — Institut für Chemie und Biochemie, FU-Berlin

Gold atoms deposited onto a clean Re($10\bar{1}0$) surface form, as a function of surface concentration, various submonolayer phases leading to $(1 \times n)$ LEED structures ($n = 3, 4, 5, 6$), the final one being a (1×1) phase associated with a pseudomorphic Au bilayer and a coverage of two monolayers ($\Theta = 2$) [1].

The first well-ordered Au overlayer structure is a (1×3) phase [1]. If we relate its coverage to the surface concentration of the full bilayer ($\Theta = 2$) we end up with a coverage $\Theta_{1\times3} = \frac{4}{3}$. LEED calculations have been performed for various Au surface geometries based on this coverage. However, a plausible ball model suggests an additional Au atom in the (1×3) unit cell, and a LEED I,V calculation has also been carried out for $\Theta_{1\times3} = \frac{5}{3}$. We will present the calculated I,V curves for both coverages and compare their structural parameters (geometrical displacements and thermal vibration amplitudes). An additional analysis of the Au(1×4) phase's experimental data will also be presented as a support to the assumption $\Theta_{1\times3} = \frac{5}{3}$.

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O 36.52 Tue 18:30 P4

Analysis of electrochemically inserted Lithium in metal electrodes — •Philipp Bach, Andreas Seemayer, and Frank Uwe Renner — Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf

Due to the very negative potential of Li, Li-ion batteries supply a high voltage and high energy density. Lithium ion batteries will continue to be the most important power source for mobile applications in the near future. For achieving longer lifetime and even higher capacity a more detailed knowledge of the basic processes is required. Li alloys with Si, Sn, or Ag provide anodes with higher capacities than the actually used graphite. We focus on the investigation of the electrochemical insertion process of Lithium into simple model anodes like polycrystalline discs or thin films. As electrolyte we use the ionic liquid 1-Butyl-1-methylpyrrolidinium bis(trifluoromethanesolfonyl)imide (PYR14TFSI) with 0.3M LiTFSI. The electrochemical processes, i.e. alloying and dealloying of the anode material, are characterised by Cyclic Voltammetry (CV). The chemical characterisation of the produced alloys is performed ex-situ by the means of Atom Probe Tomography (APT) and Secondary Ion Mass Spectrometry (SIMS). First in-situ measurements using a droplet cell for x-ray diffraction (XRD) experiments using synchrotron radiation are presented.

O 36.53 Tue 18:30 P4

Aufbau einer Magnetronsputteranlage zur Untersuchung dünner Schichten mit PAES, STM und XPS — •Elisabeth Lachner und Christoph Hugenschmidt — FRM II, TU München

In der vorliegenden Arbeit werden Oberflächenprozesse wie Bildung von Oberflächenlegierungen und Segregation untersucht. Neben Scanning Tunneling Microscopy (STM) und X-ray Photoelectron Spectroscopy (XPS) soll die extrem oberflächensensitive Positron-annihilation induced Auger-Electron Spectroscopy (PAES) zum Studium der Oberflächenprozesse genutzt werden. Mittels PAES ließ sich bereits die Segregation von Cu in Pd eindrucksvoll beobachten [Phys. Rev. Lett. 105, 207401 (2010), Mayer et al.].

Zur Herstellung von atomaren Schichten im Submonolagenbereich wird eine UHV-Probenpräparationskammer aufgebaut. Diese arbeitet mit drei Magnetronsputterkanonen, einem heizbaren Probenhalter, einem Pyrometer und einem Schichtdickencontroller. Im Rahmen dieses Beitrags soll das gesamte Spektrometer samt Erweiterungen wie eine drehbare Ausführung des Probenhalters für größere Gleichmäßigkeit der Materialdeposition vorgestellt werden.

O 36.54 Tue 18:30 P4

Vibrational properties of copper on Cu(111) — Heiner Maslosz, •Olaf Skibbe, and Annemarie Pucci — Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, D-69120 Heidelberg

In the context of understanding the properties of rough and defect-rich surfaces it is useful to be able to characterize the surfaces roughness. By the use of electron energy loss spectroscopy (HREELS) we examined the vibrational features of small amounts of copper on Cu(111) evaporated at liquid nitrogen temperature. We found after annealing to $\sim 160\,\mathrm{K}$ a vibration with an energy of 44 meV polarized perpendicular to the surface. This is an extraordinary high energy compared to the bulk phonon band. Upon annealing to temperatures above 200 K the peak disappears. The attribution of the vibration features to morphological changes upon annealing is ongoing work.

O 36.55 Tue 18:30 P4

Investigating metal phthalocyanine molecules on Cu(100) — •Sarah Fahrendorf[1], Christian Hahn[1], Frank Matthes[1], Claire Besson[1], Paul Kögerler[1,2], Claus M. Schneider[1], and Daniel E. Bürgler[1] — [1]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich — [2]Institut für Anorganische Chemie, RWTH Aachen

Magnetic molecules play an important role for the further evolution of spintronics to nanospintronics. Organic molecules, such as metal phthalocyanines, show promising properties for the field of nanospintronics due to (i) their electronic tunability e. g. by adding magnetic atoms to the centre or combining two or three single phthalocyanines, (ii) the high thermal stability and (iii) possible self-organization. For envisaged applications it is important to understand the interaction between the substrate and the molecules and its influence on the electronic and magnetic properties.

Here we study the electronic structure of single metal phthalocyanine molecules deposited on Cu(100) surfaces. We chose two different magnetic atoms and molecule configurations, namely iron phthalocyanine (FePc) and neodymium doubledecker phthalocyanine (NdPc2), to investigate the influence of the substrate on molecules with 3d and 4f like centres and different ligand environments of the central atoms. The molecules were sublimated from a Knudsen cell and in-situ characterized by surface science techniques. First results from scanning tunneling microscopy and spectroscopy are shown.

O 36.56 Tue 18:30 P4

Struktur und Dynamik von Metallclustern auf dielektrischen Substraten — •Bernhard Faber und Paul-Gerhard Reinhard — Institut für Theoretische Physik 2, Staudtstr. 7, 91058 Erlangen, Germany

Es wird die Deposition von kleinen Natriumclustern auf einer Ar(001)-Schicht, die auf einer Metallunterlage aufliegt, simuliert. Dabei wird ein hierarchisches Modell aus zeitabhängiger DFT und Molekulardynamik verwendet. Die Valenzelektronen der Natriumatome werden im Kohn-Sham Schema mit Selbstwechselwirkungskorrektur behandelt. Die Wechselwirkung zwischen den Edelgasteilchen und den Natriumionen wird durch Atom-Atom-Potentiale beschrieben und die Ankopplung an die quantenmechanischen Elektronen durch lokale Pseudopotentiale. Ein entscheidender Bestandteil des Modells ist die dynamische Polarisierbarkeit der Edelgasatome. Die optionale Metallunterlage wird durch die Methode der Bildladungen berücksichtigt.

Wir untersuchen den Einfluss der Bildladungskräfte der Metallunterlage und der Schichtdicke der Ar-Schicht auf Struktur, optischen Response und Depositionsdynamik von Na$_6$ und Na$_8$. Die Struktur der Cluster wird kaum beeinflusst; es gibt lediglich geringfügige Verschiebung des Abstands von Cluster zu Oberfläche. In der optischen Absorption bleibt die Position der Mie-Resonanz robust, wohingegen die Details der spektralen Fragmentierung sehr empfindlich auf jede Veränderung reagieren. Bei der Deposition der Cluster spielt die Bildladungskraft der Metallunterlage nur eine untergeordnete Rolle wohingegen die Dicke der Ar-Schicht die Dissipation stark beeinflusst.

O 36.57 Tue 18:30 P4

RHEED Study of grown AuSi Nanoparticles on Si(111) and deposited Cu Clusters — •Stephan Bartling, Hannes Hartmann, Vladimir Popok, Ingo Barke, Kristian Sell, Stefan Polei, Viola von Oeynhausen, and Karl-Heinz Meiwes-Broer — Institut für Physik, Universität Rostock, 18051 Rostock, Germany

The contribution focuses on *in situ* reflection high energy electron diffraction (RHEED) of grown AuSi nanoparticles on Si(111) and deposited Cu clusters. After Au deposition of >1ML on vicinal Si(111) three-dimensional gold-rich AuSi nanoparticles are formed via Stranski-Krastanov growth. A mean particle height of 5.8nm has been determined from large-scale STM images for $\approx$ 3ML Au. The RHEED diffraction pattern can be modeled by a quasi close-packed structure with rhombohedral unit cell [1]. We do not observe flat top facets reported for similar preparation conditions [2]. This is in agreement with the crystal orientation determined by RHEED.

First experimental results of RHEED investigations on deposited Cu clusters produced by a magnetron sputtering source are presented. The evolution of diffraction features for different sample treatments (heating, oxygen exposure) is discussed. The analysis is supported by ex-situ AFM measurements.

[1] S. Bartling et al., submitted to Eur. Phys. J. D

[2] E. Moyen et al., Appl. Phys. Lett. 94, 233101 (2009)

O 36.58 Tue 18:30 P4

Ultra-High Vacuum Cluster Deposition for in-situ RHEED Studies — •Hannes Hartmann, Vladimir Popok, Stephan Bartling, Ingo Barke, and Karl-Heinz Meiwes-Broer — Institut für Physik, Universität Rostock, 18051 Rostock, Germany

Clusters and nanoparticles deposited on surfaces are of significant interest for applications in electronics, data storage, spintronics, plasmonics, and catalysis. Among a variety of methods for particle production the cluster-beam technique in connection with size selection offers several advantages. Particularly magnetron sputtering is nowadays a well established technique widely used for the production of continuous cluster beams of various species. The design and construction of a compact and flexible cluster-deposition setup is presented. Key elements are a commercial magnetron-sputtering cluster source, a five-stage differential pumping scheme, online flux measurement, and simple ion guiding. It is optimized for deposition of size-selected metal clusters ranging from a few atoms to more than 20 nm in diameter on atomically clean substrates in ultra-high vacuum. Characterization is done by flux measurement and ex-situ microscopy (AFM, TEM). First results of in-situ RHEED investigations of deposited copper nanoparticles on atomically clean surfaces are presented.

O 36.59 Tue 18:30 P4

Synthesis of vanadium oxide nanoparticles and characterization by TEM — •Christina Kunzmann, Aladin Ullrich, Matthias Klemm, Michael Krispin und Siegfried Horn — Lehrstuhl für Experimentalphysik II, Universität Augsburg, D-86135 Augsburg

We have synthesized vanadium oxide nanoparticles by thermal decomposition of vanadylacetylacetonate ($VO(acac)_2$) on a highly oriented pyrolytic graphite substrate under Ar/H_2 atmosphere. Particles were analyzed by high resolution transmission electron microscopy (HRTEM) and atomic force microscopy (AFM). Chemical composition of the particles was confirmed by TEM energy dispersive x-ray analysis (EDX). Our analysis shows that the degree of crystallinity as well as the morphology depends on the reaction parameters, e.g. temperature and concentration. For low concentrations of $VO(acac)_2$ the particle size varies between 9 and 17 nm. With increasing concentration of $VO(acac)_2$ the particle size increases and particle size distribution broadens. Particles with cubic section exhibit lattice spacing in agreement with V_2O_3. In addition, for high concentration samples, rod-like particles are found, which show a different crystalline vanadium oxide phase.

O 36.60 Tue 18:30 P4

Controlled coupling of interface quantum well states — •Willi Auwärter[1], Knud Seufert[1], David Ecija[1], Niveditha Samudrala[1], Saranyan Vijayaraghavan[1], Sushobhan Joshi[1], F. Javier Garcia de Abajo[2], and Johannes V. Barth[1] — [1]Physik Department E20, Technische Universität München, 85748 Garching, Germany — [2]Instituto de Optica, CSIC, 28006 Madrid, Spain

The confinement of surface state electrons in artificial nanostructures permits exploring and visualizing fundamental aspects of quantum mechanics. Here, we introduce a new approach to engineer quantum wells by combining a scanning tunneling microscope manipulation technique with recipes for molecular self-assembly on surface-state-supporting surfaces. Following this procedure, we can not only fabricate resonators of varying size, but also build specific arrangements of quantum wells, such as dimers or one-dimensional chains. The electronic structure of such coupled systems, representing artificial molecules, is studied by local scanning tunneling spectroscopy. Hereby, the scattering characteristics of the potential walls enclosing the wells are determined by the molecules employed as barriers. In particular, we compare quantum well states in free-base and metalated porphyrin arrays on Ag(111). The experimental data on the electron confinement and the coupling of quantum wells are corroborated by boundary element method calculations. These simulations might also be used to design structures with specific electronic properties.

O 36.61 Tue 18:30 P4

Template-Assisted Growth of Regular Arrays of One-Dimensional Nanostructures using Anodic Aluminum Oxide Membranes — •Huaping Zhao[1,2], Fabian Grote[1,2], Feng Xu[1,2], Shikuan Yang[1,2], and Yong Lei[1,2] — [1]Institute of Materials Physics, University of Muenster — [2]Center for Nanotechnology, Muenster 48149

Organic one-dimensional (1D) nanostructures represent attractive building blocks for nano-scale optoelectronic devices because they behave in a unique way that differentiates them from the isolated molecule or the bulk. The synthesis of such organic nanostructures with good control of both size and morphology is still a challenge due to the weak intermolecular interactions in organic molecules compared with those in inorganic materials. Anodic aluminum oxide (AAO) membranes are excellent templates for fabricating organic 1D nanostructures with high arrangement regularity, variable length and diameter. The highly ordered nano-sized channels of the AAO templates force the organic molecules to assemble within a well-defined space. Moreover, the AAO templates are thermal and mechanical stable as well as resistant to organic solvents. By using a combination of solvent saturation and low temperature solvent annealing process, crystalline organic semiconductor nanowires were fabricated with AAO as template. Besides the organic nanostructures, ordered 1D nanostructure arrays of other materials were also synthesized in our group, including different semiconductors and metals.

O 36.62 Tue 18:30 P4

Cutting Carbon Nanotubes and Graphene — •Cornelius Thiele and Ralph Krupke — Institut für Nanotechnologie, Karlsruhe Institut für Technologie (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen

A new technique to locally oxidize carbon-based materials at the nanometer scale is presented. In an oxygen atmosphere, an electron beam is scanned across the material. Secondary electrons ionize the oxygen and induce oxidation around the focal point. Here the formation of trenches in graphene sheets and cuts across carbon nanotubes is shown. These gaps could provide means to contact single molecules. In-situ electrical measurements are used to characterize the cutting process.

O 36.63 Tue 18:30 P4

Contacting of individual InAs nanowires without photoresist — •Kilian Flöhr[1,3], Marcus Liebmann[1,3], Kamil Sladek[2,3], Hilde Hardtdegen[2,3], Thomas Schäpers[2,3], Detlev Grützmacher[2,3] und Markus Morgenstern[1,3] — [1]II. Institute of Physics, RWTH-Aachen University, 52074 Aachen — [2]Institut für Bio- und Nanosysteme (IBN-1), Forschungszentrum Jülich, 52425 Jülich — [3]Jülich Aachen Research Alliance (JARA)

We investigated methods to spacially control InAs nanowires on a substrate using micromanipulators attached to an optical microscope with the goal of producing InAs tips for scanning tunneling microscopy. The wires, which were grown by metalorganic vapor phase epitaxy (MOVPE) on a GaAs wafer without catalysts, could be picked up individually using a sharp indium tip exploiting adhesion forces. Later,

the wires were placed onto a desired position somewhere on or at the edge of a double cleaved wafer. Contacting the wires was accomplished using indium microsoldering [1] or electron beam induced deposition [2], since standard lithographic methods are not possible close to the wafer edge due to non-uniform photoresist thickness. Several variations of contacting the wires and optimizing the InAs/metal interface were tested and ohmic contacts could be realized.
[1] C. Ö. Girit and A. Zettl, Appl. Phys. Lett. 91, 193512 (2007).
[2] S. Bauerdick and C. Hierold, J. Vac. Sci. Technol. B 24, 3144 (2006).

O 36.64 Tue 18:30 P4

The resistance of single atomic steps in ultrathin Pb nanowires on Si(557) — Jan Rönspies, •Lisa Kühnemund, Svend Wiessell, and Herbert Pfnür — Leibniz-Universität Hannover, Inst. f. Festkörperphysik

We studied the local electronic transport properties of a monolayer thick Pb wire by local potentiometry with the tip of a tunneling microscope. 50-nm-wide wires on bare Si(557) were generated by direct writing with an electron beam in an ultrathin film of SiO$_2$ using the process of electron-beam-induced selective stimulated thermal desorption of oxygen (EBSTD) in combination with a shadow mask technique and macroscopic TiSi$_2$ contacts. The resistivity of this wire agrees well with expectations derived from anisotropic monolayer thick Pb films on Si(557). Although small Pb clusters nucleated during annealing and desorption of excess Pb, they had a negligible effect on the local resistive properties of the wire. Steps in the substrate of atomic height apparently do not interrupt the conducting path, but due to local scattering at step edge states increase the local resistivity by more than one order of magnitude. Furthermore, a systematic study of the resistance as a function of the lateral width of the wires revealed an effective conducting width, which is about 3 nm smaller on both sides than the geometrically determined width. In addition, we found deviations from Ohm's law at widths below 20 nm.

O 36.65 Tue 18:30 P4

Na adsorption on In/Si(111)-(4x1) nanowires: electron transport and structural properties — •Martin Babilon, Christian Thierfelder, Stefan Wippermann, and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn, 33098 Paderborn, Germany

Quasi one-dimensional structures, such as artificial atomic-scale wires, have attracted considerable attention recently [1,2]. They do not only show fascinating physical properties, but also have a large technological potential, e.g., as atomic-scale interconnects. Highly anisotropic surface superstructures are suitable model systems to explore atomic-scale wires both experimentally and computationally. The In/Si(111)-(4x1) surface [3] is probably the most intensively investigated system in this context. Here we present first-principles calculations on the adsorption geometries and the influence of Na adatoms on the Landauer conductance of these In nanowires. Our findings with regard to structural properties confirm the results by Kleinman et al. [4]. Additionally, we discuss the implications of the Na adatoms on the temperature induced (4x1) -> (8x2) phase transition [5].

[1] N. Nilius, T. M. Wallis and W. Ho, Science 297, 1853 (2002).
[2] A. Calzolari et al., Phys. Rev. Lett. 93, 096404 (2004).
[3] O. Bunk et al., Phys. Rev. B 59, 12228 (1999).
[4] J.-H. Cho et al., Phys. Rev. B 66, 075423 (2002).
[5] H. Morikawa et al., Phys. Rev. B 81, 075401(2010).

O 36.66 Tue 18:30 P4

Temperature-Dependent Ordering in Au-induced Chains on Ge(001) — Christian Blumenstein[1], •Sebastian Mietke[2], Jörg Schäfer[1], Sebastian Meyer[1], Michael Lochner[2], René Matzdorf[2], and Ralph Claessen[1] — [1]Physikalisches Institut, Universität Würzburg — [2]Institut für Physik, Universität Kassel

Atomic nanowires may be formed by self-organization on a semiconductor surface. Their structure and the resulting quasi-one-dimensional character is determined by the choice of metal adatom and the substrate material. It is commonly believed that many of these systems will undergo a Peierls instability upon cooling. Here we scrutinize nanowires realized by Au chains on Ge(001) to investigate the potential occurrence of lattice instabilities. In combining scanning tunneling microscopy with electron diffraction, we find a phase transition, notably occurring at elevated temperature. It is of second order, and leads to a complex ordering with transversal elongations in addition to the $c(8\times2)$ reconstruction. However, since it lacks the electronic prerequisites, such as a nesting condition or an energy gap, this excludes a Peierls scenario. Instead, this transition points at cooperative interactions of charge and lattice including the substrate. As important consequence, these chains remain metallic even at low temperature.

O 36.67 Tue 18:30 P4

Investigation of a Single Chiral Nano-Structure — •Paweł Woźniak[1,2], Peter Banzer[1,2], Katja Höflich[3,4], Silke Christiansen[1,3], and Gerd Leuchs[1,2] — [1]Max Planck Institute for the Science of Light, Günther-Scharowsky-Str. 1, D-91058 Erlangen, Germany — [2]Institute of Optics, Information and Photonics, University Erlangen-Nuremberg, Staudtstr. 7/B2, D-91052 Erlangen, Germany — [3]Institute of Photonic Technology, Albert-Einstein-Str. 9, D-07745 Jena, Germany — [4]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany

It was shown just recently that polarization tailored light beams can be used as a versatile tool for investigating the resonance behavior and the optical properties of single nano-structures in detail [1]. We now apply this technique to investigate the properties of single three-dimensional chiral nano-particles namely nanoscopic spirals experimentally. The use of polarization tailored light beams allows for the realization of different coupling scenarios. Due to their chirality the single nanospirals show for instance different response to left- and right-handed circularly polarized light. Experimental results for different excitation schemes and structure designs are presented.

[1] Peter Banzer, Ulf Peschel, Susanne Quabis, and Gerd Leuchs, "On the experimental investigation of the electric and magnetic response of a single nano-structure," Optics Express 18, 10905-10923 (2010)

O 36.68 Tue 18:30 P4

template fabrication of highly ordered arrays of organic semiconductor nanowires — •Christian Heckel, Stefan Ostendorp, Yong Lei, and Gerhard Wilde — Institut fuer Materialphysik, Wilhelm - Klemm - Str. 10, 48149 Muenster

Porous alumina membrane (PAM) is a widely used template for the fabrication of highly ordered arrays of one-dimensional (1D) nanostructures. The structural parameters of the PAMs are adjustable, including the pore diameter and spacing, and the thickness of the membranes. And thus the structures of the 1D nanomaterials prepared using PAMs can be controlled.

On the other hand, the investigation of organic semiconductors opens a new field of applications in computer technology like twistable displays or printing integrated circuits.

In the current work, these two technologies are combined by depositing organic n-type semiconductors into the pores of PAMs using different synthesizing processes such as molecular evaporation and solution-phase self-assembly. As a result, highly ordered arrays of organic semiconducting wires are obtained within the pores with a diameter of about 50 nm, which indicates that it is possible to fill the pores with organic materials.The properties of these "filled" membranes are characterized by measuring the electrical properties of several nanowires pooled together and also of single nanowires by AFM-based methods.

[1] Y. Lei, W. Cai, G, Wilde, Prog. Mater. Sci., 52, 465 (2007).
[2] J. Puigdollers, Thin Solid Films, 517, 6271 (2009).
[3] A. L. Briseno, Nano Lett., 7, 2847 (2007).

O 36.69 Tue 18:30 P4

Fabrication of tungsten oxide nanotube arrays in porous alumina membranes by a sol-gel-process — •Stefan Bartels[1,2], Hui Sun[1,2], Yong Lei[1,2], and Gerhard Wilde[1,2] — [1]Institut für Materialphysik, WWU Münster — [2]Center for NanoTechnology, Münster

Tungsten oxide (WO3) is a suitable material for gas sensing applications relying on the change of conductivity by adsorped molecules. Regular arrays of nanotubes provide a large surface area and promise very high sensitivity. This work presents the production of such nanotube arrays with the potential of tuning the surface area by sol-gel-deposition of WO3 in porous alumina membranes (PAM) from the precursors tungsten hexachloride (WCl6) and acetylacetone (C5H8O2). Dimensions and composition of the nanotubes are characterized by SEM and EDX, their sensing properties for CO and NO2 will be investigated.

O 36.70 Tue 18:30 P4

Selective Growth of Si Nanorods on Si Surfaces — L. Kühnemund[1], •K. Meyer auf der Heide[1], C. Tegenkamp[1], H. Pfnür[1], R. Brendel[2], and J. Schmidt[2] — [1]Leibniz Universität

Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover — [2]Institut für Solarenergieforschung Hameln, Am Ohrberg 1, 31860 Emmerthal

The growth of silicon nanorods and in particular of highly ordered arrays of nanorods on surfaces are promising concepts for improving further the efficiency of photovoltaic devices. From a fundamental point of view such antenna structures in combination with ultra-thin metallic films or quantum wires are interesting assemblies for the study of opto-electrical conversion in low dimensional systems. However, the transition between the surface and the vertically grown rods is decisive.

In this study the morphology, the chemical composition of the rods and its vicinity as well as the transport properties of single rods have been investigated by means of a combined SEM-STM system. The Si-rods were grown via the VLS mechanism using metallic clusters (Au, Al) as catalyzer and silane as CVD precursor gas. Selective growth single rod structure was realized using electron beam lithography. It was found that after growth of the rods with diameters in between 100 nm and 1 μm, the area around the rod (1-2 μm) is contaminated with Au. As such effects limit the lifetimes of electron-hole pairs in photovoltaic cells other VLS catalyst materials such as Al, which forms only shallow acceptor states in Si, have been studied as well.

O 36.71 Tue 18:30 P4

Conservation of hexagonal order during photochemical particle growth and its application to SiO_2 nanostructuring — •Axel Seidenstücker, Burcin Özdemir, Alfred Plettl, and Paul Ziemann — Universität Ulm, Institut für Festkörperphysik, 89069 Ulm (Germany)

Recently, we reported on a photochemically controlled growth of metallic nanoparticles which initially formed hexagonally ordered arrays [1]. During the growth process, however, some of the particles are displaced from their original position. In this contribution we will report on how the hexagonal order can be conserved and the particle enlargement extended up to 50 nm. It turned out that coating the Au seed particles by a thin layer of OTMS their hexagonal order is practically conserved during each photochemical growth step. The resulting ordered and size controlled particle arrays where used as a starting point for subsequent nanostructuring SiO_2 surfaces by reactive ion etching (RIE). In this way, well defined nanoscaled pillars and pores are obtained.

T. Härtling, A. Seidenstücker, P. Olk, A. Plettl, P. Ziemann and L. M. Eng, Nanotechnology 21, 145309 (2010)

O 36.72 Tue 18:30 P4

A combination of pulsed laser interference and block copolymer micelle lithography — •Fabian Enderle[1], Alfred Plettl[1], Paul Ziemann[1], Stephen Riedel[2], Johannes Boneberg[2], Paul Leiderer[2], and Elke Scheer[2] — [1]Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm — [2]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz

A basic goal of surface nanopatterning is to provide possibilities to ”write” lateral patterns decorated with e.g. metallic nanoparticles (NPs) as opposed to homogeneously decorated surfaces. The latter type of NP coating can be accomplished by exploiting the self-organization of precursor loaded diblock-copolymers forming reverse spherical micelles in apolar solvents. After optimized dip-coating a surface and removing the polymer matrix by oxygen/hydrogen plasma treatments, one finally obtains homogeneous hexagonally ordered arrays of metallic NPs. To add lateral patterning, one may try to influence the wetting behavior of the micelle containing solution. For this end, first an OTS-SAM (octadecyltrichlorosilane) is prepared on the surface and exposed to a nanosecond pulsed laser interference pattern. Above a certain energy density of the laser, the related temperature pattern will remove SAM molecules in the high temperature regions by thermal desorption. It will be demonstrated that upon dip-coating the micellar solution on top of such a laser pre-patterned surface a corresponding deposition contrast of metal NPs can be achieved.

O 36.73 Tue 18:30 P4

Gold nanoparticle arrays generated by modified Electron Beam Lithography and their applicability to plasmonic sensors — •Susan Derenko[1], Jochen Grebing[2], and Thomas Härtling[1] — [1]Fraunhofer Institute for Non-Destructive Testing, Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden

Gold nanoparticle arrays manufactured by a modified Electron Beam Lithography method are presented. The method allows to write highly ordered dot structures with a dot size of 50 nm and total area of 4 x 4 mm in a reasonable time.

The arrays are evaluated with respect to the desired application as plasmonic sensors. Therefore the uniformity of the particles created by the modified method is investigated. Using far-field optical spectroscopy the sprectral position and FWHM of the surface plasmon resonance (SPR) of the arrays are determined. Influences of plasmonic coupling effects on the SPR properties of closely packed array structures are elucidated by comparing the results to single particle SPR spectra. The experiments are conducted on arrays with different interparticle spacings.

O 36.74 Tue 18:30 P4

Accomodation of molecular guests in adaptive 2D nanoporous metal-organic networks — •David Ecija[1], Saranyan Vijayaraghavan[1], Willi Auwärter[1], Sushobhan Joshi[1], Knud Seufert[1], Claudia Aurisicchio[2], Davide Bonifazi[2], Kentaro Tashiro[3], and Johannes V. Barth[1] — [1]Physik Department E20, Technische Universität München, D-85748 Garching, Germany — [2]Department of Chemistry, University of Namur, B-5000 Namur, Belgium — [3]National Institute for Materials Science, Tsukuba 305-0044, Japan

Flexibility in host frameworks is a key issue regarding their molecular recognition capabilities. The impact of guest species on the host structure ranges from conformational variation to pronounced structural changes. Here we report the usage of a glassy supramolecular porous network on Cu(111) to spatially organize and control CO and Ce(TPP)2 guest molecules, the latter representing molecular rotors. For the assembly of the host lattice a de novo synthesized molecule with three-fold symmetry was employed, featuring three terminal pyridyl groups. By STM experiments we show the flexibility of the realized open network where a local variation of the pore shapes can be induced. In order to assess the host-guest adaptability, we dose molecular species of different size. We study the selective accommodation of the guests in pores of different shape and geometry. Whereas the host network behaves as a rigid entity in the uptake and removal of CO, preliminary results signal that the dosing of Ce(TPP)2 species entails an adaptive response of the porous network towards the guest species.

O 36.75 Tue 18:30 P4

Selforganized periodic 2D-Nanotemplates in Surfactant Mediated Epitaxy of Ge on Si(111) — •Claudius Klein, Martin Kammler, and Michael Horn-von Hoegen — Department of Physics & Center for Nanointegration Duisburg Essen (CeNIDE), University Duisburg-Essen, D-47057 Duisburg, Germany

Surfactant mediated growth of epitaxial Ge heterofilms on Si(111) is utilized to create selforganized 2-dim. ordered nano templates. Using Sb as surfactant a honeycomb pattern like reconstruction of 4 x 4 nm size is formed between 1 - 2 bilayer Ge coverage. Employing the spot width in SPA-LEED the degree of order in the honeycomb pattern has been optimized at a growth temperature of 700°C. STM studies confirm the increase of periodicity with growth temperature. Relaxed Ge films were grown using Bi as surfactant at 450°C. For coverages above 4 bilayers of Ge the lattice mismatch of 4.2% is then accommodated by the formation of a 2-dim. ordered hexagonal dislocation array confined to the hetero interface. Each dislocation is surrounded by a strain field causing a lateral and vertical distortion of the film. The vertical displacement field causes a height undulation of about 1 Å of the surface which becomes apparent in LEED by spot splitting. The lateral displacement fields have been explored in STM and their amplitude determined by highly sophisticated image analysis. Above an interfacial dislocation line the lattice parameter of the Ge film is expanded by more than 10% with respect to the bulk value. Inbetween two dislocation lines the Ge is still compressed to the Si lattice parameter.

O 36.76 Tue 18:30 P4

DFT study of Mn-oxide nanostructures on vicinal Pd surfaces — Cesare Franchini[1] and •Raimund Podloucky[2] — [1]Faculty of Physics, Univ. Vienna — [2]Faculty of Chemistry, Univ. Vienna

The research of oxide-metal hybrid structures with reduced dimensionality is of interest for nanotechnology. By means of density functional theory (DFT) we study the formation and the physical characterization of MnO_x nanostructures on the Pd (1 1 17), (1 1 19) and (1 1 21) vicinal surfaces[1]. Experimentally it is found that the deposition of 0.1 ML of Mn atoms followed by oxidation, results in a regular decoration of the Pd step edges by mono-atomic rows of MnO$_x$ structures which coexist with an oxygen-induced p(2×2) reconstruction on the flat terraces. The complete coverage of the (1 1 17) and (1 1 19) vicinal surfaces by Mn-oxide (0.75 ML) leads to the formation of a well ordered c(4×2)-Mn$_3$O$_4$ superstructure accompanied by a substrate-refaceting towards a (1 1 21) surface. On the basis of the calculated surface phase diagram and STM simulations the full structural and compositional details as well as the electronic properties of the Mn-oxide nanostructures are resolved and interpreted at low (Mn-oxide nanowires) and high (c(4×2)-Mn$_3$O$_4$) coverage.

[1] F. Li, F. Allegretti, S. Surnev and F. P. Netzer, Surf. Sci. **604**, 143-147 (2010).

O 36.77 Tue 18:30 P4

Production and electrical properties of nano and micro structures on graphite surfaces — •Lukas Patryarcha[1], Karl Bauer[1], Sven Bauerdick[2], Lars Bruchhaus[2], and Heinz Hövel[1] — [1]TU Dortmund, Experimentelle Physik I — [2]Raith GmbH, Dortmund

Nano structures on HOPG surfaces were produced by using focused Ga^+ ion beams (FIB, 10nm beam width). Nano structures were produced either using high doses by a direct milling process with a structure depth up to 300nm or after a low dose exposure by an additional oxidation process with Ar/O_2 (2% O_2) at 770K for 3h where the structure depth abruptly increases at a critical ion dose of 15-20μAs/cm^2 to values between 50-70nm dependent on the acceleration voltage. Structuring on thin (0.1μm) but large (2.5mm^2) HOPG films on an insulating mica slice create structures without electrical contact to the rest of the HOPG sample. The purpose of the project is to control the production process of these structures and to measure their physical properties using AFM and four-point measurements for nano and micro scaled structures.

O 36.78 Tue 18:30 P4

Electron Beam Induced Surface Activation Lithography on Silicon Oxide, Silicon Nitride and Titanium Oxide — •Marie-Madeleine Walz, Florian Vollnhals, Florian Rietzler, Michael Schirmer, Hubertus Marbach, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Friedrich-Alexander-University Erlangen-Nuremberg, Egerlandstr. 3, 91058 Erlangen

Recently, we were able to demonstrate that a focused electron beam can be used to locally activate SiO$_x$ to allow for a new kind of nanoscale lithography. In contrast to the established direct write technique electron beam induced deposition (EBID), where a precursor gas adsorbs on a substrate and is decomposed locally by a focused electron beam, in electron beam induced surface activation (EBISA) the e-beam is used to locally activate the surface. In a second step a precursor gas is introduced and may decompose at the activated areas. In combination with a precursor that exhibits autocatalytic growth effects, like Fe(CO)$_5$, this can be used to fabricate nanostructures on surfaces [1].

In the present work we expand the EBISA concept to other substrates, i.e, ultrathin Si$_3$N$_4$ membranes and a TiO$_2$ single crystal. The basic principle of EBISA and the corresponding experimental results will be presented and discussed.

This work was supported by the DFG through grant MA 4246/1-1.

[1] M.-M. Walz et al., Angew. Chem. Int. Ed. 49 (2010), 4669

O 36.79 Tue 18:30 P4

Growth of nanostructures for multi-tip STM investigations — •Marcus Blab, Vasily Cherepanov, and Bert Voigtländer — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology

The main field of research of a multi-tip STM is the investigation of self assembled conducting nanostructures. The study of silicide nanostructures is often a benchmark test for a multi-tip STM. Therefore, we searched for the ideal parameters to grow MnSi-nanowires on a Si(111)-7x7 surface. 2 μm long MnSi-nanowires occur at a sample-temperature of 590 °C and a low deposition rate of 0.13 ML/min. These nanowires with typical diameters and height of $\sim$20 Å are ideal to contact and investigate their electrical properties by a multi-tip STM.

Small defects in epitaxial layers can be used to search for the Landauer conductivity dipole. Defects which occur by depositing Bi on Si(111)-7x7 at RT, are of the size between 10-100 nm. To reduce the defect-size we deposit small Si-cluster on a flat Bi-layer, which change the surface state. These defects can be explored by scanning tunneling potentiometry using a multi-tip STM.

O 36.80 Tue 18:30 P4

Probe-based thermomechanical direct-writing — •Felix Holzner, Philip Paul, Cyrill Kuemin, Michel Despont, Heiko Wolf, Armin Knoll, and Urs Duerig — IBM Research GmbH, Rueschlikon, Switzerland

A probe-based patterning method is presented. The presence of a hot tip leads to a local material desorption from specific organic resists. Structures with a half-pitch of 8 nm have been fabricated. Moreover, 3D patterns can be written by controlling the amount of material removal at each pixel. The method can reach patterning speeds comparable to electron beam lithography (so far a pixel rate of 400kHz).

The poster shows the principle of the patterning process as well as studies of the kinetics of the material evaporation.

Furthermore it is shown how the written 3D structures can be used as traps to catch and align gold nanorods (25 x 75 nm) using Capillary Assembly.

O 36.81 Tue 18:30 P4

Manipulation of Rashba-split surface states in PbAg$_2$/Ag(111) by rare-gas and alkali metal adsorption — •Arne Buchter[1], Hendrik Bentmann[1], and Friedrich Reinert[1,2] — [1]Universität Würzburg, Experimentelle Physik VII, Am Hubland, D-97074 Würzburg, Germany — [2]Karlsruhe Institute of Technology, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe, Germany

Surface alloys like BiAg$_2$ or PbAg$_2$ show a huge Rashba-splitting in their 2D electronic structure. But unlike in the BiAg$_2$-case the exact size of the splitting for the PbAg$_2$-alloy is not yet clearly determined since in the latter case the spin-split bands are not fully occupied. Using angle-resolved photoelectron spectroscopy we studied the PbAg$_2$ surface alloy after Xe adsorption and evaporation of alkali metals. Xe adsorbes in a 9x9 reconstruction [1] and backfolding of the electronic bands is clearly visible. Electron doping via adsorption of alkali metals (K, Cs) allows for a continuous band-shift towards higher binding energies [2]. The aim of our study is to gain further insight into the actual size of the splitting, the character of these electronic states and to tune the spin topology at the Fermi level.

O 36.82 Tue 18:30 P4

Growth mode and evolution of electronic properties for Bi$_{1-x}$Sb$_x$ alloys on W(110) — •Thomas Eelbo, Mike Gyamfi, Marta Waśniowska, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Jungiusstr. 11a, D-20355 Hamburg

Recent experiments show that the alloy of bismuth and antimony is a prominent example for topological insulators[1]. In order to systematically study the properties of Bi$_{1-x}$Sb$_x$ alloys on W(110), we firstly report on the early stage of Bi and Sb growth on W(110). The LEED and STM measurements reveal that Bi and Sb grow ordered in the pseudocubic (001) orientation. The growth mode was found to vary with thickness and temperature of the deposition for both films. For Bi thick films we observe prominent peaks in dI/dU spectra at -0.35 eV, +0.4 eV, +0.7 eV. However, for thick films of antimony a characteristic peak is observed at +0.6 eV. Furthermore we studied the growth mode and evolution of electronic properties of Bi$_{1-x}$Sb$_x$ alloys. The LEED images for different alloys exhibit hexagonal patterns, indicating (111) surfaces and STM topographies show a two-dimensional growth mode. STS measurements performed on the Bi$_{1-x}$Sb$_x$ alloy films on W(110) are consistent with the electronic structure obtained on the single crystal surface[1].

[1] P. Roushan *et al.*, *Nature* **460**, 1106 (2009)

O 36.83 Tue 18:30 P4

Geometric spin-Hall effect of light in highly focused vector beams — •Martin Neugebauer[1,2], Peter Banzer[1,2], Thomas Bauer[1,2], Andrea Aiello[1,2], Norbert Lindlein[2], and Gerd Leuchs[1,2] — [1]Max Planck Institute for the Science of Light, Günther-Scharowsky-Str. 1, D-91058 Erlangen, Germany — [2]Institute of Optics, Information and Photonics, University Erlangen-Nuremberg, Staudtstr. 7/B2, D-91052 Erlangen, Germany

Optical angular momentum plays a key role in many fundamental and applied research areas. One example for its appearance is the spin Hall-effect of light (SHEL). The SHEL amounts to the split of a linearly polarized light beam at an interface into its two right- and left-handed circularly polarized components.

In a recent paper [1] it has been shown that in a beam observed from a tilted reference frame a polarization dependent intensity shift of the Barycenter is found. This can be interpreted as a purely geometric effect (gSHEL).

We investigate this gSHEL in highly focused vector beams. The highly focused beam consists of left-handed and right-handed circularly polarized light generated by a split aperture. We use a sub-wavelength nano-particle for probing the focal field distribution experimentally. First results of these measurements are shown and compared to analytical calculations.

[1] A. Aiello et al., PRL 103, 100401 (2009)

O 36.84 Tue 18:30 P4

Standing-wave excited hard x-ray phototemission studies on a Au-sandwiched Fe/MgO interface — Sven Döring[1], •Christoph Keutner[1], Frank Schönbohm[1], Ulf Berges[1], Daniel E. Bürgler[2], Mihaela Gorgoi[3], Franz Schäfers[3], Claus M. Schneider[2], and Carsten Westphal[1] — [1]DELTA/Experimentelle Physik I, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund — [2]IFF-9, Forschungszentrum Jülich, 52425 Jülich — [3]Helmholtzzentrum Berlin für Materialien und Energie, Albert Einstein Str. 15, 12489 Berlin

Magnetic tunnel junctions (MTJs) consisting of a thin layer-stack of Fe/MgO/Fe show a high tunnel-magneto resistance (TMR) ratio at room temperature. The strength of this effect is mainly driven by the interface and thus the Fe/MgO interface has been subject of many studies during the last years. Quite recently, calculations predicted an even higher TMR ratio for modified interfaces [1]. In that work it was proposed that a monolayer of Au at the interface prevents the oxidation of the Fe-layer, and thus an increase of the TMR effect is expected. Up to now there is no experimental evidence that a well-defined Au monolayer can be prepared with the objective of preventing the Fe oxidation at the interface. In this work we studied a Au-modified interface with standing-wave excited hard x-ray photoemission. The goal of this study was the determination of the effective roughness of the Au layer. Our data-analysis shows that Au does not grow as a protective monolayer nor any hint of FeO formation was found.

[1] J. Mathon and A. Umerski, Phys. Rev. B **71**, 220402 (2005)

O 36.85 Tue 18:30 P4

Coordination defects at the Si/SiO_2 interface investigated via ab initio g-tensor calculations — •Martin Rohrmüller, Uwe Gerstmann, and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn, 33098 Paderborn, Germany

The interface between silicon and SiO_2 and its defects such as the $\mathrm{P_b}$ centers are technologically highly relevant and intensively investigated. Electron paramagnetic resonance (EPR) gives a magnetic fingerprint of the centers including the electronic g-tensor and the hyperfine splittings.

The so-called $\mathrm{P_{b1}}$ center at the $Si(100)$ surface is characterized by a strongly anisotropic g-tensor. Interestingly, the angular average coincides exactly with the EPR-resonance found in hydrogenated μc-$Si{:}H$. In order to clarify if this coincidence is simply by chance, we calculate the elements of the electronic g-tensor for surface states and several oxidation stages from first principles, using the gauge-including projector augmented plane wave (GI-PAW) approach in the framework of density functional theory.

We find that (1) hydrogen adsorption at the $Si(100)$ surface influences the magnetic signature of the material dramatically, whereby a large variety of g-tensors is obtained. (2) After oxidation, however, the g-tensors do not change considerably. The g-tensors resemble those of hydrogenated Si surfaces if the surface atoms are coordinated in the same way. This holds for all investigated surface states and the complete EPR fingerprint suggesting this technique to probe sensitively the crystalline part of the interface structures.

O 36.86 Tue 18:30 P4

A novel electron spectrometer for surface magnon scattering — •Rajeswari Jayaraman, Lutz Baumgarten, Bernd Küpper, Harald Ibach, and Claus Michael Schneider — Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

Technical improvements in electron energy loss spectroscopy have enabled studies on the dispersion of spin waves (magnons) [1]. The previously designed spectrometer for surface magnon scattering featured a 90°/180° monochromator section and had the spin orientation perpendicular to the scattering plane and parallel to the surface [2]. Based on a calculation of the electron optical properties [3] we have designed a new electron spectrometer with spin orientation longitudinal to the electron beam and have implemented this spectrometer into an experimental set-up for studies on magnetic thin films. In agreement with theoretical calculations, a current of 3nA in direct beam has been achieved at 11meV resolution which is 6 times larger than for the previous instrument. First experimental results obtained with a new spectrometer will be reported.

[1] R. Vollmer et al., Phys. Rev. Lett. 91 (2003) 147201.

[2] H. Ibach et al., Rev. Sci. Instrum. 74 (2003) 4089.

[3] H. Ibach et al., Surface and Interface Analysis 38 (2006) 1615.

O 36.87 Tue 18:30 P4

Magnetic Fe-porphyrin on superconducting Pb (111) — •Lukas Z. Braun, Benjamin W. Heinrich, Jose I. Pascual, and Katharina J. Franke — Institut für Experimentalphysik, Freie Universität Berlin, Germany

The temperature dependent Fermi-Dirac broadening of electronic states is a physical limit of the energy resolution for Scanning Tunneling Spectroscopy on metal surfaces. A higher energy resolution can be achieved in a superconducting system due to tunneling through the well defined BCS states. Here, we studied Fe(III)-Octaethylporphyrin-Cloride adsorbed on Pb(111) at 4.8 K. At submonolayer coverage, we observed on molecular islands a magnetic fingerprint with submolecular spatial resolution.

O 36.88 Tue 18:30 P4

Structure and magnetism of Mn-tetrapyridyl porphyrin molecules on Ag(111) — Tobias R. Umbach[1], •Christian Felix Hermanns[1], Alex Krüger[1], Zechao Yang[1], Isabel Fernández-Torrente[1], Nils Krane[1], Matthias Bernien[1], Constantin Czekelius[2], Katharina J. Franke[1], Jose I. Pascual[1], and Wolfgang Kuch[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [2]Institut für Chemie und Biochemie - Organische Chemie, Freie Universität Berlin, Germany

Deposition of metal porphyrines on metallic surfaces can lead to the modification of the magnetic moment of the metal ion. We investigated a submonolayer 5,10,15,20-Tetrakis-(4-pyridyl)-porphyrin-Mn(III)-chloride (TPyP-Mn(III)-Cl) on a Ag(111) surface by Low Temperature Scanning Tunneling Microscopy (LT-STM) and X-Ray Magnetic Circular Dichroism (XMCD). Our measurements reveal that T4PyP-Mn(III)-Cl forms a self-assembled ordered phase with a small fraction of ordered second-layer molecules even for submonolayer coverage after annealing to 370 K. The first monolayer consists of domains with alternating molecular rows. The second layer forms a square lattice on top of the first monolayer. By Low Temperature Scanning Tunneling Spectroscopy (LT-STS) we identify similar resonances of the metallic ion of TPyP-Mn(III)-Cl molecules in the first and second monolayer, indicating no strong interactions with the metallic surface underneath. XMCD measurements on the same system show that the TPyP-Mn(III)-Cl molecules keep a magnetic moment upon adsorption with an easy axis along the surface normal.

O 36.89 Tue 18:30 P4

The magnetic properties of Ni on modified Cu(110) surfaces — •Michael Hohage, Mariella Denk, Daniel Queteschiner, Richard Denk, and Peter Zeppenfeld — Institut für Experimentalphysik, Johannes Kepler Universität Linz, A-4040 Linz, Austria

The magnetism and morphology of thin Ni films deposited on Cu(110) surfaces reconstructed by exposure to oxygen and nitrogen has been studied. Both, oxygen and nitrogen act as a surfactant for the Ni growth, leading to smoother films. Scanning Tunneling Microscopy (STM), as well as Reflectance Difference Spectroscopy (RDS) is used to characterize the sample properties. The sensitivity of the RDS to the polar Magneto-Optic Kerr Effect has been exploited (RD-MOKE). Contrary to the growth on pristine Cu(110), thin Ni films on oxygen covered Cu(110)-(2x1)O show a spin reorientation transition (SRT) from in-plane to out-of-plane magnetization at 9 ML Ni coverage [1], [2]. Increasing the oxygen pre-coverage to form the Cu(110)-c(6x2)O reconstruction leads to a shift of the SRT to thicker Ni-films. However, Ni films grown on the Cu-CuO stripephase at lower oxygen precoverage only exhibit an SRT after post-growth exposure to oxygen. Ni films evaporated on the Cu(110)-(2x3)N do not show an SRT as long as no coadsorption of oxygen is permitted. The origin of the magnetic properties of these systems will be discussed and in particular the crucial role of the oxygen will be addressed.

[1] Th. Herrmann et al., Phys. Rev. B 73, 134408 (2006).

[2] R. Denk et al., Phys. Rev. B 79, 073407 (2009).

O 36.90 Tue 18:30 P4

Depth Resolved Photoelectron Microscopy of Nanostructures via Soft X-Ray Standing Wave Excitation — •Florian Kronast[1], Alexander Gray[2], Christian Papp[3], See-Hun Yang[4], Alexander Kaiser[4], Farhad Salmassi[6], Eric M. Gullikson[6], Dawn L. Hilken[6], Erik H. Anderson[6], Hermann A. Dürr[1], Claus M. Schneider[5] und Charles S. Fadley[2] — [1]Helmholtz-Zentrum Berlin - BESSY II, Berlin, Germany — [2]Department of Physics, University of California, Davis, CA, USA — [3]Physical Chemistry II, University of Erlangen, Germany — [4]IBM Almaden Research Center, San Jose, CA, USA — [5]Juelich Research Center, Jülich, Germany — [6]Center for X-Ray Optics, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

We demonstrate the addition of depth resolution to the usual two-dimensional images in photoelectron emission microscopy (PEEM), with application to a square array of circular magnetic Co microdots. The method is based on excitation with soft x-ray standing-wave (SW) generated by Bragg reflection from a multilayer mirror substrate. The standing wave is moved vertically through the sample simply by varying the photon energy around the Bragg condition. Photoemission intensities as functions of photon energy were compared to x-ray optical theoretical calculations in order to quantitatively derive the depth-resolved film structure of the sample. This SW approach thus provides complementary information to the usual lateral information provided by the PEEM, and should have wide applicability to studies of magnetic nanostructures in the future.

O 36.91 Tue 18:30 P4

Investigation of magnetic properties in a multiferroic layer system — •Martin Welke[1], Remya Kunjuvettil Govind[2], Martin Trautmann[2], Vasili Hari Babu[1], Karl-Michael Schindler[2], and Reinhard Denecke[1] — [1]Wilhelm-Ostwald-Institut für Physikal. und Theoret. Chemie, Universität Leipzig, Linnestr. 2, 04103 Leipzig, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle, Germany

Systems with multiferroic properties are of interest for research since the 1960s. In the beginning single phase multiferroics were in the focus of research, whereas nowadays layer systems with a ferroelectric and a ferromagnetic component are investigated. The work presented covers the system Cobalt on Bariumtitanate (001) within SFB 762. In particular, XAS measurements of 3, 6, 9, 12, and 21 monolayer thick Co films prepared by e-beam evaporation are taken into account.

Magnetic properties are determined by X-ray magnetic circular dichroism (XMCD) at the Co L edge. The films show in-plane magnetization starting from 6 ML. It is possible to calculate the magnetic moments using the sum rule formalism. The calculated values correspond to those for Co (hcp) bulk reported in literature [1,2].

Changes to the $BaTiO_3$ substrate by heating in vacuum up to 600 °C prior to Co deposition, resulting in O vacancies and increased conductivity, do not yield significant differences for the magnetic moments. Work supported by the DFG through SFB 762.

[1] Eriksson et al., Phys. Rev. B 42 (1990) 2707

[2] Guo et al., Phys. Rev. B 50 (1994) 3861

O 36.92 Tue 18:30 P4

Two Photon Photoemission Studies of FeO-films on ZnO(0001) — •Stephan Hilgenfeldt and Michael Bauer — Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24098 Kiel, Germany

We investigated FeO films prepared on a ZnO(0001) substrate by two photon photoemission (2PPE). The FeO was produced by epitaxial growth of Fe on ZnO in ultra high vacuum and a subsequent annealing of the films to 670 K. In the 2PPE-data we were able to identify a distinct spectral feature of FeO from an unoccupied state at a binding energy of $E - E_F = +2.5\,\mathrm{eV}$ exhibiting a clear parabolic dispersion in $k_{\|}$. The nature and the properties of this electronic band will be discussed under consideration of additional time resolved 2PPE data.

O 36.93 Tue 18:30 P4

The Formation of Shockley derived Interface States at Metal-Organic Interfaces studied with 2PPE — •Manuel Marks[1], Christian H. Schwalb[1], Sönke Sachs[2], Benjamin Schmidt[1], Achim Schöll[2], Friedrich Reinert[2], Eberhard Umbach[2], and Ulrich Höfer[1] — [1]Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität Marburg, D-35032 Marburg — [2]Universität Würzburg, Experimentelle Physik II, D-97074 Würzburg

The charge carrier injection across a metal-organic interface into the active regions of a functional device is one major influence on the efficiency of organic electronics. New electronic states that emerge at such interfaces can alter these dynamical processes substantially. We applied time- and angle-resolved 2-photon photoemission (2PPE) to study the electron dynamics at structurally well characterized interfaces directly in the time domain. With adsorption of monolayer films of PTCDA and NTCDA on a Ag(111) surface strongly dispersing interface states (IS) form above the Fermi Level E_{F}. For PTCDA the inelastic electron lifetime of 54 fs indicates a significant overlap with the metal substrate and the state mainly originates from an upshifted Shockley state [1]. For NTCDA films the IS has comparable properties though lying closer to E_{F}. In the stronger chemisorbed disordered precursor phase of the PTCDA monolayer [2] an interface state emerges at $E - E_{\mathrm{F}} = 0.45$ eV. The lifetime of 63 fs and its non-dispersing behavior raise the question whether this state has more molecular character.

[1] C. H. Schwalb *et al.*, Phys. Rev. Lett. **101**, 146801 (2008)

[2] L. Kilian *et al.*, Phys. Rev. Lett. **100**, 136103 (2008)

O 36.94 Tue 18:30 P4

Two-photon photoelectron spectroscopy of graphene on SiC(0001) — •Dieter Gugel[1], Daniel Niesner[1], Florian Speck[2], Thomas Seyller[2], and Thomas Fauster[1] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen, Germany — [2]Lehrstuhl für Technische Physik, Erwin-Rommel-Straße 1, 91058 Erlangen, Germany

A monolayer of graphene grown epitaxially on the silicon face of silicon carbide was investigated using angle- and time-resolved two-photon photoelectron spectroscopy. In this measurement, the surface electrons were excited by a UV pump laser with a photon energy of 4.66 eV and a pulse duration of 58 fs. Using an IR probe puls with an energy of 1.55 eV and a pulse width of 33 fs, we determined the energy dispersion and lifetime of the lowest unoccupied image potential state. The lifetime of this state was observed to be 50 fs. Moreover, we measured the work function of the surface, which amounts to 4.5 eV.

O 36.95 Tue 18:30 P4

Time-resolved ARPES studies with high-oder harmonic radiation — Robert Carley[1], Kristian Döbrich[1], •Björn Frietsch[1,2], Cornelius Gahl[1], Martin Teichmann[1], Kai Godehusen[3], Olaf Schwarzkopf[3], Philippe Wernet[3], Frank Noack[1], and Martin Weinelt[1,2] — [1]Max-Born-Institut, Berlin — [2]Fachbereich Physik, Freie Universität, Berlin — [3]Helmholtz-Zentrum für Materialien und Energie (BESSY II), Berlin

We present characterization results of our newly developed high-order harmonics XUV source and beamline. The scope of this new setup is to provide XUV photons between 20-65 eV, at an energy resolution of a few 100 meV and a pulse duration $\geq$ 100 fs for time-resolved photoelectron spectroscopy studies of metal and semi-conductor surfaces as well as gas-phase experiments.

40-fs pulses from a commercial amplified Ti:Sapphire laser system running at 10 kHz repetition rate are focused into an argon-filled gas cell to create harmonics, currently up to the 25th order (=38.4 eV). We select the XUV wavelength and energy resolution using a toroidal grating monochromator. Our current resolution is 170 meV and the time resolution is 140 fs (both FWHM) at a reasonable harmonic yield. We performed first pump-probe experiments on the lanthanide metals Gadolinium and Terbium.

O 36.96 Tue 18:30 P4

Hot phonons in the relaxation dynamics at the Si(001) surface — •Thi Uyen-Khanh Dang[1], Christian Eickhoff[2,3], Martin Weinelt[2,3], Andreas Knorr[1], and Carsten Weber[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Berlin, Germany — [3]Freie Universität Berlin, Fachbereich Physik, Berlin, Germany

We investigate the relaxation dynamics of photo-excited carriers at the Si(001) surface. Relaxation occurs mainly from the bulk conduction band into the surface state D_{down}. We present time-resolved experimental results on the relaxation dynamics obtained via two-photon photoemission measurements. The results are compared to theoretical calculations based on the Bloch-Boltzmann-Peierls approach, where the influences of electron-phonon and electron-electron scattering are analyzed. We find that the electronic temperature remains well above the equilibrium lattice temperature for times much longer than the typical scattering times of the system (even after 10 ps). This is found to be due to strong heating of LO phonon modes due to electron relaxation in the bulk via LO phonon emission. The different contributions of the scattering channels as well as phonon bottleneck effects are discussed.

O 36.97 Tue 18:30 P4

A time-of-flight electron spectrometer for angle- and time-resolved 2PPE — •Andreas Damm[1], Anne Spende[1], Jens Güdde[1], Achim Czasch[2], Ottmar Jagutzki[2], Horst Schmidt-Böcking[2], and Ulrich Höfer[1] — [1]Fachbereich Physik, Philipps-Universität, D-35032 Marburg — [2]Institut für Kernphysik, Goethe-Universität, D-60438 Frankfurt am Main und RoentDek Handels GmbH, D-65779 Kelkheim

Many studies on surface electron dynamics employing two-photon photoemission (2PPE) would benefit from the ability to map the full two-dimensional surface bandstructure in a single time-resolved experiment. Examples include the study of quasi-elastic electron scattering within electronic surface bands or the extension of 2PPE for the generation of coherently excited electrical currents at surfaces.

Thus, we have developed a position-sensitive time-of-flight spectrometer capable of measuring the kinetic energy as well as the full parallel momentum $\vec{k}_{||}$ of low-energy electrons photoemitted from a surface with a maximum rate of few MHz. Its main components are a field-free drift tube and a delay-line detector for a position-sensitive detection. A variable drift length allows to enhance either the acceptance angle or the energy- and momentum-resolution. The energy resolution for low kinetic energy electrons as typical for 2PPE experiments is better than 10 meV even at the maximum acceptance angle of $\pm 25°$.

Investigations on the momentum-dependence of the decay of image-potential electrons on Cu(100) will be presented underlining the capabilities of this instrument.

O 36.98 Tue 18:30 P4

Time resolved desorption of atomic hydrogen from graphite induced by femtosecond laser pulses — •Robert Frigge[1], Tim Hoger[1], Henrik Witte[1], Thomas Olsen[2], Jakob Schiotz[2], and Helmut Zacharias[1] — [1]Physikalisches Institut, Universität Münster, Germany — [2]CINF, Technical University of Denmark, Denmark

The desorption of hydrogen from graphite (HOPG) is an important issue in the understanding of molecular hydrogen formation on dust particles upon irradiation. The velocity distribution of atomic hydrogen from HOPG is examined after surface excitation with fs-laser pulses at $\lambda = 400$ nm. Desorbed neutral H atoms are ionized using (2+1) REMPI via the $2s \leftarrow 1s$ transition, and are detected with a time-of-flight mass spectrometer. As a result the velocity distribution reveals a structure consisting of different maxima for fast, medium and very slow desorbed hydrogen atoms. Electron scattering calculations have been performed employing a repulsive electronic excited state and H-graphite adsorption potentials corresponding to different adsorption sites [1]. Via populating diferent vibrationally excited intermediate states by multiple scattering events velocity distributions for desorption out of different adsorption sites are obtained. A good agreement with the experimentally observed velocities is obtained. A nonlinear fluence dependence for the fast electrons, allow two pulse-correlation experiments and as a result we derive a pulse-delay dependent yield with a FWHM of about 700 fs. This correlation time indicates short lifetimes of the excited electrons and supports a calculation in the DIMET model. [1]R. Frigge et al., Phy. Rev. Lett.,104, 256102 (2010)

O 36.99 Tue 18:30 P4

Photo-induced melting of a Pb overlayer on Cu(111) observed with time- and angle-resolved XUV photoemission — •Andreas Ruffing[1], Steffen Eich[1], Adra V. Carr[2], Daniel Steil[1], Alexander Hassdenteufel[1], Margaret M. Murnane[2], Henry C. Kapteyn[2], Michael Bauer[3], Stefan Mathias[1,2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]JILA, University of Colorado and NIST, Colorado 80309 0440, USA — [3]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24908 Kiel, Germany

The electronic structure during a thermally induced melting transition was investigated by Baumberger et al. in 2004 [1]. Baumberger et al. found that the liquid film of Pb/Cu(111) shows electronic features as the persistence of a Fermi surface, the filling of band gaps, and the localization of the electron wave functions upon melting. In our experiment, we use intense femtosecond infrared pulses to photo-induce this melting transition of the Pb overlayer on Cu(111). We monitor the dynamical changes in the electronic structure as a function of time by using time- and angle-resolved XUV photoemission spectroscopy. XUV pulses are generated from high-harmonic upconversion, and are needed to access the Brillouin zone boundary, where the melting transition can be followed by a transient change of the electronic band structure.

[1] Baumberger et al., Science 306 (2004), 2221-2224

O 36.100 Tue 18:30 P4

2PPE-measurement on Cu(1 1 11) with an angle-resolving time-of-flight spectrometer — •Thomas Kunze[1,2], Jens Kopprasch[1], Martin Teichmann[1], Thorsten U. Kampen[2], and Martin Weinelt[1] — [1]Max Born Institut, Berlin, Germany — [2]SPECS GmbH, Berlin, Germany

We present two-photon photoemission measurements with the angle-resolved time-of-flight spectrometer THEMIS. The spectrometer allows us to measure the kinetic energy and wave vector parallel to the surface of the photo emitted electrons. Due to the maximum angle acceptance of +/- 15° and the usable energy range of up to more than 20 % of the passenergy, it is possible to measure a remarkable part of the band structure concurrently.

We present measurements of the image-potential states (IPS) on Cu(111) and Cu(1 1 11), a vicinal surface with (001)-terraces. For both measurements we calculated the effective mass and the binding energy of the electrons. The dispersion relations correspond to other measurements (M. Roth). Furthermore we measured the Umklapp band and the lifetime differences of the IPS depending on the parallel momentum of the photo emitted electrons of Cu(1 1 11).

O 36.101 Tue 18:30 P4

Collective electron excitations on potassium-covered Be(0001) — •Martin Jahn and Jörg Kröger — Institut für Physik, TU Ilmenau, PF 100565, DE-98684 Ilmenau, Germany

Electron-energy-loss spectroscopy (EELS) of clean Be(0001) demonstrated the existence of acoustic surface plasmons in agreement with ab initio calculations [1]. The origin of these low-energy collective excitations with a soundlike dispersion relation is the dynamical screening of surface state electrons by bulk electrons. Calculations and photoemission experiments showed that on potassium-covered Be(0001) the interaction of quantum well states with bulk electrons results in coverage-dependent acoustic surface plasmons [2]. We report on EELS measurements on potassium-covered Be(0001). The dispersion relation of the acoustic surface plasmon depending on the potassium coverage is presented. Furthermore, the influence of potassium adsorption on the ordinary surface plasmon and on the phonons of Be(0001) is investigated.

[1] B. Diaconescu et al., Nature 448, 57 (2007).

[2] J. Algdal et al., Phys. Rev. B 78, 085102 (2008).

O 36.102 Tue 18:30 P4

Adsorption of Hydrazine (N_2H_4) on Hexagonal Ice(0001): First-Principles Investigations on the Mechanism of Chirality Changes — •Pawel Rodziewicz and Bernd Meyer — Interdisciplinary Center for Molecular Materials ICMM and Computer-Chemistry-Center CCC, University of Erlangen-Nürnberg, Germany

Surfaces can have a pronounced effect on the chiral properties of adsorbed molecules. For example, it has been observed that chiral molecules spontaneously separate into domains with different chirality or that enantiopure adsorbates are transformed into racemate mixtures by lowering of the activation barrier for chirality flips. We have used hydrazine as a simple model of a chiral molecule to study possible binding sites and flips of chirality on ice(0001) surfaces. The chemical properties of hydrazine are similar to those of water. Due to the presence of electron lone pairs and N-H groups hydrazine is simultaneously a proton acceptor and a proton donor. Density functional theory (DFT) calculations and Car-Parrinello molecular dynamics (CP-MD) simulations were used to investigate the interplay between molecule-molecule and molecule-substrate interactions. Hydrazine monomers and different enantiomers of its dimers were adsorbed on the hexagonal ice (0001) surface. The adsorbed aggregates were analyzed in terms of their coordination to the surface, with special focus on identifying hydrogen bonds. Finally, the process of chirality flips was studied using coordination constrained CP-MD simulations in order to obtain free energy barriers for rearrangements of enantiomers with Gauche A into Gauche B.

O 36.103 Tue 18:30 P4

Towards time- and angle-resolved photoemission at a free-electron laser with an angle-resolving ToF spectrometer — Christian Sohrt[1], •Kerstin Hanff[1], Stefan Hellmann[1], Michael Bauer[1], Wilfried Wurth[2], Lutz Kipp[1], and Kai Rossnagel[1] — [1]Institut für Experimentelle und Angewandte Physik, Kiel, Germany — [2]Institut für Experimentalphysik and Center for Free-Electron Laser Science, Hamburg, Germany

The Free-Electron Laser (FEL) in Hamburg (FLASH) generates highly brilliant, ultrashort pulsed radiation with pulse durations down to 50 fs and photon energies up to 1000 eV. This enables unique experiments, as for example time-resolved core-level photoelectron spectroscopy. However, to establish photoelectron spectroscopy as a completely viable technique at an FEL, one has to develop a detection scheme with maximum efficiency, because the pulse repetition rates of FELs are notoriously low and the available beam time is extremely scarce. Our proposed solution is a photoelectron spectroscopy experiment based on a novel angle-resolved time-of-flight spectrometer. Compared to traditional detection schemes the instrument is expected to enhance the detection efficiency by a factor of about 200–due to the larger acceptance angle–and the temporal resolution by a factor of seven to about 100 fs–due to single-pulse detection. Thus, it will become possible to correlate core-level dynamics which is sensitive to changes in the charge distribution around specific atomic sites, with the dynamics of electrons at the Fermi surface in a single experiment. This work is supported by the BMBF (FSP 301 FLASH).

O 36.104 Tue 18:30 P4

Coupling of Pb adsorbate vibrations to Si(111) substrate studied by molecular dynamics — Sung Sakong, •Peter Kratzer, Simone Möllenbeck, Annika Kalus, Anja Hanisch-Blicharski, Martin Kammler, and Michael Horn-von Hoegen — Fakultät für Physik and Center for Nanointegration (CeNIDE), Universität Duisburg-Essen, Duisburg, Germany

The decay of low-lying vibrational modes of heavy adsorbates is best studied in the time domain. Time-resolved electron diffraction (RHEED) experiments provide evidence for a long (several ns) and a short (100 ps) time scale in the dissipation of vibrational energy of a Pb monolayer following pulsed laser irradiation. We perform density functional (DFT) calculations of a Pb/Si(111) $(\sqrt{3}\times\sqrt{3})$ surface to obtain the vibrational modes. To study the vibrational dynamics on the ns time scale, we use classical molecular dynamics with a Pb-Si interaction potential that matches the DFT data. The lattice dynamics at $T = 100$K is simulated using a large super cell with 12 nm in depth, and the lower part of the Si slab is coupled to a thermostat. As initial condition, we assume that the energy deposited by the laser has already been converted to kinetic energy of the Pb atoms. We watch how this extra kinetic energy is dissipated into the Si substrate. After averaging over many trajectories, the relaxation dynamics monitored by the mean-square displacements of the Pb adatoms can be compared to the experimental data. In conclusion, we assign the experimentally observed short time scale to the decay of the "optical" Pb–Si mode, i.e., the Pb vibration relative to the top-most Si layer.

O 36.105 Tue 18:30 P4

Dynamics of the $\beta(\sqrt{3}\times\sqrt{3}) \leftrightarrow (3\times3)$-Pb/Si(111) phase transition on the ps-timescale — •Jörg Reimann, Tim Frigge, Simone Möllenbeck, Friedrich Klasing, Martin Kammler, and Michael Horn-von Hoegen — Department of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE), University of Duisburg-Essen, D-47057 Duisburg, Germany

The structural dynamics of strongly driven phase transitions on surfaces take place on a picosecond timescale. Ultrafast time resolved electron diffraction in a RHEED (reflection high energy electron diffraction)-geometry is an excellent technique to study such processes after excitation by a fs laser pulse [1]. In a metallic adsorbat system absorption of the photons results in an excitation of the electron system. Electron-phonon coupling causes heating of the adsorbate layer and may trigger the phase transition. In order to study the dynamics of an order-disorder phase transition far away from thermal equilibrium we performed time resolved measurements on the $\beta(\sqrt{3}\times\sqrt{3}) \leftrightarrow (3\times3)$-Pb /Si(111) phase transition with $T_c = 84°$C. The Pb adlayer is excited by a 50 fs laser pulse with 800 nm at a sample temperature of 25 K. After excitation the $\beta(\sqrt{3}\times\sqrt{3})$-diffraction spot intensity drops instantaneously due to the Debye Waller effect but is followed by a sharp increase which is delayed by 30 ps. While the intensity decrease is explained by thermal heating of the adsorbate layer up to 125 K, we attribute the increase of intensity to a delayed structural phase transition triggered by the temperature rise.

[1] A. Janzen et al., Surf. Sci. 600, 4094 (2006)

O 36.106 Tue 18:30 P4

Generation, characterization and compression of pJ white-light-continuum pulses for ultrafast spectroscopy — •Daniel Wegkamp[1], Simon Wall[1], Daniele Brida[2], Stefano Bonora[2], Giulio Cerullo[2], Julia Stähler[1], and Martin Wolf[1] — [1]Fritz-Haber-Institute of the MPG, Dep. of Physical Chemistry, Berlin, Germany — [2]Politecnico di Milano, Dipartimento di Fisica, Milan, Italy

Broadband white-light-continuum pulses are widely used as a probe for optical spectroscopies, providing a probing bandwidth of several hundred nanometers in the UV, visible and IR. However, their use in ultrafast spectroscopy is limited due to the long duration of the pulses. In addition, pulse diagnostics are difficult because of their low power. We report the measurement of the group-delay of such white-light pulses with sub-nJ pulse energy. Furthermore we describe the setup and application of a deformable mirror-based compressor resulting in optimized temporal shapes of the pulses. White-light pulses are generated by self-phase modulation due to focusing of 40 fs laser pulses (800nm, provided by a 300 kHz Ti:Sa regenerative amplifier system) into a YAG crystal. The resulting pulses have durations of several hundred femtoseconds and contain spectral components ranging from near-UV to the IR. These are characterized by spectrally resolved measurement of the transient reflectivity. Compression of the pulses is achieved by adjustment of the extracted group delays [1] using the deformable mirror.

[1] Parmigiani et al. Appl. Phys. Lett. 96 (2010) 021102

O 36.107 Tue 18:30 P4

NanoESCA, a new nanospectroscopy tool with synchrotron radiation — •Marten Patt[1], Carsten Wiemann[1], Ingo Krug[1], Matthias Escher[2], Nils Weber[2], Michael Merkel[2], and Claus Michael Schneider[1] — [1]PGI-6, Forschungszentrum Jülich GmbH, Jülich, Germany — [2]Focus GmbH, Hünstetten, Germany

Nanotechnology and nanoscience are developing more and more to smaller length scales. We face the need for the characterization of surface electronic and magnetic states in these reduced dimensions with a new energy-filtered photoelectron emission microscope (PEEM), which we have recently installed at the ELETTRA synchrotron facility (Italy)[1]. The instrument features a novel electrostatic lens system with 30 kV extraction voltage, enabling spatially resolved photoelectron imaging with a lateral resolution smaller than 100 nm and combines it with a double-hemispherical energy filter [2], a single-event counting detector unit and a liquid helium cooled sample manipulator with five degrees of freedom. A second operation mode provides the mapping of the angular distribution (k-space microscopy) of the photoelectrons. We discuss the capabilities and the performance of the instrument with respect to its lateral and energy resolution, sensitivity and signal-to-noise-ratio.

[1] http://www.elettra.trieste.it/beamlines/NASP

[2] M. Escher et al., J. Electron Spectr. Rel. Phen., 144-147 (2005) 1179

O 36.108 Tue 18:30 P4

Observation of the topological state and a two-dimensional electron gas in Bi_2Se_3 by multidimensional photoemission spectroscopy — •Lupulescu C.[1,2], Ovsyannikov R.[2], Rienks E.D.L.[2], Fink J.[2], King P.D.C.[3], Baumberger F.[3], Hatch R.C.[4], Hofmann P.[4], Mi J.[4], Iversen B.B.[4], Lindblad A.[5], Svensson S.[5,6], and Eberhardt W.[1,2] — [1]Technische Universität Berlin, Berlin, Germany — [2]Helmholtz Zentrum Berlin, Berlin, Germany — [3]University of St Andrews, St Andrews, UK — [4]Aarhus University, Aarhus, Denmark — [5]MAX-lab, Lund, Sweden — [6]Uppsala University, Uppsala, Sweden

The electronic structure of Bi_2Se_3 (0001) was investigated using a new time-of-flight angle-resolved electron spectrometer (VG Scienta, ARTOF 10k). Measurements were taken at the 10m NIM beamline of BESSY II, operating in single-bunch mode. Both the topological surface state and a two-dimensional electron gas near the surface were observed. The main advantage of using this type of electron analyzer is the simultaneous mapping of both kinetic energy and angular distribution in two dimensions, ruling out various artefacts induced by sample misalignment, temperature-induced drifts, etc. Moreover, the collection of such data sets is rather fast, so that the temporal evolution of the electronic structure can be studied. Utilizing this, we study the time-dependence of band bending at the surface of Bi$_2$Se$_3$, which leads to the emergence of a two-dimensional electron gas.

O 36.109 Tue 18:30 P4

Development of a thin film spin filter optics for PEEM — •Daniel Panzer[1,2], Jan David Kuttig[1], and Gerd Schönhense[1] — [1]Institut für Physik, Johannes-Gutenberg Universität Mainz — [2]Max-Planck Institut für Polymerforschung, Mainz

Analyzing the spin polarization of electrons is a vital aspect of many experiments in nuclear, molecular, surface and solid-state physics, and of fundamental importance for investigations of ferromagnetic materials. However, combining spin detection with a laterally resolved method like PhotoEmission Electron Microscopy (PEEM) is quite demanding. One possibility is the use of low energy electron diffraction for spinfiltering of an image or a momentum distribution [1].

Here we test a new method that takes advantage of the spin dependence of the mean free path of electrons in magnetized ferromagnet. We use a tandem lens to extract electrons from a sample and project the magnified electron image onto a thin metal film that acts as a spin filter at low kinetic energies. On the opposite side the spinfiltered image is then picked up and further magnified by a regular PEEM optics.

We have successfully tested the electron optics at low magnification with a calibration sample and confirmed transmission through nm-thick layers of metals and semiconductors with a thermal emitter as electron source. The next challenge is combining photoemission, electron optics and transmission in a way that provides sufficient intensity so PEEM images can be aquired fast enough for regular use.

Funded by DFG(SCHO341/7-1); [1] Tusche et al., this conference

O 36.110 Tue 18:30 P4

High-Efficiency Multichannel-Spindetector — •Michaela Hahn, Bernd Petereit, Hans-Joachim Elmers, and Gerd Schönhense — Institut für Physik, Staudinger Weg 7, 55128 Mainz

The spinpolarisation analysis of electrons is a central demand in surface and solid state physics, especially for investigations of ferromagnetic materials. All state-of-the-art spindetectors work in a single-channel mode, i.e. monoenergetic and with only one detection angle. This leads to a very low efficiency in comparison with modern, parallel-detecting intensity analysers. We present a new type of spindetector with strongly improved efficiency by implementing a strategy for parallel multichannel detection.

The spinresolved photoelectron spectrometer comprises a hemispherical analyzer (Leybold EA10) and a helium discharge lamp (hν=21,23eV). Spindependent scattering at W(100) (asymmetry function S=0.45) yields a spinfiltered image of the analyzer exit plane, detected using a delayline detector (Surface Concept GmbH). A high-resolution spinfiltered image requires an acquisition time of minutes, whereas the same distribution with a state-of-the-art single channel detector would take several hours measuring time. A similar approach is used for the detection of spinfiltered momentum distributions [1].

Funded by Stiftung Rheinland-Pfalz für Innovation (project 886) and DFG (Scho 341/9-1)

Patent DE 10 2005 045 622 B4

[1] Ch. Tusche et al., this conference

O 36.111 Tue 18:30 P4

The High Resolution Diffraction Beamline at PETRA III - First Experiments — •Carsten Deiter, Florian Bertram, Kathrin Pflaum, and Oliver H. Seeck — DESY, Notkestr. 85, 22607 Hamburg

Since 2009 the new synchrotron radiation source PETRA III is operational. At the High Resolution Diffraction Beamline (P08) the equipment and the beam parameters are highly suited for surface and interface studies. Different sample cells with heating and cooling capability and the possibility of vacuum and gas atmosphere up to 1bar are available. These cells can be installed in the six circle diffractometer (Kohzu) for extreme angular resolution and will be supported by an UHV infrastructure with MBE preperation, structural (LEED) and chemical (AES) analysis operational in late summer 2011. The first regular user experiments have been performed and some results will be presented which show the benefits of the PETRA III beam parameters.

O 36.112 Tue 18:30 P4

NMR of buried interfaces — •Anuschka Schmitt, Matthias Buschmann, Richard Kastelik, Alexander Potzuweit, and Heinz Jänsch — Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg

We employ Xe-NMR to investigate surface phenomena by adsorbing hyperpolarized ^{129}Xe onto a helium-cooled single crystal and studying the electronic interactions of substrate and adsorbate. The high nuclear spin polarization of the adsorbed Xe-film could be transferred to buried interfaces within the substrate (which then would be accessible for further NMR experiments) via dipolar distant-field transfer. Such a transfer can be achieved by applying two rf-frequencies at the same time using a double resonant probe, integrated into an UHV system. Furthermore, an inhomogeneous magnetic structure of the Xe-film is needed, which could be provided by a geometrically structured sample in the μm range. Here, we present the development of the double resonant probe and first experiments.

O 36.113 Tue 18:30 P4

Preparation of highly polarized Xe with variable ^{129}Xe content — •Alexander Potzuweit, Matthias Buschmann, Richard Kastelik, Anuschka Schmitt, and Heinz Jänsch — Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg

We employ NMR of hyperpolarized ^{129}Xe to investigate surface phenomena. Dynamic processes at the bulk surfaces can be monitored by exchange spectroscopy (EXSY) of the bulk and surface atoms ($\Delta\sigma \approx 100$ppm). The annealing of Xe films can be investigated by line narrowing. To increase the sensitivity towards structurally caused, local inhomogeneities a small line width is favorable. In solid Xe the line width is dominated by dipolar interaction with neighboring nuclear spins. This can be substantially reduced by diluting the NMR-active isotope ^{129}Xe in the NMR-inactive isotope ^{132}Xe. With the new, improved experimental setup we will be able to provide mixtures of highly polarized ^{129}Xe and ^{132}Xe with adjustable abundances. Here we present the technical development of the apparatus and discuss first results.

O 36.114 Tue 18:30 P4

Molecule-Surface Scattering with Velocity-Controlled Molecular Beams — •Fabian Grätz[1], Daniel Engelhart[2], Henrik Haak[1], Daniel J. Auerbach[2], Alec M. Wodtke[2], and Gerard Meijer[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin — [2]Max-Planck-Institut für biophysikalische Chemie, Am Faßberg 11, D-37077 Göttingen

The production of cold molecular beams with a tunable velocity by means of pulsed electric fields, known as Stark deceleration, is now mature and convenient. At the same time, molecular beam experiments that use traditional ways of velocity manipulation have been commonly used to study different aspects of molecule-surface interactions in the regime of high kinetic energy. We present a new generation of molecule-surface scattering machine, which brings the advantages of Stark decelerated molecular beams to the field of surface physics. Using this machine, CO molecules will be scattered at surfaces, quantum-state selective with respect to both impacting and scattered molecules, while providing a tunable velocity in the range of 1000 to 20 m/s with an exceptional translational energy resolution.

O 36.115 Tue 18:30 P4

Quasiparticle energies and excitonic effects of alkali-metal fluorides — •Christoph Sommer, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster, D-48149 Münster, Germany

We present a comparative study of quasiparticle and excitonic properties of the alkali-metal fluorides LiF, NaF and KF. For the calculation of quasiparticle effects within the GW approximation, we use a localized Gaussian basis set.

Excitonic effects are obtained by solving the Bethe-Salpeter equation for an effective two-particle problem.

Furthermore, the applicability of self-interaction corrected DFT-LDA energies and wavefunctions as a substitute for computationally highly demanding quasiparticle energies in the Bethe-Salpeter equation is discussed.

The calculated optical spectra are in accord with experimental and theoretical results available in the literature for these systems.

O 36.116 Tue 18:30 P4

Methane adsorption on graphene: Influence of dispersion interaction — •Matthias Witte[1], Christian Thierfelder[1], Stephan Blankenburg[1,2], Eva Rauls[1], and Wolf Gero

Schmidt[1] — [1]Theoretische Physik, Universität Paderborn, 33100 Paderborn, Germany — [2]Eidgenössische Materialprüfungs- und Forschungsanstalt (EMPA), 8600 Dübendorf, Switzerland

Van der Waals interaction is not properly described in density functional theory within commonly used exchange-correlation functionals. Therefore several semi-empirical and ab-inito solutions have been proposed and implemented in widely used program packages. Here we use the methane-graphene interaction as benchmark system to compare the results of semiempirical dispersion correction schemes (DFT-D) [1,2] and an ab initio van der Waals density functional (vdW-DF) ansatz [3]. Møller Plesset perturbation theory (MP2) [4] calculations are used as a reference. The adsorption energy of 0.17 eV and the molecular distance of 3.28 Å obtained from the MP2 calculations are close the experimental data, while the vdW-DF scheme results either in a realistic adsorption energy or a realistic adsorption geometry, depending on the exchange-correlation functional. The present implementation of DFT-D overbinds about as much as bare DFT calculations underbind, but yields a meaningful adsorption height. [1] F. Ortmann, W.G. Schmidt and F. Bechstedt, Phys. Rev. Lett. 95, 186101 (2005) [2] S. Grimme, J. Comp. Chem. 27, 1787 (2006) [3] M. Dion, H. Rydberg, E. Schröder, D.C. Langreth and B.I. Lundqvist, Phys. Rev. Lett. 92, 246401 (2004) [4] C. Møller and M.S. Plesset, Phys. Rev. 46, 618 (1934)

O 36.117 Tue 18:30 P4

Adsorption behavior of super-heavy elements ($Z \geq 100$) and their chemical complexes on inert and metal surfaces — •Josef Anton and Timo Jacob — Inst. für Elektrochemie, Uni Ulm

One of the very interesting but on the other site also extremely challenging topics in modern chemistry concerns the properties of superheavy elements [1]. Due to their very short life times ($\sim 1\,\mathrm{s}$) one is limited to experiments on only one atom at a time, which have to be performed before the nucleus decays. Since most standard techniques of 'traditional' chemistry are not applicable, only few experimental setups are available, such as the gas-phase thermochromatography [1, 2]. In this method the volatility of a super-heavy element as well as the adsorption temperature T_{ads} of these species on the detector is measured. Adsorption enthalpies, ΔH_{ads}, can then be deduced from T_{ads} using statistical thermodynamic models and Monte Carlo simulations. In order to be able to perform accurate calculations one has to describe the motion of the electrons in a fully relativistic manner. We used our four-component DFT code [3] to determine the adoption energies of the super-heavy elements ($Z \geq 100$) and their homologues on different surfaces. After discussing the prodecure and the results, we will provide a comparison of some of the obtained trends to recent experimental studies.

[1] M. Schädel, *The Chemistry of Superheavy Elements*, Kluwer Academic Publishers, Dordrecht, 2003.

[2] M. Schädel and A. Türler, *Physik Journal*, **6**, 35 (2009).

[3] J. Anton, B. Fricke, E. Engel, *Phys. Rev. A*, **69**, 012505 (2004).

O 36.118 Tue 18:30 P4

Neural Network Potential-Energy Surfaces for Organic Molecules: First Applications to Tartaric Acid — •Sinja Klees, Tobias Morawietz, and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

First-principles calculations provide an accurate description of many systems. However, the computational costs severely limit the size of the systems that can be studied. Therefore, the development of efficient interatomic potentials is an important prerequisite for studying complex systems in molecular dynamics simulations. Neural Networks represent a class of flexible functions, which allows to construct accurate potential-energy surfaces (PESs) based on a set of reference points. To date, most Neural Network potentials have been reported for very small molecules or inorganic solids. Here, we investigate the applicability of this method to large organic molecules. Using tartaric acid as a benchmark system we show that a highly accurate PES can be constructed systematically.

O 36.119 Tue 18:30 P4

Magnetic properties of adatoms and clusters on metal surfaces, the effect of electric field on MAE — •Tamene Regassa Dasa, Pavel Ignatiev, and Valeriy Stepanyuk — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

Magnetic properties of Co adatoms, chains and mixed Co/Pt chains on Pt surfaces are investigated. This is done by non-collinear density functional theory using the fully relativistic pseudopotentials. Spin-orbit interaction is taken into account . The local magnetization and magnetic anisotropy energies of the studied nanostructures are evaluated and compared with available experimental and theoretical results. Finally, the magnetic effect of electric fields on the magnetic properties is discussed.

O 36.120 Tue 18:30 P4

polarity-induced oxygen vacancies at $LaAlO_3|SrTiO_3$ interfaces — •pengxiang xu[1], zhicheng zhong[2], and paul j. kelly[2] — [1]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

Using first-principles density functional theory calculations, we find a strong position and thickness dependence of the formation energy of oxygen vacancies in $LaAlO_3|SrTiO_3$ (LAO|STO) multilayers and interpret this with an analytical capacitor model. Oxygen vacancies are preferentially formed at p-type $SrO|AlO_2$ rather than at n-type $LaO|TiO_2$ interfaces; the excess electrons introduced by the oxygen vacancies reduce their energy by moving to the n-type interface. This asymmetric behavior makes an important contribution to the conducting (insulating) nature of n-type (p-type) interfaces while providing a natural explanation for the failure to detect evidence for the polar catastrophe in the form of core level shifts.

O 36.121 Tue 18:30 P4

Electronic structure calculations on 100,000 atoms — •Gerald Jordan, Martijn Marsman, and Georg Kresse — University of Vienna, Faculty of Physics, and Center for Computational Materials Science, Sensengasse 8/12, A-1090 Wien, Austria

We present an efficient method for tackling electronic structure calculations on the scale of 100,000 atoms, where a full diagonalization of the Kohn-Sham Hamiltonian becomes computationally unfeasible because of cubic scaling with system size. In many applications, however, one is only interested in a few states near the Fermi level. Solving the associated interior eigenvalue problem is numerically difficult and requires a realistic model of the electronic charge density.

Our approach is based on the Jacobi-Davidson method using harmonic Ritz values, which mimicks the shift-and-invert strategy to target a specific energy but avoids any explicit inversion. In contrast to the folded spectrum technique, our method easily extends to the generalized eigenvalue problems arising from the use of pseudopotentials. To construct suitable charge densities reproducing the band structure, we fit atomic charge distributions to a self-consistent reference calculation.

O 36.122 Tue 18:30 P4

Electronic structure and optical spectrum of lonsdaleite — •Johannes Büngeler, Stephan Blankenburg, and Arno Schindlmayr — Department Physik, Universität Paderborn, 33095 Paderborn, Germany

Lonsdaleite is a rare but naturally occurring allotrope of carbon. Like in diamond, each carbon atom forms four sp^3-hybridized bonds with a local tetrahedral geometry, but the overall crystal structure is hexagonal, not cubic. First discovered in fragments of the Canyon Diablo meteorite in 1967, it was originally characterized as translucent with a brownish-yellow color and a Mohs hardness of 7–8, whereas recent first-principles calculations predicted a substantially higher indentation strength than that of diamond. If confirmed, this would make lonsdaleite the hardest material known. To resolve the conflicting experimental and theoretical findings, we perform a quantitative study of the quasiparticle band structure, using the GW approximation for the nonlocal and dynamic self-energy. Subsequently, the optical absorption spectrum is calculated from time-dependent density-functional theory, including a long-range kernel to account for the electron-hole attraction and the formation of excitons. Our results show unambiguously that pure lonsdaleite crystals are completely transparent in the visible spectral range. This gives strong support to the hypothesis that the analyzed samples were contaminated by impurities and imperfections, which not only influence the color, but also reduce the hardness.

O 36.123 Tue 18:30 P4

GaN/AlN Structures with Two Dimensional Electron Gas: A

Density Functional Theory Study — Jakub Sołtys[1], Michał Łopuszyński[1], •Jacek Piechota[1], and Stanisław Krukowski[1,2] — [1]Interdisciplinary Centre for Materials Modelling, University of Warsaw, ul. Pawińskiego 5a, 02-106 Warszawa, Poland — [2]Institute of High Pressure Physics, Polish Academy of Sciences, ul. Sokołowska 29/37, 01-142 Warsaw, Poland

GaN is a promising material because of its properties: it can be used in high-temperature, high-frequency and high-power device applications. It has been shown that the GaN/AlN/GaN junction with ultra-thin AlN layer can be prepared and significant improvement in some crucial parameters over GaN/AlGaN is attained. In our work we present density functional study of the AlN/GaN high electron mobility transistor (HEMT) structure. It was shown that two dimensional electron gas (2DEG) is present at the AlN/GaN interface. Analysis of potential profiles and band structures for different thickness of AlN barier allow us to assess how the barrier affects 2DEG.. It was demonstrated that for too thin AlN barrier 2DEG is not well confined. However, for a thicker AlN barrier, the occupancy of this states is higher, and this result is consistent with the available experimental data [Dabiran et.al., Appl. Phys. Lett. 93 082111 (2008)].

O 36.124 Tue 18:30 P4

A Density Functional Theory Study of the TMG Adsorption on the GaN Surface — Maria Ptasińska[1], Jakub Sołtys[1], •Jacek Piechota[1], and Stanisław Krukowski[1,2] — [1]Interdisciplinary Centre for Materials Modelling, University of Warsaw, ul. Pawińskiego 5a, 02-106 Warszawa, Poland — [2]Institute of High Pressure Physics, Polish Academy of Sciences, ul. Sokołowska 29/37, 01-142 Warsaw, Poland

TMG (trimetylogallium) and NH3 (ammonia) are widely used reactants in the metal organic chemical vapor deposition (MOCVD) technique used in the growth of the GaN thin films. We have recently examined theoretically, with the help of the density functional theory (DFT), TMG adsorption on the GaN(0001) surface in order to study formation of bonds between Ga and N. Dangling bonds on the GaN(0001) surface were saturated with the hydrogen atoms. The slab polarization, which is due to the dangling bonds present on the GaN(0001) surface, and energy of the system in the vicinity of TMG was computed for different distances between the surface atoms and TMG. We also studied TMG diffusion on the GaN surface. As a result, the energy path for diffusion from Top N to Hollow was obtained.

O 36.125 Tue 18:30 P4

Band convergence of all-electron *GW* calculations: the extreme case of ZnO — •Christoph Friedrich, Mathias C. Müller, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Recently, Shih *et al.* [1] presented a new one-shot *GW* calculation for the band gap of wurtzite ZnO based on the pseudopotential approach. They showed that a proper convergence with respect to the number of bands used in the construction of the self-energy yields a band gap that is very close to the experimental value of 3.6 eV. This is in contrast to previous all-electron calculations where band gaps in the range 2.12–2.44 eV have been found [2]. In this work we present a *GW* calculation for ZnO that is based on the all-electron full-potential linearized augmented-plane-wave (FLAPW) method [3]. We obtain a band gap that is much larger than that of the previous all-electron calculations, but still smaller than that of Ref. 1. We go beyond their approach in two respects: we neither employ the pseudopotential nor the plasmon-pole approximation. Apart from the band convergence we also discuss the linearization error for high-lying states and how to eliminate it with local orbitals. Our results show that the band convergence is a very serious issue in the *GW* approach. ZnO is an extreme case in this respect. [1] B.-C. Shih *et al.*, Phys. Rev. Lett. 105, 146401 (2010). [2] M. Usuda *et al.*, Phys. Rev. B 66, 125101 (2002); M. Shishkin and G. Kresse, *ibid.* 75, 235102 (2007); F. Fuchs *et al.*, *ibid.* 76, 115109 (2007). [3] C. Friedrich *et al.*, Phys. Rev. B 81, 125102 (2010).

O 36.126 Tue 18:30 P4

Time-Dependent Density Functional Theory study of transfer of charge by atomic impact, a case study with C4H10 + Au — •Guillermo Avendano Franco, Myrta Grüning, and Xavier Gonze — Université catholique de Louvain, Louvain-la-Neuve, Belgium

The transfer of charge between metals and organic structures is studied using Time-dependent density functional theory (TDDFT) in a simple case of a molecule of Butane (C4H10) and an atom of gold (Au).

For a first approach to the problem we studied the transfer of charge in a dynamic dissociation of gold-Butane complex, the range of kinetic energies was between 132 Ha (3.59 keV) and 13 kHa (359 keV). In a second step we studied the effect of a collision of one atom of gold directed to one of the carbon atoms of Butane or bond between carbons.

In both cases we observe the partial or total transfer of one electron from the Butane molecule to the atom of gold, an effect that is dependent on the kinetic energies involved in the process.

O 36.127 Tue 18:30 P4

Energetics and metastability of the silicon vacancy in cubic SiC — Fabien Bruneval and •Guido Roma — CEA-Service de Recherches de Métallurgie Physique, Saclay, France

The silicon vacancy is a prominent intrinsic defect of cubic SiC (3C-SiC) to which much effort has been devoted so far, experimentally and theoretically. We calculate its properties using the state-of-art GW approximation that does not suffer from the band gap problem. The obtained formation and transition energies deviate significantly from the usual density functional theory evaluations and now compare favorably with experiment. A new assignment for the main line of photoluminescence is then proposed. We further perform GW calculations for the saddle point of reaction paths. The resulting barrier energies explain the thermal annealing experiments thanks to an original mechanism mediated by a minority charge configuration.

O 36.128 Tue 18:30 P4

KKRnano, a code for accurate density functional calculations for systems with thousands of atoms — •Rudolf Zeller, Alexander Thiess, and Stefan Blügel — Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich und JARA, D-52425 Jülich

The present state of our newly developed computer code KKRnano will be outlined. The code, which is designed for massively parallel computing, is based on the Korringa-Kohn-Rostoker (KKR) Green function method and can be applied to supercells with arbitrary atomic arrangements. KKRnano uses an iterative solution of the algebraic Dyson equation which describes the interaction between otherwise independent single atomic scattering events. Because of that efficient parallelization and reduced scaling of the computational effort (quadratically instead of cubically with the number of atoms) are easily achieved. For large systems calculations with linear scaling effort are possible if small total energy errors are admitted (less than 1 meV per atom). In particular, it will be explained how a preconditioner for the iterative solution can be constructed so that the calculations are accelerated by about a factor ten for all systems investigated so far which include metallic systems, defect levels in Si, magnetic GaN:Gd with O and N codoping and GeSbTe phase-change materials.

O 37: Invited Talk (Hubertus Marbach)

Time: Wednesday 10:15–11:00 Location: TRE Phy

Invited Talk O 37.1 Wed 10:15 TRE Phy

Writing nanostructures with a focused electron beam — •Hubertus Marbach — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

The injection of electrons can be used to trigger physical or chemical processes, like bond formation or dissociation. In our surface science approach to focused electron beam induced processing (FEBIP) we use a 3 nm diameter electron beam from a scanning electron microscope (SEM) in ultra high vacuum to locally dissociate adsorbed precursor molecules or locally change substrate properties. This approach is suitable to fabricate extremely small and pure nanostructures with lithographic control. One example are pure iron nanostructures produced by electron beam induced dissociation (EBID) of $Fe(CO)_5$ on Si(100) [1]. Systematic studies on various substrates revealed a strong influence of the nature and preparation state of the surface; among other effects electron scattering and catalytic properties must be considered. On SiO_x, we found that an electron beam can locally preactivate the sample; subsequent exposure to a precursor and autocatalytic growth allow to produce pure structures already at room temperature [2]. This represents a novel lithographic technique to generate pure nanostructures.

[1] Lukasczyk et al., Small, 4 (2008) 841.

[2] Walz et al., Angew. Chem. Int. Ed., 49 (2010) 4669.

This work has been supported by the DFG through grant MA 4246/1-1, COST Action CM0601 and COST Action D41.

O 38: [DS] Progress in Micro- and Nanopatterning: Techniques and Applications II (Focused Session, jointly with O - Organisers: Graaf, Hartmann)

Time: Wednesday 11:00–13:00 Location: GER 38

O 38.1 Wed 11:00 GER 38

Tuning the electrical conductivity of Pt-containing granular metals by postgrowth electron irradiation — •Fabrizio Porrati, Roland Sachser, Christian H. Schwalb, and Michael Huth — Physikalisches Institut, Goethe-Universität, D-60438 Frankfurt am Main, Germany

We have fabricated Pt-containing granular metals by focused electron beam induceddeposition from the $(CH_3)_3CH_3C_5H_4Pt$ precursor gas. The granular metals are made of platinum nanocrystallites embedded in a carbonaceous matrix. We have exposed the as-grown nanocomposites to low energy electron beam irradiation and we have measured the electrical conductivity as a function of the irradiation dose. Postgrowth electron beam irradiation transforms the matrix microstructure and thus the strength of the tunnel coupling between the Pt nanocrystallites. For as-grown samples (weak tunnel coupling regime) we find that the temperature dependence of the electrical conductivity follows the stretched exponential behavior characteristic of the correlated variable-range hopping transport regime. For briefly irradiated samples (strong tunnel coupling regime) the electrical conductivity is tuned across the metal-insulator transition. For long-time irradiated samples the electrical conductivity behaves like that of a metal. In order to further analyze changes of the microstructure as a function of the electron irradiation dose we have carried out atomic force microscopy (AFM) and micro-Raman measurements. These measurements reveal that by increasing the irradiation dose the matrix changes following a graphitization trajectory between amorphous carbon and nanocrystalline graphite.

O 38.2 Wed 11:15 GER 38

Ordered triple color patterns based on two dye molecules — •Wang Wenchong, Fuchs Harald, and Chi Lifeng — Physikalisches Institut and Center for Nanotechnology (CeNTech), Universität Münster, 48149 Münster, Germany

Functional, small molecular weight organic molecules have received great scientific and technological interest due to their promising potential applications in molecular electronics and optoelectronics. Since last two decades, exciting progress has been witnessed in both materials and film preparation that applied for organic field effect transistors (OFETs),light emission diodes (OLEDs), solar cells,Memories, Sensors, and so on. However, device processing techniques yielding high performances, high levels of integration and uniformity over large area are still underdevelopment. Template directed growth of molecules has been demonstrated as a promising technique for patterning,functionalizing materials at predefined areas and improving device performance.[1-3] Here, based on liquid behavior and solid solvation of molecuoes on patterned surface, the technique can further be applied to fabricate high resolution, ordered triple color patterns with only two molecules.

[1] W. C. Wang, L. F. Chi, et al, Phys. Rev. Lett.2007, 98, 225504.

[2] W. C. Wang, L. F. Chi, et al, Adv. Mat. 2009, 21, 4721.

[3] W. C. Wang, L. F. Chi, et al, Adv. Mat. 2010, 22, 2764.

O 38.3 Wed 11:30 GER 38

Artificial Hierarchical Gecko-mimicking Structures — •Michael Röhrig, Alexander Kolew, Fabian Pfannes, Matthias Worgull, and Hendrik Hölscher — Institute for Microstructure Technology (IMT), Karlsruhe Institute of Technology (KIT), Germany

Geckos have an impressive attachment system that makes them able to climb on nearly every surface. Like various other mechanisms developed by nature, the gecko effect is strongly connected to the structuring of surfaces. The toes of the Tokay Gecko for example are divided into several lamellae which are covered with millions of setae, delicate hairs which are about $100\,\mu m$ in height and $4\,\mu m$ in diameter. The setae branch into hundreds of tiny endings, the so called spatulae. Thus the gecko is capable of achieving intimate contact with smooth and rough surfaces which leads to a strong adhesion due to intermolecular forces, in particular van der Waals forces.

Mimicking these micro- and nanostructures leads to artificial dry attachment systems. *Hot embossing* is a well-suited molding technique to fabricate such biomimetic structures. In this talk a new variation of hot embossing, the so called *hot pulling* will be presented. Hot pulling allows the fabrication of fibrillar, gecko-mimicking surfaces. Beyond that, the method of measuring the adhesion of structures via AFM force distance curves by using spherical tips will be depicted.

O 38.4 Wed 11:45 GER 38

Self-arranged anodic nanostructured thin films on titanium — •Robin Kirchgeorg, Steffen Berger, and Patrik Schmuki — Institute for Surface Science and Corrosion (LKO), Department Material Science and Engineering, Fridrich-Alexander-Universität Erlangen-Nürnberg, Martensstraße 7, 91052 Erlangen, Germany

Self-organized anodic oxide nanostructures, in particular highly ordered titania nanotubes offer several interesting functional properties that have been explored in a wide field of applications, such as wettability tuning of surfaces, bio medicine, electrochromic devices, and solar energy conversion. The nanotubular oxides can be tailored, for example with respect to layer thickness, tube diameter, and other morphological, electrical or chemical properties. For many applications these patterned surfaces are at prime importance. The self-organization and growth mechanism of TiO_2 nanotubes during anodization were investigated on photolithographically masked titanium thin films. The influence of potential, time and anodization conditions on the growth mechanism of TiO_2 nanotubes are evaluated. The presentation will provide an overview on the mechanisms of growth and self-ordering of TiO_2 nanotubes.

O 38.5 Wed 12:00 GER 38

Flexible, free-standing and electrically active TiO_2 nanotubular membranes via lithographic approaches — •Sergiu P. Albu, Steffen Berger, Himendra Jha, and Patrik Schmuki — Department of Materials Science, WW4-LKO, University of Erlangen-Nuremberg, Martensstrasse 7, D-91058 Erlangen, Germany

In the presentation we show the fabrication of a new generation of TiO_2 nanotube membranes. The anodic oxide nanotube growth can be performed through a patterned Ti foil into an underlying Al metal layer [1]. After the selective dissolution of the Al/alumina layer, a very well defined both side open suspended TiO_2 nanotube layer can be obtained. Using lithographic patterning of the anodization area allows to achieve large scale, flexible and well electrically connected nanotubular flow-through membranes with fast electrical switching features over the entire membrane. The removal of the top-initiation layer is based on carrying out anodization through a slowly soluble photoresist coating [2]. These approaches facilitate a better quality and new features of the TiO_2 nanotubular structures.

[1] S. P. Albu, A. Ghicov, S. Berger, H. Jha, P. Schmuki, Electrochem. Commun. 2010, 12, 1352.

[2] S. P. Albu, P. Schmuki, Phys. Status Solidi RRL 2010, 4, 151.

O 38.6 Wed 12:15 GER 38

ALD Growth of Highly Ordered ZnO Nanotube Arrays with Tunable Structures and Their Device Applications — •Hui

Sun, Kin-Mun Wong, Stefan Bartels, Gerhard Wilde, and Yong Lei — Institute of Materials Physics and Center for Nanotechnology, University of Münster, Münster 48149, Germany

Because of the highly ordered feature, anodic alumina membranes have been widely used as nano-templates for growing one-dimensional (1D) nanostructures of various materials. The structural parameters of the template-prepared 1D nanostructures are adjustable including the size, spacing, and aspect ratio of the nanostructures. Recently, we successfully fabricated large-scale ordered arrays of ZnO nanotubes using a synthesizing route combining the template technique and atomic layer deposition (ALD) process. The advantages of the template technique together with the natures of the ALD process (e.g., precisely controllable atomic-scale growing process) results in attractive features of the obtained ZnO nanotube arrays, including tunable tube diameter, wall thickness, length and array density. These nanostructures are of extremely high and variable surface-to-volume ratio, which means that the change of surface status would affect the state of the material significantly. We believe that those constructions will largely enhance the utility of surface electronics devices, such as chemical sensors, biosensors etc., and the structure meets the requirement for conductometric semiconductor gas sensors of high sensitivity. Potential applications, such as photonic detector of super high resolution and band edge mode surface emitting laser are discussed.

O 38.7 Wed 12:30 GER 38

Surface Patterning using Nano-Templates For Realizing Highly Ordered Nanostructure Arrays with Controllable Properties — •Huaping Zhao, Shikuan Yang, Fabian Grote, Feng Xu, and Yong Lei — Institute of Materials Physics and Center for Nanotechnology, University of Muenster, Muenster 48149, Germany

Here we present the research progress of template-based surface nanopatterning techniques [1-5] in our group. Two kinds of templates were used in the surface patterning process: ultra-thin alumina membranes and monolayer polystyrene spheres. Using the templates, surface patterns of different materials with diverse shapes were synthesized. The structural parameters of the template-prepared surface patterns largely depend on those of the templates. The feature size of the building blocks of the patterns can be adjusted from the quantum size to nanoscale and microscale range [1]. The cost-effective and time-saving fabrication processes of template-based surface patterning approaches are highly desirable for industrial applications in fabricating different nano-devices, giving rise to broad applications of template-prepared surface nanostructures.

References:

1.Lei Y, Yang SH, Wu MH, et al., Chem. Soc. Rev., in press, 2010 (DOI:10.1039/ B924854B).

2. Wu MH, Wen LY, Lei Y, et al., Small, 6 (5), 695, 2010.

3. Lei Y, Cai WP, Wilde G, Prog. Mater. Sci., 52, 465, 2007.

O 38.8 Wed 12:45 GER 38

Dynamics of step bunches on vicinal surfaces: Sublimation, electromigration and transparent steps — •Marian Ivanov[1], Vladislav Popkov[2], and Joachim Krug[1] — [1]Institut für Theoretische Physik, Universität zu Köln, Köln — [2]Dipartimento di Fisica Teorica, Università degli Studi di Salerno, Salerno, Italy

Using morphological instabilities one can produce templates for nanoscale technology. One example of such an instability is step bunching, which splits a regular vicinal surface into regions of low and high density of monoatomic steps. We consider a one-dimensional step train evolving in the presence of sublimation, step-step interactions, fast kinetics and an Ehrlich-Schwoebel effect. We show that the interplay of sublimation and step-step interactions removes the conservation law for the crystal volume in the co-moving frame, which has been assumed in previous work [1,2]. As a consequence large step bunches are found to break up into smaller bunches of a characteristic size, and the monotonic coarsening dynamics of the volume-conserving model is replaced by a complex quasiperiodic pattern [3]. This interesting behavior is preserved by adding the corresponding terms due to the effect of electromigration. In the case of fast diffusion we consider a recently introduced model for transparent steps [4] and present simulation results for the evolution of the bunch geometry.

[1] V. Popkov, J. Krug, Europhys. Lett. 72, 1025 (2005) [2] V. Popkov, J. Krug, Phys. Rev. B 73, 235430 (2006) [3] M. Ivanov, V. Popkov, J. Krug, Phys. Rev. E 82, 011606 (2010) [4] B. Ranguelov, S. Stoyanov, Surf. Sci. 603, 2907 (2009)

O 39: Focussed session: Theory and computation of electronic structure: new frontiers III (jointly with HL, DS)

Time: Wednesday 11:15–13:00 Location: TRE Phy

O 39.1 Wed 11:15 TRE Phy

Dynamical magnetic excitations of nanostructures from first-principles — •Samir Lounis[1,2], Antonio Costa[3], Roberto Muniz[3], and Douglas Mills[1] — [1]Department of Physics and Astronomy, University of California Irvine, California, 92697 USA — [2]Institut für Festkörperforschung and Institut for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [3]Instituto d Fisica, Universidade Federal Fluminense, 24210-340 Niteroi, Rio de Janeiro, Brazil

Within the framework of time-dependent density functional theory combined with the Korringa-Kohn-Rostoker Green function formalism, we present a real space methodology to investigate dynamical magnetic excitations from first-principles [1]. We set forth a scheme which enables one to deduce the correct effective Coulomb potential needed to preserve the spin-invariance signature in the dynamical susceptibilities, i.e. the Goldstone mode. We use our approach to explore the spin dynamics of 3d adatoms and different dimers deposited on a Cu(001) surface[1] and a Cu(111) surface [2] with emphasis on their decay to particle-hole pairs.

Research supported by the U. S. Depart. of Energy through grant No. DE-FG03-84ER-45083. S. L. thanks the A.v. Humboldt Foundation for a Feodor Lynen Fellowship. R.B.M. acknowledges support from CNPq and FAPERJ, Brazil.

[1] Lounis *et al.* Phys. Rev. Lett. **105**, 187205 (2010); Lounis *et al.* arXiv:1010.1293. [2] Khajetoorians et al. arXiv:1010.1284v2.

O 39.2 Wed 11:30 TRE Phy

Magnetic order of LaVO$_3$/SrVO$_3$ superlattices — •Cosima Schuster[1], Ulrike Lüders[2], Udo Schwingenschlögl[3], and Raymond Fresard[2] — [1]Institut für Physik, Universität Augsburg, D-86135 Augsburg — [2]Laboratoire CRISMAT, UMR CNRS-ENSICAEN(ISMRA) 6508, FR3095 Caen — [3]KAUST, PCSE Division, P.O. Box 55455, Jeddah 21534, Saudi Arabia

While stable ferromagnetic ground states are predicted based on model calculations their experimental realizations are scarce. Experimental data obtained on LaVO$_3[m]$/SrVO$_3[1]$ superlattices show that these systems remain magnetic above room temperature for particular values of m, in contrast to the solid solutions with the same composition. To clarify the magnetic and orbital order in these heterostructures, we perform electronic structure calculations based on density functional theory. First, we discuss the magnetic and orbital order of strained LaVO$_3$, for the c/a ratio of the heterostructure, where two types of ordering are nearly degenerate. While both g-type and c-type antiferromagnetic ordering within the LaVO$_3$ favour a non-magnetic interface in case of odd m and a ferromagnetic interface in case of even m, the orbital ordering perpendicular to the interface is different in both cases. A detailed discussion of the particular combinations of the magnetic and orbital order at the interface is given.

O 39.3 Wed 11:45 TRE Phy

First-principles quantum-mechanical methods for full prediction of NMR parameters in fluorides — •Aymeric Sadoc[1], Florent Boucher[1], Mamata Biswal[2], Monique Body[2], and Christophe Legein[2] — [1]Institut des matériaux Jean Rouxel (IMN) - Université de Nantes, CNRS, 2 rue de la houssinière, BP 32229, 44322 Nantes, France — [2]Institut de Recherche en Ingénierie Moléculaire et Matériaux Fonctionnels (IRIM2F) - Université du Maine, CNRS, Avenue Olivier Messiaen, 72085 Le Mans, France

^{19}F magic angle spinning (MAS) NMR is a powerful structural tool for complex fluoride crystalline materials having multiple crystallographic sites since ^{19}F (I=1/2) isotropic chemical shift (δ_{iso}) is very sensitive to the environment of the fluorine atom. However, in many cases, several fluorine sites have the same multiplicity preventing an unambiguous experimental assignment. Simulation of the response to an external magnetic field is then necessary to complete the analysis. The relation of the measured δ_{iso} values with the calculated isotropic chemical shieldings (σ_{iso}) is needed to interpret of NMR spectra.

^{19}F σ_{iso} values were calculated for alkali, alkaline earth and rare earth of column IIIB fluoride compounds using the GIPAW method implemented in the CASTEP software. Using DFT-PBE, we have established a linear relation between ^{19}F calculated σ_{iso} and experimental δ_{iso} values which enables full prediction of ^{19}F NMR spectra. In the case of complex NMR spectra, this calibration curve is successfully applied for the attribution from first-principles quantum-mechanical of ^{19}F chemical shifts.

O 39.4 Wed 12:00 TRE Phy

Ab-initio study of MnO and NiO in various crystal structures – The failure of (semi)local density functionals — •Andreas Schrön, Claudia Rödl, and Friedhelm Bechstedt — IFTO, FSU Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Transition-metal oxides (TMOs) are of great interest for applications in e.g. dilute magnetic semiconductors (DMSs) which are supposed to allow for transparent ferromagnets with high critical temperatures. One of the most promising host materials is ZnO which crystallizes in the wurtzite structure. Although TMOs have been investigated a long time experimentally, their theoretical description is still unsatisfying.

The semilocal generalized-gradient approximation (GGA) to density functional theory (DFT) works well for many materials. Here we demonstrate that this approach predicts the wrong ground-state crystal structure for MnO, since it does not account sufficiently for the electron correlation effects in materials with strongly localized electrons. It is usually assumed, that approaches including an additional on-site Coulomb interaction U (GGA+U) or non-local exchange contributions like the hybrid functional HSE03 cure this failure.

The relative energetic ordering of the rock-salt, zinc-blende, and wurtzite crystal structures are investigated for various magnetic orderings. It is shown that neither GGA nor the HSE03 hybrid functional yields the experimentally observed ground-state structure. However, agreement with experiment is obtained if the GGA+U functional with $U > 4$ eV is applied. For NiO, on the other hand, all three functionals yield rock-salt as the equilibrium crystal structure.

O 39.5 Wed 12:15 TRE Phy

Laser-induced ultrafast demagnetization: First-principles analysis of Elliott-Yafet processes — •Karel Carva[1,2] and Peter M. Oppeneer[2] — [1]Department of Condensed Matter Physics, Charles University, Ke Karlovu 5, CZ-12116 Prague 2, Czech Republic — [2]Department of Physics and Materials Science, Uppsala University, Box 530, SE-75121 Uppsala, Sweden

The laser-induced ultrafast demagnetization phenomenon has attracted a lot of attention since the first successful experiment on the fs timescale in 1996. However even now it is still far from being understood on the microscopic level. A number of possible microscopic mechanisms have been proposed.

Here we concentrate on Elliott-Yafet spin relaxation due to to electron-phonon scattering in Ni. The spin-flip probability associated with electron-phonon scattering in Ni has been estimated - employing the ab initio band structure - to be larger than expected. We calculate the spin-flip Eliashberg function based on ab initio electron-phonon coupling matrix elements to obtain the spin-flip probability with much higher accuracy. We extend this method to the regime of non-equilibrium electron distributions relevant for ultrafast processes. We find significant differences between the efficiency of this spin relaxation mechanism for highly non-equilibrium electron distributions pumped by the laser and thermalized ones (not in equilibrium with lattice).

O 39.6 Wed 12:30 TRE Phy

Momentum Distribution and Renormalization Factor in Sodium and the Electron Gas — •Valerio Olevano — Institut Neel, CNRS & UJF, Grenoble, France

The homogeneous electron gas or jellium is one of the most fundamental models, canonical workbench to test different many-body theoretical approaches. Although really simple, still is very close to real solids, especially alkali metals, and sodium is one of its nature's closest realization. Here we present theoretical and also experimental results on the momentum distribution and the quasiparticle renormalization factor in sodium. From an x-ray Compton-profile measurement of the valence-electron momentum density, we derive its discontinuity at the Fermi wavevector. This yields for the first time an accurate measure of the renormalization factor, one of the most important quantities in many-body theory, that we compare with GW and quantum Monte Carlo calculations performed both on crystalline sodium and on the homogeneous electron gas. Our calculated results are in good agreement with the experiment.

References: S. Huotari, J. A. Soininen, T. Pylkkänen, K. Hämäläinen, A. Issolah, A. Titov, J. McMinis, J. Kim, K. Esler, D. M. Ceperley, M. Holzmann, and V. Olevano, Phys. Rev. Lett. 105, 086403 (2010).

O 39.7 Wed 12:45 TRE Phy

Construction of low energy Hamiltonians using maximally localized Wannier functions — •Roman Kovacik and Claude Ederer — School of Physics, Trinity College Dublin, Ireland

The theoretical description of correlated electron systems, such as e.g. transition metal oxides, is often based on effective tight-binding (TB) models. A systematic way to obtain realistic TB model parameters from first principles calculations is the construction of maximally localized Wannier functions (MLWFs) [1]. The corresponding TB representation is given by the real space Hamiltonian matrix elements in the MLWF basis. We address two important issues: i) how many orbitals to include in the basis set for the TB model representation, and ii) what is the most appropriate reference point to connect the model and Kohn-Sham band structures (i.e. should the Kohn-Sham band structure be considered as "non-interacting" or as mean-field approximation to the interacting case). We use $LaMnO_3$, a prototype material for correlation-driven phenomena, as an example for the construction of model Hamiltonians. In particular, we compare a TB description based only on effective Mn e_g bands with a description that explicitly includes also the O p bands, and we analyze the effects of the Hubbard U and the Jahn-Teller distortion on the corresponding TB parameterizations. In addition, we discuss the suitability of different types of Wannier functions for the calculation of TB parameters.

[1] I. Souza, N. Marzari, and D. Vanderbilt, PRB 65, 035109 (2001).

O 40: Metal substrates: Adsorption of organic / bio molecules V

Time: Wednesday 11:15–13:00 Location: PHY C213

O 40.1 Wed 11:15 PHY C213

Bonding and metalation of 2H-TPP on the Cu(111) surface- a multitechnique study — •Katharina Diller[1], Florian Klappenberger[1], Klaus Hermann[2], and Johannes V. Barth[1] — [1]Physik Department, E20, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

We report on the interaction of free base tetraphenylporphyrin (2H-TPP) molecules with the Cu(111) surface studied with a multitechnique approach combining x-ray photoelectron spectroscopy (XPS) and near-edge x-ray absorption fine structure spectroscopy (NEXAFS) measurements with density functional theory (DFT) calculations. After the adsorption of 2H-TPP on Cu(111) at room temperature the spectroscopic signatures (XPS and NEXAFS) depend on the molecular coverage. Near to a saturated monolayer NEXAFS indicates a strongly deformed macrocycle and electron transfer into the LUMO. XPS reveals that the adsorbate is a free base porphyrin. After annealing both XPS and NEXAFS data show the signature of a metalloporphyrin with a relaxed macrocycle. DFT calculations corroborate the peak assignment used for the analysis of the XPS and the NEXAFS data and provide information on the electronic structure of isolated 2H-TPP and Cu-TPP molecules.

O 40.2 Wed 11:30 PHY C213

Metalation of tetrapyridylporphyrin with Cu atoms on

Au(111): aspects of structure and reactivity — •Jie Xiao[1], Martin Schmid[1], Min Chen[1], Ziliang Shi[2], Nian Lin[2], Tatyana Shubina[3], Timothy Clark[3], Hans-Peter Steinrück[1], and Michael Gottfried[1] — [1]Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Erlangen, Germany — [2]Hong Kong University of Science and Technology, Hong Kong, China — [3]Universität Erlangen-Nürnberg, Computer-Chemie-Centrum, Erlangen, Germany

The reaction between a submonolayer of tetrapyridylporphyrin (2HTPyP) on Au(111) and co-deposited Cu atoms was studied by temperature-dependent X-ray photoelectron spectroscopy (XPS) and scanning tunneling microscopy (STM). The Cu atoms undergo two simultaneous reactions with 2HTPyP: (1) Metalation of the porphyrin core and (2) coordination by pairs of pyridyl groups of adjacent 2HTPyP molecules. At 300 K, the metalation reaction (1) leads mainly to a metastable initial complex, Cu-2HTPyP, in which Cu remains in the zero oxidation state. At elevated temperatures, Cu is oxidized by the porphyrin ligand, forming copper(II) tetrapyridylporphyrin (CuTPyP). Further details of the complex reaction mechanism are revealed by DFT calculations. The coordination reaction (2) leads to the formation of a 2D metal-organic coordination network, which gradually degrades at higher temperatures due to bulk diffusion of Cu, resulting in close-packed molecular monolayer stabilized by intermolecular hydrogen bonds. Supported by the Deutsche Forschungsgemeinschaft through SFB 583 and by the Alexander von Humboldt Foundation.

O 40.3 Wed 11:45 PHY C213

Adsorption behaviour of CoPc and CoTMPP on Cu(110) and Cu(110)-(2x1)O — •Daniel Queteschiner, Mariella Denk, Michael Hohage, and Peter Zeppenfeld — Institute of Experimental Physics, Johannes Kepler University Linz, A-4040 Linz, Austria

The geometric arrangement of cobalt-phthalocyanine (CoPc) and cobalt-tetra(4-methoxyphenyl)porphyrin (CoTMPP) on the Cu(110) and Cu(110)-(2x1)O surface was investigated for coverages up to 1 ML by a combination of reflectance difference spectroscopy (RDS), low energy electron diffraction (LEED), and scanning tunneling microscopy (STM).

On Cu(110) both molecules adsorb at room temperature in a 2D-gas. Upon cooling to $T = 14$ K CoTMPP condenses into a well-ordered structure while for CoPc the gas phase is maintained.

On the oxygen reconstructed Cu surface, however, both CoPc and CoTMPP form well-ordered structures even at room temperature. Continuing the growth up to the saturated ML, the CoTMPP layer undergoes two coverage driven transitions between distinct superstructures.

O 40.4 Wed 12:00 PHY C213

DFT Calculations on the Electronic Interaction of Iron-Phthalocyanine with the Ag(111)-Surface — •Martin Callsen[1,2] and Eckhard Pehlke[2] — [1]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel

Organic molecules adsorbed on metal-surfaces play an important role for the functionalization of surfaces or as candidates for electronic devices in the emerging field of nano-electronics. As such metal-phthalocyanines (MPc) are an intensely studied model-system, both experimentally in STM/STS-measurements and theoretically by density functional theory (DFT) calculations. For the latter it is known that there are still problems concerning the correct treatment of dispersion interactions and the exact description of excitation spectra of organic molecules. For this reason a detailed comparison with experiments will be helpful. Iron-phthalocyanine (FePc) adsorbed on the Ag(111)-surface has been investigated by spin-polarized total energy calculations employing DFT as implemented in the VASP-code. The PAW-pseudopotential-method has been applied and as approximation for the xc-functional GGA-PBE has been used. To account for dispersion interactions the empirical C_6/R^6-ansatz [1] has been applied.

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

O 40.5 Wed 12:15 PHY C213

Stabilization by rotational entropy - A general attribute of 'large' adsorbates? — •Thomas Waldmann[1], Harry E. Hoster[1,2], and R. Jürgen Behm[1] — [1]Ulm University, Institute of Surface Chemistry and Catalysis, 89069 Ulm, Germany — [2]Current address: Technische Universität München, Centre for Electromobility, 50 Nanyang Drive, Singapore 637553

Large molecules have in general considerable moments of inertia. At sufficiently high temperatures and not too high coverages this can lead to a stabilization of the adlayer by rotational entropy, as shown, e. g., in a recent thermal desorption (TPD) study [1] of the bisterpyridine derivative 2,4'-BTP on graphite (HOPG). In this presentation we used 2,4'-BTP on Ag(111) as a model system, where this behavior was directly observed by scanning tunneling microscopy (STM) at 300 K. Domains of freely rotating 2,4'-BTP molecules are in a dynamic equilibrium with static disordered 2D islands $(2,4'\text{-BTP})_n$ (n>1) and individual molecules (n=1) stabilized by lateral (N...H) and vertical (N...Ag) interactions [2]. Evaluating a large number of molecules in STM images, we determined the mean energy difference between the rotating and the non-rotating adsorbates in the 2D islands. The stabilization by rotational entropy is compared with that of other typical small (O_2, N_2, acetylene) and large (benzene, PTCDA, 3,3'-BTP, HBDC, MPc) adsorbates at 300 K.

[1] M. Roos et al., PCCP 12, 812 (2010).

[2] T. Waldmann et al., ChemPhysChem 11, 1513 (2010).

O 40.6 Wed 12:30 PHY C213

Interplay of acceptor and donor species in charge-transfer complexes — •Tobias R. Umbach[1], Isabel Fernández-Torrente[1], Janina Ladenthin[1], Michael Kleinert[1], Robert Drost[1], Riccardo Rurali[2], Jose I. Pascual[1], and Katharina J. Franke[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Institut de Ciència de Materiales de Barcelona (ICMAB),Consejo Superior de Investigaciones Científicas (CSIC), Campus de Bellaterra, 08193 Bellaterra (Barcelona), Spain

The redistribution of charge between donor and acceptor species plays a key role for tuning the electronic functionality of organic compounds. By low temperature scanning tunneling microscopy and spectroscopy (LT-STM, LT-STS) we investigate molecular layers of the donor acceptor complexes Na-TCNQ, Na-TNAP, TTF-TNAP and TTF-TCNQ on a Au(111) surface. Due to the presence of the metallic surface the amount of charge transfer (CT) and its localization can differ from the bulk system. Both TTF-TCNQ and Na-TCNQ exhibit a CT of one electron, demonstrated by the presence of the Kondo resonance. In the case of Na-TCNQ the electron is localized at the Na-CN bond, whereas for TTF-TCNQ it lies in the conjugated lowest unoccupied molecular orbital. By changing the molecular acceptor the CT can be varied. TCNQ offers a lower electron affinity and higher symmetry compared to TNAP. In contrast to the first two systems, Na-TNAP as well as TTF-TNAP show no Kondo resonance, evidencing an even or non-integer CT.

O 40.7 Wed 12:45 PHY C213

STM/STS-Study of Spiro-DPO molecules on Au(111) up to two monolayers coverage — •Michael Waelsch[1], Benjamin Herath[1], Tobat P. Saragi[2], Josef Salbeck[2], and René Matzdorf[1] — [1]AG Experimentalphysik 2, Oberflächenphysik — [2]AG Makromolekulare Chemie und Molekulare Materialien, Universität Kassel

In the Spiro-DPO-molecule an arylamine group (acceptor) is linked to an oxadiazole group (donor) via a spiro-C-atom. Coverages of 1/10...2 ML of the organic semiconductor Spiro-DPO have been investigated with STM/STS at 4.7 K. Large islands of homochiral molecules were observed, whose internal double-row structure is oriented in an ± 10° angle relative to the Au-crystal axes. Spatially resolved tunneling spectra show different LUMO-energies of the donor/acceptor groups of one molecule.

O 41: Plasmonics and Nanooptics IV

Time: Wednesday 11:15–13:00 Location: WIL A317

O 41.1 Wed 11:15 WIL A317

Steering and Negative Refraction of Surface Plasmon Beams — •Benedikt Stein, Jean-Yves Laluet, Eloïse Devaux, Cyriaque Genet, and Thomas W. Ebbesen — ISIS, Université de Strasbourg & CNRS, 8 allée Gaspard Monge, 67000 Strasbourg, France

Surface plasmon polaritons have raised renewed interest over the past decade for their potential in optical devices and circuits [1]. Inspired by the design principles of photonic bandgap materials [2,3], we have studied the propagation of surface plasmon beams through singly and doubly periodic metallic gratings. Large beam steering effects are experimentally revealed by probing the isofrequency surfaces related to propagating Bloch waves inside the gratings. In particular, negative refraction is demonstrated close to the Bragg condition. We also analyze how the local structure of the isofrequency surface can amplify the sensitivity of surface plasmon based refractive-index sensors [4].

[1] Barnes, W. L.; Dereux, A.; Ebbesen, T. W. *Nature* 2003, 424, 824
[2] Zengerle, R. *Journal of Modern Optics* 1987, 34, 1589
[3] Russell, P.S.J. *Phys. Rev. A.* 1986, 33, 3232
[4] Stein, B.; Laluet, J.-Y.; Devaux, E.; Genet, C.; Ebbesen, T. W. *Phys. Rev. Lett.*, in press

O 41.2 Wed 11:30 WIL A317

Far-field optical characterization of ultrafast plasmon propagation in nanostructures — •Christian Rewitz[1], Thomas Keitzl[1], Philip Tuchscherer[1], Jer-Shing Huang[2], Peter Geisler[3], Bert Hecht[3], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg — [2]Department of Chemistry, National Tsing Hua University, Hsinchu 30013, Taiwan — [3]Nano-Optics and Biophotonics Group, Department of Experimental Physics 5, University of Würzburg, Am Hubland, 97074 Würzburg

Our goal is to characterize and control the propagation of ultrafast excitations in optical nanocircuits. For this purpose, the technique of spectral interferometry (SI) is combined with a microscope setup. This allows for a full characterization (amplitude and phase) of an ultrafast pulse emitted at the output of a nanocircuit. The input and output of the nanostructure can be addressed with a diffraction-limited resolution. As a first experiment, we investigate the propagation of plasmons in silver wires with nanometer radial and micrometer longitudinal dimensions. Once the excitation pulse is focused on one end of a wire, part of the energy is converted into a propagating plasmon mode. Upon propagation the plasmon is modified by dispersion and attenuation that is specific to the nanostructure. After the plasmon is converted into a radiative far-field mode at the other end of the wire the field is collected by the microscope objective and can be fully characterized via SI. Thus, specific plasmonic properties of the nanostructure can be determined. One of them is the propagation speed of the plasmon.

O 41.3 Wed 11:45 WIL A317

Ultrafast optical nonlinearities in hybrid metal-semiconductor nanostructures — •Parinda Vasa[1], Robert Pomraenke[1], Giovanni Cirmi[2], Elenora De Re[2], Wei Wang[1], Stephan Schwieger[3], David Leipold[3], Erich Runge[3], Giulio Cerullo[2], and Christoph Lienau[1] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany — [2]IFN-CNR, Dipartimento di Fisica, Politecnico di Milano, Milano, Italy — [3]Institut für Physik and Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, Germany

Understanding and manipulating the interactions between quantum emitters and surface plasmon polaritons (SPPs) is the key to designing and implementing novel nano-optical devices. We report the measurements of ultrafast optical nonlinearity resulting from the strong interaction between SPPs on a gold grating and excitons in either a semiconductor QW or a J-aggregated cyanine dye. The hybrid structures are characterized by linear reflectivity measurements and exhibit enhanced SPP-exciton coupling. The nonlinearity is investigated by low-temperature, angle-resolved, ultrafast pump-probe spectroscopy under different excitation schemes. Strong optical excitation drastically alters the hybrid nanostructure response by transiently changing the exciton density. A significant shift in the polariton resonance wavelength and changes in the response time are observed. The results are explained within a semi-classical density matrix formalism. Such a strong ultrafast nonlinear interaction between SPPs and excitons will be of key importance in adding active functionality to plasmonic devices.

O 41.4 Wed 12:00 WIL A317

Characteristics of the Electron Emission from Metal Nanotips due to Ultrashort Laser Pulses — •Steve Lenk and Erich Runge — Institut für Physik und Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, 98693 Ilmenau, Germany

We investigate the electron emission process from sharp gold nanotips illuminated by ultrashort femtosecond laser pulses theoretically. The emission processes under discussion for few-femtosecond laser pulses are multiphoton emission [1] and optical field emission [2]. We calculate the probability current from a numerical solution in two spatial dimensions of an initial-value problem [3] via an exponential split-operator method and a real-space product-formula algorithm [4]. The time-dependent electromagnetic potentials used for the study of the electron emission are derived from a finite-difference time-domain method calculation. We observe spatial emission spot changes dependent on the bias voltage as well as different time characteristics due to different laser pulse powers. The electric field and the photoelectron current are compared to experimental results.

[1] C. Ropers, D. Solli, C. Schulz, C. Lienau, and T. Elsaesser, Phys. Rev. Lett. **98**, 043907 (2007).
[2] P. Hommelhoff, C. Kealhofer, and M. Kasevich, Phys. Rev. Lett. **97**, 247402 (2006).
[3] S. Glutsch, *Excitons in Low−Dimensional Semiconductors*, Springer Heidelberg (2004).
[4] H. De Raedt, Comp. Phys. Rep. **7**, 1 (1987).

O 41.5 Wed 12:15 WIL A317

Theory of ultrashort plasmon pulse generation by mode-locked surface plasmon polariton lasers — •Kwang-Hyon Kim, Anton Husakou, and Joachim Herrmann — Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Max-Born-Str. 2a, 12489 Berlin

Amplification of surface plasmon polaritons (SPP) by embedding a dielectric with a gain medium is of great importance for a variety of applications including surface spectroscopy, imaging and information processing. By adding a feedback and a fast modulator, mode-locked lasing of SPPs becomes possible. In this contribution, we extend a semiclassical theory of surface plasmon polariton lasers to the case of mode-locked SPP lasers. In the considered scheme feedback is provided by a Bragg reflector of SPPs, and the SPP laser is composed of a metal film deposited on a polymer host as well as a saturable absorber layer and a gain layer. We investigate mode-locking characteristics, such as pulse duration and peak intensity, in dependence on the layer thickness of the metal film and the absorber layer, the pump intensity, and densities of gain and absorber molecules. We consider the dyes R6G as gain and DQOCI as saturable absorber and predict the possibility of SPP pulse generation with maximum peak intensity of more than 500 GW/cm^2 and shortest pulse duration of 280 fs.

O 41.6 Wed 12:30 WIL A317

Spatiotemporal nanofocusing in random nanostructures achieved by time-reversal, adaptive optimization, and optimal open-loop control of ultrashort laser pulses — •Dominik Differt[1], Javier Garcia de Abajo[2], Christian Strüber[1], Dmitri Voronine[1,3], and Walter Pfeiffer[1] — [1]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — [2]Instituto de Optica, CSIC, Serrano 121, 28006 Madrid, Spain — [3]Department of Physics, Texas A&M University, 4242 TAMU, College Station, USA

Because of the reciprocity of electromagnetic wave propagation the time-reversal of a wave emitted from a nanoemitter embedded in a random scattering environment should refocus in space and time at the emitter site. If only partial waves, e.g. one particular planar wave component, of the outgoing wave are time-reversed this nanolocalization of the back-propagated wave is not perfect. Here we investigate the degree of spatiotemporal nanolocalization of time-reversed partial planar waves. The chosen nanostructure consists of two nanoemitter particles embedded in a random assembly of metallic nanospheres acting as scattering environment. A multiple elastic scattering of multipole expansion (MESME) code is used for solving Maxwell's equations in frequency domain. The degree of nanolocalization varies significantly and depends critically on which partial planar wave is time-reversed. In addition, direct adaptive optimization or optimal open-loop control of the spatiotemporal nanofocusing of planar waves at the emitter position exhibits a much higher degree of nanolocalization.

O 41.7 Wed 12:45 WIL A317

Investigating Ag Nanostructures by TOF-PEEM using High Harmonic Radiation — •Soo Hoon Chew[1], Frederik Süssmann[2], Christian K. Späth[1], Alexander Guggenmos[2], Yingying Yang[2], Jürgen Schmidt[1], Adrian Wirth[2], Sergey Zherebtsov[2], Michael Hofstetter[2], Matthias F. Kling[2], Mark I. Stockman[3], Ferenc Krausz[2], and Ulf Kleineberg[1] — [1]Department of Physics, Ludwig Maximilian University of Munich, Garching, Germany — [2]Max Planck Institute of Quantum Optics, Garching, Germany — [3]Georgia State University, Altanta, USA

We demonstrate first experimental results on imaging plasmonic nanostructures by Time-of Flight-Photoelectron Emission Microscope (TOF-PEEM) in combination with Extreme Ultraviolet (XUV) attosecond pulses from a High Harmonic Generation source. The 1 kHz coherent attosecond XUV radiation is produced by ionizing neon atoms with waveform-controlled near-infrared (0.6 mJ, 5 fs) laser pulses and spectrally filtered at 93 eV by means of a multilayer mirror. We have characterized various polycrystalline Cu microstructures and Ag nanostructures using these ultrashort XUV pulses by TOF-PEEM with a spatial resolution approaching 100 nm. The electron energy spectrum have been investigated at different sample positions and energy filtering has been applied to improve image resolution. The experiments demonstrate first steps towards the temporal characterization of nanoscaled localized surface plasmon fields in a femtosecond optical-pump/attosecond XUV-probe experiments.

O 42: Graphene II

Time: Wednesday 11:15–12:45 Location: WIL B321

O 42.1 Wed 11:15 WIL B321

Graphene edge magnetism for spintronics applications: Dream or Reality? — •Jens Kunstmann[1], Cem Özdogan[2], Alexander Quandt[3,4], and Holger Fehske[3] — [1]Institute for Materials Science, TU Dresden, 01062 Dresden, Germany — [2]Department of Computer Engineering, Cankaya University, Ankara, Turkey — [3]Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, Germany — [4]School of Physics, University of the Witwatersrand, South Africa

We critically discuss the stability of edge states and edge magnetism in zigzag edge graphene nanoribbons (ZGNRs). We point out that magnetic edge states might not exist in real systems, and show that there are at least three very natural mechanisms – edge reconstruction, edge passivation, and edge closure – which dramatically reduce the effect of edge states in ZGNRs or even totally eliminate them. Even if systems with magnetic edge states could be made, the intrinsic magnetism would not be stable at room temperature. Charge doping and the presence of edge defects further destabilize the intrinsic magnetism of such systems. We conclude that edge magnetism within graphenes ZGNRs is much too weak to be of practical significance, in particular for spintronics applications. [1] J. Kunstmann, C. Özdoğan, A. Quandt, H. Fehske, arXiv:1007.2602 (2010).

O 42.2 Wed 11:30 WIL B321

Electronic properties of graphene superlattices in a strong magnetic field — •George Pal, Walter Apel, and Ludwig Schweitzer — Physikalisch-Technische Bundesanstalt (PTB), Bundesalee 100, 38116 Braunschweig, Germany

The application of 1-dimensional periodic potentials to graphene leads to new and unexpected phenomena. For example, new Dirac points are induced in the band structure whose positions are controlled by the ratio between the strength and the period of the superlattice potential. Also, the conductivity shows strong resonances when new zero energy states appear.

When graphene superlattices are placed in a magnetic field, the system is described by three length scales: the lattice constant, the period of the superlattice, and the magnetic length. When the parameters of the system are tuned such that these three characteristic lengths are commensurable, then the band structure is modulated in an unique way which has important consequences for the electronic and transport properties.

We study theoretically the electron properties of graphene superlattices in a perpendicular magnetic field within the lattice model. We show that the band structure changes dramatically depending on the ratio between the magnetic length and the superlattice period. Moreover, for certain strengths of the superlattice potential, additional energy gaps open in the Landau bands, which may lead to unusual plateau sequence in the Hall conductivity.

O 42.3 Wed 11:45 WIL B321

Mechanically-induced transport switching effect in graphene-based nanojunctions — Takazumi Kawai[1], Markus Poetschke[2], •Claudia Gomes da Rocha[2], Yoshiyuki Miyamoto[1], Stephan Roche[3], and Gianaurelio Cuniberti[2] — [1]Green Innovation Research. Laboratoriess, NEC Corp., 34 Miyukigaoka, Tsukuba, Ibaraki, Japan — [2]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany — [3]Centre d' Investigacio en Nanociencia i Nanotecnologia (ICN-CSIC), UAB Campus, E-08193 Bellaterra, Spain

We present a theoretical study suggesting a novel type of electronic switching effect, driven by the geometrical reconstruction of nanoscale graphene-based junctions. We considered junction structures which have alternative metastable configurations transformed by rotations of local carbon dimers. The use of external mechanical strain allows a control of the energy barrier heights of the potential profiles and also changes the reaction character from endothermic to exothermic or vice-versa. The reshaping of the atomic details of the junction encode binary electronic ON or OFF states, with ON/OFF transmission ratio that can reach up to 100000. Our results suggest the possibility to design modern logical switching devices or mechanophore sensors, monitored by mechanical strain and structural rearrangements.

O 42.4 Wed 12:00 WIL B321

Charged collective excitations and SU(4) symmetry in graphene — •Andrea Fischer[1], Rudolf Römer[1], and Alexander Dzyubenko[2,3] — [1]University of Warwick, Coventry, UK — [2]California State University Bakersfield, California, US — [3]General Physics Institute, Russian Academy of Sciences, Moscow, Russia

We show that graphene in a strong magnetic field with partially filled Landau levels sustains charged collective excitations, which are bound states of three-particle complexes [1]. Some of these states are optically bright and may be detected in spectroscopy experiments, enhancing the current understanding of electron-electron interactions in graphene. Indeed, such states have recently been seen at zero magnetic field in an ARPES study [2]. The states can be classified using the geometrical symmetries - non-commutative magnetic translations and generalized rotations - in addition to the dynamical SU(4) symmetry in graphene. From the SU(4) symmetry point of view, such excitations are analogous to bound states of two quarks and one antiquark with four flavours. Using Young diagram techniques, we determine the multiplet structure and establish a flavour optical selection rule to identify the bright states for experimental studies.

[1] A.M. Fischer, R.A. Römer and A.B. Dzyubenko, arXiv: 1005.3277

[2] A. Bostwick *et al.*, Science **328**, 999 (2010)

O 42.5 Wed 12:15 WIL B321

Electronic structure of graphene twist stacks — •Sam Shallcross[1], Sangeeta Sharma[2], and Oleg Pankratov[1] — [1]Lehrstuhl fur Theoretische Festkorperphysik, Staudstr. 7-B2, 91058 Erlangen, Germany. — [2]Max-Planck Institute for Microstructure Physics, Weinberg 2, 06120 Halle, Germany.

We present a study of graphene stacks consisting of an ordered sequence of pairs of twisted layers - the graphene twist stack; extending previous work on the graphene twist bilayer [1,2]. We find that this remarkable system entails a fundamental mixing of dimensionalities: while the twist stack spectrum is generated by an ensemble of *independent effective twist bilayer* Hamiltonians, the wavefunctions are products of *bilayer* wavefunctions and standing electron waves in the stacking direction, and thus extend over many layers of the stack. These have the property that of the ensemble of Dirac cones that constitute the twist stack band structure, it is those topologically closest to single layer graphene that dominate the surface region. We further examine the impact of stacking disorder, finding that these results are robust for moderate stacking fault density. With these results we are able to explain some of the striking differences between the physics of graphene grown on the C-face of SiC, and the by now well studied model of this system, the graphene twist bilayer.

[1] S. Shallcross, S. Sharma, E. Kandelaki, and O. A. Pankratov, Phys. Rev. B, 81:165105, 2010.

[2] S. Shallcross, S. Sharma, and O. A. Pankratov, Phys. Rev. Lett., 101:056803, 2008.

O 42.6 Wed 12:30 WIL B321

Selective chemisorption of graphene-like molecules on the Si(111) 7×7 surface: A theoretical study — •Janos Kiss, Thomas Gruhn, and Claudia Felser — Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg-Universität, D-55099 Mainz, Germany

Graphene and porous graphene are very promising materials, which have been widely studied for electronic applications. Because of their improved properties, in the future it is expected, that graphene, porous graphene and graphene-like molecules will replace silicon. Despite its superior material properties, however, the field-effect transistors based on graphene or graphene nanoribbons build so far via top-down approaches have low on/off ratios. On the other hand, molecular nanotransistors build with precisely know atomic structures resembling graphene were synthesized only very recently. In order to pave the way towards the industrial fabrication of molecular nanotransistors, we have investigated the chemisorption of graphene-like molecules on the 7×7 reconstructed Si(111) surface via density functional theory (DFT) calculations. We found, that Si(111) is a very promising candidate to serve as substrate for the large-scale fabrication of coronene-based molecular transistors. Moreover, our calculations show, that various adsorbate molecules prefer specific binding sites on the Si(111) surface. By following the template of the Si(111) substrate, the molecules selectively adsorb and form a well defined two-dimensional grid with a 1×1 surface pattern.

O 43: Surface Dynamics II

Time: Wednesday 11:15–12:15 Location: WIL B122

O 43.1 Wed 11:15 WIL B122

Field induced noise spectra in ion traps — •H.R. Sadeghpour[1], A. Safavi-Naieni[1,2], P. Weck[3], and P. Kral[1,4] — [1]ITAMP, Harvard-Smithsonian CfA, Cambridge, MA 02138 — [2]Dept. of Physics, MIT, Cambridge, MA 02139 — [3]Dept of Chemistry, UNLV, Las Vegas, NV — [4]Iqoqi, Austrian Academy Of Sciences, Insbruck, Austria

Electric field noise from fluctuating dipoles adsorbed on surfaces is a significant problem in a number of subfields of physics, ranging from precision measurements, nanomechanics and measurements of weak forces. We describe a first-principles calculations of the dipole properties fluctuating on surfaces, and the electric field noise spectral dependence on distance, frequency and temperature of the ion trap. We discuss implications for the ion trap experiments.

O 43.2 Wed 11:30 WIL B122

Anisotropy in time-resolved electron diffraction of bismuth films — •Carla Streubühr, Manuel Ligges, Thorsten Brazda, Uwe Bovensiepen, Ping Zhou, and Dietrich von der Linde — Universität Duisburg-Essen, Deutschland

With time-resolved electron diffraction we have investigated the excitation and relaxation of lattice vibrations in thin bismuth films after optical excitation with femtosecond laser pulses. Due to the property of the transmission electron diffraction from thin films, we are able to observe several diffraction orders at the same time. This provides us a complete view of the atomic motion.

The experiments showed a change in the diffraction intensity up to 300 ps after optical excitation, which depends on the azimuth angle of the diffraction order. This anisotropy depends on the polarization of the excitation pulses. We attribute this anisotropic intensity change to the excitation of polarized lattice vibrations by optical pulses. Possible excitation mechanisms of these lattice vibrations are impulsive stimulated Brillouin- or Raman- scattering.

O 43.3 Wed 11:45 WIL B122

Optical-induced CDW-phase-transition in $1T$-TiSe$_2$ probed by Time-Resolved High Harmonic Photoemission — •Timm Rohwer[1], Stefan Hellmann[1], Martin Wiesenmayer[1], Christian Sohrt[1], Ankatrin Stange[1], Matthias Kalläne[1], Stefan Mathias[2], Kai Rossnagel[1], Lutz Kipp[1], and Michael Bauer[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel — [2]JILA, University of Colorado and NIST, Boulder, USA

Time- and angle-resolved photoemission was employed to monitor the ultrafast dynamics consequent to the photoexcitation of a charge density wave (CDW) phase in the transition metal dichalcogenide $1T$-TiSe$_2$. The application of XUV high harmonic pulses (43 eV) allows us to record photoemission transients covering the full size of the first Brillouin zone. The excitation fluence dependence of the ultrafast breakdown of a (2×2×2) superstructure characteristic for the $1T$-TiSe$_2$ CDW phase was investigated and response times up to values less than 30 fs were observed. The origin of this breakdown is assigned to a build up of electronic screening by the transient generation of free charge carriers.

O 43.4 Wed 12:00 WIL B122

How Fast Does a Lead Monolayer Cool? — •Annika Kalus, Simone Möllenbeck, Sung Sakong, Anja Hanisch-Blicharski, Martin Kammler, Peter Kratzer, and Michael Horn-von Hoegen — Department of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE), Universität Duisburg-Essen, D-47057 Duisburg, Germany

We employ ultra fast time-resolved electron diffraction to analyze the vibrational dynamics of adsorbates on surfaces on a ps-timescale upon excitation by a fs laser pulse. Surface sensitivity is achieved by a reflection geometry of high energy electrons (RHEED) and time resolution by a pump probe setup.

Two different reconstructions of Pb on Si were prepared: the $(\sqrt{3} \times \sqrt{3})$ reconstruction with a coverage of 4/3 monolayers (ML) and the $(\sqrt{7} \times \sqrt{3})$ reconstruction with a coverage of 1.2 ML. All experiments were performed at 90K. Upon excitation with 50fs laser pulses at 800nm both reconstructions show a sharp drop of intensity in all reconstruction spots due to the Debye-Waller effect. The intensity reversibly recovers on two different time scales. The short time constant of 100ps is attributed to the deexcitation of the Si-Pb mode with an energy of 4meV and is in good agreement with molecular dynamic simulations. The long time constant of 3ns is assigned to a low frequency Pb-Pb mode with an energy of 2meV. The weak coupling of this mode to the Si substrate is explained by the small overlap of this mode with the density of phonon states in Si. The vibrational amplitude of these excited modes shows a strong non-linear dependence on the laser fluence.

O 44: Nanostructures at surfaces: Dots, particles, clusters, arrays III

Time: Wednesday 11:15–13:15 Location: WIL C107

O 44.1 Wed 11:15 WIL C107

Ultra-high dense array of magnetic quantum dots on a GdAu$_2$ template — •Laura Fernandez[1], Alberto Cavallin[2], Frederik Schiller[3], Stefano Rusponi[2], Martina Corso[1], Maider Ormaza[4], Harald Brune[2], and Enrique Ortega[1,3,4] — [1]DIPC, San Sebastián, Spain — [2]EPFL, Lausanne, Switzerland — [3]CFM-CSIC, San Sebastián, Spain — [4]UPV, San Sebastián, Spain

The growth of magnetic nanoparticles on surfaces by auto-organization processes represents a flexible and powerful alternative to obtain high-density, patterned magnetic storage media. Here, we report on the growth of a dense array of magnetic Co dots on a GdAu$_2$ surface alloy. We show that this GdAu$_2$ surface alloy behaves as an excellent template to achieve dot arrays with very high areal densities up to 54 Teradots/inch^2. Magnetic properties were analyzed by UHV-MOKE and XMCD revealing in-plane remanent magnetization.

O 44.2 Wed 11:30 WIL C107

Atomically flat single-crystalline gold nanostructures for plasmonic nanocircuitry — J.-S. Huang[1], P. Geisler[1], C. Brüning[1], J. Kern[1], J.C. Prangsma[1], X. Wu[1], •Thorsten Feichtner[1], J. Ziegler[1], P. Weinmann[1], M. Kamp[1], A. Forchel[1], P. Biagioni[2], and B. Hecht[1] — [1]Wilhelm-Conrad-Röntgen-Center for Complex Material Systems, University of Würzburg, Germany — [2]CNISM - Dipartimento di Fisica, Politecnico di Milano, Italy

Deep subwavelength integration of high-definition plasmonic nanostructures is of key importance for the development of future optical nanocircuitry. So far the experimental realization of proposed extended plasmonic networks remains challenging, mainly due to the multi-crystallinity of commonly used thermally evaporated gold layers. Resulting structural imperfections in individual circuit elements drastically reduce the yield of functional integrated nanocircuits. Here we demonstrate the use of very large but thin chemically grown single-crystalline gold flakes. After immobilization on any arbitrary surface, they serve as an ideal basis for focused-ion beam milling. We present high-definition ultra-smooth gold nanostructures with reproducible nanosized features over micrometer lengthscales. By comparing multi- and single-crystalline optical antennas we prove that the latter have superior optical properties which are in good agreement with numerical simulations.

O 44.3 Wed 11:45 WIL C107

Fabrication and Characterization of Well-Aligned Zinc Oxide Nanowire Arrays and their realizations in Schottky-Device Applications — •Kin Mun Wong[1], Liaoyong Wen[2], Yaoguo Fang[2], Fabian Grote[1], Hui Sun[1], and Yong Lei[1] — [1]Institute of Materials Physics and Center for Nanotechnology, University of Muenster — [2]Institute of Nanochemistry and Nanobiology, Shanghai University, Shanghai 201800, China

Highly ordered arrays of vertical zinc oxide (ZnO) nanowires (NWs) or nanopores were fabricated in our group by first thermal evaporating a thin film of gold on the ultrathin alumina membrane (UTAM). The UTAM was then utilized as a substrate for the growth of the ordered arrays using a chemical vapour deposition (CVD) process. Alternatively, a modified CVD process was also used to fabricate ultra-long ZnO NWs with the length of the nanowire exceeding 100 micrometres. Subsequently, densely packed arrays of ZnO NWs Schottky diodes were synthesized by transferring the long NWs on a substrate using a dry contact printing method and the electrical contacts were made on the NWs with a photolithographic process. The interesting electrical properties of the ZnO NWs, diodes or other metal oxide NWs such as the field emission, electron transport and piezoelectric properties were characterized by current-voltage or by other appropriate measurements.

1. L. Y. Wen, Z. Z. Shao, Y. G. Fang, K. M. Wong, Y. Lei, L. F. Bian, and G. Wilde, Appl. Phys. Lett. 97, 053106 (2010).

O 44.4 Wed 12:00 WIL C107

Surface Nano-Patterning in Realizing Large-Scale Ordered Arrays of Metallic Nanoshells with Controllable Structures and Properties — •Shikuan Yang[1,2], Feng Xu[1,2], Nina Winkler[1,2], Huaping Zhao[1,2], and Yong Lei[1,2] — [1]Institute of Materials Physics, University of Muenster — [2]Center for Nanotechnology

Surface patterns of metallic nanostructure arrays play an important role in many application areas such as surface-enhanced Raman scattering sensors, lithium-ion batteries, solar cells, and optical devices. Here we present an innovative surface nano-patterning technique in our group for realizing large-scale ordered arrays of metallic spherical nanoshells with well-defined structures. Sliver nanoshell arrays are synthesized using polystyrene sphere templates by an electrophoretic process. The fabricated Ag nanoshell arrays have a high controllability of the structural parameters, including the diameter, the surface roughness, and the inter-shell spacing. And the properties of the synthesized nanoshell arrays can be controlled based on the adjustment of the structural parameters. As an example, tunable surface-enhanced Raman scattering and localized surface plasmon resonance of the nanoshell arrays are demonstrated by controlling the structural parameters. The presented surface nano-patterning technique is a general fabrication process in achieving not only metallic nanoshell arrays, but also nanoshell arrays of other materials, such as semiconductors and metallic oxides.

O 44.5 Wed 12:15 WIL C107

Electrochemical formation of Self-Organized Superlattice Nanotube Arrays - Embedding Heterojunctions into Nanotubes Walls — •Wei Wei[1], Himendra Jha[1], Guang Yang[2], Erdmann Spiecker[2], and Patrik Schmuki[1] — [1]Department of Materials Science WW-4 (LKO), University of Erlangen-Nuremberg, Erlangen, Germany — [2]Center for Nanoanalysis and Electron Microscopy, University of Erlangen-Nuremberg, Erlangen, Germany

In recent years, a simple and convenient approach to form ordered transition metal oxide nanotubes arrays, i.e. self-organized electrochemical growth method, has attracted wide interests.In present work, we demonstrate how this simple anodization technique can be used to produce highly defined superlattice oxide nanotube arrays on metallic substrates. Under optimized growth conditions, a self-organization process occurs that yields 3D ordered nanotube arrays with regular nm-spaced modulations in the tube wall composition.An example will be shown where we prepared TiO2/Ta2O5 confined heterojunction nanotubes arrays, each of which contains approx. 100 periods of modulated pairs. The electronic properties in the tube wall alternate with a sub-20nm precision, which yields a significant phonon confinement effect. These structures are also expected to drastically enhance efficiencies in charge transfer devices. The process, however, is versatile (transferrable to a broad range of metal oxide junctions), allows tuning of the tube and superlattice geometry, neither requires UHV conditions, nor expensive equipment, and due to its parallel processing nature, it can easily be scaled up.

O 44.6 Wed 12:30 WIL C107

Surface Patterning Technique using Polystyrene Sphere Templates for Fabricating Diverse Nanostructures and Broad Applications — •Feng Xu, Shikuan Yang, Fabian Grote, Huaping Zhao, and Yong Lei — Institute of Materials Physics and Center for Nanotechnology, University of Muenster

Surface nano-patterning is a necessary step in many real device applications ranging from electronics to optics, data storage, sensing and display areas. Various protocols are adopted to synthesize surface nano-patterns, such as electron beam lithography, optical lithography, focused ion beam etching and so on. Template-based methods can be utilized for parallel surface nano-patterning with advantages such as high through-put and low-cost of surface nanostructures. Among them, monolayer polystyrene (PS) sphere template is powerful in preparing various surface nano-patterns with different topologies and composed of different building blocks. In our group, through heating Au-coated PS sphere arrays in a very controllable way, nanodot arrays can be acquired. These fabricated surface nano-patterns show intriguing optical properties, which include multiple surface plasmon resonance (SPR) bands and strong infrared absorption. These unique optical properties are very important in biological related application areas. Moreover, the full structural controllability of the surface nano-patterns supplies a possible way to investigate the relation of the sensing and surface-enhanced Raman scattering (SERS) performances to the structural parameters. This is important in the exploration of the fabrication of SERS and SPR-based sensing substrates with ultra-high sensitivities.

O 44.7 Wed 12:45 WIL C107

Surface nano-structuring utilizing porous anodic alumina membranes; to the limits and beyond — •Stefan Ostendorp, Yong Lei, and Gerhard Wilde — Institute of Materials Physics and Center for Nanotechnology, University of Münster, 48149 Münster, Germany

Porous anodic alumina membranes (PAAMs) have been intensively investigated for more than two decades, especially for their applications as masks or templates for fabricating various nano-structures of regular hexagonal arrays of wires and tubes. In addition ultra-thin alumina membranes (UTAMs) are used as deposition masks for nano particles. The spacing of the hexagonal structure of PAAMs and UTAMs can be modified within certain limitations, that had been reported in the literature. So far there were only several *allowed* combinations of parameter values reported that lead to highly regular porous structures during the anodization process of the underlying aluminum foil. Here we present our latest results concerning the extension of these limits to larger interpore distances and pore sizes and concerning the ability to create structures with desired spacing. For this purpose, we combined two well known methods during the anodization process, which now allows adjusting the structural parameters beyond the previous known limitations, what is of great importance to device applications based on PAAM- and UTAM- prepared functional nanostructures.

O 44.8 Wed 13:00 WIL C107

Environment Controlled De-wetting Kinetics of Rh-Pd Bilayer Thin Films — •Gintautas Abrasonis[1], Sebastian Wintz[1], Maciej Oscar Liedke[1], Funda Aksoy[2], Zhi Liu[2], Karsten Kuepper[3], Matthias Krause[1,4], and Sibylle Gemming[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA. — [3]Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm, Germany — [4]Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden, Germany

The control of morphology and surface composition of nanoalloys is the key factor in order to tune or to extend the range of their optical, magnetic and chemical properties. Therefore it is one of the major tasks in nanoalloy materials science. The de-wetting dynamics and kinetics dependence of a Rh-Pd bilayer/alloy thin film model system on chemical environment (CO and NO) is investigated in-situ by means of high pressure x-ray photoelectron spectroscopy. Independently of the initial state, the film surface shows an enrichment of Pd upon heating in vacuum. De-wetting caused by heating in NO or CO shows significant differences in the surface chemical composition evolution and, consequently, in the de-wetting onset temperature. Alternating exposure to NO or CO results in the surface enrichment with either Rh or Pd, respectively, and subsequent film rupture. The results are discussed on the basis of the interplay between thermodynamic and kinetic factors. The study demonstrates the effect of the chemical environment on the morphology as well as on the composition of supported nanostructures.

O 45: Oxides and insulators: Adsorption II

Time: Wednesday 11:15–13:00 Location: WIL C307

O 45.1 Wed 11:15 WIL C307

Atomic scale manipulation of single molecules on ultrathin insulating films using an STM — •Ingmar Swart, Tobias Sonnleitner, and Jascha Repp — Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

On metallic and semiconducting substrates, atoms and molecules can be manipulated controllably on the atomic scale by the tip of a scanning tunnelling microscope (STM) or atomic force microscope (AFM), allowing the creation of nano-engineered structures. In recent years, ultrathin insulating films have been used in STM studies to decrease the electronic coupling between the adsorbate and the underlying substrate. In contrast to manipulation on metal substrates, the use of traditional lateral manipulation modes cannot be successfully applied to molecules on ultrathin insulating films, due to the unfavorable diffusion barrier to binding energy ratio: it is relatively easy to pick the molecule up from the surface with the STM tip compared to successful lateral manipulation. On insulating films, inelastic excitation is relatively efficient due to the increased life-time of the additional charge. Inelastic excitation can result in lateral motion of the molecule. We studied the inelastic excitation for different parameters to gain control over the direction of the lateral motion. By using this new manipulation scheme we can form well-defined and stable structures consisting of several molecules. The mechanical stability of such structures is evidenced by the motion of the entire complex upon excitation.

O 45.2 Wed 11:30 WIL C307

On the influence of molecular symmetry on surface diffusion — Tobias Sonnleitner, Ingmar Swart, •Niko Pavliček, Andreas Pöllmann, and Jascha Repp — Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Symmetries govern many fields of physics and chemistry. In the case of molecules adsorbed on single-crystal surfaces the symmetry of the combined adsorbate-substrate system is decisive for its properties. For example, in spectroscopy symmetry arguments are the basis of many selection rules. However, in diffusion there do not exist such things as selection rules that completely forbid certain diffusion steps. This raises the question how big structural differences that reduce the symmetries have to be, in order to have a significant influence on the surface-potential landscape.

Here, we address the issue of how diffusion of molecules is influenced by the molecular symmetry in a systematic manner using a scanning tunneling microscope. To this end, we investigated π-conjugated molecules for which four symmetry distinct isomers exist on an insulating surface. Despite minute changes in the molecular structure in such a weakly interacting system we find that the surface-potential landscape is governed by the molecular symmetry. Indeed, the four isomers exhibit four distinctly different diffusion patterns, as evidenced by diffusion movies.

O 45.3 Wed 11:45 WIL C307

Determining the Exact Adsorption Configuration of a Chiral Metal-Organic Complex on a Bulk Insulator — •Alexander Schwarz[1], Knud Lämmle[1], Tom Trevethan[2], Matthew Watkins[2], Alex Shluger[2], and Roland Wiesndanger[1] — [1]Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, 20355 Hamburg, Germany — [2]University College London, Gower Street , London WC1E6BT, United Kingdom

Determining the exact position and geometry of an adsorbed molecule is crucial to understand the chemical and physical properties of a particular molecule-surface system. Here we present a high-resolution non-contact atomic force microscopy (NC-AFM) study of Co-Salen, a paramagnetic, low symmetry, chiral Schiff base metal-organic complex, deposited on NaCl(001), a prototypical bulk insulator [1]. The experimental results are compared to theoretical calculations.

By utilizing a metallic tip and resolving individual banana-shaped molecules, while simultaneously obtaining atomic resolution on the substrate, we find that the central Co atoms always sits on top of a Cl ion. This adsorption site is confirmed by theoretical calculations. Moreover, we could identify 16 orientations of the molecule on NaCl(001). The molecule axis is rotated by about ±5° away from either <110>- or <100>-directions. These 16 low energy configurations are also predicted by theory and reflect the fourfold symmetry of the surface as well as the chirality of the molecule.

[1] K. Lämmle, *et al.*, Nano Lett. **10**, 2965 (2010).

O 45.4 Wed 12:00 WIL C307

Ab-initio calculations of the adsorption energy of physisorbed molecules on ionic surfaces — •Beate Paulus, Carsten Müller, and Lukas Hammerschmidt — Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin

The standard density functional methods have their difficulties with describing dispersion forces, especially the long-range van der Waals interactions. Therefore there is a need of highly accurate results especially for physisorbed systems. The method of increments [1] provides a tool to calculate the correlation contribution to the adsorption energy at the coupled cluster level.It is based on the expansion of the correlation energy in terms of localized orbital groups,the Hartree-Fock treatment is performed for the extended systems.

Here we want to present the application of open-shell adsorbants like NO and gold atoms on ceria surfaces, and the adsorption of small molecules on magnesium fluorid surfaces.

[1] B. Paulus, Phys. Rep. 2006, 428, 1 (review); C. Müller, B. Herschend, K. Hermansson, B. Paulus, J. Chem. Phys. 2008, 128, 214701., C. Müller, K. Hermansson, B. Paulus, Chem. Phys. 2009, 362, 91., C. Müller, B. Paulus, K. Hermansson, Surf. Science 2009, 603, 2619.

O 45.5 Wed 12:15 WIL C307

Controlling the charge-state of single molecules — Ingmar Swart, •Tobias Sonnleitner, and Jascha Repp — Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg

The chemical and physical properties of atoms and molecules adsorbed on surfaces are influenced by several factors, such as molecule-substrate and molecule-molecule interactions. In this context, especially the charge state of adsorbates is of great importance, since it governs various properties, such as the spin-state, the interaction with other adsorbates and the substrate. Here, we present an STM study on single molecules adsorbed on an ultrathin NaCl film supported by a Cu surface. The use of an ultrathin insulating NaCl film electronically decouples the molecules from the metallic substrate. The molecules exhibit two states with considerably different conductance, which are associated with two different charge states. This is evidenced by changes in the scattering of the interface state, as well as spectroscopic data. The charge state of a molecule can be controlled by adding or removing a single electron to or from the molecule with the STM tip, analogous to what has previously been shown for individual metal atoms. Most importantly, both states are stable, that is, an additional charge will remain on the molecule until it is removed by a voltage pulse of opposite polarity. We demonstrate how one can generalize the charge state control to other molecules. Furthermore, we demonstrate how the tunneling barrier is modified by the presence of an additional charge with intramolecular resolution.

O 45.6 Wed 12:30 WIL C307

A comparative study of small Si and Sn clusters On MgO Surface: An ab-initio approach — •Sudip Chakraborty[1], Chiranjib Majumder[2], and Subhash V Ghaisas[1] — [1]Department of Electronic Science,University of Pune,Pune-411007,India — [2]Chemistry Division,Bhabha Atomic Research Center,Trombay-400085,Maharashtra

One of the essential aspects of the architecture of a surface-based electronic device is that the substrate should preferably be an insulator (wide band gap), which enables more than one electrical contact to the adsorbed species. In this respect, the MgO surface (001) could serve as an excellent model system for exploring nanoscale electronic architectures with its inert and catalytic nature.Here we report the atomic and electronic structures of Silicon and Tin clusters(number of atoms =1-6,9)on the Magnesium Oxide(MgO) surface using DFT calculation. The primary focus of this study is to understand the nature of interaction between Si/Sn and MgO substrate,which in turn will affect the geometries and electronic properties of Si/Sn clusters which are of technological relevance.The results reveal that for both the cases the single Si/Sn atom prefers to be adsorbed on the top of oxygen on the surface and hollow sites. The adsorption mechanism is completely driven by the adsorbed atom interaction with the MgO surface. The shapes of gas phase clusters get distorted on adsorption on the surface. We have also calculated the Projected Density of States(PDOS) from which we can get the hybridization as well as the charge transfer of the total system after adsorption of ad-atoms (Si/Sn).

O 45.7 Wed 12:45 WIL C307

Adsorption of Au and Pd on a hematite surface — •Adam Kiejna and Tomasz Pabisiak — Institute of Experimental Physics, University of Wrocław, Wrocław, Poland

The adsorption of sumonolayer Au and Pd atoms at the two most stable (0001) surfaces of hematite, one being terminated by oxygen and the other by iron, is studied by spin-density functional theory. The changes in configuration caused by adsorption and the adsorption energy in different sites and for different Au and Pd coverages are investigated. The results show that both Au and Pd bind strongly to hematite surfaces and induce large changes in their geometry. In most stable Au and Pd adsorption sites the adsorbate atoms form threefold bonds with surface oxygen atoms. The binding is stronger for Pd than Au and for both adsorbates is distinctly stronger at the oxygen- than at the iron-terminated surface. The adsorbate interactions with substrate iron and oxygen atoms and their contributions to bonding are discussed based on the calculated local density of states and the electron charge transfer. The effect of on-site Coulomb interactions is briefly discussed based on the calculations performed within DFT+U scheme.

O 46: Surface magnetism I (jointly with MA)

Time: Wednesday 11:15–13:30 Location: CHE 184

O 46.1 Wed 11:15 CHE 184

Structural and magnetic investigations of Fe_3Si/GaAs(001) — •Sani Noor, M. Samet Özkan, and Ulrich Köhler — Experimentalphysik IV, AG Oberflächen, Ruhr-Universität Bochum

Fe_3Si has got magnetic and electric properties that make it a possible candidate as a spin aligning material in spintronic devices. Thus, it is of great interest to investigate its growth behaviour on semiconductor substrates.

In this contribution we present growth studies of the system Fe_3Si/GaAs(001) as measured by STM. Atomic resolution reveals long range ordering alongside a lattice structure that is to be compared with theory. The influence of varying growth temperatures and post annealing on the surface morphology has been investigated. We find that under the appropriate parameters layer-by-layer growth can be achieved. Magnetic analysis was performed by angular dependent in situ MOKE. While the uniaxial anisotropy remains unaffected by the growth temperature the coercive field scales with it. In order to determine the magnetic moment the samples were measured with SQUID magnetometry. It appears that the magnetic moment shows a dependence on the layer thickness.

O 46.2 Wed 11:30 CHE 184

Scattering behaviour of single non-magnetic and magnetic impurities buried under a Cu(100) surface — •Henning Prüser[1], Martin Wenderoth[1], Piet E. Dargel[2], Alexander Weismann[1], Robert Peters[2], Thomas Pruschke[2], and Rainer G. Ulbrich[1] — [1]IV. Physikalische Institut, Georg-August Universität Göttingen, Germany — [2]Institut für Theoretische Physik, Georg-August Universität Göttingen, Germany

It has been recently shown [1] that the anisotropy of the copper Fermi surface leads to a strongly directional propagation of quasi particles called electron focusing. This effect gives access to individual bulk impurities in a metal that were previously assumed to be "invisible" due to charge screening. Following this idea we have investigated the energy-dependent scattering characteristics for single isolated atoms of Ag, Co and Fe buried under a Cu(100) surface using low temperature scanning tunnelling spectroscopy (STS). For the case of a non-magnetic Ag impurity a Friedel oscillation in the local density of states is observed. For a magnetic Fe or Co impurity the Kondo effect influences strongly the energy-dependent scattering behaviour. We present a theoretical interpretation of the measured signatures using a combined approach of band structure and many-body numerical renormalization group calculations. The obtained results are in excellent agreement with the rich spatially and spectroscopically resolved experimental data. This work was supported by DFG SFB 602 Project A3.

[1] A. Weismann et al., Science 323, 1190 (2009)

O 46.3 Wed 11:45 CHE 184

First-principles study of the magnetic interaction in single atom contacts — •Cesar Lazo, Paolo Ferriani, and Stefan

Heinze — Institute of Theoretical Physics and Astrophysics, University of Kiel, Germany

The miniaturization of spintronic devices towards the limit of single atoms calls for an understanding of the interaction and electron transport in atomic-scale contacts. Such structures are extreme cases, where the typical dimensions are comparable to the Fermi wavelength and a fully quantum mechanical description is required. Based on density functional theory calculations, we investigate single atom contacts formed by an antiferromagnetic Cr-tip of a scanning tunneling microscope (STM) and a magnetic atom adsorbed on a metallic surface. We analyze the exchange interaction between tip and adatom from the tunneling to the contact regime and explain a spin-valve effect observed with an STM [1]. Furthermore, we characterize the geometric properties of the contact as the tip approaches the sample, and show that the relaxations in the system can be related to the measured spin-polarization [1].

[1] M. Ziegler et al. in preparation

O 46.4 Wed 12:00 CHE 184

Spin-Resolved Investigations of the Exchange Split Gd Surface and Image-Potential State — •Beatrice Andres[1,2], Kristian Döbrich[1], Marko Wietstruk[1], Anke B. Schmidt[3], Markus Donath[3], and Martin Weinelt[1,2] — [1]Max-Born-Institut, 12489 Berlin — [2]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin — [3]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster

The study of image-potential states (IPS) in front of ferromagnetic surfaces provides information about the magnetic properties of surfaces and thin films. Recent investigations on IPS revealed exchange splittings ΔE_{ex} in Fe, which persist even above the Curie temperature T_{C} [1].

Gd(0001) exhibits a d-derived surface state (SS) with $\Delta E_{\mathrm{ex}} > 0$ above T_{C} [2]. We used the occupied majority spin component of this state to populate the first ($n = 1$) image potential state on a 100-Å-thick Gd film on W(110) with the second harmonic of our Ti:Sa laser ($h\nu$ = 3.30 eV). By probing with the fundamental IR pulse ($h\nu$ = 1.65 eV), we investigated the binding energy and exchange splitting of the IPS as a function of the temperature.

[1] M. Pickel *et. al.*, *Phys. Rev. Lett.* **104**, 237204 (2010).

[2] M. Getzlaff *et al.*, *J. Magn. Magn. Mater.* **184**, 155 (1998).

O 46.5 Wed 12:15 CHE 184

Magnetic signature of surface defects at nanodiamonds — •Nora Jenny Vollmers, Uwe Gerstmann, and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn

The n-type doping of diamond has been a long-standing issue, which recently gained attention in the context of nanodiamonds. Attempts of doping with nitrogen failed to result in the Electron paramagnetic Resonance (EPR) fingerprints expected from bulk material. Instead, the nanodiamond signals show a much larger deviation from the free-electron g-value and are believed to be related to intrinsic, carbon inherited defects. However, the absence of the bulk-like EPR spectra does not mean that nitrogen is not incorporated at all. The N atoms could be built in predominantly at or at least close to the surfaces yielding EPR spectra, very different from those measured in the bulk.

In this work, we elucidate the situation by investigating the magnetic signature of paramagnetic defects in the nanodiamonds. We use the gauge-including projector augmented plane wave (GI-PAW) approach [1, 2] to calculate the hyperfine splittings and the elements of the electronic g-tensor. Taking the C(100) surface as a first model system, a possible contribution of nitrogen is discussed by comparing EPR parameters for different N incorporation depths: Incorporated directly at the surface, N gives rise to surface states similar to intrinsic carbon dangling bond-like states. Otherwise N is able to introduce surface conductivity as demonstrated by calculated effective mass tensors.

[1] Ch.J. Pickard, F. Mauri, Phys. Rev. Lett. 88, 086403 (2002).

[2] U. Gerstmann et al., phys. stat. sol. (c) 7, 157 (2010).

O 46.6 Wed 12:30 CHE 184

Realizing Spin Logic Atom by Atom — •Alexander Khajetoorians, Bruno Chilian, Jens Wiebe, and Roland Wiesendanger — Institute of Applied Physics, Hamburg University, Jungiusstrasse 11, 20355 Hamburg, Germany

Scanning tunneling microscopy (STM) has emerged as a leading technique which can address single atom magnetism with high energy and spatial resolution. With the development of sub-Kelvin high-magnetic field STM, two complementary methods, namely spin-polarized scanning tunneling spectroscopy (SP-STS) and inelastic STS (ISTS), can address the fundamental properties of individual magnetic impurities at surfaces [1-2]. We use a map of the distance-dependent RKKY interaction between Fe atoms on Cu(111) obtained by SP-STS to engineer complex magnetic nanostructures with tailored magnetic properties with atomic manipulation. By combining constructed antiferromagnetic structures with spin frustration, we realize an atomic-scale logic device which functions solely on the spin-degrees of freedom of its magnetic constituents.

[1] A. A. Khajetoorians, B. Chilian, J. Wiebe, S. Schuwalow, F. Lechermann, and R. Wiesendanger, Nature 467, 1084 (2010).

[2] A. A. Khajetoorians, S. Lounis, B. Chilian, A. T. Costa, L. Zhou, D. Mills, J. Wiebe, and R. Wiesendanger, arXiv:1010.1284v2 (2010).

O 46.7 Wed 12:45 CHE 184

Magnetic anisotropy of Co and Ni adlayers on diamond and GaAs surfaces: an ab-initio study — •Bernd Stärk, Peter Krüger, and Johannes Pollmann — Westfälische Wilhelms-Universität, Münster, Germany

We present ab-initio investigations of magnetic transition-metal multilayers on semiconductors. In our work, we focus on the description of noncollinear magnetic systems and their magnetic anisotropy. To this end, we employ density functional theory in the framework of both LDA and GGA using a basis set of Gaussian orbitals.

Adsorption of Co/Ni adlayers on C(111)/C(001)-(1x1) surfaces is distinguished by a very small lattice mismatch. For one adlayer we find the metal adatoms to be localized in positions saturating all surface dangling bonds. They form strong covalent bonds with the substrate atoms that markedly reduce the magnetic moment at the interface and can even change the direction of the easy axis of magnetization as compared to the free standing monolayer. Furthermore, we find a strong dependance of anisotropy energies on the number of adlayers.

Secondly, we also discuss Ni on GaAs surfaces. Recent experiments suggest [1] that Ni grows epitaxially in bcc structure on GaAs(001) and that its magnetic properties strongly deviate from the bulk fcc case. We present a thorough investigation of possible atomic structures for this system and their magnetic properties.

[1] C. S. Dian *et al.*, PRL 94, 137210 (2005).

O 46.8 Wed 13:00 CHE 184

A spin polarizing electron mirror for spin-resolved photoelectron microscopy — •Christian Tusche, Martin Ellguth, A. Akin Ünal, Aimo Winkelmann, Alexander Krasyuk, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik Halle, D-06120 Halle, Germany

We report on a novel imaging spin-filter for electrons, that allows the parallel detection of the electron spin-polarization over a two-dimensional field of view. The spin-filter is installed in our momentum microscope, consisting of a photoelectron emission microscope (PEEM) optics and a double hemispherical imaging energy analyzer. After the energy analyzer, a reciprocal image is 90 degrees reflected at a tungsten (100) surface. Spin contrast is obtained due to the spin-dependent reflection probability of low energy electrons, while the angle of incidence is conserved in the outgoing elastic (00) diffraction spot [1]. This geometry transfers the full PEEM image, whereas the spatial information is encoded by small deviations of the angel of incidence.

We demonstrate that the magnetic domain structure of cobalt films grown on Cu(100) can be imaged with a resolution better than 500 nm, limited by the natural domain wall width (≈ 400 nm [2]) of the film. The intensity asymmetry, defined by $A = [M^{+} - M^{-}]/[M^{+} + M^{-}]$, shows sharp maxima and minima as a function of the scattering energy in the range between 15 eV and 90 eV, whereas a maximum scattering asymmetry of up to A=45% is found.

[1] German Patent DE102005045622B4 (2009)

[2] A. Berger and H. P. Oepen, Phys. Rev. B **45**, 12596 (1991)

O 46.9 Wed 13:15 CHE 184

(SP)VLEED: Experimental access to the spin-dependent surface barrier — •Kathrin Wulff, Anke B. Schmidt, and Markus Donath — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster

We present the first spin-polarized very-low-energy electron-diffraction (SPVLEED) measurements on a ferromagnetic system.

The fine structures, which appear in intensity vs. energy $I(V)$ profiles of elastically reflected electrons [1], are sensitive to the shape of the surface-barrier potential. On the vacuum side far from the surface, the potential resembles the well-known Coulomb-like shape, while, on the crystal side, it merges the inner potential. In theoretical calculations the transition region, i.e. the surface barrier, is usually described by a parameterized phenomenological model. Our experiment gives access to exactly this transition region.

On Co/Cu(001) we found a significant spin dependence of the reflected intensities that varies strongly with incidence and azimuth angles. It should be noticed that the spin-dependent reflectivity of very-low-energy electrons from ferromagnetic surfaces has recently been utilized in electron spin polarimeters [2,3].

[1] R.O. Jones, P.J. Jennings, Surf. Sci. Reports **9**, 165 (1988) ; [2] A. Kakizaki *et al.*, Rev. Sci. Instrum. **79** (2008) 123117 ; [3] A. Winkelmann *et al.*, Rev. Sci. Instrum. **79** (2008) 083303

O 47: Gaede Prize talk (Philip Hofmann)

Time: Wednesday 14:00–14:45 Location: TRE Phy

Prize Talk O 47.1 Wed 14:00 TRE Phy

Spin-split metallic surface states on semimetals and topological insulators — •Philip Hofmann — Department of Physics and Astronomy, Interdisciplinary Nanoscience Center Aarhus University, 8000 Århus C, Denmark

The surfaces of Bi, Sb and the so-called topological insulators (TIs) all share the property that their electronic structure is metallic, in sharp contrast to the bulk which is either semimetallic (Bi, Sb) or semiconducting (TI). The main reason for the existence of the metallic surface states is not bond-breaking but the loss of inversion symmetry at the surface, combined with a strong spin-orbit interaction. The surface states are almost completely non-degenerate with respect to the electron's spin and this has interesting consequences for their electron dynamics. Indeed, the surface states on TIs are predicted to exhibit a number of novel and exotic physical phenomena and have potential applications in spintronics and quantum computing. In this talk I will review some basic properties of spin-split surface states, relate the findings on semimetal surfaces to topological considerations and discuss the similarities and differences of surface states on semimetals and topological insulators.

O 48: Focussed session: Theory and computation of electronic structure: new frontiers IV (jointly with HL, DS)

Time: Wednesday 15:00–17:00 Location: TRE Phy

Topical Talk O 48.1 Wed 15:00 TRE Phy

Progress in diffusion quantum Monte Carlo calculations — •Richard Needs — Cavendish Laboratory, J J Thomson Avenue, Cambridge CB3 0HE, UK

My group has developed the CASINO code [1] for performing variational and diffusion quantum Monte Carlo calculations. Fixed-node diffusion quantum Monte Carlo is the most accurate method known for calculating the energies of large many-particle quantum systems. The key ingredient is an accurate trial many-body wave function which controls the statistical efficiency and accuracy of the calculations. Accurate wave functions can be obtained by building correlation effects on top of mean field descriptions such as density functional theory or Hartree-Fock theory. About 80% of the correlation energy can typically be included by multiplying the mean-field determinant by a Jastrow factor which is small when electrons are close together and tends to unity at large separations. Such wave functions provide an excellent description of electron correlation in closed shell molecules but are often not much better than density functionals for small open shell systems. The wave functions of open shell systems can, however, be greatly improved by introducing more determinants, pairing functions, and backflow transformations, and extremely good results can be obtained. The calculations are expensive but the polynomial scaling with system size allows calculations for 1000 or more particles. The discussion of the methodology will be illustrated by recent applications to atoms, molecules and extended systems.

[1] http://www.tcm.phy.cam.ac.uk/~mdt26/casino2.html

O 48.2 Wed 15:30 TRE Phy

N^3 implementation for molecules and clusters of Hedin's GW scheme — •Dietrich Foerster[1], Peter Koval[2], and Daniel Sanchez-Portal[2] — [1]CPMOH, University of Bordeaux 1, Cours de la Liberation 351, Talence, France — [2]Centro de Fisica de Materiales, Paseo Manuel Lardizabal, 5, Donostia-San Sebastian, Spain

In the context of organic semiconductors it is useful to be able to predict key properties of their molecular constituents, such as their lumo and homo levels.

To make such predictions possible, we developed a new implementation of Hedin's GW approach for one-electron Green's function that scales like N^3 rather than N^4 with the number of atoms (see also the contribution by Peter Koval).

We achieved an N^3 scaling by using a local basis in the space of dominant orbital products.

This local basis has already been applied in a TDDFT code and it is also suitable in the Bethe Salpeter approach. To accelerate calculations in these frameworks for large molecules, we reanalyze the product basis and reduce its dimension.

O 48.3 Wed 15:45 TRE Phy

Applications of a dominant product basis in many-body perturbation theory — •Peter Koval[1], Dietrich Foerster[2], and Daniel Sanchez-Portal[1] — [1]Centro de Fisica de Materiales, Paseo Manuel Lardizabal, 5, Donostia-San Sebastian, Spain — [2]CPMOH, Universite Bordeaux 1, Cours de la Liberation 351, Talence, France

The knowledge of excitation properties of molecules is crucial in developing organic semiconductor devices. Many-body perturbation theory is one of the most promising theories for characterization of excitations in electronic systems. In particular, Hedin's GW approximation for one-electron Green's function is capable of calculating lumo and homo of molecules with $O(N^3)$ computational complexity like TDDFT (see the contribution of Dietrich Foerster).

In this work, we implement the Hedin's G_0W_0 approximation on top of DFT calculations performed with SIESTA [1] code. We apply a dominant product technique [2] to span the space of orbital products and to reduce the dimensionality of dielectric matrix.

We discuss several results for ionization potentials and electron affinities of large molecules, revealing strengths and limitations of our implementation.

[1] J. M. Soler, E. Artacho, J. D. Gale, A. García, J. Junquera, P. Ordejón, D. Sánchez-Portal, J. Phys. **C 14**, 2745 (2002).

[2] P. Koval, D. Foerster, and O. Coulaud, J. Chem. Theory Comput. **6**, 2654 (2010); and references therein.

O 48.4 Wed 16:00 TRE Phy

Using Finite Element method to tackle the Hartree-Fock equations — •Amélie Fau and Denis Aubry — MSSMat laboratory, Ecole Centrale Paris

It is well know that the Schrödinger equation cannot be solved exactly, except maybe for very simple cases, as it represents a many-body interaction problem. However, it is possible to derive approximations of the Schrödinger equation from variational principles. The Hartree-Fock equations are then generally solved thanks to a set of basis functions, e.g. Gaussians, Slater-type orbitals or plane waves.

To avoid to impose a general form to the approximate wave function, we use localized trial functions. We consider here the Finite Element Method as a new approach to solve these Hartree-Fock equations. We shall present the main properties of our computations with the different advantages and drawbacks involved by this strategy. We will present numerical results about different electronic systems: such as atoms or molecules (LiH, BeH2).

O 48.5 Wed 16:15 TRE Phy

Finite-basis correction applied to the optimized effective potential within the FLAPW method — •Christoph Friedrich, Markus Betzinger, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The optimized-effective-potential (OEP) method is a special technique to construct local exchange-correlation (xc) potentials from general orbital-dependent xc energy functionals. Recently, we showed that particular care must be taken to construct local potentials within the all-electron full-potential augmented-plane-wave (FLAPW) approach. In fact, we found that the LAPW basis had to be converged to an accuracy that was far beyond that in calculations using conventional functionals, leading to a very high computational cost. This could be traced back to the convergence behavior of the density response function: only a highly converged basis lends the density enough flexibility to react adequately to changes of the potential. In this work we derive a numerical correction for the response function, which vanishes in the limit of an infinite, complete basis. It is constructed in the atomic spheres from the response of the basis functions themselves to changes of the potential. We show that such a finite-basis correction reduces the computational demand of OEP calculations considerably: the local potential converges at much smaller basis sets than before and its construction becomes numerically stable. We also discuss a similar correction scheme for *GW* calculations.

O 48.6 Wed 16:30 TRE Phy

A conventional, massively parallel eigensolver for electronic structure theory[1] — •V. Blum[1], M. Scheffler[1], R. Johanni[2], H. Lederer[2], Th. Auckenthaler[3], Th. Huckle[3], H.-J. Bungartz[3], L. Krämer[4], P. Willems[4], B. Lang[4], and V. Havu[5] — [1]Fritz Haber Institute, Berlin — [2]RZ Garching — [3]TU München — [4]BU Wuppertal — [5]Aalto University, Helsinki

We demonstrate a robust large-scale, massively parallel conventional eigensolver for first-principles theory of molecules and materials. Despite much research into $O(N)$ methods, standard approaches (Kohn-Sham or Hartree-Fock theory and excited-state formalisms) must still rely on conventional but robust $O(N^3)$ solvers for many system classes, most notably metals. In particular, our eigensolver overcomes parallel scalability limitations where standard implementations of certain steps (reduction to tridiagonal form, solution of reduced tridiagonal eigenproblem) can be a serious bottleneck already for a few hundred CPUs. We demonstrate scalable implementations of these and all other steps of the full generalized eigenvalue problem. Our largest example is a production run with 1046 Pt (heavy-metal) atoms [1] with converged all-electron accuracy in the numeric atom-centered orbital code FHI-aims,[2] but the implementation is generic and should easily be portable to other codes. [1] P. Havu *et al.*, Phys. Rev. B **82**, 161418 (2010). [2] V. Blum *et al.*, Comp. Phys. Comm. **180**, 2175 (2009). [1] ELPA research consortium, funded by German Ministry of Research and Education (BMBF). http://elpa.rzg.mpg.de

O 48.7 Wed 16:45 TRE Phy

Accurate and efficient density-functional calculations for the electronic entropy — •Rudolf Zeller — Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich

The calculation of the electronic entropy S(T) as function of temperature is a numerically demanding problem for metallic systems because S(T) depends logarithmically on the Fermi-Dirac distribution which varies rapidly near the Fermi level. Therefore, very accurate Brillouin zone samplings are usually needed.

I will present a technique based on complex energy contour integration and show how significant reduction of the number of sampling points can be achieved and how the problem of undetermined phases of complex valued logarithms can be avoided. The technique exploits the analytical properties of the Green function of the single-particle Kohn-Sham equation and has been implemented within the full-potential Korringa-Kohn-Rostoker method, where the use of Lloyd's formula guarantees fast convergence with respect to the angular momentum cutoff.

As a by-product I obtain a broadening scheme for total energy calculations with error elimination up to the sixth power of T. I will also explain particular advantages of Fermi-Dirac broadening (besides its direct physical significance) compared to other broadening schemes.

O 49: Metal substrates: Adsorption of organic / bio molecules VI

Time: Wednesday 15:00–17:15 Location: PHY C213

O 49.1 Wed 15:00 PHY C213

Investigation of the CuPc/PTCDA interface on Ag(111) — •Benjamin Stadtmüller, Ingo Kröger, Christoph Kleimann, Tamoki Sueyoshi, Sergey Subach, and Christian Kumpf — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and JARA-Fundamentals of Future Information Technology

One crucial issue for improving organic electronics is the understanding of interfaces between different functional materials. While recently interfaces between metal contacts (i.e., noble metal surfaces) and active organic layers were investigated intensively, only few studies so far focused on the interface between different organic materials. In this context we investigated the adsorption of copper-II-phthalocyanine (CuPc) on a closed monolayer of perylen-tetracarboxylicacid dianhydride (PTCDA) on Ag(111). Using high resolution low energy electron diffraction (SPA-LEED) we could show that at room temperature the CuPc molecules form a diluted, disordered layer, similar to the case of direct adsorption on Ag(111). Upon cooling (<-150°C) or increasing coverage (close to one monolayer) phase transitions to ordered structures occur. These ordered phases are compared with the adsorption of CuPc on Ag(111) in first and second layer. Furthermore, UV photoemission experiments are reported, which allow to reveal the electronic properties of the interfaces. The experiments nicely demonstrate the strong impact of structure and composition of the first adsorbate layer (which is in direct contact to the Ag surface) on the properties of the second molecular layer.

O 49.2 Wed 15:15 PHY C213

Charge transfer from a metal to a strong electron acceptor molecule through an organic spacer-layer — •Patrick Amsalem[1], Jens Niederhausen[1], Johanes Frisch[1], Andreas Wilke[1], Benjamin Bröker[1], Antje Vollmer[2], Ralph Rieger[3], Klaus Müllen[3], Jürgen P Rabe[1], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Brook-Taylor-Str. 6, 12489 Berlin, Germany — [2]HZB-BESSY II, Albert-Einstein-Str. 15., 12489 Berlin, Germany — [3]Max Planck Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

We investigate the possibility for electrons to tunnel from a metal surface to a strong electron acceptor molecule through an inert organic layer used as spacer. We report photoemission measurements performed on one monolayer (ML) hexaaza-triphenylene-hexacarbonitrile (HATCN) deposited under ultrahigh vacuum conditions on Ag(111) precovered with 1ML tris(8-hydroxyquinoline)aluminium (Alq3). The valence spectra reveal a density of states (DOS) in the vicinity of the Fermi-level which is attributed to the filling of the HATCN lowest unoccupied molecular orbital derived state, resulting from a charge transfer from the Ag(111). Indications that this DOS is located at the very surface are given by the intensity variations of the molecular level valence features as a function of the emission angle. These variations match well with the expected signal attenuation in photoemission, allowing to conclude that the low-energy DOS arises from HATCN molecules located at the very surface. Work function changes are set in relation to the observed charge transfer.

O 49.3 Wed 15:30 PHY C213

Elucidating the adsorption mechanism of isophorone on the Pd(111) surface — •Wei Liu, Aditya Savara, Wiebke Ludwig, Swetlana Schauermann, Xinguo Ren, Alexandre Tkatchenko, Hans-Joachim Freund, and Matthias Scheffler — Fritz-Haber-Institut der MPG

We present a joint theoretical and experimental study of the structural, vibrational, and chemical properties of isophorone ($C_9H_{14}O$) on the Pd(111) surface. Experimental vibrational spectroscopy and temperature-programmed desorption data indicate that both the pure isophorone and dehydrogenated moieties coexist on the surface below 400 K. To elucidate the underlying adsorption and dehydrogenation processes, we carried out density-functional theory (DFT) calculations with and without accounting for the long-range van der Waals (vdW) interactions. The PBE+vdW method [1] significantly changes the potential energy surface compared to the standard PBE, altering both the height and the tilt angle of the molecule with respect to the surface. We identify the reaction pathway from the weakly chemisorbed $C_9H_{14}O$ gas-phase reactant to the strongly chemisorbed dehydrogenated products, both by a direct elimination of hydrogen atoms closest to the Pd(111) surface and by *ab initio* molecular dynamics simulations. The coexistence of different isophorone moieties on the Pd(111) surface is attributed to an interplay of covalent and van der Waals bonding, along with zero point motion, and kinetic effects.

[1] A. Tkatchenko and M. Scheffler, Phys. Rev. Lett. 102, 073005 (2009).

O 49.4 Wed 15:45 PHY C213

Conformations of tetra(phenyl)porphyrine on Au(111): identification by experiment and theory — •Felix Hanke[1], Johannes Mielke[2], Leonhard Grill[2], and Mats Persson[1] — [1]University of Liverpool, Liverpool, UK — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

The on-surface synthesis of covalently coupled networks of tetra (phenyl)-porphyrines (TPP) on Au(111) [1] is a significant step toward custom-designed molecular structures. This is particularly useful as single TPP molecules adsorbed on Au(111) and imaged with a scanning tunneling microscope show several distinct configurations, which could be used for information storage. Here we present a combined density functional (DFT) and scanning tunneling microscopy study to elucidate the nature of the observed conformers. They differ in the internal structure of the porphyrin core which can be either flat or buckled. We further assess the importance of accounting for dispersion interactions in the adsorbate-surface coupling by comparing DFT results using the van der Waals density functional (vdw-DF) [2] and the PW91 functional. While the vdw-DF is found to significantly alter both adsorption height and binding energy of TPP, it hardly affects either its internal geometry or the electronic structure, suggesting that TPP is largely decoupled from the substrate.

[1] L. Grill *et al.*, Nature Nanotech., **2** 687 (2007). [2] J. Klimeš is acknowledged for his implementation of the vdw-DF density functional.

O 49.5 Wed 16:00 PHY C213

Electronic Decoupling in Monolayer and Multilayer: Fe-Phthalocyanine on Ag(111) — •Thiruvancheril Gopakumar[1], Thomas Brumme[2], Jörg Kröger[1], Cormac Toher[2], Giovanni Cuniberti[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, D-01069 Dresden, Germany

Electronic properties of Fe-phthalocyanine (FePc) molecules in ultrathin films on Ag(111) have been investigated by scanning tunnelling spectroscopy and density functional calculations. Single FePc molecules show a broad signature of Fe d orbitals. However, in a two-dimensional ordered superstructure spectroscopic contributions from individual d_{z^2} and d_{xz}/d_{yz} orbitals are resolved. Calculations suggest that an increased molecule-surface distance in the superstructure and a change of the Ag(111) surface electronic structure cause the spectral changes, which are consistent with a partial electronic decoupling of the molecules from the substrate. A progressive evolution towards a gap around the Fermi level is observed for molecules atop the first and second molecular layer.

Financial support by the Deutsche Forschungsgemeinschaft through SFB 677 is acknowledged.

O 49.6 Wed 16:15 PHY C213

Phase separation of cobalt- and 2H-tetraphenylporphyrin on Cu(111): A Scanning Tunneling Microscopy Study — •Stefanie Glässel, Elisabeth Zillner, Florian Buchner, Michael Röckert, Michael Stark, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058

The understanding of the adsorption behavior of large organic molecules on surfaces is a prerequisite to utilize their functional properties either in single-molecule devices or in self-assembled supramolecular architectures. In this regard the discrimination of the corresponding molecule-molecule and molecule-substrate interactions are in the center of our scanning tunneling microscopy (STM) study at room temperature. While tetraphenylporphyrins (TPP) are known to form ordered square phases and intermix well on Ag(111) [1], on Cu(111) the separation of CoTPP and 2HTPP is observed [2]. This can be explained by the domination of attractive T-type interactions between adjacent CoTPP molecules and the domination of site specific molecule-substrate interactions for 2HTPP on Cu(111); the observed behavior can conclusively be interpreted as due to a coordinative bond between the iminic nitrogens and copper surface atoms.

This work has been funded by the DFG through Sonderforschungsbereich 583.

[1] F. Buchner et al., Phys. Chem. Chem. Phys., 2010, 12, 13082-13090. [2] F. Buchner et al., submitted

O 49.7 Wed 16:30 PHY C213

The adsorption geometry and bonding properties of PTCDA on Ag(110) — •Oliver Bauer[1], Giuseppe Mercurio[2], Sergey Subach[2], Benjamin Fiedler[1], Christoph H. Schmitz[1], Frank Stefan Tautz[2], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Bonn — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, und JARA-Fundamentals of Future Information Technology

The vertical bonding distance of an adsorbate to the underlying surface can be regarded as a quantity related to the strength and the chemisorptive character of the bond. The Normal-Incidence X-ray Standing Wave (NIXSW) technique has recently been used to determine the bonding distance of perylene-3,4,9,10-tetracarboxylic acid dianhydride (PTCDA) on (111) coinage metal surfaces [1]. In addition, we have investigated the adsorption geometry of PTCDA in the monolayer regime on the more open Ag(110) surface: We find a bonding distance of the perylene core to the substrate which is significantly smaller than the sum of the vdW radii of both Ag and C, indicating a strong chemical interaction. Furthermore, the PTCDA molecule adsorbs in an arc-like geometry with the O atoms being even closer to the surface than the perylene core. This hints at strong local, covalent Ag-O intercations. The experimental results are discussed in the framework of the Newns-Anderson model and the recent finding, that for coinage metal (111) surfaces the adsorption height of PTCDA correlates with the work function of the bare substrate [1]. Supported by the DFG and the ESRF. [1] a.o. A. Hauschild et al., PRB 81 (2010) 125432.

O 49.8 Wed 16:45 PHY C213

Experimental & theoretical study of a perylene derivative on Cu(111): insight into the bonding mechanism — •Mihaela Enache[1], Jonas Björk[2], Manfred Matena[3], Jorge Lobo-Checa[3], Lutz Gade[4], Thomas Jung[5], Mats Persson[2], and Meike Stöhr[1] — [1]University of Groningen, Netherlands — [2]University of Liverpool, UK — [3]University of Basel, Switzerland — [4]University of Heidelberg, Germany — [5]Paul-Scherrer-Institute, Switzerland

By utilizing the concepts of supramolecular chemistry, remarkable results for molecular self-assembly on surfaces have been presented. The outcome of the self-assembly process is known to be affected by the fine tuning of different parameters which have a direct influence on the interplay between intermolecular and molecule-substrate interactions. In our case we studied the influence of temperature by annealing the sample. STM investigations of a perylene derivative (TAPP) deposited on Cu(111) held at -100°C showed that the molecules do not form an ordered arrangement. Annealing at room temperature results in the formation of a herringbone arrangement while the molecules interact with each other via vdW forces. After annealing at 150°C, a metal coordinated rectangular network is obtained which is commensurate to the substrate [1]. By performing XSW measurements, the vertical adsorption geometry for both phases of TAPP on Cu(111) was determined and such insight into the interplay between intermolecular and molecule-substrate interaction is gained. The findings are supported by DFT calculations. [1] Matena et al., Chem. Eur. J., 16, 2079 (2010)

O 49.9 Wed 17:00 PHY C213

Assembly and manipulation of rotatable cerium-porphyrinato sandwich complexes on a surface — •Saranyan Vijayaraghavan[1], David Ecija[1], Willi Auwärter[1], Knud Seufert[1], Felix Bischoff[1], Kentaro Tashiro[2], and Johannes V. Barth[1] — [1]Physik Department, E20 Technische Universität München, Garching, Germany — [2]National Institute for Materials Science (NIMS) ,1-1 Namiki, Tsukuba 305-0044, Japan

The characterization and engineering of molecular nanostructures on surfaces is of great interest, especially the development of metal-directed assembly protocols with suitable linkers and metal atoms combined on well-defined surfaces. Porphyrin molecules are ideal building blocks for these surface anchored nanostructures. Particularly interesting are tetrapyrrole-derived sandwich compounds comprising rare-earth metal centres. Here we report a novel route to synthesize such Bis(porphyrinato)cerium double-deckers (Ce(TPP)2) and Tris(porphyrinato) cerium triple-deckers (Ce2(TPP)3 directly on a Ag(111) surface under UHV conditions by exposing a porphyrin precursor layer to a beam of Ce atoms. The double and triple-decker compounds are studied by scanning tunneling microscopy (STM) topographic measurements, including a comparison with Ce(TPP)2 layers generated by molecular beam epitaxy. Moreover, we address the motion of double- and triple-decker moieties in specific environments: the top porphyrin of each molecular species can be rotated by STM manipulation. Such complexes can have important applications like single molecule magnets or field effect transistors.

O 50: Plasmonics and Nanooptics V

Time: Wednesday 15:00–17:00 Location: WIL A317

O 50.1 Wed 15:00 WIL A317

Optical Nanoantennas for Ultrafast Spectroscopy of Single Nanoparticles — •Thorsten Schumacher[1,2], Daniela Ullrich[1,2], Kai Kratzer[1,2], Mario Hentschel[1,2], Harald Giessen[2], and Markus Lippitz[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]4th Physics Institute, University of Stuttgart

Nonlinear spectroscopy investigates the deviations from linear light-matter interaction. The already weak signals are reduced further when single nanoobjects such as quantum dots, molecules, or nanoparticles are investigated. Here, we demonstrate how such an extremely weak nonlinear signal can be enhanced by an optical nanoantenna. For this purpose we use the transient optical response of a mechanically oscillating single gold nanodisc. Our antenna is another gold nanostructure which is placed closely next to the small disc. In this configuration we find a strong plasmonic coupling what can be described by a plasmon hybridization model and numerical simulations. Our calculations show how this plasmonic interaction cause a transfer of the weak nonlinear response of the nanoparticle to the much stronger antenna signal. With ultrafast pump-probe spectroscopy we verify the theoretical predictions and show a measured signal enhancement by a factor of 10, what is in good agreement with our simulations. Finally we can give an outlook for more advanced antenna structures to further increase the enhancement factor.

O 50.2 Wed 15:15 WIL A317

Connecting antennas, waveguides and couplers in nanoplasmonics — •Arian Kriesch[1,2,3], Jing Wen[1,2], Daniel Ploss[1,2,3], Peter Banzer[1,2], and Ulf Peschel[1,2] — [1]MPI für die Physik des Lichts, Erlangen, Germany — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [3]Erlangen Graduate School in Advanced Optical Technologies (SAOT)

Subwavelength, plasmonic waveguides open the way to the manipulation of light in photonic circuits at the nanoscale. However, they demand new techniques to efficiently transfer light from the far-field into these highly confined waveguide modes. Recent technological progress has enabled the fabrication of plasmonic metal gap waveguides on dielectric substrates with a width in the range of a few tens of nanometers as well as connected optical nanoantennas by Focussed Ion Beam (FIB) and e-beam lithography. We present experimental measurements of the properties of such waveguides, namely transmission and bend losses, which are compared to Finite Element Method (FEM) calculations. Our optimized optical antennas (coupling efficiency from the far-field to waveguide ≈ 15%) allow for efficient, selective coupling to single waveguides. Utilizing these antennas together with a setup for high-numerical-aperture focal scanning, we have demonstrated and quantitatively analyzed the coupling between closely adjacent waveguides, thus realizing discrete diffraction and coupling effects in nanoplasmonic waveguide arrays. Efficient optical antennas, low loss bent waveguides and interwaveguide couplers are each a building block in future highly confined plasmonic nanocircuitry.

O 50.3 Wed 15:30 WIL A317

Spiral Optical Nanoantenna — •Daniel Dregely, Martin Schäferling, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, D-70569 Stuttgart, Germany

Advances in nanofabrication in the past years allowed for adaption of concepts of the radiofrequency and microwave regime to optical wavelengths [1]. Recently, the road has been opened towards more complex antenna geometries suitable for tailoring light emission on the nanoscale [2,3]. Self-complementary structures are commonly used in the high frequency regime to transmit and receive signals over a broad frequency range.

We investigate a self-complementary spiral nanoantenna for the optical wavelength range. The structure has different handedness for opposite incident directions of light. Albeit being planar, its emission cone is normal to the surface. We study experimentally the optical properties in transmission and reflection for circularly polarized light. Numerical simulations confirm our measurements and give insight to the near-field response of our structure.

References:

[1]P. Mühlschlegel et al., Science 308, 1607 (2005)

[2]T. Kosako, Y. Kadoya, and H. F. Hofmann, Nature Photonics 4, 312-315 (2010)

[3]A. G. Curto et al., Science 329, 930-933 (2010)

O 50.4 Wed 15:45 WIL A317

Plasmonic sensing using multipolar infrared antenna resonances — •Frank Neubrech[1], Daniel Weber[1], Jörg Bochterle[1], Gui Han[2], Tadaaki Nagao[2], and Annemarie Pucci[1] — [1]Kirchhoff-Institute for Physics, Heidelberg University, Germany — [2]National Institute for Materials Science, Tsukuba, Japan

Excited resonantly, antenna-like nanostructures confine the electromagnetic radiation on the nanoscale and therefore enhance the electromagnetic field in their vicinity, which can be exploited for surface enhanced infrared spectroscopy. The only precondition is a good match between the fundamental resonant excitation of the nanoantenna and the vibrational signal of the adsorbate of interest. But not only the near field of the fundamental mode can be used to enhance vibrational signals, but also multipolar modes (l=3, 5, 7) as we will show in this contribution. We performed infrared spectroscopic measurements of nanoantennas supported by a silicon wafer with a natural SiO_2 layer. For parallel polarized light and at a good match of the fundamental resonance mode of the antenna with the SiO_2 phonon, the SiO_2 surface phonon-polariton signal is enhanced. Its line shape reveals a Fano-type interaction with the antenna resonance. Detuning the nanoantenna by increasing its length leads to a decrease of the SiO_2 signal due to the frequency dependence of the antenna resonance. For even longer antennas the SiO_2 signal increases again and reaches a second maximum if the multipolar l=3 excitation of the nanoantenna matches the excitation frequency of the SiO_2 phonon-polariton.

O 50.5 Wed 16:00 WIL A317

Dispersion engineering in a plasmonic microcavity through mode interaction — •Liwei Fu[1], Heinz Schweizer[1], Thomas Weiss[1,3], Philipp Schau[2], Karsten Frenner[2], Wolfgang Osten[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]Institut für Technische Optik and Research Center SCoPE, University of Stuttgart, Germany — [3]LASMEA, Université Blaise Pascal, F-63177 Aubière Cedex, France

Microcavities provide the possibility to control and enhance light-matter interaction, which is indispensable for future quantum optical communication [1]. Microcavities with two identical periodically corrugated metallic mirrors supporting surface plasmon polaritons can further confine optical fields into a subwavelength regime. In this report, we demonstrate that mode interactions between surface plasmons and a microcavity mode can be used to tune mode dispersion, which is essential for light matter interaction. We study here numerically how the surface plasmons interact with the cavity modes in both near and far field regimes in a metallic meander cavity via tuning the excitation strength of the surface plasmons [2].

[1] K. J. Vahala, "Optical microcavities," Nature 424, 839 (2003).

[2] L. Fu, H. Schweizer, T. Weiss, and H. Giessen, "Optical properties of metallic meanders," J. Opt. Soc. Am. B 26, B111 (2009).

O 50.6 Wed 16:15 WIL A317

Cavity-enhanced localized plasmonic resonance sensing — •Ralf Ameling, Lutz Langguth, Mario Hentschel, Martin Mesch, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

We present a method to enhance the sensing properties of a localized plasmon resonance sensor. The concept is based on the combination of localized plasmons in nanostructures and a photonic microcavity. Metal nanorods that are placed at Bragg distance above a metal mirror form a Fabry-Pérot microcavity and constitute a coupled photonic-plasmonic system. The localized plasmon resonances of the nanorods and the phase shifts upon plasmon excitation are extremely sensitive to changes of the refractive index of the material surrounding the nanorods. Compared to the plasmonic nanorods alone, the coupled photonic-plasmonic system allows for a much more sensitive detection of small refractive index changes. We experimentally demonstrate our method with water and glucose solution. Our concept can be applied to many localized plasmonic sensor structures (e.g., colloidal systems such as nanostars) and will considerably increase their sensing properties. Potential applications in the fields of biotechnology, medical diagnostics, or pharmacology including biomolecule detection as well as real-time monitoring of chemical reactions or molecular kinetics might benefit from this concept.

O 50.7 Wed 16:30 WIL A317

Simulating EELS Spectra using the Discontinuous Galerkin Time Domain Method — •Christian Matyssek[1,2], Jens Niegemann[3], Wolfram Hergert[2], and Kurt Busch[3] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany — [2]Institute of Physics, von-Seckendorff-Platz 1, 06120 Halle, Germany — [3]Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT), D-76128 Karlsruhe, Germany

Electron Energy Loss Spectroscopy (EELS) was recently used to examine single metal nano particles[1] and also systems of particles[2,3]. Frequently, the calculation of these spectra is done in frequency domain, e.g. using the Boundary Element Method[1]. We present the calculation of EEL spectra using the Discontinuous Galerkin Time Domain (DGTD) method, which is well approved in photonics calculations[4]. The numerical results are compared to analytical results that are available for spheres. The influence of substrates on the surface-plasmon excitation is studied. Application of nonlinear material models will be discussed.

[1] Nelayah et al., Nat. Phys. 3, 348 (2007)
[2] Chu et al., Nanotech. 20, 235705 (2009)
[3] Sigle et al., Opt. Lett. 34, 2150 (2009)
[4] Niegemann et al., Phot. and Nanostr. 7, 2 (2009)

O 50.8 Wed 16:45 WIL A317

Release of the fluorescent dye DAPI via photothermal dissociation of programmable DNA-gold-nanoparticle networks — •Malte Linn[1], Anne Buchkremer[2], Maximilian Reismann[1], Ulrich Simon[2], and Gero von Plessen[1] — [1]Inst. of Physics (IA), RWTH Aachen University, Germany — [2]Institute of Inorganic Chemistry, RWTH Aachen University, Germany

The optical excitation of particle plasmons in gold nanospheres by means of laser light enables a highly localised and contact free heating of the nanoparticles and their immediate surroundings. This effect can be exploited to control temperature-sensitive biochemical reactions. In this work, it is used for the selective release of the DNA-intercalating fluorescent dye 4',6-diamidino-2-phenylindole (DAPI). Here, the release is realized via the photothermal dissociation of networks consisting of DNA-linked gold nanoparticles using focused cw-laser light (532 nm wavelength). Since the DAPI molecules only intercalate into DNA double strands, these molecules are released from the networks due to the photothermal controlled dehybridisation of the DNA into single strands. This process can be spectroscopically observed by measuring the fluorescence intensity, since the fluorescence of DAPI stored in the networks is suppressed by the nearby nanoparticles (fluorescence quenching). By using layer-by-layer networks, consisting of nanoparticles linked by different types of DNA, both a well-defined network structure and a step-by-step release of molecules can be realized. The principle shown here might be the basis for a remote release process of medical agents of future medicines.

O 51: Graphene III

Time: Wednesday 15:00–17:15 Location: WIL B321

O 51.1 Wed 15:00 WIL B321

A graphene phase transition induced by compressing nanomembranes using STM. — •Alexander Georgi[1], Dinesh Subramaniam[1], Christian Pauly[1], Torge Mashoff[1], Ludger Wirtz[2], Viktor Geringer[1], Marcus Liebmann[1], Marco Pratzer[1], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B, Otto-Blumenthal-Straße, RWTH Aachen University and JARA-FIT, 52074 Aachen — [2]IEMN, Dept. ISEN, B.P. 60069, 59652 Villeneuve d'Ascq Cedex.

The variety of the different carbon allotropes is due to the energetic similarity between the sp^2 and sp^3 band. Even a metastable 3d structure of sp^2 bands called K$_4$ has been proposed [1].

Applying forces to a graphene flake exfoliated on SiO$_2$ using an STM-tip the valleys of the intrinsic rippling can be lifted [2]. The induced compression during lifting leads to a transition from flat hexagonal graphene to a triangular appearence probably representing a buckled hexagonal structure resembling a diamond-like arrangement of the atoms. Further lifting leads to a reduction of the compression and a corresponding switch-back to the unbuckled phase. For valleys with 1.5 nm^2, a buckling amplitude of 5 pm has been deduced, which is only 10% of the buckling within a 2d-diamond crystal. The phase transition cannot be reproduced by DFT Calculations so far.

[1] Itoh *et al.*, Phys. Rev. Lett. **102**, 055703 (2009).
[2] Mashoff *et al.*, Nano Lett. **10**, 461 (2010).

O 51.2 Wed 15:15 WIL B321

Local transport measurements on folding graphite and multilayer graphene on SiO2 by a four-probe scanning tunneling microscope — •Shiro Yamazaki, Tobias Spitz, Oswald Pietzsch, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Germany

Unique electrical transport properties of carbon-based materials such as graphite and graphene have attracted great research interest over a long period of time [1,2]. Mechanically-exfoliated microscopic graphite and multi-layer graphene on SiO2 exhibit sub- micron-scale unique structural defects such as various kinds of layer folding. We have measured the local electrical resistance at folding sites, using a variable-temperature UHV-based four-probe scanning tunneling microscope equipped with a high-resolution UHV scanning electron microscope. We have succeeded in detecting the electrical current flowing along a graphite folding sheet. The folding part exhibits a higher resistance than flat areas. We changed a square-like folding to a triangle-like one by mechanically pushing the tip toward the folding part. The electrical resistance has been compared before and after the manipulation of the folding. [1] K. Krishnan et al., Nature 144, 667 (1939); [2] K. S. Novoselov et al., Nature 438, 197 (2005).

O 51.3 Wed 15:30 WIL B321

Raman spectroscopy on graphene on insulator surfaces — •Hanna Bukowska, Florian Meinerzhagen, Sevilay Akcöltekin, Markus Neubert, Volker Buck, and Marika Schleberger — Universität Duisburg-Essen, Fakultät für Physik, Lotharstraße 1, 47058 Duisburg, Germany

Raman spectroscopy is a powerful nondestructive method to investigate graphene sheets. We prepare graphene on different substrates: SiO_2 as well as the insulators $SrTiO_3$, TiO_2, and Al_2O_3. We measure the Raman spectra of all those samples for single-, bi-, fewlayer graphene and graphite. The 2D peak of the Raman spectrum evolves clearly with the number of layers. It reflects the changes in the electronic structures and any substrate-induced changes. The D peak is solely activated by presence of morphological defects - here we verify the quality of our graphene. We compare virgin and modificated graphene which was irradiated with swift heavy ions. Finally, in the future we want to study graphene transistors prepared on two of the above mentioned substrates, where any difference in charge carrier doping should show up in a change of the G peak.

O 51.4 Wed 15:45 WIL B321

Polarized Raman scattering of graphene nanoribbons — •Nils Scheuschner[1], Bernat Terrés[2], Christoph Stampfer[2], and Janina Maultzsch[1] — [1]Institut für Festkörperphysik, TU Berlin, Germany — [2]JARA-FIT, Institute of Bio and Nanosystems, Forschungszentrum Jülich and II. Institute of Physics, RWTH Aachen University, Germany

Understanding the physics of graphene nanoribbons is a key requirement to build novel nanoelectronic devices on the basis of graphene. Resonant Raman spectroscopy is a powerful tool for the investigation of carbon nanomaterials, in particular for studying both their vibrational and electronic properties. Moreover it allows to investigate the electron phonon coupling. Polarization depended Raman scattering can also give information about the edge configuration of graphene nanostructures. We present Raman line scans on lithographically defined and etched single-layer graphene nanoribbons at different incident polarization angles. The length of the nanoribbons is in the range of 1.5-2 micrometer and the width ranges from 100-500 nm. We discuss the dependence of the Raman intensity on the polarization.

O 51.5 Wed 16:00 WIL B321

Illuminating the dark corridor in graphene: polarization dependence of angular resolved photoemission spectroscopy on graphene — •Isabella Gierz[1], Jürgen Henk[2], Hartmut Höchst[3], Christian R. Ast[1], and Klaus Kern[1,4] — [1]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle (Saale), Germany — [3]Synchrotron Radiation Center, University of Wisconsin-Madison, Stoughton, WI 53589, USA — [4]IPMC, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

We have used s- and p-polarized synchrotron radiation to image the electronic structure of epitaxial graphene near the K-point of the 2D Brillouin zone by angular resolved photoemission spectroscopy (ARPES). Part of the experimental Fermi surface is suppressed due to the interference of photoelectrons emitted from the two equivalent carbon atoms per unit cell of graphene's honeycomb lattice [1]. We will show that by rotating the polarization vector, we are able to illuminate this 'dark corridor' indicating that the present theoretical understanding is oversimplified. Our measurements are supported by first-principles photoemission calculations, which reveal that the observed effect persists in the low photon energy regime.

[1] E. L. Shirley, L. J. Terminello, A. Santoni, and F. J. Himpsel, Phys. Rev. B **51**, 13614 (1995)

O 51.6 Wed 16:15 WIL B321

Plasmon electron – hole resonance in epitaxial graphene — •Thomas Langer[1,2], Jens Baringhaus[1], Christoph Tegenkamp[1], Herbert Pfnür[1], and Hans Werner Schumacher[2] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, D-30167 Hannover — [2]Physikalisch -Technische Bundesanstalt, D-38116 Braunschweig

The sheet plasmon in epitaxially grown graphene on SiC(0001) has been studied by means of angle resolved high resolution electron energy loss spectroscopy. Most interestingly, the dispersion reveals a dip, which can be assigned to quasiparticle dynamics. The effect is characteristic for pristine graphene and depends on the chemical potential but not on temperature and roughness. By assuming an resonant coupling between the 2d plasmon and an inter-band electron-hole pair excitation (so-called plexciton) the dip in the dispersion can be quantitatively explained using the Drude model of the dielectric function and the nearly free 2d electron gas model of Stern. The relation between this dip and the chemical potential becomes apparent by adsorption experiments performed with F4-TCNQ molecules, which reduces the carrier density and lowers the Fermi level. As expected the dip in the dispersion as well as the signature of the enhanced damping in the FWHM shifts to the lower k_F-values. Remarkably, the average slope of the dispersion remains unchanged, although the electron density at E_F is reduce. Obviously, the coupling of the plasmon mode with the loss channels leads to an effective integration over the electron density around E_F with a width proportional to the measured FWHM of the plasmon mode.

O 51.7 Wed 16:30 WIL B321

Phonon-Plasmon Dispersion of Graphene and Quasi-Freestanding Graphene on 6H-SiC(0001) — •Michael Endlich[1], Roland J. Koch[1,2], Thomas Haensel[1], Thomas Seyller[2], and Juergen A. Schaefer[1,3] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, PF 100565, 98684 Ilmenau, Germany — [2]Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Germany — [3]Department of Physics, Montana State University, P.O. Box 173840, Bozeman, MT 59717-3840, USA

We report on a comparison between the strongly coupled phonon-plasmon modes of graphene and hydrogen-intercalated monolayer graphene epitaxially grown on 6H-SiC(0001). The dispersion of these modes have been simulated within a simple dielectric model. As a result, the quasi-freestanding character of the hydrogen-intercalated graphene has been corroborated. From the model it is possible to derive essential values of the graphene such as charge carrier density, effective mass and mobility, which are important for technological applications like high frequency transistors. Furthermore, the existence of silicon-hydrogen and carbon-hydrogen stretching and bending vibrations indicate not only a saturation of Si-dangling bonds at the interface, as it has been previously reported in the literature.

O 51.8 Wed 16:45 WIL B321

Plasmarons in Quasi-Freestanding Doped Graphene Observed through Photoemission — Aaron Bostwick[1], Florian Speck[2], Thomas Seyller[2], •Karsten Horn[3], Marco Polini[4], Reza Asgari[5], Allan McDonald[6], and Eli Rotenberg[1] — [1]ALS, Lawrence Berkeley Lab, USA — [2]Technische Physik, Uni Erlangen, Germany — [3]Fritz Haber Institute, Max Planck Society, Berlin, Germany — [4]CNR and Scuola Normale Superiore Pisa, Italy — [5]Institute of Research in Fundamental Sciences, Teheran, Iran — [6]Department of Physics, University of Texas, Austin USA

The unusual conical band structure of graphene leads to a zero-energy band gap at a single Dirac crossing point. By measuring the spectral function of charge carriers in quasi-freestanding graphene with ARPES, we showe that at finite doping, this well-known linear Dirac spectrum does not provide a full description of the charge-carrying excitations. We observed composite plasmaron particles, which are bound states of charge carriers with plasmons, the density oscillations of the graphene electron gas; such quasiparticles were predicted more than forty years ago, but their experimental confirmation so far has proven elusive. We show that the Dirac crossing point is resolved into three crossings: the first between pure charge bands, the second between pure plasmaron bands, and the third a ring-shaped crossing between charge and plasmaron bands. This observation resolves a controversy about the existence of a gap at the Dirac point in graphene on SiC(0001).

O 51.9 Wed 17:00 WIL B321

Electron spectrum of epitaxial graphene monolayers — •Oleg Pankratov, Stephan Hensel, and Michel Bockstedte — Lst. Theoretische Festkörperphysik, Universität Erlangen, Staudtstr 7B2, 91058 Erlangen.

Epitaxial graphene on SiC possesses, quite remarkably, an electron spectrum similar to that of free-standing samples. Yet, the coupling to the substrate, albeit small, should affect the quasiparticle properties. Whether the graphene-substrate interaction opens an energy gap has been a long debate with experimental estimates ranging from 0 to 0.3 eV [1,2]. Using symmetry analysis, we derive a modified Dirac-Weyl Hamiltonian for graphene epilayers [3]. To determine the numerical values of the Hamiltonian parameters we performed *ab initio* calculations for a model (5×5) comensurable interface structure. We find that for the epilayer on the C-face the Dirac cone remains intact, whereas for epilayers on the Si-face the band splitting is about 30 meV. At certain energies, the Dirac bands are significantly distorted by the resonant interaction with interface states, which should lead to mobility

suppression, especially on the Si-face.
[1] T. Seyller *et al.*, Phys. Status Solidi B **245**, 1436 2008
[2] S. Y. Zhou *et al.*, Nature Mater. **6**, 770 (2007).
[3] O. Pankratov, S. Hensel, and M. Bockstedte, Phys. Rev. B **82**, 121416 (2010).

O 52: Nanostructures at surfaces: Wires, tubes

Time: Wednesday 15:00–17:15 Location: WIL B122

O 52.1 Wed 15:00 WIL B122

Surface and Interface Characterization of III-V Semiconductor Nanowires — •Rainer Timm, Martin Hjort, Edvin Lundgren, Lars Samuelson, and Anders Mikkelsen — The Nanometer Structure Consortium, Dept. of Physics, Lund University, Sweden

III-V Semiconductor Nanowires have attained strong interest due to their unique properties and tremendous possibilities for device application. They are characterized by an extreme surface-to-volume ratio, so that their surface properties or interface properties in core-shell nanowire heterostructures are crucial for the entire device behavior.

Recently, we have obtained first atomically resolved images of different InAs nanowire surfaces using scanning tunneling microscopy (STM) [1]. Here, we combine STM and scanning tunneling spectroscopy (STS) measurements to directly link local structural and electronic properties of InAs and InP nanowire heterostructures.

A promising application of InAs nanowires are high-speed metal-oxide-semiconductor (MOS) devices [2]. The exact chemical composition of the nanowire-oxide interface is crucial for the MOS device performance. We have therefore studied the reduction of the native oxide on InAs upon deposition of high-k dielectric thin films and the resulting interface properties using X-ray photoemission spectroscopy for planar InAs substrates [3] as well as for InAs nanowires. A clear reduction of various oxide states is observed, also depending on nanowire crystal structure and InAs surface orientation.

[1] E. Hilner *et al.*, Nano Lett. **8**, 3978 (2008). [2] S. Roddaro *et al.*, APL **92**, 253509 (2008). [3] R. Timm *et al.*, APL **97**, 132904 (2010).

O 52.2 Wed 15:15 WIL B122

Photochemical tuning of the conductivity of DNA-platinum cluster chains — •Christiane Schuster[1], Thomas Härtling[2], Lukas Eng[3], and Michael Mertig[1] — [1]Technische Universität Dresden, Professur für Physikalische Chemie, Mess- und Sensortechnik, 01062 Dresden — [2]Fraunhofer Institute for Non-Destructive Testing, 01109 Dresden — [3]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden

We present a self-assembly based method for the fabrication of conductive DNA-based nanowires. By means of chemical functionalization, DNA molecules were engineered into the gaps of $3-5\,\mu$m wide Au finger electrode arrays. Photo-induced metal deposition was then applied to grow about 5 nm Pt clusters along the molecules. At this stage, the resulting discontinuous cluster chains showed no electrical conductivity. Hence, we "welded" the Pt clusters by further photo-induced deposition of gold into the interparticle gaps and finally obtained continuous, electrically conducting nanowires. The photochemical reduction of gold takes place from a $HAuCl_4$ solution and is catalyzed by the platinum clusters. Exploiting this catalytic activity, we obtain high spatial selectivity of the photo-induced deposition process far below the diffraction limit. Experiments were carried out on an inverted microscope, using a laser for inducing the reduction reaction, and a white-light illumination for monitoring the deposition process. The wires were analyzed by atomic force microscopy and conductivity measurements which proofed the high spatial selectivity of the method as well as the electrical quality of the wires.

O 52.3 Wed 15:30 WIL B122

One-dimensional Mn atom chains templated on a Si(001) surface — •Sigrun A. Köster[1], James H. G. Owen[1], François Bianco[1], Alex M. P. Sena[2], David R. Bowler[2], and Christoph Renner[1] — [1]University of Geneva, Switzerland — [2]University College London/London Centre of Nanotchnology, UK

Single-atom chains on a wide gap substrate are a very attractive embodiment of a truly one-dimensional system to explore the remarkable physical properties emerging in such low dimensions. We present self-assembled single-atom Mn chains on a Si(001) surface with Bi nanolines, which serve to increase greatly the average length of the Mn chains. They grow perpendicular to the Si(001) dimer rows, at densities which can be adjusted by means of the growth parameter. High resolution scanning tunneling microscopy (STM) micrographs are in perfect agreement with density functional theory (DFT), providing detailed insight into the chain structure. We further discuss low temperature STM spectroscopy and spin dependent DFT modeling suggesting Mn-chains are indeed a suitable candidate to observe electronic and magnetic properties in one-dimension experimentally.

O 52.4 Wed 15:45 WIL B122

The In/Si(111)-(4×1)/(8×2) surface – A fascinating model system for 1D conductors — •Stefan Wippermann, Simone Sanna, and Wolf Gero Schmidt — Lehrstuhl für Theoretische Physik, Universität Paderborn, D-33095 Paderborn

One-dimensional (1D) electronic systems are currently intensively investigated for both fundamental and technological reasons. The ordered array of In nanowires that self-assembles at the Si(111) surface is an extremely popular model system for such 1D electronic systems. It shows an intriguing temperature-induced metal-insulator (MI) transition below 120K from (4×1) to (8×2) translational symmetry. The low-temperature (LT) ground state of the nanowires as well as the driving force and mechanism of the phase transition remain controversial, however.

Here we present an overview of recent *ab initio* optical response and free-energy calculations [1] that allow for the unambiguous determination of the ground-state geometry. Soft shear and rotary phonon modes are shown to describe the structural transformation between the LT and the room-temperature (RT) geometry. The MI transition is explained as a triple-band Peierls instability. The phase transition is caused by the subtle interplay between the lower total energy of the insulating (8×2) ground state and the larger vibrational and electronic entropy of the less tightly bound and metallic RT (4×1) phase.

[1] S Wippermann *et al.* PRL **98**, 026105 (2007) + PRL **100**, 106802 (2008) + PRL **102**, 226805 (2009) + PRL **105**, 126102 (2010)

O 52.5 Wed 16:00 WIL B122

Comparative Study of the Growth of Nonacosan-10-ol Wax Tubules of Lotus (Nelumbo nucifera) Leaves on Gold (111) and HOPG Surface — •Sujit Kumar Dora and Klaus Wandelt — Institute for Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, D-53115, Bonn, Germany

A comparative study of self-assembly of nonacosan-10-ol tubules derived from lotus (Nelumbo nucifera) leaves on gold (111) and HOPG surface is presented. Even though the average time period of tubule formation is ≈ 2-3 hours, however, the orientation of tubules differed on both substrates. On HOPG, a vertical orientation of tubules was found whereas on gold (111) tubules are arranged in a horizontal fashion with respect to the surface. Taking into account the surface properties of HOPG and gold (111) where both are nonpolar, crystalline as well as hydrophobic, the different orientation of tubules on these surfaces clearly indicated that none of the surface properties are responsible for the tubule orientation. This also provokes another question whether HOPG is a good material to mimic natural surfaces.

O 52.6 Wed 16:15 WIL B122

Growth behaviour of Ge nanowires grown homoepitaxially by means of MBE — •Jan Schmidtbauer, Roman Bansen, Torsten Boeck, and Thomas Teubner — Leibniz Institute for Crystal Growth, 12489 Berlin, Germany

Germanium has gained renewed interest within recent years for aggressively scaled Si CMOS as well as Si photonics technologies. The reasons are given by the facts that: (*i*) Ge is compatible with Si process technology, (*ii*) it has higher hole concentration and mobility compared to many III-V semiconductor materials and (*iii*) its band gap value matches the wavelength of typical telecommunication infrastructure. With respect to the later application we investigated germanium nanowires as promising structures for low-band-gap photonics devices compatible with Si CMOS process technologies.

We studied the influence of different types of Ge substrates on growth direction, growth rate and shape of MBE grown Ge nanowires. In particular, homoepitaxial growth of the nanowires was compared using (100), (110) and (111) oriented germanium substrates. In all cases, the experiments revealed preferential growth in ⟨110⟩ direction. A clear dependency of the growth rate on the inclination of nanowires towards the surface normal was shown. This growth behaviour is explained by different amounts of material that contribute to nanowire growth through direct impingement on the sidewalls of the nanowire. To understand the nature of the preferential growth in ⟨110⟩ direction TEM studies are presented. Furthermore, a model is proposed to explain this behaviour.

O 52.7 Wed 16:30 WIL B122

Template-Fabrication of Highly Ordered MnO2 One-Dimensional Nanostructure Arrays and their Device Applications as Super-Capacitors — •Fabian Grote[1,2], Jingjing Xu[1,2], Huaping Zhao[1,2], and Yong Lei[1,2] — [1]Institute of Materials Physics, University of Muenster — [2]Center for Nanotechnology, Muenster 48149, Germany

MnO2 is a promising candidate for future applications in supercapacitors, especially for nano-structured MnO2 that might result in a high specific capacitance of the super-capacitor. Moreover, it is highly desirable to prepare highly ordered arrays of MnO2 nanostructures so that the properties (e.g., electrochemical property) can be controlled. Recently, using anodic alumina membranes as templates, we fabricated regular arrays of MnO2 one-dimensional nanostructures, including nanotubes and nanowires. The morphology and microstructures of the synthesized nanostructures were characterized by scanning electron microscopy and transmission electron microscopy. Electrochemical properties of the highly ordered MnO2 nanostructure arrays were investigated for super-capacitor application.

O 52.8 Wed 16:45 WIL B122

Tin dioxide nanowire gas sensor for detection of the toxic gases CO, H2S and SO2 — •Elise Brunet[1], Christian Griessler[1], Giorgio Mutinati[1], Stephan Steinhauer[1], Anton Koeck[1], Christian Edtmaier[2], and Wolf-Dieter Schubert[2] — [1]AIT Austrian Institute of Technology GmbH, Health & Environment Department, Nano Systems, Vienna, Austria — [2]Institute of Chemical Technologies and Analytics, Vienna University of Technology, Vienna, Austria

Metal oxide-based gas sensors rely on changes of electrical conductance due to interactions between the surrounding gas and the sensing layer. This sensing layer is most commonly a polycrystalline tin dioxide (SnO2) thin film. However, single crystalline SnO2 nanowires have higher chemical resistance and thermal stability and are therefore of great interest for highly sensitive gas detecting devices. We present nanosensors based on single crystalline SnO2 nanowires, which are very sensitive to the highly toxic gases CO, H2S and SO2. A SnO2 thin film is deposited by spray pyrolysis on a SiO2/Si substrate and further tempered 1h at 900°C in Ar-atmosphere resulting in the growth of single crystalline SnO2 nanowires. The sensing performance of the nanowire sensor is presented. Exposure to 260ppm CO leads to a sensitivity of 1.5% at 300°C. In presence of 1,5ppm H2S the highest sensitivity of 25% is obtained at 250°C and the sensor response to 27ppm SO2 reaches a sensitivity of 8% at 400°C. The specific responses achieved from the nanowire sensor at different temperatures are crucial for a selective detection of the toxic gases CO, H2S and SO2.

O 52.9 Wed 17:00 WIL B122

Synthesis, characterization and gas sensing applications of CuO nanowires — •Stephan Steinhauer[1], Elise Brunet[1], Christian Griessler[1], Marcus Milnera[1], Giorgio Mutinati[1], Anton Köck[1], Christian Edtmaier[2], Wolf-Dieter Schubert[2], Christian Gspan[3], and Gerald Kothleitner[3] — [1]Health & Environment Department, Nano Systems, AIT Austrian Institute of Technology GmbH, Vienna, Austria — [2]Institute of Chemical Technologies and Analytics, Vienna University of Technology, Vienna, Austria — [3]Institute for Electron Microscopy and Fine Structure Research, Graz University of Technology, and Centre for Electron Microscopy Graz, Graz, Austria

A powerful strategy to improve sensor performance of metal oxide based gas sensors is the implementation of single-crystalline nanowires as sensing elements due to the high surface to volume ratio. Thermal oxidation is a convenient solution for growth of single-crystalline cupric oxide (CuO) nanowires with high aspect ratios. SEM and TEM analysis showed different growth characteristics when varying the oxidation temperature, the oxygen concentration, the relative humidity and the substrate. Single-crystalline CuO nanowires with lengths between 0.5 micrometer and 40 micrometer and diameters from 20 nanometer to 120 nanometer have been fabricated. In particular, high-aspect ratio CuO nanowires have been employed as gas sensing elements and their sensitivity to carbon monoxide and hydrogen sulfide has been successfully demonstrated. For hydrogen sulfide, the nanowire gas sensor is even able to detect a concentration as low as 1 ppm.

O 53: Solid / liquid interfaces III

Time: Wednesday 15:00–16:45 Location: WIL C107

O 53.1 Wed 15:00 WIL C107

The adsorption and in situ characterization of viologen monolayers at copper/electrolyte interfaces. — •Emilia Sak[1], Ralf Troff[2], Christoph Schalley[2], and Klaus Wandelt[1] — [1]Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr.12, 53115 Bonn, Germany — [2]Institute Chemistry and Biochemistry, Free University of Berlin, Takustr.3, 14195 Berlin, Germany

Different redox-active 1,1'-Dibenzyl-4,4'-bipyridinium (or "viologen") molecules (DBV) adsorbed on a chloride - modified Cu(100) electrode have been studied by means of cyclic voltammetry (CV) and in-situ scanning tunneling microscopy (STM). At anodic potentials unsubstituted DBV forms a laterally well ordered quadratic array of dicationic "cavitand" ensembles which at negative potentials transformes into a stripe phase of π-stacked monocation radicals. Likewise with Dimethyl-DBV (DMDBV) a pair of redox peaks P1/P1' (-305 mV / -240 mV) is found which is accompanied by a transition form a "cavitand" to a dimer phase. Quite in contrast, Tetrametyl-DBV (TMDBV) does not show redox peaks in CV and, accordingly, only a "cavitand" phase. Also the adsorption kinetics of all three molecules is significantly different, it slows down with increasing methylation.

O 53.2 Wed 15:15 WIL C107

Adsorption of TMPy-porphyrin on iodine-modified Pt(100) electrodes — •Klaus Stallberg[1,2] and Winfried Daum[1,2] — [1]Institute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — [2]NTH School for Contacts in Nanosystems

The adsorption of free-base meso-tetra(N-methyl-4-pyridyl)porphyrin (TMPyP) cations on Pt(100)$(\sqrt{2} \times 5\sqrt{2})$I electrode surfaces in 0.1 M $HClO_4$ was studied in situ with STM and cyclic voltammetry (CV). To facilitate ordered porphyrin adsorption under electrochemical conditions, the Pt(100) surface was precovered with a monolayer of iodine. With a porphyrin surface coverage of 0.7 ML, ordered $(5\sqrt{2} \times 5\sqrt{2})$ superstructures were observed only on parts of the surface indicating a high mobility of the adsorbed molecules. Ordered porphyrin structures were preferentially detected on defect-free terraces but not at the line defects of specifically structured iodine adlayers [1]. The characterization of TMPyP adsorption by means of their pronounced redox current peaks in CV turned out to be complicated: CV experiments performed with porphyrin adlayers adsorbed under different experimental conditions suggest that initially adsorbed molecules may have a low 'redox activity' which increases in time. A possible relation of the increase of this activity with a protonation of TMPyP in acidic electrolytes will be discussed.

[1] B. Braunschweig et al., Surf. Sci. 603 (2009) 3361

O 53.3 Wed 15:30 WIL C107

Self-organized Porphyrin monolayers on iodine-modified noble metal surfaces — •Michael Schneider[1], Thomaz Kosmala[2], and Klaus Wandelt[1,2,3] — [1]Institut für Physikalische Chemie und Theoretische Chemie, University of Bonn, Wegelerstr. 12 D-53115, Bonn, Germany — [2]Institute of Experimental Physics, University of Wroclaw, Maxa Barna 9, 50-204, Wroclav, Poland — [3]Department of Physics, University of Rome Tor Vergata, Via Delle Ricerca Scientifica 1, 00133 Rome, Italy

In the field of template chemistry, new and interesting phenomena can be discovered at noble metal /electrolyte interfaces in the presence of anions and molecules as function of electrode potential. The spontaneous self-assembly of organic molecules is considered a promising *bottom-up* technique in nanotechnology to create surface patterns and electronic devices. Porphyrins, for example, are important organic compounds for potential applications in cancer therapy, or as catalysts and sensors. Halide-modified noble metal surfaces are suitable substrates due to their long range order. Moreover, iodide anion layers on Au(111)-surfaces show electrocompression and phase transitions depending on the electrode potential.

Our studies with in-situ STM and cyclic voltammetry not only reproduce previous works about Tetra(N-methyl-4-pyridyl)-porphyrin molecules (TMPyP) on iodide-modified gold and copper surfaces, but firstly reveal new TMPyP phases on gold not previously described, and secondly are extended to bimetallic Cu/Au surfaces providing new template properties.

O 53.4 Wed 15:45 WIL C107

Competing Phase Transition in Binary Viologen Layers on Cl/Cu(001) — •Martino Saracino[1], Nguyen Thi Minh Hai[2], Peter Broekmann[2], and Klaus Wandelt[1] — [1]Institute of Physical and Theoretical Chemistry, Bonn University, Wegelerstr. 12, D-53115 Bonn — [2]Interfacial Electrochemistry Group, Department of Chemistry and Biochemistry, Bern University, Freiestr. 3, CH-3012 Berne

In-situ STM and cyclic voltammetry are employed to analyze the competing adsorption of Diphenyl- (DPV) and Dibenzylviologen (DBV) on a chloride precovered Cu(001) surface. This model system for similar N-containing aromatic molecules is studied for the significant role of this type of organic and inorganic additives in metal plating processes. DPV^{2+} is reduced even at most anodic potentials to the monocationic radical DPV$^{+\bullet}$ and forms a full monolayer of a hydrophobic π-stacked stripe-phase, preventing the post-adsorption of the di-cationic DBV^{2+}. Lowering the concentration of DPV in solution till only a submonolayer coverage with mono-cationic π-stacked DPV$^{+\bullet}$ stripes is obtained permits the co-adsorption of the less stable di-cationic DBV^{2+} in its characteristic quadratic cavitand structure next to the DPV$^{+\bullet}$ stripe-phase. Lowering the electrode potential to the DBV^{2+} reduction potential at -250mV$_{RHE}$ leads first to a complete replacement of the more stable DPV$^{+\bullet}$ stripe-phase by a π-stacked stripe-phase of mono-cationic DBV$^{+\bullet}$. The resulting proximity of DBV$^{+\bullet}$ stripes and DBV^{2+} cavitands now permits the decay of the cavitand-phase starting at the domain boundaries to the mono-cationic DBV$^{+\bullet}$ stripe-phase, which finally fully covers the whole surface.

O 53.5 Wed 16:00 WIL C107

co-operative adsorption of TMA-alcohol mixture controlled by sonication time — •Nguyen Thi Ngoc Ha[1], Thiruvancheril G. Gopakumar[2], and Michael Hietschold[1] — [1]Solid Surfaces Analysis Group, Institute of Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Trimesic acid (TMA) dissolved in alcoholic solvents shows linear pattern of straight-chain aliphatic alcohols co-adsorbed with TMA on highly oriented pyrolytic graphite (HOPG). According to literature the detailed structure of these patterns depends on the number of carbon atoms in the alkyl chain of alcohols, the so called odd-even effect. In odd alcoholic solvents, dimer rows of TMA molecules are interacting with interdigitating alcohol molecules in a nearly perpendicular (86°) manner with respect to the direction of the TMA tapes, and the alkane chains of alcohols oriented orthogonally with respect to HOPG surface. However, in aliphatic alcohols with even number of carbon atoms dimer rows of TMA interact with alcohol molecules with an angle of 64° and alcoholic molecules adsorbed parallel on HOPG surface. By adjusting the sonication time of TMA-alcohol mixture, here we show that the geometry of adsorption pattern, packing density etc. of TMA and alcohol molecules can be controlled within one type of alcoholic solvent.

O 53.6 Wed 16:15 WIL C107

Quantitative studies of adsorbate diffusion and interactions at Cu(100)-electrolyte interfaces by in situ Video-STM — •Andriy Taranovskyy, Sophie Guézo, Yaw-Chia Yang, Hisayoshi Matsushima, Tunay Tansel, and Olaf Magnussen — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel, Germany

Quantitative data for adsorbate tracer diffusion and adsorbate-adsorbate interactions at solid-liquid interfaces were obtained from the analysis of high-speed in situ STM data [1,2]. Here we present a comparison of the results for lead, sulphur and methyl thiolate adsorbates on Cu(100) electrodes in 0.01 M HCl. Even though the mobility of these different adsorbate species can differ by one or two orders of magnitude, it exhibits a similar potential dependence, with the hopping rates increasing towards negative electrode potentials. This could be explained by the strong influence of the coadsorbate layer on the hopping process. Furthermore, the adsorbate-adsorbate interactions of sulphur and thiolate depend on the lattice direction, whereas those of lead are attractive for the nearest and next nearest sites, as expected for metal adatoms.

[1] T. Tansel, O.M. Magnussen, Phys. Rev. Lett. 96, 026101 (2006).
[2] A. Taranovskyy, T. Tansel, O.M. Magnussen, Phys. Rev. Lett. 104, 106101 (2010).

O 53.7 Wed 16:30 WIL C107

Adsorption of phthalocyanine molecules on an iodide modified cu(100) electrode studied by means of in-situ stm and ex-situ xps — •Thanh Hai Phan[1], Stephan Breuer[1], Uwe Hahn[2], Thomas Torres[2], and Klaus Wandelt[1,3,4] — [1]Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, D-53115 Bonn, Germany — [2]Departamento de Quimica Organica C-I-305, Universidad Autonoma de Madrid, Campus de Cantoblanco, 28049 Madrid, Spain — [3]Institute of Experimental Physics, University of Wroclaw, Maxa Borna 9, 50-204, Wroclaw, Poland — [4]Department of Physics, University of Rome Tor Vergata, Via Della Ricerca Scientifica 1, 00133 Rome, Italy

A combination of CV, in-situ STM and ex-situ XPS studies were performed to gain information about an iodide modified Cu(100) electrode surface exposed to an acidic electrolyte containing a redox-active phthalocyanine (abbreviated as [ZnPcPyMe]$^{+4}$). In the CV, four single electron transfer steps were observed, which lead to the formation of tri-, di-, and mono-cations, respectively. The XPS data reveal not only the strong adsorption of molecules, but also the replacement of the zinc atoms by hydrogens. The well-ordered self-assembled adlayer of metal-free phthalocyanine seen in STM forms a (quasi) square-shaped lattice (angle of 92 ± 2°, intermolecular distance of 19.5Å) which coincide neither with the iodide nor with the copper lattice underneath. A detailed molecular structure model is proposed in agreement with the experimentally observed pattern.

O 54: Particles and clusters I

Time: Wednesday 15:00–16:15 Location: WIL C307

O 54.1 Wed 15:00 WIL C307

Gold clusters at finite temperature: influence of fluxionality on ligand adsorption — •Luca M. Ghiringhelli, Elizabeth C. Beret, Jörg Meyer, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Metal clusters, in particular in relation with their catalytic properties, have been the object of intensive experimental and theoretical studies, in the recent years. A great deal of effort has been devoted by many theoretical groups to understanding the zero kelvin properties of such clusters. Here, by focusing on small gas phase Au$_N$ clusters ($3 \leq N \leq 20$) and their interaction with CO and O$_2$ as a showcase, we illustrate a methodology for the study of small clusters and their interaction with atoms and molecules at finite temperature. We combine all-electron density functional theory, including scf-density dependent van-der-Waals tail corrections, with finite temperature sampling techniques, like Biased MD and Parallel Tempered MD. We find an unusual flexibility of the clusters, at room and lower temperature. At certain sizes, Au_N clusters at room temperature are liquid droplets. This has an important implication, when accounting for the dynamics of ligand adsorption. One has to consider that the energy released by an exothermic ligand adsorption heats up the newly formed complex, and the equilibration with the environment is much longer than the typical timescale for conformational rearrangement. In this respect, the very concept of a preferred adsorption site in the bare cluster might be meaningless.

O 54.2 Wed 15:15 WIL C307

Small-Angle X-ray Scattering (SAXS) for metrological size determination of nanoparticles — •Gudrun Gleber[1], Michael Krumrey[1], Armin Hoell[2], Levent Cibik[1], Stefanie Marggraf[1], and Peter Müller[1] — [1]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin — [2]Helmholtz-Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin

To measure the size of nanoparticles, different measurement methods are available but their results are often not compatible. In the framework of an European metrology project we use Small-Angle X-ray Scattering (SAXS) to determine the size and size distribution of nanoparticles in aqueous solution, where the special challange is the traceability of the results.

The experiments were performed at the Four-Crystal Monochromator (FCM) beamline in the laboratory of Physikalisch-Technische Bundesanstalt (PTB) at BESSY II using the SAXS setup of the Helmholtz-Zentrum Berlin (HZB). We measured different particles made of PMMA and gold in a diameter range of 200 nm down to about 10 nm. The aspects of traceability can be classified in two parts: the first is the experimental part with the uncertainties of distances, angles, and wavelength, the second is the part of analysis, with the uncertainty of the choice of the model used for fitting the data. In this talk we want to show the degree of uncertainty, which we reached in this work yet.

O 54.3 Wed 15:30 WIL C307

Control of ultrafast photoinduced processes at graphene-supported metal clusters — •Kira Hinrichs, Mihai Vaida, and Thorsten Marco Bernhardt — Institute of Surface Chemistry and Catalysis, University of Ulm, Albert-Einstein-Allee 47, 89069 Ulm, Germany

A new experimental setup is presented which enables the control of the laser-induced photodissociation of molecules on graphene supported metal cluster nano-structures. Graphene is employed as a substrate providing a geometric template to obtain a regular array of clusters with equal size and distance for the investigation of field localization effects.

The temporal control of the processes at this system is archieved by photodissociation and detection of the adsorbed probe molecule methyl bromide via femtosecond laser pump-probe mass spectrometry with resonance enhanced multi-photon ionization.

For the additional spatial resolution the fate of the photodissociation products on the surface after the reaction is analyzed by scanning tunneling microscopy. The combination of methyl product mass spectrometry and local surface analysis opens new possibilities to optimize laser pulse shapes for enhanced photoreaction and selective field localization at the surface.

O 54.4 Wed 15:45 WIL C307

Reactive forcefield for simulating gold surfaces and nanoparticles — •Donato Fantauzzi, John Keith, Josef Anton, and Timo Jacob — Ulm University, Albert-Einstein-Allee 47, D-89069 Ulm, Germany

Due to its special physicochemical properties Gold has reached a wide range in modern-day applications, e.g. in electronics, nanotechnology, and catalysis. This has stimulated many experimental and theoretical studies in the past decades. Unfortunately, theoretical contributions on the QM level of theory are restricted by the computational expense, motivating the development of empirical atomistic interaction potentials to rapidly simulate atomic-level phenomena on larger-scale systems [1]. However, the parametrization of these (semi-)empirical potentials to specific physical data often limits their transferability.

In our work we report how to construct a ReaxFF (reactive forcefield) potential from first-principles for broad material applications. After comparing this reactive forcefield to other available forcefields reported in literature, we show that this potential is capable of reproducing qualitatively and quantitatively binding energies and diffusion barrier profiles for surface processes, as well as bulk equations of state. A strict transferability test on effective cohesive energies of molecular clusters indicated the capability to not only study bulk and single crystal surfaces, but also the morphology of Au nanoparticles [2].

[1] M. S. Daw, and M. I. Baskes, *Phys. Rev. Lett* **50**, 1285 (1983) [2] J. A. Keith, D. Fantauzzi, T. Jacob, A. C. T. van Duin, *Phys. Rev. B* **81**, 235404 (2010)

O 54.5 Wed 16:00 WIL C307

CO adsorption on neutral iridium clusters — •Christian Kerpal, Daniel Harding, Gerard Meijer, and André Fielicke — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin

The adsorption of carbon monoxide on neutral iridium clusters in the size range of $n = 3$ to 21 atoms is investigated with infrared multiple photon dissociation spectroscopy. The spectra are obtained by irradiating a molecular beam containing $\mathrm{Ir}_n\mathrm{CO}$ complexes with intense, tunable IR radiation from the Free Electron Laser for Infrared eXperiments (FELIX) and measuring the changes induced in the mass distribution. For each cluster size only a single ν(CO) band is present with frequencies in the range between 1962 cm^{-1} ($n = 8$) and 1985 cm^{-1} ($n = 18$) which can be attributed to an atop binding geometry. This behaviour is compared to the CO binding geometries on clusters of other group 9 and 10 transition metals as well as to that on extended surfaces. The preference of Ir for atop binding is rationalized by relativistic effects on the electronic structure of the later $5d$ metals.

O 55: Surface magnetism II (jointly with MA)

Time: Wednesday 15:00–16:45 Location: CHE 184

O 55.1 Wed 15:00 CHE 184

Hyrogen-induced Kondo effect for Co/Pt(111) — •Quentin Dubout, Fabian Calleja Mitja, Markus Etzkorn, Anne Lehnert, Laurent Claude, Pietro Gambardella, and Harald Brune — Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

We present 0.4 K Scanning Tunneling Spectroscopy (STS) results on hydrogenated Co adatoms on Pt(111). Molecular H dosage creates two Co-H adsorption complexes with comparable abundance. Type I displays very large (~40 %) inelastic conductance steps that originate from vibrations, as evidenced by their shift when substituting H by D. Type II displays smaller (~5 %) conductance steps at higher energies, again due to H vibrations, together with a large conductance peak at the Fermi level. This feature is attributed to the Kondo effect. Its splitting in magnetic fields up to 8 Tesla identifies the Co-H complex as a S = 1/2 system, whereas clean Co/Pt(111) has a spin of 1 and shows no Kondo effect. H-adsorption has been reported to quench the Kondo effect, here we show that it can produce it.

O 55.2 Wed 15:15 CHE 184

Magnetic and structural investigations of thin ferromagnetic CrSb layers on GaAs(110)/GaAs(001) — •Carsten Godde and Ulrich Köhler — Institut für Experimentalphysik IV / AG Oberflächen, Ruhr-Universität Bochum, Germany

In this contribution we present structural and magnetic measurements of thin CrSb layers on GaAs(110) and GaAs(001) surfaces. These systems are of great interest because of their possible use as spin aligner for spin injection in semiconductors. Thin CrSb layers up to 4 ML thickness grow in the metastable zinc blende structure on GaAs and keep ferromagnetic properties and structural stability up to high annealing temperatures which is interesting for enabling better crystalline quality. We investigate the growth of CrSb on the GaAs surfaces at different coverages and annealing temperatures by STM, LEED and

SQUID magnetometry. The CrSb films are co-deposited on the GaAs substrate by MBE at a deposition temperature of 250°C with a codeposition ratio of Cr and Sb: 1:6. On the GaAs(110) surface STM shows for a 3ML CrSb deposition a closed film of rectangular and rooflike islands elongated in $[1\bar{1}0]$-direction of substrate with increasing tendency towards a flat continuous morphology with height variations in the monolayer range after thermal processing at 300°C for 45min. These flat areas are characterized by a atomic fishbone row structure in $[1\bar{1}0]$-direction. SQUID magnetometry measurements show ferromagnetic characteristics of the thin CrSb layers with a magnetic moment per atom of $\approx 3\ \mu_B$.

O 55.3 Wed 15:30 CHE 184

Fe/GaAs(001) and MgO/Fe/GaAs(001) epitaxial systems: A spin- and angle-resolved photoemission study — •Daniel Gottlob[1,2], Lukasz Plucinski[1], Carsten Westphal[2], and Claus M. Schneider[1] — [1]Forschungszentrum Jülich GmbH — [2]Technische Universität Dortmund

Spintronics is an inportant field of current Solid State Research and memory units based on Magnetic Tunnel Junctions (MTJs) are now within reach. In MTJ's the nature of the electronic structure at the interface determines the spin-selectivity of the tunneling process, and thereby the magnetorestive potential of the MTJ.

Electronic interface states can influence the tunneling process in epitaxial MTJs especially for thinner tunnel barriers. The research that has been done at Beamline 5, DELTA, Dortmund in the context of a Diploma thesis focussed on the electronic structure of Fe/GaAs(001) and MgO/Fe/GaAs(001) and a surface/interface state of these systems. The samples have been prepared *in situ* by molecular beam epitaxy and characterized by LEED and Auger spectroscopy.

The electronic structure was probed in two different regions of the Brillouin zone, which have been chosen for reference (normal emission, Γ point) and the expectation of the surface state (21° off normal) that has been seen on Fe/W(001) in a previous study [1]. Measurements on the MgO capped iron sample have been conducted to confirm whether the surface state does transform into an interface state.

[1] L. Plucinski, Y. Zhao, C.M. Schneider, B. Sinkovic, and E. Vescovo; Phys. Rev. B 80, 184430 (2009)

O 55.4 Wed 15:45 CHE 184

Itinerant Nature of Atom-Magnetization Excitation by Inelastic Scanning Tunneling Spectroscopy — Alexander Khajetoorians[1], Samir Lounis[2], Bruno Chilian[1], Antonio Costa[3], Lihui Zhou[1], Douglas Mills[2], Sergej Schuwalow[4], Frank Lechermann[4], •Jens Wiebe[1], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, Hamburg University, Germany — [2]Department of Physics and Astronomy, University of California Irvine, USA — [3]Instituto de Física, Universidade Fedeal Fluminense, Niterói, Brazil — [4]I. Institute for Theoretical Physics, Hamburg University, Germany

We have performed single-atom magnetization curve (SAMC) measurements [1] and inelastic scanning tunneling spectroscopy (ISTS) on Fe atoms adsorbed on a semiconducting [2] and a metallic substrate [3]. ISTS reveals magnetization excitations whose lifetime strongly depends on the type of substrate. In the semiconducter case the lifetime is relatively long. In the metallic case the lifetime decreases upon application of a magnetic field and the SAMCs show a broad distribution of magnetic moments. The experimental observations are quantitatively explained by the decay of the magnetization excitation into Stoner modes of the itinerant electron system as shown by newly developed theoretical modeling [3].

[1] F. Meier *et al.*, Science **320**, 82 (2008).

[2] A. A. Khajetoorians *et al.*, Nature **467**, 1084 (2010).

[3] A. A. Khajetoorians *et al.*, arXiv:1010.1284v2.

O 55.5 Wed 16:00 CHE 184

Magnetism of ultrathin Fe layers on BaTiO$_3$(001) — •Remya Kunjuveettil Govind[1], Vasili Hari Babu[2], Federica Bondino[3], Marco Malvestuto[3], Martin Trautmann[1], Karl-Michael Schindler[1], and Reinhard Denecke[2] — [1]Institut fur Physik, Martin-Luther-Universität Halle-Wittenberg — [2]Wilhelm-Ostwald-Institut fur Physikalische und Theoretische Chemie, Universität Leipzig — [3]IOM CNR, Laboratorio Nazionale TASC, Area Science Park, Basovizza, Italy

Multiferroic systems are promising candidates for switching magnetization using voltages. Layered systems from ultrathin magnetic films on ferroelectric substrates are model systems. In this study ultrathin layers of Fe are deposited on a BaTiO$_3$(001) substrate and characterized by XPS, AES, NEAXFS and LEED. X-ray circular dichroism (XMCD) measurements in remanent magnetization show no magnetization for thicknesses up to 6 Å, in contrast to theoretical predictions [1]. From 8 to 28 Å, the XMCD spectra clearly show in-plane magnetization and the XMCD spectra look like bulk Fe. However, the dichroism is smaller and values for orbital and spin magnetic moments derived from a sum rule analysis are significantly smaller than bulk values. Possible reasons for this behavior, like partial oxidation of the Fe layer or non-uniform layer growth will be discussed.

[1] M. Fechner et al., Phys. Rev. B 78 (2008) 212406; M. Fechner et al., Phys. Stat. Sol. B 1 (2010) 8.

O 55.6 Wed 16:15 CHE 184

Quantum-well-states in a copper/cobalt/copper heterostructure — •Philipp Kloth[1], Martin Wenderoth[1], Henning Prüser[1], Alexander Weismann[2], and Rainer G. Ulbrich[1] — [1]IV. physikalisches Institut, Georg-August Universität Göttingen, 37077 Göttingen — [2]IEAP, Christian-Albrechts-Universität zu Kiel, 24098 Kiel

The morphological and electronic properties of a copper/cobalt/copper hetero-structure have been investigated by LEED, AES and STM/STS. We focus on the structural dependent electronic features, that could be observed for different preparation methods.

The samples are prepared and analyzed under UHV-conditions. Cobalt and copper films are deposited onto a (100)-copper single crystal by electron beam evaporation. The growth of both materials at room and LN2 temperature with a subsequent annealing step reveals different surface morphology. Furthermore a considerable diffusion between the interfaces takes place during the deposition process - even at low temperatures.

Due to the finite thickness of just a few monolayers the copper film on top of the sample exhibits the formation of quantum-well-states which can be identified by STS. The crossover to smoother hetero-structures by growing at low temperatures leads to a change in the energetic behaviour of those states. This is explained by the anisotropic electron propagation of copper [1]. This work is supported by the SFB 602 TP A3.

[1] A. Weismann et al., Science 323, 1190 (2009)

O 55.7 Wed 16:30 CHE 184

Observing the Spin of an Individual Mn$_{12}$ Molecule — •Steffen Kahle[1], Zhitao Deng[1], Charlène Tonnoir[1], Nicha Thontasen[1], Gordon Rinke[1], Nikola Malinowski[1], Alicia Forment Aliaga[1], Stephan Rauschenbach[1], Markus Ternes[1], and Klaus Kern[1,2] — [1]MPI for Solid State Research, Stuttgart — [2]EPFL, Lausanne, Switzerland

The Mn$_{12}$-acetate$_{16}$ molecule (Mn$_{12}$) is considered a prototypical single molecular magnet (SMM) because its high spin measured in bulk is commonly attributed as spin of the individual molecules [1]. To confirm this we want to measure the spin of an individual Mn$_{12}$ molecule.

We are able to gently deposit Mn$_{12}$ molecules on different metal substrates by electrospray ion beam deposition [2]. STM images show intact and individual addressable molecules, which can be resolved with submolecular resolution.

Low temperature (1K) scanning tunneling spectroscopy on top of the molecule adsorbed on bare metal is featureless near E_F. This changes when we decouple the molecule from the metal adding a BN layer on the substrate before deposition. We now observe symmetric inelastic tunneling features around E_F in the range of a few mV, which is ascribed to spin flip excitations. The excitation is delocalized evenly over the whole molecule supporting the giant-spin model.

This proofs the existence of a molecular spin, thus confirming the SMM nature of individual Mn$_{12}$ molecules on the surface.

[1] R. Sessoli *et. al.*, **Nature** 365, 141, (1993).

[2] N. Thontasen *et. al.*, **J. Phys. Chem. C** 114, 17768, (2010).

O 56: [DS] Progress in Micro- and Nanopatterning: Techniques and Applications III (Focused Session, jointly with O - Organisers: Graaf, Hartmann)

Time: Wednesday 15:00–17:00 Location: GER 38

O 56.1 Wed 15:00 GER 38

Femtosecond laser induced recrystallization and ablation of hydrogenated amorphous silicon films — •Babak Soleymanzadeh[1], Christian Strüber[1], Helmut Stiebig[1,2], and Walter Pfeiffer[1] — [1]Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — [2]Malibu GmbH & Co. KG, Böttcher Str. 7, 33609 Bielefeld, Germany

Ultrashort laser pulses offer new and fascinating possibilities in the field of laser material processing. Here we investigate the femtosecond laser induced recrystallization and ablation of hydrogenated amorphous silicon films (300 nm thickness) grown on glass substrates by large area (>1 m^2) plasma-enhanced chemical-vapor deposition. At laser fluences of <40 mJcm^{-2} (800 nm, <100 fs pulse duration) recrystallization of the amorphous silicon layer is observed in spatially resolved Raman micro-spectroscopy. The fluence dependence of this recrystallization indicates that a nonlinear excitation mechanism is responsible. At slightly higher fluences the amorphous silicon thin-film is ablated. Scanning electron microscopy and energy-dispersive X-ray spectroscopy (EDX) is applied to investigate the ablation process for various laser fluences. The prospect of using femtosecond laser induced material processing in silicon thin-film photovoltaics is discussed.

O 56.2 Wed 15:15 GER 38

Photothermal Laser Micro- and Nanoprocessing of Mesoporous Gold — •Lina Schade[1], Mareike Mathieu[1,2], Monika Biener[2], Juergen Biener[2], and Nils Hartmann[1] — [1]Fakultät für Chemie, NETZ, CeNIDE, Universität Duisburg-Essen, Universitätsstr. 5, 45141 Essen, Germany — [2]LLNL, Livermore, CA 94550, USA

In recent years, mesoporous gold has gained significant attention as a novel material in actuation, sensing and catalysis. The particular properties of this material result from its spongelike open-cell morphology with pore sizes of about 25 nm. Techniques which allow one to engineer mesoporous gold on a micro- and nanoscale, of course, are of high interest in view of fundamental studies and technical applications. Common annealing procedures, for example, provide a means to adjust the pore size in the range of 50 - 600 nm and investigate size dependent properties, such as the enhancement effect in surface enhanced Raman spectroscopy (SERS) [1]. Here we report on a photothermal laser technique for micro- and nanoprocessing of mesoporous gold [2]. A focused beam of a cw-laser with a wavelength of 532 nm and a 1/e spot size of 1.4 microns is used to locally anneal the substrate surface and fine tune the pore structure. This allows one to fabricate porous gradients on micrometer length scales. In addition, thiol-based self-assembled monolayers provide unique opportunities to functionalize these porous structures [2]. Prospects in SERS measurements and other applications are discussed.

[1] S.O Kucheyev, et al., Appl. Phys. Lett. 89 (2006) 053102.

[2] M. Mathieu, N. Hartmann, NJP, in press.

O 56.3 Wed 15:30 GER 38

Photothermal laser patterning of buried polymer interfaces — •Anja Schröter, Steffen Franzka, and Nils Hartmann — Fakultät für Chemie, CeNIDE and NETZ, Universität Duisburg-Essen, Universitätsstr. 5, 45141 Essen, Germany

Covalent attachment of polymer films provides a versatile means to taylor chemical and physical surface properties. Alternative to the approach of growing a polymer on a surface [1], here we report on a facile and flexible photothermal procedure for local grafting of thin polymer films to solid surfaces. Surface-oxidized silicon samples are coated with alkylsiloxane monolayers. After wet-chemical treatment in order to form azide-terminated monolayers a thin polymer film is spin-coated on top of the monolayer. Local irradiation with a focused beam of a diode-pumped solid-state laser at a wavelength of 532 nm thermally activates the azide groups at the buried polymer interface and leads to local covalent attachment of the polymer. Subsequently, polymer material, which is not coupled to the surface, is removed via sonication. The influence of incident laser power and irradiation time is investigated. At a 1/e focal spot diameter of 2.1 microns dots with diameters close to 1 micron can be fabricated. This procedure allows for rapid large-scale patterned attachment of a wide spectrum of polymers.

[1] M. Mathieu, A. Friebe, S. Franzka, M. Ulbricht, N. Hartmann, Langmuir 25 (2009) 12393.

O 56.4 Wed 15:45 GER 38

Photothermally induced chemical patterning of organic monolayers on oxide-free silicon substrates — •Martin Przyklenk[1], Benjamin Klingebiel[1], Luc Scheres[2], Han Zuilhof[2], and Nils Hartmann[1] — [1]Fakultät für Chemie, CeNIDE, NETZ, Universität Duisburg-Essen, Universitätsstr. 5, 45141 Essen — [2]Laboratory of Organic Chemistry, Wageningen University, Dreijenplein 8, 6703 HB Wageningen, The Netherlands

Patterned self-assembeld organic monolayers (SAMs) are widely used as templates to build up complex functional surface structures. A simple routine for nanopattering of organic monolayers down to 100 nm and below relies on photothermal processes [1,2]. In photothermal processing a focused laser beam is used to locally heat the substrate and initiate thermal decomposition of the monolayer. Here we use a simple photothermal procedure for direct chemical functionalization of organic monolayers [1]. Oxide-free silicon samples are coated with alkyl and alkenyl monolayers [2]. Through irradiation with a focused beam of an argon ion laser at a wavelength of 514 nm in gaseous bromine local bromination of the monolayer takes place. Mechanistic aspects and prospects of photothermal routines in micro- and nanofabrication of multifunctional organic monolayers are discussed.

[1] B. Klingebiel, A. Schröter, S. Franzka, N. Hartmann, ChemPhysChem 10 (2009) 2000.

[2] L. Scheres, B. Klingebiel, J. ter Maat, M. Giesbers, H. de Jong, N. Hartmann, H. Zuilhof, Small 6 (2010) 1918.

O 56.5 Wed 16:00 GER 38

Pattern transfer on large samples using a sub-aperture reactive ion beam — •André Miessler, Agnes Mill, Jürgen W. Gerlach, and Thomas Arnold — Leibniz-Institut für Oberflächenmodifizierung (IOM), Permoserstrasse 15, D-04318 Leipzig, Germany

In comparison to sole Ar ion beam sputtering Reactive Ion Beam Etching (RIBE) reveals the main advantage of increasing the selectivity for different kind of materials due to chemical contributions during the material removal. Therefore RIBE is qualified to be an excellent candidate for pattern transfer applications. The goal of the present study is to apply a sub-aperture reactive ion beam for pattern transfer on large fused silica samples. Concerning this matter, the etching behavior in the ion beam periphery plays a decisive role.

Using CF$_4$ as reactive gas, XPS measurements of the modified surface exposes impurities like Ni, Fe and Cr, which belongs to chemically eroded material of the plasma pot as well as an accumulation of carbon (up to 40 atomic percent) in the beam periphery, respectively. The substitution of CF$_4$ by NF$_3$ as reactive gas reveals a lot of benefits: more stable ion beam conditions in combination with a reduction of the beam size down to a diameter of 5 mm and a reduced amount of the Ni, Fe and Cr contaminations. However, a layer formation of silicon nitride handicaps the chemical contribution of the etching process. These negative side effects influence the transfer of trench structures on quartz by changing the selectivity due to altered chemical reaction of the modified resist layer. Concerning this we investigate the pattern transfer on large fused silica plates using NF$_3$-sub-aperture RIBE.

O 56.6 Wed 16:15 GER 38

Swift Heavy Ion Beam Shaping Of Sub-Micron Structures — •R. Ferhati[1], N. Guilliard[1], T. Weishaar[1], S. Amirthapandian[1], M. Fritschke[2], L. Bischoff[2], and W. Bolse[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart — [2]Forschungszentrum Dresden

Already in 1983 it was discovered, that swift heavy ion (SHI) irradiation of metallic glasses results in anisotropic deformation (shrinking along the beam direction expansion in perpendicular directions) [1]. We have employed this "hammering effect" to reshape sub-micrometer structures by SHI bombardment under proper variation of the beam incidence angle. Utilizing the focused ion beam (FIB) technique, a rectangular grid with varying lateral distances of 100 to 5000 nm was cut into a 100 nm thick NiO- resp. ZnO-film from their surfaces down to the oxidized Si-substrate, in order to produce small oxide "ashlars".

The samples were then irradiated under grazing incidence and continuous azimuthal target rotation with 1.4 GeV U- (NiO) and 0.95 GeV Au-ions (ZnO), respectively, in our new in-situ SEM at the UNILAC accelerator of GSI [2]. After certain fluence steps, the irradiation was stopped and one and the same spot was analyzed by means of SEM in order to investigate the evolution of the irradiated objects. Depending on their initial size complex structures (egg-, cone-, pillar-, forceps-, tooth-like) were formed, which can only be understood if besides the hammering effect deformation due to surface tension and yield stress are taken into account. [1] S. Klaumünzer, G. Schumacher, Phys. Rev. Lett. 51 (1983), [2] S. Amirthapandian, et al., Rev.Sci.Instr. 81, (2010)

O 56.7 Wed 16:30 GER 38

Surfactant driven self-organized surface patterns by ion beam erosion — •Hans Hofsäss and Kun Zhang — II. Physikalisches Institut, Universität Göttingen, 37077 Göttingen, Germany

Self-organized pattern formation on surfaces by ion beam erosion and driven by metal surfactant atoms is discussed. Si substrates were irradiated with 5 keV Xe ions at normal incidence and ion fluences up to 5x10^{17} Xe^+/cm^2 under continuous deposition of surfactant atoms. In the absence of surfactants uniform flat surfaces are obtained. With surfactants pronounced patterns like dots, combinations of dots and ripples as well as ripples with about 100 nm wavelength are generated. The surfactant coverage and deposition direction determine the pattern type and the pattern orientation, respectively. A critical steady-state coverage for onset of dot formation and onset of ripple formation is between about 10^{15} and 5x10^{15} atoms/cm^2. With increasing ion fluence the pattern contrast increases but the pattern type remains unchanged. The surface region consists of a thin amorphous metal silicide layer with high metal concentration in the ripple and dot regions. Pattern formation is explained by ion induced diffusion and phase separation of the initially flat amorphous silicide layer and subsequent ion beam erosion with composition dependent sputter yield. Directed deposition of metal surfactant causes preferential deposition and shadowing and determines the final pattern orientation and morphology. First results on the dynamic behaviour of the ripples are presented.

O 56.8 Wed 16:45 GER 38

Dynamics of surfactant induced ripple patterns on Si generated by ion beam erosion — •Kun Zhang, Hans Hofsäss, Hans-Gregor Gehrke, and Oliver Göpfert — II.Physikalisches Institut, Universität Göttingen, 37077 Göttingen, Germany

Some metallic surfactants induce pronounced dot and ripple patterns on Si substrates during normal and near normal ion incidence sputter erosion. In the absence of metal co-deposition uniform flat surfaces are obtained. It is known that surface ripples generated by ion beam erosion at glancing ion incidence propagate across the surface. In this work we investigate the propagation of ripple patterns triggered by surfactant atoms and a possible correlation between ripple propagation and directed deposition of surfactant atoms. Si substrates were irradiated with 5 keV Xe ions at normal ion incidence under continuous deposition of Fe or Mo surfactant atoms. With surfactants pronounced patterns like dots, combinations of dots and ripples as well as ripples with about 100 nm wavelength and up to 12 nm in height are generated. The dynamics of patterns, in particular the propagation of ripples across the surface with increasing ion fluence was investigated using sequential ion irradiation and scanning electron microscopy analysis. Specific regions on the irradiated samples were identified using thin marker grooves prepared by focused ion beam milling. Using pattern recognition methods we are able to determine the fluence dependent shift of the ripple patterns with respect to the marker grooves. We find dynamic patterns with a propagation velocity of about 0.7 nm per 10^{15} ions/cm^2. A qualitative model for the ripple propagation is presented.

O 57: Nanotribology

Time: Wednesday 16:30–17:00 Location: WIL C307

O 57.1 Wed 16:30 WIL C307

Driven colloidal monolayers on periodic and quasiperiodic substrate potentials as model systems for nanotribology — •Thomas Bohlein, Jules Mikhael, and Clemens Bechinger — 2. Physikalisches Institut, Universität Stuttgart, Germany

Tribology - the science of interacting surfaces in relative motion - is of great importance for all technical applications where moving bodies are in contact. Experimental tools such as the friction force microscope enable the investigation of frictional processes at atomic scales. Here we present a study which allows to probe friction on the micrometer range. We experimentally study the sliding behavior of a two dimensional colloidal crystal interacting with periodic and quasiperiodic light induced substrate potentials created by overlapping several laser beams. Translations of the sample cell correspond to applying a lateral force on the crystal in any desired direction. The crystal's response is then studied in real space by digital video microscopy. We observe high friction for periodic commensurate systems, whereas for periodic incommensurate and quasiperiodic systems the static friction force almost vanishes, giving rise to superlubric sliding states. In a final step, we examine the effect of phononic and phasonic excitations of the quasiperiodic substrate potential on the sliding friction.

O 57.2 Wed 16:45 WIL C307

Frictional duality of metallic nanoparticles: Influence of particle morphology, orientation, and air exposure — •Dirk Dietzel[1], Michael Feldmann[1], Udo D. Schwarz[2], Ivan Stich[3], Jan Brndiar[3], and Andre Schirmeisen[1] — [1]Institute of Physics and Center for Nanotechnology, University of Muenster — [2]Department of Mech. Engineering, Yale University, New Haven, USA — [3]Institute of Physics, Slovak Academy of Sciences,Bratislava

The contact area dependence of the interfacial friction experienced during the translation of Sb nanoparticles deposited on a graphite substrate is studied under different conditions using the tip of an atomic force microscope as manipulation tool. In vacuum a dual behavior of the friction-area curves is found, characterized by the observation that some particles exhibit friction below the detection limit while other similarly sized particles showed constant shear stress. Detailed investigations prove the reproducibility of this effect, revealing that neither the particle's morphology nor their alignment relative to the substrate lattice influence the findings [1]. In contrast, we observe that temporary exposure to ambient air can lead to a drastic increase in the particle's friction. This finding highlights the strong effect of interface contamination, which is also considered the reason for the frictional duality observed in UHV. To further elucidate the contamination mechanisms, simulations by DFT modelling have been performed for different kinds of conceivable contaminants. These simulations help to get a grasp on the degree and nature of the interface contamination affecting the experiments. [1] Dietzel et al. Phys. Rev. B. 82, 035401 (2010)

O 58: [DS] Plasmonics and Nanophotonics (jointly with HL and O)

Time: Wednesday 17:15–19:15 Location: GER 38

O 58.1 Wed 17:15 GER 38

Simulation of second harmonic generation from split ring resonators with the Discontinuous Galerkin Time Domain method — •Yevgen Grynko, Torsten Meier, and Jens Förstner — Universität Paderborn, Warburger Str. 100, 33098 Paderborn

We report our results of the application of the Discontinuous Galerkin Time Domain (DGTD) method [1] for the simulation of the linear and non-linear response of plasmonic nanostructures. We use DGTD as it has a number of attractive features including adaptive grid refinement and nonlinear stability. In this work, we consider an array of U-shaped split ring resonators. Metallic dispersion is described with a current density equation based on the representation of electron dynamics in terms of electron plasma. It includes linear Drude terms and nonlinear terms for the Lorentz force and convective acceleration of the electron flow. The nonlinear part of the equation causes the doubling of the transmitted frequency leading to the the SH peak in the spectrum. Switching between the terms shows that the "convective" term plays the main role in the observed phenomena. The strength of the the SH peak is comparable to the values reported previously in the experiments [2] and FDTD simulations [3].

[1] J. S. Hesthaven, T. Warburton, 2002, J. Comp. Phys., 181, 186-221. [2] M. W. Klein, et al., 2007, Opt. Express, 15, 5238. [3] Y. Zeng, et al., 2009, Phys. Rev. B 79, 235109-1 - 235109-9.

O 58.2 Wed 17:30 GER 38

Analysis of optimization techniques for coherent optical control in nanostructures — •Tobias Fankhänel, Torsten Meier, and Jens Förstner — University of Paderborn, Department of Physics and CeOPP, Warburger Str. 100, D-33098 Paderborn, Germany

We compare the efficiency of optimization approaches for shaping coherent optical control in nanostructures. The optical response of various structures is calculated using the Finite-Difference Time-Domain (FDTD, [1]) method. Standard optimization algorithms (L-BFGS gradient method [2], genetic algorithm [3]) are used to maximize target function like the flux transmission or spatio-temporal response; the algorithms' convergence time and computational effort is analyzed.

[1] A. Taflove, S. C. Hagness. Computational electrodynamics: the finite-difference time-domain method, third edition (Artech House Inc., Norwood 2005)

[2] J. Nocedal. Updating Quasi-Newton Matrices with Limited Storage (1980), Mathematics of Computation 35, pp. 773-782.

[3] GALib, http://lancet.mit.edu/ga/

O 58.3 Wed 17:45 GER 38

Two state lasing from a quantum dot laser — •Diana Khabipova, Kathy Lüdge, Niels Majer, and Eckehard Schöll — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We investigate the emission properties of a quantum dot (QD) laser with two confined electron and two hole levels, respectively. Our microscopically based rate equation model for quantum dot lasers [1] is extended by including the first excited state of the QDs as a second lasing state besides the ground state. The model treats separately the dynamics of QD electrons and holes, photon densities of the ground and excited state lasing, respectively, and the electron and hole densities in the 2D wetting layer as carrier reservoir. The carrier-carrier scattering rates include the direct capture from the wetting layer into the ground and excited state as well as relaxation processes from excited to ground state. The influence of the energy differences between the excited state, ground state, and wetting layer on the turn-on dynamics is investigated. We analyse also the effect of the excited state upon the relaxation oscillations, their turn-on delay and damping rate. Furthermore we study the excited state dynamics under thermal heating conditions and for different device dimensions.

[1] K. Lüdge, R. Aust, G. Fiol, M. Stubenrauch, D. Arsenijevic, D. Bimberg, and E. Schöll, IEEE J.Quantum Electron. 46, 12, 1755 (2010).

O 58.4 Wed 18:00 GER 38

Analytical approach to modulation properties of quantum dot lasers — •Kathy Lüdge[1], Evgeny Viktorov[2], Thomas Erneux[2], and Eckehard Schöll[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Universite Libre de Bruxelles, Optique Nonlineaire Theorique, Campus Plaine, C.P. 231, 1050 Bruxelles, Belgium

We analyze a microscopically based rate equation model for quantum dot lasers. The model separately treats the dynamics of electrons and holes, and the carrier-carrier scattering rates depend nonlinearly on the wetting layer carrier densities [1]. Our objective is to determine analytical expressions for the relaxation oscillation frequency and damping rate. To this end, we consider the Class B limit of the five rate equations and apply asymptotic techniques. We consider two cases corresponding to either equivalent or drastically different decay rates for the electrons and holes. We show how they contribute to increase the relaxation oscillation damping rate compared to the damping rate of the conventional laser and that there exist optimal conditions on the control parameters in order to observe maximum damping.

[1] K. Lüdge, E. Schöll, IEEE J.Quantum Electron. 45, 1396 (2009).

O 58.5 Wed 18:15 GER 38

Periodic Nanostructures: Spatial dispersion mimics chirality — •Bruno Gompf[1], Julia Braun[1], Thomas Weiss[1], Harald Giessen[1], Martin Dressel[1], and Uwe Hübner[2] — [1]Physikalisches Institut and Research Center SCOPE, Universität Stuttgart — [2]Institut für Photonische Technologien, Jena

The underlying idea of metamaterials is that it should be possible to construct artificial materials with completely new effective dielectric properties from nanometer-sized photonic atoms. One of these new fascinating properties is, for example, the recently achieved optical activity in photonic metamaterials. In our work we demonstrate that even a simple isotropic metal-dielectric nanostructure, i.e., a subwavelength hole array on a square lattice in a semitransparent Au film, rotates the polarization state at oblique incidence, but this behaviour cannot be explained by effective optical parameters. The structure was characterized by Mueller matrix spectroscopic ellipsometry at various angles of incidence and azimuthal orientations in the energy range of 0.73 to 4.6 eV. For the additional theoretical simulations, we employed a Fourier modal approach. To visualize the theoretical and experimental results, we plot the matrix elements in polar coordinates. Already from a brief look at the off-diagonal elements, it becomes obvious that the hole array mixes different incoming polarization states upon reflection in a complex way, which can not be explained by purely dielectric optical constants. It can be shown that for our square array even a bi-anisotropic model must fail. Rather spatial dispersion has to be taken into account.

O 58.6 Wed 18:30 GER 38

New transparent conductive metal based on polymer composite — •mehdi keshavarz hedayati[1], mohammad jamali[1], thomas strunkus[2], vladimir zaporochentko[2], franz faupel[2], and mady elbahri[1,3] — [1]Nanochemistry and Nanoengineering, Institute for Materials Science, Faculty of engineering, Christian-Albrechts-University of Kiel — [2]Multicomponent Materials, Institute for Materials Science, Faculty of engineering, Christian-Albrechts-University of Kiel — [3]Helmholtz-Zentrum Geesthacht GmbH, Institute of Polymer Research, Nanochemistry and Nanoengineering

Currently great efforts are made to develop new kind of transparent conductors (TCs) to replace ITO. In this regard different materials and composites have been proposed and studied including conductive polymers, carbon nanotubes (CNTs), metal grids, and random networks of metallic nanowires. But so far none of them could be used as a replacing material, since either they are either fragile and brittle or their electrical conductivity is below the typical ITO. Thin metallic films due to their high electrical conductivity could be one of the best replacing materials for ITO, however their poor transparency makes their application as TCs limited. Here we design and fabricate a new polymeric composite coating which enhances the transparency of the thin metal film up to 100% relative to the initial value while having a high electrical conductivity of typical metals. Therefore our proposed device has a great potential to be used as new transparent conductor.

O 58.7 Wed 18:45 GER 38

A self-assembly route to mesoporous Bragg reflectors — •Stefan Guldin[1], Matthias Kolle[1], Morgan Stefik[3], Richard Langford[1], Dominik Eder[2], Ulrich Wiesner[3], and Ullrich Steiner[1] — [1]Physics Department, Cavendish Laboratory, University of Cambridge, UK — [2]Materials Science Department, University of Cambridge, UK — [3]Materials Science Department, Cornell University, Ithaca, NY, USA

Mesoporous distributed Bragg reflectors (MDBRs) consist of a periodic lattice of alternating high and low refractive index, while exhibiting porosity on the sub-optical length scale. MDBRs have great potential as sensing materials in biology and chemistry, as adsorption and desorption of gas phase molecules lead to reversible changes in the refractive index of the stack. Optoelectronics is another promising field of applications. MDBRs can be used as light harvesting element in excitonic solar cells. When infiltrated with light emitting polymers, MDBRs have exhibited distributed feedback lasing.

We present a new route for the fabrication of MDBRs which relies on the self-assembling properties of the block copolymer PI-*b*-PEO in combination with sol-gel chemistry to finely tune porosity and pore size in the resulting inorganic material. Stacking-up multiple layers of alternating refractive index results in a fast and reliable assembly of a continuous network with well defined interfaces. The outcome are MDBRs of high quality optical properties even when built from a single material, in our case TiO_2.

O 58.8 Wed 19:00 GER 38

Launching Surface Plasmons by Carbon Nanotube Photoluminescence — •Nicolai Hartmann[1], Johann Berthelot[2], Alexandre Bouhelier[2], and Achim Hartschuh[1] — [1]Department Chemie and CeNS, Ludwig-Maximilians-Universität München, Germany — [2]Département Nanosciences, Laboratoire Interdisciplinaire Carnot Bourgogne, Université de Bourgogne, Dijon, France

We report on the excitation of propagating surface plasmons in metal films and waveguides via photoluminescence emission from semiconducting single-walled carbon nanotubes. Upon excitation in the visible regime a single carbon nanotube acts as a directive near-infrared point dipole source for surface plasmons propagating along the direction of the nanotube axis. To investigate this behaviour we used leakage radiation microscopy [1,2]. The excitation of propagating surface plasmons manifests itself by a narrow emission of leakage radiation in Fourier space appearing at angles according to the surface plasmon resonance. In real space we observe the exponential decay of the intensity along the propagation direction of the plasmon. Propagation lengths between 11 and 13 μm could be extracted and supported by calculations, depending on the thickness of the dielectric spacer layer separating carbon nanotubes and metal film. Combining surface plasmon coupling with electroluminescence from carbon nanotubes [3] opens up the possibility to create an electrically driven plasmon source.

[1] B. Hecht, et.al., Phys. rev. Lett. 77, 1889 (1996) [2] M. Böhmler, et.al., Opt. Express 18, 16443 (2010) [3] P. Avouris, et.al., Nat. Photonics 2, 341 (2008)

O 59: Poster Session III (Nanotribology; Polymeric biomolecular films; Organic electronics and photovoltaics, Covalent networks on surfaces; Phase transitions; Particles and clusters; Transparent conductive oxides)

Time: Wednesday 17:30–21:00 Location: P3

O 59.1 Wed 17:30 P3

Nanoscale hotspot formation in an energetic material during friction — Alexander Kovalev and •Heinz Sturm — BAM - Federal Inst. Mat. Res. Testing, FG "Scanning Probe Microscopy, Tribology and Wear Protection", 12200 Berlin

The chemical-mechanical decomposition of energetic materials is not fully understood, and the initial decomposition steps are not firmly established yet. The nanoscale formation of the hot-spot on 2,4,6-trinitrophenol (TNP) single crystal has been studied using atomic force microscopy (AFM). Indentation and plowing AFM techniques were used for destructive modification of TNP crystal surface. Microcrystals of TNP were grown on a gold substrate by fast evaporation from aqueous saturated solution. During friction we observed features of TNP crystal at the nanoscale which are difficult to explain from the macroscopic point of view of explosion. Occasionally, the hotspot has occurred spontaneously during the scanning process. According to the accepted knowledge of chemical reaction/decomposition of energetic materials the main decomposed substances are gases CO2 and NO2. But, in our experiments, agglomerated solid particles have been occurred on a surface of TNP crystal. It is known that TNP has two polymorph structures. Additionally, partially decomposed TNP may have still a phenyl ring, so pi- pi-complexes may be formed. However, we observed that friction at the nanoscale does not stimulate spontaneous decomposition. The observed behaviours of energetic materials at the nanoscale need further elucidation.

O 59.2 Wed 17:30 P3

Transition from Static to Kinetic Friction of Nanoparticles — •Michael Feldmann[1], Dirk Dietzel[1], Udo D. Schwarz[2], and André Schirmeisen[1] — [1]Institute of Physics and Center for Nanotechnology, University of Münster, Germany — [2]Department of Mechanical Engineering, Yale University, New Haven, USA

On macroscopic scales a phenomenological difference between static and sliding friction forces is routinely observed for contacts between solid surfaces. But does this hold true for nanoscopic contacts as well? We investigated this fundamental question through manipulation of thermally evaporated antimony nanoparticles over atomically flat HOPG substrates with the tip of a friction force microscope (FFM) [1]. In contrast to direct measurements with the FFM tip the manipulation of nanoparticles has important advantages of providing very well defined contact areas as well as enabling the precise measurement of static friction. A novel approach to nanoparticle manipulation, called 'tip-on-top' technique, allowed us to vary the lateral forces exerted on individually chosen particles in very small increments. This was achieved by scanning the FFM tip on top of the particle while slowly increasing the applied normal force. The results clearly show a transition between frictional states, corresponding to static and sliding friction. Interestingly, we observe a hysteresis when switching from the static friction to the sliding friction regime and back. We found that the ratio between the static and kinetic friction forces for individual particles is 1/2 independent of their size, in agreement with theoretical predictions. [1] Dietzel et al., Appl. Phys. Lett. 95, 53104 (2009)

O 59.3 Wed 17:30 P3

Simulations of friction force microscopy on KBr(001) based on ab-initio forces — •Christine Wieferink, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, WWU Münster

We report on ab-initio based simulations of friction force microscopy on the KBr(001) surface at zero and nonzero temperature. To simulate sliding friction we employ an extended three-dimensional Prandtl-Tomlinson model. The microscopic part of the tip is modeled by K^+ and Br^- terminated tips. We use a tip-surface interaction potential, which is calculated within the local-density approximation of density-functional theory and supplemented by long-range van der Waals interaction resulting from the macroscopic part of the tip. The loading force acting on the tip enters the equation of motion separately from all other forces so that it can be changed at will. We find smaller sliding friction for the K^+ compared to the Br^- tip. Especially we observe a very low sliding friction for the K^+ tip at loading forces up to 1.5 nN.

O 59.4 Wed 17:30 P3

Wear experiments on the nanoscale — •Johannes Sondhauss[1,2] and André Schirmeisen[1,2] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Center for Nanotechnology (CeNTech), University of Münster, Münster, Germany

The basic mechanisms of wear at the nanoscale are of large interest, e.g., for the lifetime limitations of moving mechanical components in MEMS. So far it was not possible to derive macroscopic wear behavior from fundamental processes on small scales. The atomic force microscope (AFM) has been recently proved useful to model a single sliding asperity in order to study wear processes on the atomic scale [1]. It was found that nanoscale wear is dominated by an atom-by-atom loss process which can be modeled by a thermally activated bond breaking process. In this work we performed several wear experiments using different Si-tips sliding for distances from a few hundreds of μm to about 2m on a silicon oxide surface. We varied the applied normal load and performed measurements under ambient conditions and in UHV. The change of the tip radius due to wear was determined from the adhesion force at different sliding distances. As a further channel we simultaneously measured the friction force acting between tip and sample. Our results seem to agree with the model, that frictional stresses lower the barrier for breaking an atomic bond and thus are jointly responsible for the observed characteristic wear rates at the nanoscale.

[1] Gotsmann and Lantz, Phys. Rev. Lett. 101, 125501 (2008)

O 59.5 Wed 17:30 P3

Wear measurement by friction force and dynamic force microscopy — Özhan Ünverdi[1], •Tobias Meier[1], Jan-Erik Schmutz[2,3], and Hendrik Hölscher[1] — [1]Institute for Microstructure Technology (IMT), Karlsruhe Institute of Technology, P.O. box 3640, 76021 Karlsruhe, Germany — [2]Center for Nanotechnology (CeNTech), Heisenbergstr. 11, 48149 Münster, Germany — [3]Physikalisches Institutm Westfälische Wilhelms Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

For measuring nano-scale wear, we introduce a new technique using friction force and dynamic force microscopy. As the cantilever resonance frequency depends on mass of the tip, we can measure the increase or decrease of the tip's worn mass down to some picograms due to the resonance frequency shift of the cantilever. By attaching a small sphere to the upper end of the cantilever's tip we can detect the nano-wear of several material combinations with this approach.

O 59.6 Wed 17:30 P3

Self-assembly of pyridine-substituted alkanehiols on gold — •Hicham Hamoudi[1], Katrin Döring[2], Heinrich Lang[2], and Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany — [2]Lehrstuhl für Anorganische Chemie, Technische Universität Chemnitz, Straße der Nationen 62, 09111 Chemnitz, Germany

High-resolution X-ray photoelectron spectroscopy, near-edge X-ray absorption fine structure spectroscopy, and infrared reflection absorption spectroscopy were used to study the properties of SAMs of aminomethyl-di(2-pyridyl)-11-mercaptoundecanamide (C10AP1), 4-(aminomethyl)pyridine-11-mercaptoundecanamide (C10AP2), and 2-(aminomethyl)pyridine-11-mercaptoundecanamide (C10AP3) prepared on Au(111) substrates. Whereas all molecules formed well-defined SAMs, their structural and electronic properties were found to be noticeably different depending on (i) either ortho- or para-attachment of the terminal pyridine moiety to the molecular chain and (ii) the number of the pyridine units in the tail group. The highest order was found in the C10AP3 SAM where the alignment of the SAM constituents seemed to be additionally strengthened by intramolecular interaction. Further, the branching of the characteristic pre-edge absorption resonances in the C K-edge spectra of the SAMs is distinctly different for the cases of the ortho- or para-attachment of pyridine, which could be explained by the different coupling of the electronic and vibrational excitations in both cases.

O 59.7 Wed 17:30 P3

On the surface tension of ionic liquids — •Claudia Kolbeck[1], Julia Lehmann[3], Kevin R. J. Lovelock[4], Till Cremer[1], Natalia Paape[2], Peter Wasserscheid[2], Andreas P. Fröba[3], Florian Maier[1], and Hans-Peter Steinrück[1] — [1]LS Physikalische Chemie II, FAU Erlangen, D — [2]LS Chemische Reaktionstechnik, FAU Erlangen, D — [3]SAOT, FAU Erlangen, D — [4]School of Chemistry, University of Nottingham, UK

The interface between ionic liquids (ILs) and gases plays a vital role in many applications such as gas separation and heterogeneous catalysis. An understanding of the surface properties of ILs is thus essential for developing new and commercially favourable systems for industrial applications. To probe the influence of the cation and anion on the surface tension of ILs nine $[\mathrm{Tf_2N}]^-$-based and twelve $[\mathrm{C_8C_1Im}]^+$-based ILs were measured with the pendant drop method. When increasing the alkyl chain length in the $[\mathrm{C}_n\mathrm{C_1Im}][\mathrm{Tf_2N}]$ series (n = 1, 2, 4, 6, 8, 10, 12), an initial decrease in surface tension is observed whereas for alkyl chain lengths greater than n = 8 the surface tension reaches a plateau. Functionalizing the alkyl chains with ethylene glycol groups results in a higher surface tension. For the dependence of surface tension on the chemical nature of the anion, relations are only found for subgroups of the studied ILs. Surface tension values are discussed with respect to intermolecular interactions and surface composition as determined by angle resolved X-ray photoelectron spectroscopy. - Supported by the DFG through SPP 1191 and by the Cluster of Excellence - Engineering of Advanced Materials.

O 59.8 Wed 17:30 P3

Azobenzene thin film growth on surfaces of layered materials — Eric Ludwig[1], •Torben Johannsen[1], Thomas Strunskus[2], Alexei Nefedov[3], Christof Wöll[3], Lutz Kipp[1], and Kai Rossnagel[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel — [2]Institut für Materialwissenschaft, Universität Kiel, D-24098 Kiel — [3]Institut für Funktionelle Grenzflächen, Karlsruher Institut für Technologie, D-76344 Eggenstein-Leopoldshafen

NEXAFS and ultraviolet photoelectron spectroscopy have been used to determine the layer growth and structural properties of azobenzene adsorbed on layered compounds. We used metallic $\mathrm{TiTe_2}$ and semiconducting $\mathrm{HfS_2}$ as substrates to elucidate the influence of different electronic structures. Due to weak van der Waals-like coupling between the layers both materials serve as excellent substrates for the analysis of adsorbed photoswitches and their possible switching behavior. NEXAFS measurements were performed at BESSY (beamline HE-SGM). UPS measurements were done with a He gas-discharge lamp ($h\nu = 21.22$ eV) and a hemisperical photoelectron analyzer.

Results indicate different growth modes on semiconducting and metallic substrates. Partial reversible photoswitching of the multilayer system was observed on the semiconducting substrate. On the metallic substrate no switching was observed, presumably due to stronger absorbate-substrate interactions. This work was supported by the DFG through SFB 677.

O 59.9 Wed 17:30 P3

Combined study of interface and device properties of a solid state dye sensitized solar cell — •Julia Maibach, René Hock, Thomas Mayer, and Wolfram Jaegermann — Technische Universität Darmstadt, Department of Material Science, Surface Science Devision, Petersenstr. 32, 64287 Darmstadt

We present the combined photoelectron spectroscopic and photoelectric characterization of a solid state dye sensitized solar cell (SDSC). The aim of this study is the development of a model system that allows a direct correlation of PES determined interface properties to global IV-measurements of the complete optoelectronic device.

The samples consist of a nanoporous $\mathrm{TiO_2}$ layer on FTO, which was sensitized with a metal free organic dye developed by BASF. As a hole transport material spiro-OMeTAD doped with the organic salt Li-TFSI was used. Both the dye and the hole conductor were applied via drop coating at normal pressure under clean Ar atmosphere within a glass cell integrated to the UHV system. The $\mathrm{TiO_2}$/dye and the $\mathrm{TiO_2}$/dye/spiro-OMeTAD interfaces were characterized using synchrotron induced photoelectron spectroscopy (SXPS) at BESSY. From these measurements the band diagram of the energy converting interface is derived which shows that driving forces for the relevant charge transfer processes are given in the investigated $\mathrm{TiO_2}$/dye/spiro-OMeTAD system. To perform the IV-measurements a gold contact was sputtered on top of the hole conductor of the SXPS-sample. Despite the unusual preparation for a SDSC the resulting solar cell shows a photo current density of 0,72 mA/cm^2 under AM1,5 illumination.

O 59.10 Wed 17:30 P3

Multi-plasmon enhancement of thin film organic solar cells — •Adam Williamson[1], Erich Runge[1], Eadaoin McClean[2], and Dominic Zerulla[2] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]University College Dublin, Belfield, Dublin 4, Ireland

A theoretical, two-dimensional (2D), periodic nano-structured design for thin film organic solar cells is presented. In this design the superposition of two periodic silver plasmonic gratings is seen to strongly increase the absorptive dissipation around two selectable wavelengths in the sub bandgap region. Finite-difference time domain (FDTD) calculations were found to be comparable to analytical predictions of the plasmon dispersion relation for the system which were calculated with an averaged dielectric permittivity. A method for tuning the strength of the generated plasmons is demonstrated by controlling the ratio of silver to active material within the grating layer. Profile cross-sections illustrate areas of the active layer exhibiting an increase of 40 times the absorptive dissipation compared to a non-grating cell structure. The areas of strongest increase in absorptive dissipation are visible next to the cell exit interfaces, as desired for a reduction in recombination losses.

O 59.11 Wed 17:30 P3

Adsorption Calorimetry of Conjugated Organic Molecules on Metal Surfaces — •Ole Lytken, Hans-Jörg Drescher, Fabian Bebensee, Hans-Peter Steinrück, and J. Michael Gottfried — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II

Traditional experimental methods for determining adsorption energies, such as temperature programmed desorption (TPD) and equilibrium adsorption isotherms, rely on desorption. However, on many metal surfaces large conjugated organic molecules, such as PTCDA and pentacene, decompose at elevated temperatures before or simultaneously with desorption. Discussions about relative bond strengths are, therefore, typically based on indirect arguments, such as the height of the adsorbed species above the surface as measured with normal incidence X-ray standing waves (NIXSW) or chemical shifts in spectroscopic techniques such as X-ray photoelectron spectroscopy (XPS). Unlike the more traditional methods, nanojoule adsorption calorimetry does not require desorption of the molecules; instead, the heat of adsorption is measured directly as an adsorption-induced temperature change of the sample. We will describe the construction of such a calorimeter at the Universität Erlangen-Nürnberg. Support from the Alexander von Humboldt Foundation is gratefully acknowledged.

O 59.12 Wed 17:30 P3

Preparation and spectroscopic study of self-assembled monolayers of a functionalized perylene dye on SiO_2 — •Deb Kumar Bhowmick[1], Nabi Aghdassi[1], Steffen Linden[1], André Devaux[2], Luisa De Cola[2], and Helmut Zacharias[1] — [1]Westfälische-Wilhelms Universität, Physikalisches Institut, Wilhelm-Klemm Straße 10, 48149 Münster, Germany — [2]Westfälische Wilhelms-Universität, Physikalisches Institut, Mendelstrasse 7, 48149 Münster, Germany

Polyaromatic hydrocarbons (PAHs) are the focus of our attention because of their characteristically high fluorescence quantum yield, their sensitivity properties of their local environment and ability to accesses a wide range of photophysical and electrochemical properties. A perylene derivative, N-benzyl perylene-3,4:9,10-tetracarboxylic-3,4-anhydride-9,10-imide was synthesized. A self-assembled monolayer of this dye was prepared on the aminopropyl triethoxy silane (linker molecule) modified quartz (SiO_2) surface by an imide bond between the NH_2 group of the linker molecule and the acid anhydride group of the dye. The covalent attachment on the surface was verified by X-ray photo emission spectroscopy and FT-IR spectroscopy. UV absorption and steady-state fluorescence were measured both in the adsorbate and in the solution phase of the dye. Characteristic differences in both phases of the UV absorption, fluorescence spectrum and fluorescence lifetime are observed and will be discussed.

O 59.13 Wed 17:30 P3

Coherent phonons: an ultrafast probe of the VO_2 **phase transition** — •Laura Foglia[1], Simon Wall[1], Daniel Wegkamp[1], Joyeeta Nag[2], Richard F. Haglund[2], Julia Stähler[1], and Martin Wolf[1] — [1]Fritz-Haber Institut der MPG, Dep. of Physical Chemistry, Berlin, Germany — [2]Dep. of Physics and Astronomy, Vandebilt University, Nashville, TN, USA

The nature of the insulator to metal transition in VO_2 at 340 K has been a matter of controversy, since both lattice distortion and electronic correlations play a crucial role. Understanding the ultrafast dynamics of the *photoinduced* phase transition (PPT) may elucidate the contributions of electrons and lattice to the process. We present transient reflectivity data showing a strong change in the coherent phonon spectrum crossing the critical fluence $\Phi_c = 6.2$ mJ/cm^2, which can be explained by two scenarios: (i) The PPT is driven by the increase of the lattice temperature due to energy transfer from the photoexcited electrons. (ii) The sudden electronic excitation is sufficient to alter the symmetry of the lattice potential, even before ionic motion occurs. In a pump-pump-probe experiment we excite coherent phonons to monitor the changes of the lattice symmetry on a femtosecond time scale. Below Φ_c, we are able to coherently control the amplitude of the oscillations by changing the delay between the two pump pulses. Above threshold, this is not possible; on the contrary, the dynamics after the 2^{nd} pump pulse is comparable to the one of the thermally induced metallic phase. These results suggest that the PPT begins with a lattice potential symmetry change due to the strong electronic excitation.

O 59.14 Wed 17:30 P3

Time-resolved core-level photoelectron spectroscopy — •Christian Oberer, Martin Michelswirth, Hatem Dachraoui, Jochen Vieker, Tobias Milde, Norbert Müller, and Ulrich Heinzmann — Molecular and Surface Physics, University of Bielefeld

An experimental setup based on a combination of few femtosecond EUV pulses from high-harmonic generation, with time-of-flight (TOF) analysis of the emitted photoelectrons. A selection of the 61th harmonic 95 eV from the harmonic spectrum of the light source is achieved with a multilayer Mo/Si double mirror monochromator. Our data present a clear demonstration of the potential of femtosecond time-resolved core-level photoelectron spectroscopy to directly study ultrafast dynamical processes at surfaces and in condensed matter systems.

O 59.15 Wed 17:30 P3

Post-deposition annealing induced reduction of γ**-**Fe_2O_3 **ultra thin films studied by XRD** — •Florian Bertram[1], Carsten Deiter[1], Kathrin Pflaum[1], Matrin Suendorf[2], Christian Otte[2], and Joachim Wollschläger[2] — [1]Hamburger Synchrotronstrahlungslabor am Deutschen Elektronen-Synchrotron, Notkestr. 85, 22607 Hamburg — [2]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück

Due to their magnetic and catalytic properties iron oxide thin films are of interest for both applications and fundamental research. In both cases precise control of the oxide phase is crucial. Here, we present the effect of the post deposition annealing (PDA) in high vacuum on a 8nm γ-Fe_2O_3 film epitaxially grown by molecular beam epitaxy on MgO(001). The reduction from γ-Fe_2O_3 to FeO could be monitored by *in-situ* XRD measurements at the MgO (002) bulk reflection. By these measurements we could show that the reduction is occurring in two steps. First the film is reduced to Fe_3O_4 with the phase transition completed around 360°C. Afterwards the film is reduced to FeO which is completed at about 410°C.

O 59.16 Wed 17:30 P3

Nanoparticle impact on a W(110) surface — •Wolfgang Rosellen, Hendrik Bettermann, and Mathias Getzlaff — Institute of Applied Physics,University Duesseldorf

Deposited clusters and nanoparticles become more and more interesting from a technological point of view due to their size dependent electronic and magnetic properties. Therefore it is important to have access to the structure of these deposited particles. We will show that the deposition event itself is primarily responsible concerning the shape of the particles. In molecular dynamical simulation by Haberland et al. different kinetic energies result in a softlanding process of the particles without deformation due to themalization up to an implantation of particles into the substrate surface. In our experiments we investigate nanoparticles with different sizes and deposition energies. The particles are preformed in the gas phase by a UHV compatible Arc Ion Cluster Source (ACIS) being developed for softlanding condition. The kinetic energy of the particles are far below 1eV/atom. For mass and therefore size selection an electrostatic quadrupole is used at the exit of the particle source. This is possible due to 50% of all particles are positively or neagtively charged. Our investigations are carried on a bare W(110) surface. The deposited nanoparticles, mainly Fe, Co and their alloy are investigated by the means of Scanning Tunneling Microscope under UHV conditions. To gain a deeper insight into the landing process we will discuss the resulting shape of charged nanoparticles after accelerating the particles in an electrostatic field to prevent the nanoparticles from softlanding.

O 59.17 Wed 17:30 P3

Thermally activated decay of size selected clusters on thin C_{60} **films** — •Stefanie Duffe[1], Niklas Grönhagen[1], Lukas Patryarcha[1], Benedikt Sieben[1], Chunrong Yin[2], Bernd von Issendorff[2], Michael Moseler[2,3,4], and Heinz Hövel[1] — [1]TU Dortmund, Experimentelle Physik I — [2]Universität Freiburg, Fakultät für Physik — [3]Fraunhofer Institute for Mechanics of Materials IWM — [4]Freiburg Material Research Center

Metal nanoparticles supported by thin films are important for molecular electronics, biotechnology and catalysis, among other fields. Here we demonstrate a mechanism for the penetration of thin films and other nanoscopic barriers which is different from mere diffusion. Mass selected clusters from Ag_{55}^+ to $Ag_{923\pm9}^+$ were soft landed at 165 K on graphite (HOPG) and Au(111) covered with 1 and 2 monolayers (ML) C_{60}. Imaging by STM at 77 and 5 K showed that the clusters have extremely narrow cluster height distributions at low temperature [1]. Using C_{60}/HOPG or 2 ML C_{60}/Au(111) the cluster heights are stable for more than 12 h at room temperature, whereas for 1 ML C_{60}/Au(111) $Ag_{309\pm3}$ clusters decayed and penetrated the C_{60} film [2]. Atomistic calculations reveal a process by which the clusters decay atom by atom through 1 ML C_{60}/Au(111). These results demonstrate that a metallic substrate exerts attractive forces on metallic nanoparticles which are separated from the substrate by a single monolayer of C_{60} molecules.

[1] S. Duffe et al., Eur. Phys. J. D **45**, 401 (2007)

[2] S. Duffe et al., Nature Nanotechnology **5**, 335 (2010)

O 59.18 Wed 17:30 P3

The height of Ag_N **clusters on** C_{60} **films studied for N=55 to N=147** — •Niklas Grönhagen[1], Natalie Miroslawsik[1], Kolja Mende[1], Stefanie Duffe[1], Bernd von Issendorff[2], Michael Moseler[2,3,4], and Heinz Hövel[1] — [1]TU Dortmund, Experimentelle Physik I — [2]Universität Freiburg, Fakultät für Physik — [3]Fraunhofer Institut für Werkstoffmechanik, Freiburg — [4]Freiburger Materialforschungszentrum

Mass selected clusters from Ag^{+}_{55} to $Ag^{+}_{138\pm2}$ were soft landed at 77 K on C_{60}/Au(111) and imaged with STM at 77 K. Up to 9 deposition spots were imaged on a single sample using a new cluster focusing device. We were able to separate the spots clearly. The cluster heights are constant up to Ag^{+}_{80} which can be explained assuming an icosahedrical shape for Ag^{+}_{55} and the formation of caps of silver atoms at the rim of the clusters for larger sizes. Every single height between Ag^{+}_{80} and Ag^{+}_{88} has been deposited and analysed. However the resolution of our cluster machine had to be taken into account. A remarkable change in height occurs between Ag^{+}_{84} and Ag^{+}_{87}. An additional monolayer formed at the top cluster facet might be responsible. Ag^{+}_{87}, Ag^{+}_{88} and Ag^{+}_{95} have the same height, $Ag^{+}_{110\pm2}$ and $Ag^{+}_{138\pm2}$ are larger and approach the height of the closed shell icosahedral cluster $Ag^{+}_{147\pm2}$.

O 59.19 Wed 17:30 P3

Ag clusters in polymer PDMS: UV-VIS absorption and XANES — •Kamil Latussek[1], Sabrina Hoffmann[1], Stefanie Duffe[1], Christian Sternemann[1], Ralph Wagner[2], and Heinz Hövel[1] — [1]TU Dortmund, Experimentelle Physik I, Otto-Hahn-Str. 4, 44221 Dortmund, Germany — [2]BU Wuppertal, Fachbereich C - Fachgruppe Physik - Materialwissenschaften, Gaußstraße 20, 42097 Wuppertal, Germany

Optical properties of noble metal clusters and nanostructures such as their UV-VIS absorption band alter significantly with size, shape and interparticle spacing as well as with the properties of the local environment. The possible amount of noble metal clusters deposited on a SiO_2 substrate is limited by the process of beginning coalescence to larger particles and electromagnetic coupling. Depositing these clusters into a matrix such as a polymer yields the possibility to investigate a much higher amount of separated particles. The plasmon resonance of Ag clusters in PDMS before and after exposure to air is examined using optical spectroscopy [1]. Then the same clusters are examined with XANES at the Ag L_3 edge [2].

[1] U. Kreibig et al., Optical Investigations of Surfaces and Interfaces of Metal Clusters, In: Advances in Metal and Semiconductor Clusters Vol. 4, (ed. M.A. Duncan), JAI press Inc., 345 (1998).

[2] P. Behrens et al., Z. anorg. allg. Chem. 625, 111 (1999).

O 59.20 Wed 17:30 P3

Heterostructural Interfaces: Structural and Electronic Properties of ZnO/Si from First Principles — •Benjamin Höffling, André Schleife, and Friedhelm Bechstedt — IFTO and ETSF, FSU Jena, Germany

The growth in computational power has greatly increased the possibilities and applications of parameter-free calculations. Ever more complex systems can be accurately modeled using ab-initio computational methods. One of the great challenges that remains is the construction of realistic geometric models of these systems. Interfaces between materials of different crystal structures are particularly challenging to model within the confines of repeated-supercell methodology. Since ZnO is being widely used as a transparent electrode in Si-based photovoltaics, the interface with silicon is of particular interest.

We present a method based on coincidence lattices and Density Functional Theory (DFT) calculations to create geometric models for heterostructural interfaces and construct a model structure for the interface between diamond structure Si and wurtzite ZnO. We then use this model to predict electronic properties using both DFT and modern quasiparticle theory based on hybrid functionals within the HSE03+GW approach. We predict band level alignment and the nature and location of electronic interface states. Our results concerning structural and electronic properties are compared to experimental and theoretical findings.

O 60: Poster Session IV (Solid/liquid interfaces; Semiconductors; Oxides and insulators; Graphene; Plasmonics and nanooptics; Electronic Structure; Surface chemical reactions; Heterogeneous catalysis)

Time: Wednesday 17:30–21:00 Location: P4

O 60.1 Wed 17:30 P4

Investigation of the growth of thin Ionic Liquid films on Au(111) and HOPG — •Marcel Marschewski[1], Evgenij Pachomov[1], Oliver Höfft[2], Wolfgang Maus-Friedrichs[1], and Frank Endres[2] — [1]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Mechanische Verfahrenstechnik, TU Clausthal, Arnold-Sommerfeld-Str. 6, 38678 Clausthal-Zellerfeld, Germany

Ionic liquids (IL) are a highly interesting group of solvents for electrochemical processes; mainly due to the combination of their high electrical conductivity, their electrochemical stability and their ability to dissolve a wide range of compounds [1]. Due to the low vapour pressure ionic liquids can be used in ultra high vacuum. We present our results on the growth of thin films imidazolium - based ionic liquids on Au(111) and HOPG. These were studied by electron spectroscopy using ultraviolet photoelectron spectroscopy (UPS, HeI) and metastable atom induced electron spectroscopy (MIES). We have prepared monolayers of [RMIm]Tf2N; (R stands for Ethyl- and Octyl-chains) on the substrates by vapour deposition. For Au(111) we find hints for a reorientation of [OMIm] cation during the growth of the first two monolayers. In addition we have investigated the behaviour of evaporated silver on [EMIm]Tf2N monolayers on HOPG. We find that due to the ionic liquid films the silver particles size is increased compared to silver on clean HOPG. [1] F. Endres, S. Zein El Abedin, Phys. Chem. Chem. Phys., 8 (2006) 2101

O 60.2 Wed 17:30 P4

Potential dependent structural transition of heptyl viologen on Cu(100) studied by in situ STM and IRRAS — •Melanie Röefzaad[1], Min Jiang[2], and Klaus Wandelt[1] — [1]Institute for Phys. Chem., University of Bonn, Germany — [2]Inst. Bioenergy and Bioprocess Technology,Chinese Academy Sciences, P.R. China

The potential dependent adsorption structure of heptyl viologen (1,1*-Diheptyl-4,4*-bipyridinium, DHV) on a chloride precovered Cu(100) electrode has been investigated by Cyclic Voltammetry (CV), in situ electrochemical STM and IR-Reflection Absorption Spectroscopy (IRRAS). The redox-active DHV molecule exhibits pairs of current waves in CV measurements which are ascribed to two typical one-electron transfer steps and phase transformation processes. Between +200 and -100 mV, an ordered 2D dot-array structure in STM images emerges on the Cl- modified Cu(100) electrode surface. One-electron reduction of the dication around -150 mV causes a phase transition from a dot-array assembly to a stripe pattern in STM images which has a double layer structure. With a decrease of the applied electrode potential, the structure of the adlayer undergoes a subsequent change from the double layer phase to a closed packed monolayer of stripes. Orientation analysis with IRRAS of the bipyridine moiety reveals a slight tilt of the long molecular axis to the surface in the dicationic phase and a parallel orientation in the mono cationic striped phases. Calculation of the average angle of the alkyl chains hints to an orientation along the surface within the dot structure while protruding out of the more closely packed stripe phase.

O 60.3 Wed 17:30 P4

Phase transitions of adsorbed viologen monolayers in the presence and absence of specifically adsorbed halides — •Knud Gentz, Min Jiang, and Klaus Wandelt — Institute for Physical und Theoretical Chemistry, Uni Bonn

The structure and stability of self-assembled organic monolayers are scientifically and technologically very timely research subjects. In those cases where larger organic molecules may not be intact volatile and therefore not be deposited by vapor deposition, adsorption from solution may be an alternative route. Here we present results on heptylviologen layers on HOPG and Cu(1 0 0) surfaces as obtained with cyclic voltametry and in-situ scanning tunneling microscopy in solution. Heptylviologen was adsorbed on the HOPG- and Cu(1 0 0) electrode surfaces from a supporting electrolyte. In the CV spikes characteristic of surface phase transitions of HV monolayers on HOPG were observed. The STM images clearly show a stripe structure on the surface in the regime negative of the spike peaks indicating the presence of the radical cationic phase $HV^{\bullet+}$ stabilized by π–π-interaction of the individual molecules. On HOPG a single row and a double row structure were found showing a herringbone-like arrangement of the molecules. Additionally, on copper a second layer adsorption of HV molecules was observed the concentration and structure of which depending on the applied electrode potential. In the regime positive of the spike peak an ordered viologen layer was observed only on copper, where chloride is specifically adsorbed on the surface, which stabilizes the dicationic species on the positively charged electrode.

O 60.4 Wed 17:30 P4

Tunneling Current Driven Electrodeposition of Metals onto n-Si(111):H — •Sebastian Jakob and Werner Schindler — Physikdepartment, Lehrstuhl E20, Technische Universität München, James-Franck-Straße, D-85748 Garching bei München

Electrochemical (EC) metal deposition onto Silicon surfaces should be impossible at potentials of the n-Si(111):H electrode lying above the flatband potential due to the electron depletion at the Silicon suface. Here, we show in sophisticated *in-situ* EC-STM experiments in great detail that electrodeposition onto n-Si(111):H occurs at potentials positive with respect to the flatband potential, although obviously not found in conventional STM experiments at the solid/ liquid interface. By STM imaging and in high-resolution cyclic voltammetry we observe a deposition/ dissolution of metal, determined by the corresponding Nernst potential of the metal. We explain this behaviour by electrodeposition originating from tunneling currents through the electron depletion zone at the n-Si(111):H surface.

O 60.5 Wed 17:30 P4

Ionic Liquid on Cu(100) studied by X-ray Photoelectron Spectroscopy — •Ellen Fischermeier and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

Room temperature Ionic Liquids have attracted a lot of attention during the last years due to their extraordinary physical and chemical properties. As a number of important processes depend on the properties of the interface between Ionic Liquid and substrate, it is crucial to gain a deeper insight into the Ionic Liquid/surface interactions.

In this study films of [EMIm][Tf$_2$N] of different thickness were deposited under UHV-conditions by physical vapor deposition on well defined Cu(100) single crystal surfaces using a home-built evaporator. These samples were studied by X-ray Photoelectron Spectroscopy under different emission angles.

We focus on the growth behavior of the films and the radiation induced changes observed in the Ionic Liquid and compare the results obtained at different layer thickness.

O 60.6 Wed 17:30 P4

Copper electrodeposition and additives: from underpotential deposition to bulk growth — •Yuriy Yanson, Joost Frenken, and Marcel Rost — Leiden University, Leiden, the Netherlands

Cu electrodeposition at different stages on Au(111) surface is accessed in-situ on atomic scale by means of our newly developed fast electrochemical STM. We show the effect of industrially used additives, such as bis-(3-sodiumsulfopropyl) disulfide (SPS) and polyethylene glycol (PEG), on the Cu deposit. The EC-STM results are complemented by electrochemical measurements and discussed in the light of current state of knowledge on electrodeposition and molecular processes involving the additives.

O 60.7 Wed 17:30 P4

EC-STM investigation of self-organized Porphyrin layers on an iodide-modified Au(111) surface — •Tomasz Kosmala[1,2], Michael Schneider[2], Aleksander Krupski[1], and Klaus Wandelt[1,2] — [1]Institute of Experimental Physics, University Wroclaw, plac Maksa Borna 9, 50-204 Wrocław, Poland — [2]Institute of Physical and Theoretical Chemistry, University Bonn, Wegelerstr. 12 , 53115 Bonn, Germany

The self-assembly of Tetra(N-methyl-4-pyridyl)-porphyrin molecules (TMPyP) on an iodide- modified Au(111) surface has been studied by means of Cyclic Voltametry (CV) and in-situ Electrochemical Scanning Tunneling Microscopy (EC-STM).

The iodine precovered Au(111) surface was found to be a good substrate for the self-assembly of highly ordered layers of porphyrin cations from solution [1,2].

Unlike the Itaya group [1,2], however, we have prepared the iodine precoverage on Au(111) in situ and found the iodine layer to be stable at potential even below the first reduction potential of adsorbed TMPyP. As a consequence we were able to monitor interesting structural phase transitions as a consequence of the molecular redox-processes, which could not be seen in the previous work [1,2].

[1] M. Kunitake, N. Batina, and K. Itaya, Langmuir, vol. 11, no. 7, pp. 2337 - 2340, (1995).

[2] M. Kunitake, U. Akiba, N. Batina, and K. Itaya, Langmuir, vol. 13, no. 6, pp. 1607 - 1615, (1997).

O 60.8 Wed 17:30 P4

Fast switching of the electrochromism in thin films of a perfluoroalkyl-substituted phthalocyanine — Stefanie Nagel[1], Martin Lener[1], •André Dragässer[1], Robert Gerdes[2], Sergiu Gorun[2], and Derck Schlettwein[1] — [1]Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de — [2]Department of Chemistry and Environmental Science, New Jersey Institute of Technology, Newark, NJ 07102, USA

Thin films of metal complexes of octakisperfluoro(isopropyl)-phthalocyanine ($F_{64}Pc$) vapour-deposited on indium tin oxide electrodes were studied at negative potentials in contact to LiCl aqueous electrolyte solutions. In situ monitoring of the absorption spectra of the films during electrochemical reduction revealed electrochromic characteristics which are of possible interest for applications in displays or as smart windows. Electroneutrality of the films was preserved by intercalation of Li^+ ions. The technically relevant speed of switching the absorbance characteristics by an applied potential depends on both electron conduction and ion diffusion in the matrix. The switching speed was studied by a variation of the scan rate in cyclic voltammetry and by potential step experiments. The observed charge flow and spectral changes are discussed both in view of relevance of the decisive sample parameters and a possible technical application.

O 60.9 Wed 17:30 P4

Density functional calculation of electronic surface structure and Fe adsorption on ZnO (0001) and (000$\bar{1}$) — •Sougata Pal, Torben Jasper-Toennies, Michael Hack, and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel, Germany

The structure and electronic properties of the ZnO(0001) and ZnO(000$\bar{1}$) surfaces as studied by density functional calculations will be presented. The stability of the surface has already been investigated by various groups [1,2,3]. The electronic surface band structure, however, in particular the existence of surface states and the differences between experimental band dispersion for both terminations, still appears to pose open problems [4,5]. To address these issues, we compare Kohn Sham band structures and electrostatic potentials close to the surface for the relaxed (1x1)-surface, (2x2) vacancy reconstructions, and surfaces with pits. In particular the effect of the bending of the electrostatic potential at the surface on the eigenstates is quantified.

Comparing the adsorption energies of Fe atoms for various adsorption sites on ZnO(000$\bar{1}$), the fcc hollow position turned out to be energetically favorable. The oxidation state of the Fe atom is derived from the projected density of states.

[1] G. Kresse *et al.*, Phys. Rev. B **68**, 245409 (2003).
[2] M.-H. Du *et al.*, Phys. Rev. B **78**, 155424 (2008).
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O 60.10 Wed 17:30 P4

Different bandstructures of for- and backward buckled π-bonded chains of the Si(111)-2×1 surface reconstruction revealed by STS-measurements — •Karolin Löser, Martin Wenderoth, Thomas K. A. Spaeth, and Rainer G. Ulbrich — IV. Physikalisches Institut, Georg-August Univ. Göttingen, Germany

According to the Pandey model, the π-bonded chains of the Si(111)-2×1 surface reconstruction might be buckled either for- or backward but it is extremely hard to distinguish the buckling types as the energetic difference is very small [1] and the projection of the atomic positions is exactly the same seen from above the surface. Because of this, STM cannot be used to determine the buckling type directly.

To gain access to information on the buckling type we exploit the boundaries between domains of differently reconstructed π-bonded chains as a tool to reveal displacements of the chains. Thus, with high-resolution STM and STS measurements of π-bonded chains on cleaved Si(111)-2×1 samples in the UHV, we can not only proof the co-existence of for- and backward buckled π-bonded chains but also study the local Density of States (LDOS) of differently buckled π-bonded chains. We find that two different LDOSs for the two buckling types, one of them has a smaller bandgap than the other, which fits well with calculations [2] that predict the backward buckled π-bonded chains to have a slightly smaller bandgap. We acknowledge financial support by the DFG via project WE 1889/3.

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[2] S. H. Lee and M. H. Kang. Phys. Rev. B 54 (3), 1482(1996)

O 60.11 Wed 17:30 P4

STM characterization of MOVPE-prepared silicon surfaces — Peter Kleinschmidt, Sebastian Brückner, •Johannes Luczak, Oliver Supplie, Anja Dobrich, Henning Döscher, and Thomas Hannappel — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

The clean Si(100) surface reconstructs by forming dimers, thus reducing the number of dangling bonds at the surface. In the MOVPE environment hydrogen is commonly used as process gas, which leads to a monohydride silicon surface with a 2×1 unit cell consisting of H-Si-Si-H dimers. Even so, the quality of the surface can vary dramatically depending on process conditions. In general, annealing in hydrogen leads to a two-domain surface structure with monoatomic steps, where the resulting structure also strongly depends on misorientation. We find process conditions for preparation of Si(100) surfaces with 0.1°, 2° and 6° offcut where a strong preference for one domain is obtained, making the resulting surfaces ideal substrates for III-V-on-Si epitaxy. A process consisting of deoxidation, homoepitaxial buffer layer growth and annealing is found to result in D_A-type double layer steps for 0.1°, and D_B-type double layer steps for 6° offcut. The identical process leads to single layer steps for 2° offcut. Here, we obtain D_A-type double layer steps by a modified process which includes a slow cooling phase after the annealing step. Our results, verified by scanning tunneling microscopy, low energy electron diffraction and Fourier-transform infrared spectroscopy, are in sharp contrast to the clean and the hydrogenated Si(100) surface prepared in UHV.

O 60.12 Wed 17:30 P4

Thermal stability of thin HfO_2 films on plasma nitrided Si(100) — •Katharina Skaja[1,2], Frank Schönbohm[1,2], Daniel Weier[1,2], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Fakultät Physik - Technische Universität Dortmund, Otto-Hahn-Str. 4, D 44221 Dortmund, Germany — [2]DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D 44227 Dortmund, Germany

Thin dielectric films such as HfO_2 grown on Si(100) are interesting for metal-oxide semiconductor MOS devices, because HfO_2 has a high dielectric constant. Up to 750 °C HfSi increases in the HfO_2/Si layer stack, which creates unwanted conductive states. To avoid the formation of HfSi an amorphous Si_3N_4 diffusion barrier can be grown between the HfO_2 film and the silicon substrate. The ultrathin Si_3N_4 films were grown on the Si(100) surface by nitrogen plasma which was provided from a special plasma source. Different thicknesses of Si_3N_4 interlayers were prepared in-situ and the HfO_2 films were grown on top of the sample by electron beam evaporation. The film thicknesses were determined by ARXPS meassurements. The samples were flash heated for 1 minute at several temperatures. After each annealing step the chemical properties of the system HfO_2/Si_3N_4/Si(100) were checked by photoelectron spectroscopy (PES). For temperatures up to 750 °C the HfO_2 layer remains unchanged. For higher temperatures a further signal could be observed in the spectra, due to the chemical shift in the Hf 4f signal to higher kinetic energies. This new component could be identified as $Hf_{x_1}Si_{x_2}O_{x_3}N_{x_4}$. The $Hf_{x_1}Si_{x_2}O_{x_3}N_{x_4}$ appears to be stable up to 850 °C.

O 60.13 Wed 17:30 P4

Adsorption of metalorganic molecules on metal-semiconductor systems — •Christian Brand, Jędrzej Schmeidel, Wei Chen, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Germany

The controlled implementation of single molecules in appropriate contact assemblies is the ultimate realization of an ultra-small device structure. Besides extremely high integration densities the functionalities of the devices are adjustable by chemical synthesis. However, the interaction of the molecule with its environment is decisive.

The adsorption of ferrocene-1,1'-dithiol (FDT) on Ag-$\sqrt{3}$ reconstructions on nominally flat and vicinal Si(111) substrates has been studied. The FDT was chosen because of its large conductance and high structural flexibility with respect to rotation of the two cyclopentadienyl (Cp) rings. The reconstruction is a prototype of a highly conductive low dimensional electron gas on a technologically relevant substrate. The adsorption of intact molecules takes place predominantly at defect sites, e.g. vacancy and step structures. Submolecular resolution showing the Cp-ring structure was obtained at perfect terrace sites. Due to chemisorption of the S-atoms at hollow sites the molecule axis is oriented parallel to the substrate. The initial rotational flexibility is frozen and only tow different rotated configurations were found. The adsorption geometry is confirmed by VASP calculations. Recently, Ag reconstructions on Si(557) substrates have been used. The effect of the uniaxial step configuration towards the adsorption of the FDT molecules will be discussed.

O 60.14 Wed 17:30 P4

Investigation of Bis(phthalocyaninato)lutetium(III) on HOPG by STM, STS and DFT — •Lars Smykalla, Pavel Shukrynau, Marius Toader, and Michael Hietschold — Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany

We report results obtained on ordered layers of Bis(phthalocyaninato)-lutetium(III) ($LuPc_2$) on highly oriented pyrolytic graphite (HOPG) by using a variable temperature scanning tunneling microscope (STM) at 30K in UHV. These double decker phthalocyanine molecules were deposited by OMBE at low rates. Through slight annealing self-assembled highly ordered islands of $LuPc_2$ were formed which show a close packed square structure governed by molecule-molecule interactions. Experiments with submonolayer coverage and multilayer coverage were carried out to investigate the epitaxy of the molecular layers on the substrate, the stacking behaviour and tilting of molecules relative to the layer. Very high resolved STM-images at negative bias voltage show intra-molecular features which are in very good agreement with the appearance of the highest occupied molecular orbital (HOMO) of $LuPc_2$ gained by density functional theory (DFT). Tip-sample-distance-dependent tunneling spectroscopy was applied to study the electronic properties of the ordered molecular layers of $LuPc_2$ on HOPG and the influence of the tip and the electric field. To identify the peaks in the normalized conductance spectra DFT calculations were performed and a comparison of the energy levels with STS shows a good agreement of the HOMO-LUMO-gap.

O 60.15 Wed 17:30 P4

Surface photovoltage investigation of gold chains on Si(111) by two-photon photoemission — •Sebastian Otto, Kerstin Biedermann, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

We present surface photovoltage measurements on Si(111)-(7×7) with monoatomic gold chains. The gold coverage was varied between zero and 0.6 ML, where the Si(111)-(5×2)-Au reconstruction covers the surface completely.

During the two-photon photoemission experiments the p- or n-doped samples were illuminated by infrared (IR, $E_{IR} = 1.55$ eV) and ultraviolet (UV, $E_{UV} = 4.65$ eV) laser pulses. For all coverages the photovoltage was determined for sample temperatures of 90 K and 300 K by variation of the IR and UV laser power.

P-doped as well as n-doped Si(111) wafers show a linear dependence of the photovoltage on gold coverage. This stands in contrast to scanning tunneling spectroscopy measurements [1], which show a coverage-independent photovoltage over a wide coverage range for n-doped wafers. While for p-doped wafers our experimentally determined photovoltage is in agreement with previous reports, for n-doped wafers the observed values are lower than expected.

[1] K. Sell et al., phys. stat. sol. (b) **1087**, 247 (2010)

O 60.16 Wed 17:30 P4

C_2 inclusion by C_{60} in thin films deposited on HOPG — Seyithan Ulas, Dmitry Strelnikov, Daniel Löffler, Patrick Weis, •Artur Böttcher, and Manfred M. Kappes — Karlsruher Institut für Technologie, Institut für Physikalische Chemie, Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany

The deposition of hyperthermal C_2^- anions onto C_{60} films has been studied by means of mass spectrometry, thermal desorption spectroscopy (MS), ultraviolet photoionization spectroscopy (UPS), atomic force microscopy (AFM) and Raman spectroscopy. The inclusion of C_2

dimers by C_{60} cages manifests itself by the sublimation of the C_{62}, C_{64} and C_{66} cages as well as by pronounced modifications of the thermal, electronic and vibronic properties of the C_{60} films. The most efficient reaction channel: the formation of volatile C_{62} species depends on the deposition conditions. Its yield, y(C_{62}), does not overcome 10^{-2} per C_2. UPS and Raman spectra of the C_2/C_{60} layers supported by DFT calculations indicate the formation of polymeric network based on -C_{60}-C_2-C_{60}- chains as well as C_{62} (and -C_{62}-C_{62}- chains) as two prevailing inclusion channels. Thermal desorption spectra reveal coherent sublimation of C_{60} and C_{62} what implies that thermal decomposition of the -C_{60}-C_2-C_{60}- oligomeric chains is the common dissociative reaction step. In temperature range 750 - 975 K the thermal decomposition of the -C_{60}-C_2-C_{60}- oligomeric chains competes with the thermally activated inclusion of the C_2 into C_{60} cages resulting in non-IPR C_{62} cages arranged in semiconducting network. At higher temperatures the network becomes converted predominantly into conducting carbon chains of fused C_{62} cages.

O 60.17 Wed 17:30 P4

Karlsruher Institut für Technologie, Institut für Physikalische Chemie, Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany — Seyithan Ulas, Dmitry Strelnikov, Daniel Löffler, Patrick Weis, •Artur Böttcher, and Manfred M. Kappes — Karlsruher Institut für Technologie, Institut für Physikalische Chemie, Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany

Thin monodisperse films consisting of non-IPR C_{58} fullerene cages have been deposited onto HOPG by exploiting the soft-landing of mass-selected C_{58}^{+} ions. The ions have been created by performing the electron-impact induced fragmentation/ionization of IPR C_{60} cages. In analogy to IPR fullerenes the doping of the C_{58} films by alkali metals (e.g. Cs) leads to the formation of alkali-metal-based fullerides. The mass spectra taken during the sublimation of CsxC58 phase reveal well distinguishable three components, C_{56}, C_{58} and C_{60}. Both new components, C_{56} and C_{58}, indicate the transfer of the C_2 unit from a C_{58} to the adjacent one, $C_{58} + C_{58} \rightarrow C_{56} + C_{60}$ as a process competing with the breakage of the intercage bonds constituted by non-IPR sites (e.g. 2AP-2AP). The doping Cs atoms located in vicinity of the intercage bonds weaken them significantly and consequently facilitate the high-temperature C_2 transfer. The yield of the $C_{58} \rightarrow C_{60}$ conversion depends on the doping degree x and reaches a level of 10^{-2} per C_{58} deposited.

O 60.18 Wed 17:30 P4

Photocatalytic CO_2 reduction on dye sensitized TiO_2 — •Leo Pöttinger[1] and Thomas Bürgi[2] — [1]Im Neuenheimer Feld 253, D-69117 Heidelberg — [2]30 Quai Ernest-Ansermet, CH-1211 Genève 4

Reducing the greenhouse gas CO_2 and substituting fossil fuels are challenging tasks for the future. The photocatalytic recycling of CO_2 to hydrocarbons with sunlight as renewable energy is therefore investigated. Attenuated total reflection infrared (ATR-IR) spectroscopy was used to probe a thin layer of porous TiO_2. In the first step "in-situ" adsorption experiments of CO_2 and dyes with exposure to UV and visible light were performed. Furthermore metal co-catalysts were added to enhance the photocatalytic activity. The ATR-IR measurements show stable carbonates on the TiO_2 nanoparticles after purging the CO_2 saturated aqueous solution with pure water. After irradiation with UV light the carbonate bands vanish. The same characteristics can be observed with dye sensitized TiO_2 and visible light exposure. The increase of new bands could be a hint of intermediate products in the multiple electron process towards methanole.

O 60.19 Wed 17:30 P4

III-V semiconductors for photoelectrochemical applications: surface preparation and characterization — •Dominic Fertig, Birgit Schächner, Wofram Calvet, Bernhard Kaiser, and Wolfram Jaegermann — TU Darmstadt, Fachbereich Materialwissenschaft, Fachgebiet Oberflächenforschung

III-V semiconductors are promising reference systems for photoelectrochemical energy conversion. Therefore we have studied the influence of different acids and acidic solutions on the etching of p-doped galliumarsenide and gallium-phosphide single crystal surfaces. From our experiments we conclude, that etching with HCl and subsequent annealing up to 450°C gives the best results for the removal of the carbonates and the oxides without affecting the quality of the sample. By treating the surfaces with "piranha"-solution ($H_2SO_4 : H_2O_2 : H_2O$/7:2:1), the creation of an oxide layer with well defined thickness can be achieved. For the creation of an efficient photoelectrochemical cell, Pt nanoparticles have been deposited from solution. These surfaces are then characterized by photoelectron spectroscopy and AFM. Further electrochemical measurements try to correlate the effect of the surface cleaning and the Pt deposition on the photoactivity of the GaAs- and GaP-semiconductors.

O 60.20 Wed 17:30 P4

The growth of ultra thin Praseodymia oxide films on boron-passivated Si(111) surfaces — •Henrik Wilkens, Alexander Knobeler, Sebastian Gevers, Nina Jeppesen, Daniel Bruns, Thomas Weisemoeller, and Joachim Wollschläger — FB Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany

Silicon on insulator (SOI) CMOS technology already have an enormous commercial impact with Si dioxide as insulating material. Alternative insulating materials are in the focus of investigation to integrate semiconductors for system on chip (SOC) solutions that cannot be built on Si alone.

Due to its good insulations characteristics and a high dielectric constant, praseodymium oxide is an interesting candidate for such applications. To prevent the formation of silicate at the substrate-oxide interface it is essential to use passivated silicon substrates. In this work the influence of boron-passivation is investigated. Prior to praseodymium oxide evaporation by molecular beam epitaxy the Si substrate surface was passivated by boron via evaporation of boric acid and subsequent annealing of the substrate to 900°C. In situ Spot Profile Analysis Low Energy Electron Diffraction (SPA-LEED) and Auger Electron Spectroscopy (AES) were used to characterize the surface structure and morphology. Additional Ex-situ X-Ray Reflectivity (XRR) and X-Ray Diffraction (XRD) analyses were performed. The results show that at a substrate temperature of 500°C a single crystalline oxide film is formed.

O 60.21 Wed 17:30 P4

Optical Second-Harmonic Generation at the GaP/Si(001) interface — •Kristina Klass, Johannes Reimann, Gerson Mette, Wolfgang Stolz, Kerstin Volz, and Ulrich Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität Marburg, D-35032 Marburg

Due to similar lattice constants (a = 0.54 nm) GaP as a compound semiconductor can be grown on Si without significant lattice mismatch. The combination of Silicon with GaP-based direct III/V semiconductors is of great interest for the realization of optoelectronics based on this well understood substrate. We have employed optical second-harmonic generation (SHG) as a non-invasive and contactless method to characterize the GaP/Si(001) interface. Femtosecond laser pulses are focused on a thin sample which can be rotated around its z-axis. Irradiation and detection of different polarizations as well as variation of the angle of incidence yield access to different tensor elements of the second-order nonlinear susceptibility tensor. The investigated samples show surprisingly strong variation of the SHG response depending on growth condition and the Si(001) substrate structure. In particular, we find a strong 2-fold symmetric SHG-component which is correlated to the presence of double height steps and an almost single-domain Si(001) substrate.

O 60.22 Wed 17:30 P4

Electron pair emission from NiO(100) — •Changhui Li, Lucie Behnke, Frank O. Schumann, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany

The study of electron pair emission from surface upon electron or photon impact allows to study the electron-electron correlation, which plays an important role to determine the electronic and magnetic properties of materials, especially for strongly correlated systems. We present a first electron pair emission study from a strongly correlated system, namely NiO. We have grown ultrathin NiO(100) films on Ag(100) following standard procedures. We excite the sample with a primary electron beam in the energy range energies (E_p=35-85 eV). Compared with Ag, the coincidence count rate of NiO is about 7 times larger and the secondary electrons make much larger contributions in the electron pair emission. The sum energy spectra of the pairs shows structure which we can relate to the valence band structure. The way the available energy is shared among the electrons depends strongly on the primary energy. For E_p in the range 35-54 eV, the electrons prefer unequal energy sharing, whereas equal energy sharing is adopted for higher primary energies.

O 60.23 Wed 17:30 P4

The chemisorption of hydrogen molecules on CaO films — •Sebastian Dahle[1], Henning Munkert[1,2], and Wolfgang Maus-Friedrichs[1,3] — [1]Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Metallurgie, TU Clausthal, Robert-Koch-Str. 42, 38678 Clausthal-Zellerfeld, Germany — [3]Clausthaler Zentrum für Materialtechnik, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany

The oxide and hydroxide species of Calcium and the underlying reaction processes are of great technological interest. Even the hydration of burnt limestone is just barely predictable. Our investigations start with the preparation of the Calcium oxide and hydroxide species in a clean ultra high vacuum (UHV) environment. During the development of in-vacuo preparation methods of Calcium hydroxide, the adsorption of hydrogen molecules has been investigated. We have found that hydrogen leads to the formation of hydroxide groups, which appears to be unlikely due to thermodynamics at the first glance. Furthermore, hydrogen apparently acts as catalyst for the hydroxidation of a complete Calcium oxide film through water impinging on the surface out of the residual gas. These effects have been studied with Metastable Induced Electron Spectroscopy (MIES), Ultraviolet Photoelectron Spectroscopy (UPS) and X-ray Photoelectron Spectroscopy (XPS).

O 60.24 Wed 17:30 P4

Ab initio calculations on the adsorption energy of NO on TiO_2(110) — •Marie Arndt and Thorsten Klüner — Theoretische Chemie, Carl von Ossietzky Universität Oldenburg, PO Box 2503, 26111 Oldenburg

Catalytic surface reactions are an essential section in the technical industries. Especially photocatalytic reactions on metaloxide surfaces became more and more important since the last decade. The focus of theoretical and experimental analysis lies on the adsorption- and desorption-processes going on onto the substrate surface. In this context, the semiconductor titaniumdioxide has proved as an outstanding photocatalyst. In this study we use *ab initio* calculations to characterize the adsorption of NO on a rutile(110) surface. We use an embedded cluster model of type $Ti_9O_{18}Mg_7^{14+}$ to describe the electronical ground state of this open-shell system. Using the *Molcas* quantum chemistry package, the aim lies in finding the global minimum of the adsorption energy. Within our model we are able to regard six degrees of freedom, the desorption coordinate z, the polar angle θ, the azimuth angle ϕ, the two lateral coordinates x and y and the inner NO distance r. On RMP2-level an BSSE corrected adsorption energy of -0.57 eV at a distance from NO to rutile of 3.0 Å was found. The result affords first insight to the NO-TiO_2-system and this study serves as a basis for further studies concerning excited states involved in the desorption processes within this interesting adsorbate-substrate complex.

O 60.25 Wed 17:30 P4

Organic Molecules on Wide-Gap Insulating Surfaces from First-Principles — •Wei Chen, Karthiga Kantasamy, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

We investigate the adsorption of benzoic acid and its various phenolic derivatives on wide-gap insulators (e.g. NaCl and KCl surfaces) from first-principles, in an effort to demystify the contact charging effect between salt mines mixed with organic molecules. While Kohn-Sham density functional theory (KS-DFT) becomes a *de facto* standard for the predictions of ground-state properties, it is far from being perfect and the standard semi-local density functional approximations suffer from several limitations, such as the notorious *gap problem* and the neglect of the prevalent long-range *van der Waals* interaction in the weakly bonded systems. Moreover, the problem of electronic excitations are beyond the scope of KS-DFT. In this work, a variety of *ab initio* methods are adopted at the respective level of theory, from KS-DFT (with hybrid functionals and dispersion force corrections) to Hedin's *GW* approximation and ultimately the two-particle Bethe-Salpeter equation. The important roles of the long-range correlations, *surface defects* and the *excitonic effect* are presented in the context of the molecule-insulator interfaces.

O 60.26 Wed 17:30 P4

LEED I(V) analysis of CO and N_2 physisorption on the NaCl(100) surface — •Jochen Vogt and Helmut Weiss — Chemisches Institut der Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Carbon monoxide and N_2 physisorbed on the NaCl(100) surface have been considered in the past as model systems for orientational order-disorder phase transitions in two dimensions [1,2]. Although CO and N_2 are isoelectronic, the lateral intermolecular potential of adsorbed CO is governed by dipole-dipole interaction, while in the case of N_2 quadrupole-quadrupole interaction is the leading electrostatic term. Low-energy electron diffraction experiments (LEED) prove, that upon cooling below 35 K the lattice symmetry in the system CO/NaCl(100) changes from a (1×1) to a (2×1). However, few is known about the adsorbate structure from an experimental point of view. We report a LEED I(V) structure analysis of CO/NaCl(100) and N_2/NaCl(100), guided by density functional theory (DFT-D/PBE) calculations. Although predicted by theory [2], our experiments do not support a disorder/order phase transition (1×1)→(2×1) for N_2/NaCl(100) above 18 K.

[1] W. Rzysko, A. Patrykiejew, K. Binder, Phys. Rev. B 76 (2007), 195409

[2] A. K. Sallabi, D. Jack, Phys. Rev. B 62 (2000), 4841

O 60.27 Wed 17:30 P4

LEED and FTIR spectroscopy studies of CO_2 adsorption at NaF(100) — •Stephan Härtel, Anne Möller, Jochen Vogt, and Helmut Weiss — Chemisches Institut der Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

In the present work the adsorption system CO_2-NaF(100) was investigated by means of low-energy electron diffraction (LEED) and Fourier transform infrared (FTIR) spectroscopy. According to LEED I(V) analysis the clean NaF(100) surface shows hardly any deviation from the ideal bulk structure but enlarged vibrational amplitudes [1]. Different from other alkali halide cleavage planes such as NaCl(100) or KCl(100) up to now there are few data available dealing with the adsorption behaviour of molecules on this surface. The LEED patterns of CO_2-covered NaF(100) show no evidence for a superstructure but just a decreased intensity of the substrate spots. Apparently the adsorbed molecules do not form a long range order. This result is comparable to that for CO_2 adsorption on LiF(100) and KBr(100). However there are also alkali halide surfaces such as e.g. NaCl [2] where a superstructure could be observed. The adsorption/desorption behaviour was also studied by recording isotherms and isobars by FTIR spectroscopy from which the heat of adsorption was calculated to be $28.6 \pm 2.9\,\mathrm{kJ/mol}$ which is comparable to the corresponding values in the above mentioned homologous systems.

[1] S. Härtel, J. Vogt, and H. Weiss, Surf. Sci., **604**, 1996 - 2001 (2010)

[2] J. Vogt and H. Weiss, J. Chem. Phys., **119**, 1105 (2003)

O 60.28 Wed 17:30 P4

Luminescence of PTCDA on epitaxial KCl films on Ag(100) — M. Müller, •A. Paulheim, C. Marquardt, and M. Sokolowski — Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstraße 12, 53115 Bonn, Germany

On surfaces of the wide gap dielectric materials the luminescence of organic molecules can be studied in great detail. Thin films of the molecule perylence-3,4,9,10-tetracarboxylic acid dianhydride (PTCDA) were vacuum deposited on epitaxial KCl films on Ag(100). The structural and optical properties were investigated by spot-profile-analysis low energy electron diffraction (SPA-LEED) and by photoluminescence- (PL) and PL excitation spectroscopy (PLE). We investigated molecules in the limit of isolated entities and of a completed monolayer. The SPA-LEED measurements reveal the know quadratic unit cell of the monolayer with the molecules arranged in a brickwall-structure [1]. The optical spectra exhibit a dominating 0-0 transition and well resolved vibronic modes. The transition energy of molecules embedded in a completed monolayer phase is redshifted with respect to that of isolated molecules. In addition, we analyzed the polarization of the emitted light and were able to determine the azimuthal orientation of the organic molecules in both phases with respect to the KCl(100) surface. From these data we achieve detailed information on the role of the intermolecular coupling on the optical properties of the layers. Supported by the DFG through the research group 557. [1] T. Dienel, C. Loppacher, S. C. B. Mannsfeld, R. Forker, and T. Fritz, Advanced Materials 20, 959 (2008)

O 60.29 Wed 17:30 P4

FUNCTIONALIZATION OF THE TIO_2 (110) SURFACE BY TEREPHTHALIC ACID TOWARD THE MOF GROWTH — •Michael Naboka, Alexei Nefedov, and

Christof Wöll — Institute of Functional Interfaces, Karlsruher Institute of Technology, D- 76344 Eggenstein-Leopoldshafen, Germany

Chemically functionalized surfaces play an important role in many nanotechnological applications. A functionalization of TiO2 surface by adsorption of TPA (C6H4(COOH)2) molecules has already been studied previously. It was shown that TPA has a flat orientation at low coverages and up-standing carboxyl-terminated orientation at high coverages. This up-standing orientation at the coverage of one monolayer means that the this system may found similar application to carboxyl-terminated self assembling monolayers. Metal Organic Frameworks (MOFs) is a class of material where metal ions are bound together with organic ligands forming the 2D or 3D porous structure. In addition to the use of MOFs as powders there is currently a significant interest to anchor and grow them on functionalized surfaces. The first steps in this direction were made on the TPA-functionalized TiO2(110) surface. For this purposes the stability of the TPA/TiO2 (110) system was tested by exposing it to the nitrogen atmosphere and subsequent NEXAFS measurements. After that the sample was immersed in the copper trifluoroacetate solution. The obtained structure was studied by NEXAFS and XPS.

O 60.30 Wed 17:30 P4

FUNCTIONALIZATION OF THE TiO_2 (110) SURFACE BY TEREPHTHALIC ACID TOWARD THE MOF GROWTH — •Michael Naboka, Alexei Nefedov, and Christof Wöll — Institute of Functional Interfaces, Karlsruher Institute of Technology, D- 76344 Eggenstein-Leopoldshafen, Germany

Chemically functionalized surfaces play an important role in many nanotechnological applications. A functionalization of TiO_2 surface by adsorption of TPA ($C_6H_4(COOH)_2$) molecules has already been studied previously. It was shown that TPA has a flat orientation at low coverages and up-standing carboxyl-terminated orientation at high coverages. This up-standing orientation at the coverage of one monolayer means that the this system may found similar application to carboxyl-terminated self assembling monolayers. Metal Organic Frameworks (MOFs) is a class of material where metal ions are bound together with organic ligands forming the 2D or 3D porous structure. In addition to the use of MOFs as powders there is currently a significant interest to anchor and grow them on functionalized surfaces. The first steps in this direction were made on the TPA-functionalized TiO_2(110) surface. For this purposes the stability of the TPA/TiO_2 (110) system was tested by exposing it to the nitrogen atmosphere and subsequent NEXAFS measurements. After that the sample was immersed in the copper trifluoroacetate solution. The obtained structure was studied by NEXAFS and XPS.

O 60.31 Wed 17:30 P4

Growth of Co-Salen on NiO(001) at submonolayer coverages: A non-contact atomic force microscopy study — •Josef Grenz, Alexander Schwarz, Johannes Hattendorff, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, 20355 Hamburg

Co-Salen is a planar metal-organic Schiff base complex and known for its oxygen affinity. In a previous study we investigated the adsorption of this molecule on NaCl(001) [1,2]. The observed island growth mode indicates a rather weak molecule-surface interaction. As a result the molecular ordering within the islands is the same as in bulk Co-Salen, where the building blocks are dimers, which form a monoclinic unit cell.

Interestingly, on NiO(001), which also crystallizes in the rocksalt structure, a layer-by-layer growth is observed. Such a growth mode suggests a larger molecule-substrate interaction than on NaCl(001), most likely due to the above-mentioned oxygen affinity of Co-Salen. The measured island heights at submonolayer coverages indicate also dimers as building blocks. However, the shapes of the islands are rather irregular. In this presentation the influence of the substrate temperature on the island shape as well as the molecular ordering within the island will be discussed.

[1] S. Fremy *et al.*, Nanotechnology **20**, 405608 (2009).

[2] K. Lämmle *et al.*, Nano Lett. **10**, 2965 (2010).

O 60.32 Wed 17:30 P4

Distinction of the $SrTiO_3/NdGaO_3$ surface termination by phase resolved Second Harmonic Generation — •Thomas Fink[1], Andrea Rubano[1], Tim Günter[1], Domenico Paparo[2], Carmela Aruta[2], Fabio Miletto Granozio[2], Umberto Scotti Di Uccio[2], Lorenzo Marrucci[2], and Manfred Fiebig[1] — [1]HISKP, University of Bonn, Germany — [2]CNR-INFM Coherentia, Università Frederico II, Napoli, Italy

The development of new oxide heterostructures, like $LaAlO_3/SrTiO_3$, requires to control the substrate surface termination. Under normal conditions, a TiO_2 termination of $SrTiO_3$ is favored. However, recent experiments demonstrated that a SrO termination can be achieved by epitaxially growing the $SrTiO_3$ on a $NdGaO_3$ substrate.

Second Harmonic Generation (SHG) is an ideal tool for studying surface phenomena, since it is sensitive to surface-induced symmetry breaking. Furthermore, it allows to directly image the sample surface. Here, we report on SHG imaging of the $SrTiO_3$ /$NdGaO_3$ surface using amplified femtosecond laser pulses. For 24 unit cells of $SrTiO_3$ epitaxially grown on $NdGaO_3$, two distinct types of domains with a length scale of about 500 μm, are observed. By interference with a reference signal, we measured a 180° SHG phase shift and an additional intensity difference between both of them. The phase shift can be directly assigned to the termination of $SrTiO_3$. Thus, phase-resolved SHG is an ideal tool in order to distinct different surface terminations, opening new possibilities to control the oxide interface electronic property.

O 60.33 Wed 17:30 P4

Growth mode, morphology, and reducibility of CeO_2(111) thin films on Cu(111) — Filip Dvořák[1], Oleksandr Stetsovych[1], Michael Steger[2], El Miloudi Cherradi[2], Iva Matolínová[1], Natalya Tsud[1], Michal Škoda[1], Tomáš Skála[3], •Josef Mysliveček[1], and Vladimír Matolín[1] — [1]Charles University, Faculty of Mathematics and Physics, V Holešovičkách 2, Praha 8, Czech Republic — [2]Heinrich-Heine-Universität, Institut für Experimentelle Physik der kondensierten Materie, Universitätsstrasse 1, Düsseldorf, Germany — [3]Sincrotrone Trieste SCpA, Strada Statale 14, km 163.5, Basovizza-Trieste, Italy

We investigate morphology and degree of reduction in model oxide system CeO_2 (ceria) on Cu(111) using scanning tunneling microscopy and photoelectron spectroscopy. We identify growth mechanisms of ceria on Cu(111) - formation of incomplete oxide interfacial layer and formation of three-dimensional ceria pyramids by stacking of monolayer-high islands. Using these mechanisms we control the coverage, the number of open monolayers, and the step density of ceria thin films on Cu(111). Annealing in vacuum allows us to control besides the morphology also the degree of ceria surface reduction. We find a correlation between surface reduction and morphological stability in annealed ceria layers. Oriented and stoichiometric thin films of ceria on Cu(111) can be prepared at temperatures as low as 150 °C and 250 °C. Both the morphology and the degree of reduction of these films readily change with increasing temperature, which must be accounted for in evaluating temprature-programmed experiments with ceria on Cu(111).

O 60.34 Wed 17:30 P4

Growth and electronic structure of $MgO_{1-x}N_x$ on Mo(001) investigated by scanning tunneling microscopy/spectroscopy — •Martin Grob, Christian Pauly, Mike Pezzotta, Marco Pratzer, and Markus Morgenstern — II. Physikalisches Institut B, Otto-Blumenthal-Straße, RWTH Aachen University and JARA-FIT, 52074 Aachen

Theoretical calculations [1] predict nitrogen-doped MgO being a ferromagnetic half metal. Therefore we investigated $MgO_{1-x}N_x$ films on Mo(001) by scanning tunneling microscopy (STM) and spectroscopy (STS) at room temperature. The films were prepared by evaporation of magnesium in oxygen/nitrogen atmosphere. A concentration of up to $x = 6\,\%$ has been achieved in films up to 11 monolayers. Similarities and differences of pristine MgO and $MgO_{1-x}N_x$ were observed by STM. The electronic structure measured by STS differs in a significant way, showing additional states appearing in the band gap of MgO. The influence of the Mo substrate taking affect as a catalizer for N-dissociation is discussed as well as possible solutions in order to prepare N-doped MgO bulk for further magnetic investigations.

[1] P. Mavropoulos, M. Ležaić, and S. Blügel, Phys. Rev. B **80**, 184403 (2009).

O 60.35 Wed 17:30 P4

Photoelectron spectroscpoy of ultrathin epitaxial rare earth oxides on silicon — •Dominik Schwendt and Hans Jörg Osten — Institut für Materialien und Bauelemente der Elektronik, Leibniz Universität Hannover, Hannover, Deutschland

Thin crystalline rare earth oxide layers are a promising candidate as future high-k materials replacing silicon dioxide in various MOS applications. In order to integrate these new materials into CMOS technology, a good knowledge of the silicon - oxide interface and growth behaviour of the rare earth oxides is mandatory. Epitaxial growth not only avoids recrystallization during post-growth annealing steps but also provides good interface engineering options.

Here, we present an in situ study of the molecular beam epitaxy of rare earth oxides on silicon substrates. The growth process was monitored using reflection high-energy electron diffraction. Photoelectron spectroscopic measurements of the layers were taken at different growth stages showing the change of the electronic state of the oxide. Thus we can estimate the way the oxide layer is bound to the silicon and also draw conclusions on the successful suppression on interfacial layers.

O 60.36 Wed 17:30 P4

PTCDA monolayer growth on epitaxial graphene — •Matthias Meissner, Bernd Schröter, and Torsten Fritz — Institute of Solid State Physics, University of Jena, 07743 Jena, Germany

As a model system for organic epitaxy on graphene we have investigated the epitaxy of 3,4,9,10-perylenetetracarboxylic dianhydride (PTCDA) on epitaxial graphene (EG) with Low Energy Electron Diffraction (LEED), Angle-Resolved Ultraviolet Photoelectron Spectroscopy (ARUPS) and Scanning Tunneling Microscopy (STM). Graphene was grown by thermal decomposition of 6H-SiC(0001) in an argon atmosphere at ambient pressure [1]. For a PTCDA monolayer on EG, a new point-on-line phase has been discovered, beside that phase known already from the epitaxy of PTCDA on graphite(0001) [2]. ARUPS measurements coincide well with theoretical and experimental UPS data on thick PTCDA films [3] and show additionally a complete lack of dispersion in the PTCDA bands within experimental accuracy, confirming a weak intermolecular overlap of wave functions.

[1] K. V. Emtsev et al., Nature Materials **8**, 203 (2009).

[2] C. Ludwig et al., Physik B Condensed Matter **86**, 397 (1992).

[3] I. G. Hill et al., Chemical Physics Letters **317**, 444 (2000).

O 60.37 Wed 17:30 P4

EELS study of epitaxial graphene/Ni(111) and graphene/Au/Ni(111) — •Alexander Generalov[1], Konstantin Simonov[2], Karsten Horn[1], and Yuriy Dedkov[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]V.A. Fock Institute of Physics, St. Petersburg State University, St. Petersburg, Russia

Due to its surface sensitivity, the electron energy loss spectroscopy in reflection mode (REELS) with electron beam of low primary energy is very suitable for investigation of true and quasi two-dimensional (2D) systems. The goal of the present work is the comparative study of strongly bonded graphene/Ni(111) and quasi free standing graphene/Au/Ni(111) systems by means of REELS spectroscopy.

The graphene/Ni(111) system was prepared via thermal decomposition of ethylene C_2H_4 on the Ni(111) single crystal surface. The 2 ML Au layer was intercalated underneath graphene on Ni(111) via thermal annealing of the Au/graphene/Ni(111) system. After intercalation of gold under graphene the features in EELS spectrum which are characteristic of graphene/Ni(111) interface disappear and shift of π plasmon to the lower loss energy is observed indicating the transition of initial system of strongly bonded graphene on Ni(111) to a graphite like state. Application of the free-electron model for the dependence of surface plasma frequency on density of free carriers to our experimental results gives the value of graphene doping from Ni(111) substrate to be about of 0.05e per carbon atom relative to quasi free standing graphene on Au/Ni(111).

O 60.38 Wed 17:30 P4

Electronic scattering at defects in graphene investigated by scanning tunneling microscopy — •Marco Pratzer, Alexander Georgi, Viktor Geringer, Christian Pauly, Dinesh Subramaniam, Torge Mashoff, Marcus Liebmann, and Markus Morgenstern — II. Physikalisches Institut B, Otto-Blumenthal-Straße, RWTH Aachen University and JARA-FIT, 52074 Aachen

We investigated the electronic scattering pattern appearing at different types of defects in monolayer graphene by scanning tunneling microscopy (STM) at 5 K. The graphene sample has been prepared by exfoliation on a SiO_2-substrate and electrically contacted by indium microsoldering.

First the electronic scattering pattern appearing at a monolayer-bilayer step edge has been investigated. Using FFT-filtering a $\sqrt{3}\times\sqrt{3}$ interference pattern could be separated from the atomic corrugation, which is characteristic for the graphene intervalley scattering. The amplitude of the interference pattern decreases with increasing energy. This is caused by the growth of the equipotential lines in k-space leading to the overlap of more wave vectors and partially to a destructive interference. Further we could identify different types of point defects and their characteristic local density of states. In addition to adsorbates on top of the graphene lattice and carbon vacancies we found defects located below the graphene flake at the SiO_2 substrate. The interference pattern caused by this type of defects could be suppressed by lifting up the graphene flake from the substrate using tip induced forces.

O 60.39 Wed 17:30 P4

Vibrational spectroscopy of atomic hydrogen adsorbed on graphene — •Hyunil Kim, Thorsten Balgar, and Eckart Hasselbrink — Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany

Graphene is a promising candidate as an alternative material for future electronic devices. Thus, graphene is an very interesting system to study its properties.

Our research is focused on vibrational excited absorbates on solid state surfaces by means of VIS/IR sum frequency generation (SFG). Here we present studies on the vibrational stretching mode of atomic hydrogen on graphene. We compare our results with DFT calculations, done by Sakong et al. SFG spectroscopy offers high interface sensitivity and allows for analysing such adsorbat systems.

We generate the graphene by the chemical vapor deposition process (CVD) of ethylene on Ir(111) in an ultra high vacuum chamber. The vibrational spectroscopy is realized by a ps-lasersystem with an optical parametric generator/difference frequency generator (OPG/DFG).

S. Sakong and P. Kratzer, J. Chem. Phys. 133, 054505 (2010).

X. Han, T. Balgar and E. Hasselbrink, J. Chem. Phys. 130, 134701 (2009).

J. Coraux et al., New J. Phys. 11 (2), 023006 (2009).

O 60.40 Wed 17:30 P4

Micro Four-Point-Probe Conductivity Measurements on Graphene — •Edward Perkins, Bjarke Jørgensen, Liv Hornekaer, and Philip Hofmann — Institut for Fysik og Astronomi, Aarhus Universitet, Ny Munkegade 120, Aarhus 8000C, Denmark

Four-point-probe measurements are a well-known technique for measuring conductivity independent of contact resistances. In these experiments, we apply this method at the micrometer scale to investigate surface transport. By varying the separation and geometry of the contacts it is possible to distinguish between two-dimensional and three-dimensional conductivity. This technique thus allows us to study the details of transport at surfaces in a wide range of materials.

Measurements from epitaxial graphene on silicon carbide at room temperature and 77 K are presented. The characteristic two-dimensional transport is analysed and compared to transport in other materials. Simulations of the potential are also considered with a view to understanding the details of the conductivity profile.

O 60.41 Wed 17:30 P4

Growth of uniaxial graphene nanostructures by self-assembly — •Jens Baringhaus, Thomas Langer, Herbert Pfnür, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, 30167 Hannover, Germany

Graphene nanostructures such as ribbons and dots are building blocks for any graphene based device architecture. Furthermore, the controlled fabrication of nanostructures allows to study the feedback of defects towards the peculiar transport properties seen in perfect 2d templates. Among others the epitaxial growth of graphene on prepatterned SiC is a promising strategy for growing such nanostructures on insulating substrates.

Using vicinal 4H-SiC(0001) substrates (4°miscut) the in-situ graphitization process has been monitored by spot profile analysis LEED and angle resolved electron energy loss spectroscopy (ELS). At first for temperatures above 1200° step bunching sets in. The flat terrace sites are in the order of 20 nm, thus, the initial structural anisotropy in not reflected in the plasmon dispersion of graphene. In a second approach uniaxial mesa structures of 6H-SiC(0001) ($1\mu m$ in width) were fabricated by means of photolithography and reactive ion etching (RIE). Heating of the substrate induces step flow and the development of inclined nano-facets. At high temperatures silicon desorbs predominantly from these nano-facets leading to the formation of graphene ribbons. The structure and plasmon properties are analyzed by SEM, STM and EELS. In addition, also first transport properties will be presented.

O 60.42 Wed 17:30 P4

Growth of Graphene on Ir(100) — •Pascal Ferstl, Matthias Gubo, Lutz Hammer, and M. Alexander Schneider — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Graphene monolayers have been grown on a variety of different metal substrates with hexagonal symmetry. In contrast, the growth on substrates with square symmetry remains rather unexplored so far. Therefore, we have studied graphene growth on a Ir(100) surface by means of LEED and STM. Both, temperature programmed growth (TPG) and chemical vapour deposition (CVD) at various temperatures were tested with C_2H_4 as reacting gas. For TPG we find as a function of the reaction temperature a sequence of different superstructures indicative of the stepwise hydrocarbon decomposition towards surface carbide. Randomly oriented graphene islands are formed for temperatures above 700°C. By CVD at 700 - 900°C graphene forms domains oriented along the [001] direction, with an angular tolerance below ±4°. There are no indications for a Moiré structure from the LEED pattern. In contrast, ethylene deposition at higher temperatures (900 - 1300°C) leads to a preferential alignment of the graphene layer 5° off [001]. Also, a complex Moiré pattern is observed in LEED. In STM we find two graphene phases for all deposition temperatures: one being essentially flat, while the other shows a linear corrugation with an amplitude of up to 3 Å and a lateral spacing of about 22 Å. Possible structural models will be discussed.

O 60.43 Wed 17:30 P4

Inhomogeneous electronic properties of monolayer graphene on Ru(0001) — •Mike Gyamfi, Thomas Eelbo, Marta Waśniowska, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, 20355 Hamburg

Understanding properties of the interface between graphene and a metal surface has recently gained considerable attention. In case of Ru(0001) the linear dispersion of monolayer graphene is not preserved due to the hybridization between C and Ru orbitals at the interface [1]. In order to get access to the electronic structure inside the Moiré pattern of graphene we performed spatially resolved STS at low temperature. We report on direct evidences for variations of the electronic properties regarding the exact position of the carbon atoms with respect to Ru atoms and the corrugation within the subunit cell. The shape of dI/dU spectra is quite similar on all parts of the Moiré pattern, the spectra differ only by a slight shift, $\Delta E = 30$ meV, of the peak position at -0.4 eV and its intensity. This small energy difference is related to the carbon and Ru atoms' hybridization upon growth of graphene on the Ru surface. A detailed analysis revealed that the dominant peak at -0.4 eV originates from a *d*-like Ru bulk state.

[1] T. Brugger *et al.*, *Phys.Rev.B* **79**, 045407 (2009)

O 60.44 Wed 17:30 P4

Controlled fabrication of nanocrystalline graphene films on insulating substrates — •Nils-Eike Weber[1], Rainer Stosch[2], Armin Gölzhäuser[1], and Andrey Turchanin[1] — [1]Physik supramolekularer Systeme und Oberflächen, Fakultät für Physik, Universität Bielefeld — [2]Physikalisch-Technische Bundesanstalt, Braunschweig

We report on the fabrication and characterization of nanocrystalline graphene films on insulating substrates. Graphenoid (graphene like) carbon nanosheets with a thickness of 1 nm were made by the electron beam induced cross-linking of aromatic self-assembled monolayers. When transferred onto insulating substrates, the graphenoid sheets were converted into nanocrystalline graphene by thermal annealing. We used thermal annealing in an argon atmosphere to produce large area (cm square or larger) films of nanocrystalline graphene with a well defined thickness on silicon oxide wafers and quartz glass. The electrical conductivity was measured at room temperature by four point probe measurements. The structure and chemical composition were studied by X-ray photoelectron and Raman spectroscopies. Since the electrical conductivity, thickness and optical properties of the graphene films can be well controlled, the suggested method opens broad prospects for the fabrication of transparent conductive coating.

O 60.45 Wed 17:30 P4

Mechanically stacked 1 nm thick carbon nanosheets: 2D layered materials with tunable optical, chemical and electrical properties — Christoph Nottbohm[1], Andrey Turchanin[1], André Beyer[1], Rainer Stosch[2], •Matthias Büenfeld[1], Andreas Winter[1], and Armin Gölzhäuser[1] — [1]Physik supramolekularer Systeme und Oberflächen, Fakultät für Physik, Universität Bielefeld — [2]Physikalisch-Technische Bundesanstalt, Braunschweig

Carbon nanosheets are mechanically stable free-standing two-dimensional materials with a thickness of ˜1 nm and well defined physical and chemical properties. They are made by radiation induced cross-linking of aromatic self-assembled monolayers. Here we present a route to the scalable fabrication of multilayer nanosheets with tunable electrical, optical and chemical properties. Stacks up to five nanosheets with sizes of ˜1 cm2 on oxidized silicon were studied. Their optical characteristics were investigated by optical microscopy, UV/Vis reflection spectroscopy and model calculations. Their chemical composition was studied by X-ray photoelectron spectroscopy. The samples were then annealed in ultra high vacuum at various temperatures up to 1100 K. A subsequent investigation by Raman, X-ray photoelectron and UV/Vis reflection spectroscopy as well as by electrical four-point probe measurements demonstrates that the layered nanosheets transform into nanocrystalline graphene. This structural transformation is accompanied by changes in the optical properties and electrical conductivity and opens up a new path for the fabrication of ultrathin functional conductive coatings.

O 60.46 Wed 17:30 P4

An analytical approach to the spectrum of π electrons in bilayer graphene nanoribbons and nanotubes — •Julius Ruseckas[1], Gediminas Juzeliunas[1], and Igor Zozoulenko[2] — [1]Institute of Theoretical Physics and Astronomy, Vilnius University, A. Goštauto 12, LT-01108 Vilnius, Lithuania — [2]Solid State Electronics, ITN, Linköping University, 601 74 Norköping, Sweden

We present an analytical description of π electrons of a finite size bilayer graphene within a framework of the tight-binding model. The considered bilayered structures are characterized by a rectangular geometry and have a finite size in one or both directions with armchair- and zigzag-shaped edges. An exact analytical description of the spectrum of π electrons in the zigzag and armchair bilayer graphene nanoribbons and nanotubes is provided. The exact solution of the Schrödinger problem, the spectrum and wave functions, has been obtained and used to analyze the density of states and the conductance quantization.

O 60.47 Wed 17:30 P4

Electronic and structural properties of hydrogen-intercalated monolayer graphene on SiC(0001) — •Stiven Forti[1], Camilla Coletti[1], Konstantin Emtsev[1], Dong Su Lee[1], Alexei Zakharov[2], Jurgen H. Smet[1], and Ulrich Starke[1] — [1]Max-Planck-Institute for Solid State Research, Heisebergstr. 1, 70569 Stuttgart, Germany — [2]MAX-lab, Lund University, Lund, S-22100, Sweden

The growth of epitaxial graphene on SiC is one of the most promising techniques to provide large area, homogeneous graphene. In this work we demonstrate the possibility to combine the growth of epitaxial graphene under Ar atmosphere [1] with the capability of decoupling the carbon interface layer from the substrate by means of hydrogen intercalation [2] to obtain large area, homogeneous, free standing and undoped graphene on top of SiC(0001). The quality of the graphene samples is demonstrated by a variety of surface science experiments. AFM shows a morphology with regular steps and large terraces. Low defect concentration is revealed by Raman spectroscopy. LEEM highlights the homogeneity of the electronic structure on a micrometer scale with nanometer resolution. High-resolution ARPES shows extremely sharp bands with the dispersion of a free-standing monolayer graphene, confirming the good quality of the graphene obtained via this process and therefore demonstrating the effective decoupling of the carbon layer from the SiC substrate. [1] K.V. Emtsev et al., Nat. Mat. 8, 203(2009), [2] C. Riedl et al., PRL 103, 246804(2009).

O 60.48 Wed 17:30 P4

Kelvin probe and atomic force microscopy of pristine and irradiated graphene sheets — •Oliver Ochedowski, Benedict Kleine Bussmann, Sevilay Akcöltekin, and Marika Schleberger — Universität Duisburg-Essen, Lotharstr. 1 47048 Duisburg

We have prepared graphene by mechanical exfoliation on SrTiO3 and TiO2 single crystalline surfaces and transferred them into an Ultra-Hgih-Vacuum system. By using an atomic force microscope and the

Kelvin probe technique the contact potential differences (CPD) of graphene are mapped. The CPD is directly linked to the work function and is used to study doping effects induced by the substrate, adsorbates, water as well as laser and particle irradiation.

We show that graphene on SrTiO3 exhibits an accumulation of carriers corresponding to n-type doping and that water underneath the graphene decreases this effect. Irradiating graphene with laser light at a wavelength of 514,5 nm (5 mW, spot size: 1 micrometer^2), leads to a cleaning effect already after 5 minutes, followed by the formation of defects after about 10 minutes. Furthermore, we present KPFM measurements of graphene irradiated with swift heavy ions under glancing angles of incidence.

O 60.49 Wed 17:30 P4

Graphene and graphene nanodots on Ir(111) — •Andreas Zusan[1], Philipp Leicht[1], Muriel Sicot[1], Mikhail Fonin[1], Yuriy S. Dedkov[2], and Karsten Horn[2] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz — [2]Fritz-Haber-Institut der Max-Planck Gesellschaft, 14195 Berlin

The investigation of the electronic properties of graphene nanostructures is one of the most fundamental requirement on the route towards graphene based nanoelectronics. Within these studies a weak chemical bonding between the carbon monolayer and the substrate is required. For this purpose we used an Ir(111) substrate for the preparation of quasi-freestanding graphene and graphene nanodots by the decomposition of hydrocarbons. The topographic properties as well as the local electronic properties were studied by means of scanning tunneling microscopy and scanning tunneling spectroscopy. The nanodots exhibit a typical size of about 15 to 25 nm and show the well known Moiré superstructure. The edges of the nanodots are predominantly running along the main crystallographic directions of the Ir(111) substrate and the edge structure was determined to be of a zigzag type.

O 60.50 Wed 17:30 P4

Local electronic structure of graphene on SiC(0001) studied by scanning tunneling microscopy and spectroscopy — •Thomas Druga, Martin Wenderoth, and Rainer G. Ulbrich — IV. Physikalisches Institut, Georg-August-Universität Göttingen

In this work we present a low temperature (6K) scanning tunneling microscopy study of mono- and bilayer graphene on the silicon-terminated 6H-SiC(0001) surface. The untreated crystals were electrically contacted exsitu by tantalum foils. After annealing at base pressure of $1 * 10^{-10}$ mbar at 500°C for several hours the samples were graphitized between 1350°C and 1450°C by direct current heating. This preparation technique results in graphitized surfaces of mainly mono- and bilayer graphene up to a few hundred nm. Atomically resolved topographies of monolayer graphene show the honeycomb structure of the graphene layer, the 6x6 periodicity and disordered adatom features induced by the underlying interface layer [1]. These features have a strong influence on lateral resolved differential conductivity maps dI/dV(x,y) measured by scanning tunneling spectroscopy (STS) and demonstrate the necessity of a high lateral resolution to study the electronic properties of graphene. On bilayer graphene dI/dV - spectra show in addition to spectral features observed by other groups [e.g. 2] atomic scale modulations according to the 6x6 periodicity. This work was supported by the DFG as part of SFB 602 Tp A7.

[1] Rutter et al. Phys. Rev. B 76, 235416 (2007) [2] Lauffer et al. Phys.Rev. B 77, 155426 (2008)

O 60.51 Wed 17:30 P4

Production Nitrogen Doped Graphene on Ni(111) Surface — •Wei Zhao, Junfa Zhu, Oliver Höfert, Karin Gotterbarm, Christian Papp, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

Graphene, the 2D-carbon network is considered as one of the most promising candidates for the post-silicon semiconductor materials.[1] Referring to the classic semiconductor research route, introducing hetero-atoms to the graphene sheet will modify the electronic properties and make it possible to use it in realistic applications. Therefore, nitrogen doped graphene sheets on a Ni(111) surface were prepared by low energy nitrogen sputtering of graphene below 150 K and also directly by exposure of the Ni(111) surface to pyridine at elevated temperatures. Applying in-situ high resolution X-ray photoelectron spectroscopy, the structure and thermal stability of N-doped graphene sheets on Ni(111) were investigated. It is found that at 900 K the graphitic-N and the pyridinic-N dominate the nitrogen doped parts in the sputtered graphene layers, of which the nitrogen concentration is $\sim$ 1.5%. For the graphene sheet prepared from exposure to pyridine pyridinic-N is the main structure element found. Here we achieve a doping of with $\sim$ 1.7% of nitrogen. Moreover a closer examination of the thermal stability of these layers was conducted.

Support is acknowledged from the BMBF (05 ES3XBA/5) and the Cluster of Excellence "Engineering of Advanced Materials". [1]Novoselov, K.S., et al. Science, 2004. 306(5696).

O 60.52 Wed 17:30 P4

Ambipolar doping in quasi-free epitaxial graphene on SiC(0001) controlled by Ge intercalation — •Konstantin Emtsev[1], Alexei Zakharov[2], Camilla Coletti[1], Stiven Forti[1], and Ulrich Starke[1] — [1]Max-Planck Institute for Solid State Research, Stuttgart, Germany — [2]MAX Lab, Lund University, Lund, Sweden

Growth of graphene on single crystals of SiC is considered among the most promising routes for large scale graphene fabrication [1]. Recently we have shown that the electronic structure of graphene on SiC(0001) can be tailored by controlling the atomic structure of the interface [2]. In the present work we utilized the intercalation phenomenon to introduce atomically thin layers of germanium at the interface between the graphene-like $(6\sqrt{3}\times6\sqrt{3})$R30°-reconstructed buffer layer and the SiC surface. The expanded interface decouples the graphene from the SiC surface structurally and electronically. A quasi-free standing graphene monolayer develops and shows moderate p- or n-doping depending on the amount of Ge intercalated. We present a detailed study of the structural and electronic properties of such films. The samples were characterized by high resolution ARPES and XPS. In addition, microscopic properties of Ge-intercalated graphene films were investigated in detail by means of low-energy electron microscopy (LEEM). Importantly, relatively low temperatures required for the intercalation have enabled us to capture the transformation process by LEEM in situ in real-time. [1] P.N. First et al., MRS Bulletin, 35, 296 (2010). [2] C. Riedl et al., Phys. Rev. Lett. 103, 246804(2009)

O 60.53 Wed 17:30 P4

YIELD and Kelvin probe study of graphene — •Samir Mammadov, Jürgen Ristein, and Thomas Seyller — Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Germany

Subject of this study is the investigation of the work function and photo-YIELD of epitaxial graphene(EG) films. Two types of samples were investigated: regular EG films and H-intercalated EG films, referred to as quasi-freestanding graphene (QFG). EG films were formed by thermal decomposition on the Si-face of n-type 6H-SiC substrates and QFG samples were formed by subsequentially intercalating EG samples by hydrogen.

The work function was determined precisely for each type of samples.The YIELD spectra of the different samples display significant variation which will be discussed in details.

O 60.54 Wed 17:30 P4

Self-assembly of Pt, Ru and bimetallic PtRu clusters on Ru(0001) supported monolayer graphene — •Albert K. Engstfeld[1], Christoph U. Lorenz[1], Ottavio B. Alves[1], Harry E. Hoster[1,2], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — [2]Current address: Technische Universität München, Centre for Electromobility, 50 Nanyang Drive, Singapore 637553

The Moiré-type nm-scale patterns of graphene monolayers on metal single crystals were recently shown to allow facile fabrication of ordered arrays of virtually monodisperse metal nanoclusters by simple metal vapour deposition in UHV [1-3]. In view of a potential utilization as structurally well defined model systems in electrocatalysis, with extremely small metal clusters, we have tested the possibility of preparing Ru and bimetallic PtRu clusters by an analogous procedure. Based on statistically evaluated STM images, we will report on the nucleation behaviour of Ru and Pt clusters respectively and its consequences on bimetallic PtRu cluster growth, depending on the evaporation sequence of the two metals.

[1] A.T. N'Diaye et al., New J.Phys. 11, 2009, 103045.

[2] Yi Pan et al., Appl.Phys.Lett. 95, 2009, 093106.

[3] K. Donner and P. Jakob, J.Chem.Phys. 131, 2009, 164701.

O 60.55 Wed 17:30 P4

Intrinsic Voltage Rectification in a Graphene Nano Device — •Robert Göckeritz[1], Jörg Pezoldt[1], and Frank Schwierz[2] —

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Recently, voltage rectification effects at GHz frequencies have been observed in three-terminal junctions (TTJ) based on III-V heterojunctions. In the present work, such effects at DC voltages are reported for the first time in TTJs made of epitaxially grown graphene. Most notably, our T-shaped TTJ devices show a pronounced rectification behavior already at room temperature.

The graphene was grown on SiC using a high temperature process at 1800°C under atmospheric pressure applying a carbon capping technique prior to growth. The 50 nm wide and 500 nm long graphene devices were patterned by electron beam lithography. Raman spectroscopy revealed the fingerprint of graphene and AFM, XPS and electrical measurements have been performed.

The reported room-temperature rectification in graphene TTJs may pave the way for new applications of graphene in electronics.

O 60.56 Wed 17:30 P4

Raman spectroscopy of quasi-freestanding monolayer graphene — •Felix Fromm, Florian Speck, Martin Hundhausen, and Thomas Seyller — Universität Erlangen-Nürnberg, Lehrstuhl für Technische Physik, 91058 Erlangen, Germany

The epitaxial growth of graphene on silicon carbide (SiC) by thermal sublimation of silicon in an argon atmosphere is a promising method to produce high quality graphene layers. We focus here on the mechanical properties of graphene samples produced by converting the $(6\sqrt{3}\times 6\sqrt{3})R30^\circ$ reconstructed surface into a quasi-freestanding graphene monolayer on hydrogen terminated SiC. Raman spectroscopy of graphene is well suited to determine mechanical strain by measuring the frequency shifts of phonon modes. We evaluate the strain from the shift of the 2D peak in the Raman spectrum. Intercalation of the $(6\sqrt{3}\times 6\sqrt{3})R30^\circ$ surface reconstruction at 550°C results in tensile strained graphene. The size of strain however is reduced with prolonged intercalation time. After intercalation at higher temperature the obtained graphene layers show much smaller tensile strain.

O 60.57 Wed 17:30 P4

Gas permeation in graphenoid nanomembranes — •Nils Mellech[1], Xianghui Zhang[1], Elina Oberländer[1], André Beyer[1], Edgar Hansjosten[2], Roland Dittmeyer[2], and Armin Gölzhäuser[1] — [1]Faculty of Physics, Bielefeld University, Postfach 10 01 31, 33501 Bielefeld, Germany — [2]Karlsruhe Institute of Technology, Institute for Micro Process Engineering (IMVT), Karlsruhe, Germany

Permeation and selectivity measurements with helium and argon are carried out on freestanding nanomembranes of cross-linked self-assembled mono- and multilayers. The monolayers of 1,1'-biphenyl-4-thiol and 4'-nitro-1,1'-biphenyl-4-thiol are prepared on gold on mica and cross-linked by electron irradiation which results in layer thicknesses of approximately 1 nm. Afterwards the nanomembranes are transferred either onto millimeter-sized polished sintered porous steel substrates or onto a micron-sized opening in a silicon nitride window on silicon substrates. The latter samples are investigated with an ultrahigh vacuum permeation measurement system based on a quadrupole mass spectrometer. The nanomembranes seal the UHV chamber from the high pressure feed gas side of the system and remain stable for days under pressures up to 30 kPa. The nanomembranes on the porous substrates are characterized by a gas flow measurement system. The membranes cover the pores and substantially reduce the gas flow. Permeation properties of the nanomembranes are discussed based on the measured data.

O 60.58 Wed 17:30 P4

Experimental indication of quantum mechanical effects in surface enhanced IR-spectroscopy? — •Jörg Bochterle[1], Frank Neubrech[1], Annemarie Pucci[1], Dominik Enders[2], and Tadaaki Nagao[2] — [1]Kirchhoff-Institute for Physics, Heidelberg, Germany — [2]Institute for Material Science, Tsukuba, Japan

The conduction electrons of metal nanoparticles can be collectively excited by incident electromagnetic radiation. Their resonance frequency strongly depends on the geometric dimensions of the particles and can be tuned from the classical radio frequencies up to the visible range. Such resonantly excited localized surface plasmon-polaritons are accompanied by an electromagnetic nearfield enhancement at the surface. In the infrared spectral range these huge local fields can be applied to the enhancement of infrared vibrations of molecules. Using this technique with gold nanostripes, attomol sensitivity has been achieved.

In this contribution we look at the signal enhancement of the carbon monoxide (CO) stretching vibration of physisorbed CO ice on gold nanoantennas on silicon substrates under ultrahigh vacuum conditions. The signal changes with increasing CO layer thickness are measured in situ and exhibit a behavior differing from the classical expectations. While in the classical description the nearfield is monotonically increasing with decreasing distances to the surface, the quantum description of the localized plasmon resonance exhibits such monotonic increase only down to a certain distance and then decreases for smaller distances to the surface.

O 60.59 Wed 17:30 P4

Infrared optical properties of gold nanoantenna arrays — •Daniel Weber[1], Frank Neubrech[1], Han Gui[2], Dominik Enders[2], Tadaaki Nagao[2], and Annemarie Pucci[1] — [1]Kirchhoff Institute for Physics, Heidelberg, Germany — [2]National Institute for Materials Science, Tsukuba , Japan

Antenna-like gold nanoparticles are proven to be well-suited for spectroscopic applications due to their tuneable plasmonic properties. Excited resonantly by electromagnetic radiation, they are able to strongly enhance the local electromagnetic field. This effect can be exploited for example for surface-enhanced infrared (IR) spectroscopy, making the detection of very small amounts of molecules possible. Although the investigation of single particles is possible, well-arranged arrays of nanoantennas promise to have greater potential for possible sensor applications since the overall sensitivity can be increased if several nanoantennas interact. In this paper, we report on the IR optical properties of gold nanoantenna arrays and show the dependence of characteristic resonance parameters from the geometrical arrangement of the antennas on the substrate. The stripe-like, polycrystalline gold nanoantennas with rectangular cross-sections were produced by electron beam lithography on silicon wafers. The resonance characteristics were extracted from spectroscopic measurements with our IR microscope. Special focus herein is on interaction between nanoantennas in direction perpendicular to the long particle axis. It is shown that beginning from a crucial distance, the optical properties change dramatically if the gap between the nanoantennas is further decreased.

O 60.60 Wed 17:30 P4

Cutting gold nanoantennas by focused ion beams — •Daniel Weber[1], Frank Neubrech[1], Han Gui[2], Dominik Enders[2], Tadaaki Nagao[2], and Annemarie Pucci[1] — [1]Kirchhoff Institute for Physics, Heidelberg, Germany — [2]National Institute for Materials Science, Tsukuba , Japan

Gold nanowires (nanoantennas) are plasmonic particles of great interest due to the possibility of tuning their ability to strongly enhance the local electromagnetic field from the THz to the visible range by mainly changing the length. Furthermore, coupling of nanoparticles can lead to even higher enhancement of the local field compared to invidual particles. One very promising approach is an arrangement of two nanoantennas which are separated by a very small gap (few nm) between their tip ends. We tried to prepare such nanosized gaps by applying focused ion beam (FIB) milling. Stripe-like, polycrystalline gold nanoantennas were produced by electron beam lithography on silicon wafers and subsequently cut in the middle by FIB. It turned out that the question if the nanoantennas are really separated cannot be answered by scanning electron microscopy or FIB imaging. However, measuring the infrared optical response of such prepared dimers provides a non-contacting, non-destructive, and easy method to prove the successful cut. Alternative methods like cross-sectional transmission electron microscopy and energy dispersive spectroscopy were also applied to confirm the findings from IR spectroscopic measurements.

O 60.61 Wed 17:30 P4

Modelling of Optical Nanoantennas for Nonlinear Spectroscopy — •Daniela Ullrich[1,2], Thorsten Schumacher[1,2], Harald Giessen[2], and Markus Lippitz[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]4th Physics Institute, University of Stuttgart

The null-field method (also known as the T-Matrix approach) is a powerful tool to simulate the light scattering by single and compound particles. Here, we demonstrate that our nonlinear transient transmission measurements on single as well as antenna-coupled gold nanoparticles can be modelled numerically using the null-field method. This allows us to further optimize the optical nanoantennas with the help of the simulations. Additionally, other materials such as aluminium or silver can be included. We compare the predicted behavior to our measurements on the optimized antenna structures. Finally we show that the numerical model can be adapted to describe plasmon-enhanced sensing using dielectric nanoparticles.

O 60.62 Wed 17:30 P4

Optical properties of gold nanorings prepared by different lithography methods — •Yuliya Fulmes[1], Kai Braun[2], Christian Schäfer[1], Andreas Horrer[1], Dominik Gollmer[1], Dai Zhang[2], Alfred Meixner[2], Dieter Kern[1], and Monika Fleischer[1] — [1]Institute of Applied Physics, University of Tuebingen, 72076 Tuebingen, Germany — [2]Institute of Physical and Theoretical Chemistry, University of Tuebingen, 72076 Tuebingen

Gold nanorings feature a variety of optical phenomena and exhibit a size- and shape-dependent resonance wavelength tuneable over a wide range in the visible and near-infrared spectrum. Different approaches have been pursued for the preparation of gold nanorings. In the first one, the individual rings are fabricated from a thin gold layer by HSQ e-beam lithography followed by angular argon ion milling. In the second one, Au rings are produced using colloidal lithography. A gold film is evaporated onto polystyrene particle coated substrates. During argon ion milling secondary sputtering of material creates a gold shell around the sides of the particles, which are removed afterwards. In the third approach, the patterns are defined in PMMA by e-beam lithography. Gold rings are obtained after a standard lift-off process of a gold layer which was deposited after development of PMMA. Using the above-mentioned methods it is possible to structure gold nanorings of many desirable sizes and geometries. The optical properties of the structures under excitation with an electromagnetic field are simulated by means of finite element methods and investigated in a parabolic mirror confocal microscope.

O 60.63 Wed 17:30 P4

SEIRS with gold nanoantennas towards health diagnostics — Frank Neubrech[1], Daniel Weber[1], Jörg Bochterle[1], Wolfgang Petrich[1], •Annemarie Pucci[1], Javier Aizpurua[2], Enzo Di Fabrizio[3], and Marc Lamy De La Chapelle[4] — [1]Kirchhoff Institute for Physics, Heidelberg, Germany — [2]Donostia International Physics Center, Donostia-San Sebastian, Spain — [3]Italian Institute of Technology, Genoa, Italy — [4]University Paris 13, Bobigny, France

It is well established, that plasmonic oscillations in metal nanorods efficiently enhance near-field under resonant conditions. In the infrared, fundamental antenna-like resonance can be used for surface-enhanced infrared spectroscopic (SEIRS) studies. In the project NANOANTENNA we optimize such system for application of SEIRS to the detection of rare biomolecular disease indicators in the human blood. Accordingly, as first step, a biocompatible material combination was identified and secondly, the resonance condition is optimized.

O 60.64 Wed 17:30 P4

Volume plasmon modes in Ag@Au core-shell nanoparticles — Katja Höflich[1], Aliaksei Dubavik[2], Nikolei Gaponik[2], Silke Christiansen[1], Alexander Eychmüller[2], Lukas M. Eng[3], and •Thomas Härtling[4] — [1]Max-Plack-Institut für Mikrostrukturphysik, 06120 Halle, Germany — [2]Physikalische Chemie und Elektrochemie, TU Dresden, 01062 Dresden, Germany — [3]Institut für Angewandte Photophysik, TU Dresden, 01062 Dresden, Germany — [4]Fraunhofer Institut für Zerstörungsfreie Prüfverfahren, 01109 Dresden, Germany

In the case of special nanoparticle geometries like e.g. spherical nanoshells and cylindrical core-shell structures, classical light can not only excite surface plasmons, but also volume plasmon modes [1, 2]. We investigate the properties of such a volume mode in core-shell Au@Ag nanoparticles which we find manifested as an UV extinction peak in the plasmonic spectrum. Analytical calculations with varied dielectric functions for the particle shell demonstrate that the mode occurs if the permittivity of the shell vanishes. We furthermore provide both theoretical and experimental proof that in contrast to surface plasmon modes the spectral position of the volume mode is independent of the core-shell geometry. To this end, we calculated and prepared Au@Ag particles with different geometries and compare their extinction spectra. [1] K. Höflich, U. Gösele, C. Christiansen, Phys. Rev. Lett. 103, 087404 (2009) [2] K. Höflich, U. Gösele, C. Christiansen, J. Chem. Phys. 131, 164704 (2009)

O 60.65 Wed 17:30 P4

Fabrication and Application of Nanostructured Substrates for Surface Enhanced Raman Spectroscopy — •Sabrina Darmawi, Limei Chen, Torsten Henning, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Giessen

Detecting single nanoparticles or small concentrations of particles within a chemical complex has become more and more important. With the application of manufactured nanoparticles, such as oxides, in our daily products, concerns about our safety and their impact on us increase. In order to detect metal oxides, such as ZnO or TiO_2, a greatly sensitive approach of detection is necessary. With surface enhanced Raman Spectroscopy (SERS) the weak Raman signal can be amplified considerably. This can be achieved by a pattern of rhomb arrays that are transferred on a silicon substrate via electron beam lithography. As an alternative pathway to the subtractive method, the additive technique (lift-off) is used by evaporating silver or gold layers on the developed structure. Interactions between the analyte and the metallic lateral tip nanostructured surface lead to plasmonic excitations which cause a high electromagnetic field enhancement at the tips of the rhombs. For purposes of testing, engineered nanoparticles such as ZnO are deposited on the structured substrate. The resulting system is investigated by SERS and we will report on the dependence of the Raman signal on the tip parameters.

O 60.66 Wed 17:30 P4

Quantum-size effects on the dielectric response of metal clusters — •Koray Koksal[1,2], Yaroslav Pavlyukh[2], and Jamal Berakdar[2] — [1]Physics Department, BitlisEren University, Bitlis, 13000, Turkey — [2]Institüt für Physik, Martin-Luther-Universitat Halle-Wittenberg, Heinrich-Damerow-Strasse 4, 06120 Halle, Germany

We present analytical and numerical techniques and calculations for the quantum, dielectric response of metal clusters and elucidate the dependencies on the clusters size and topology. The calculations have been performed for Al, Ag and Cu clusters. We will discuss possible ways for the experimental verification on the basis of scanning tunneling spectroscopy [1] and electron energy loss spectroscopy [2] and also point out the relevance to nano-plasmonics.

[1] L. Limot, E. Pehlke, J. Kröger, and R. Berndt, Phys. Rev. Lett. 94, 036805 (2005)

[2] J. W. L. Eccles, U. Bangert, M. Bromfield, P. Christian, A. J. Harvey and P. Thomas, J. Phys.: Conf. Ser. 241, 012090 (2010)

O 60.67 Wed 17:30 P4

Observing optical transitions inside an STM junction: a study on field emission resonances and molecular wires — •Gunnar Schulze, Thomas Sirtl, Marten Piantek, Jingcheng Li, Katharina Franke, and Jose Ignacio Pascual — Institut für Experimentalphysik, Freie Universität Berlin, Berlin, Germany

Light emitted from direct optical transitions of tunneling electrons in a scanning tunneling microscope (STM) junction can provide rich information about electronic systems. Resulting spectra reflect the interaction of plasmonic and electronic degrees of freedom and can reveal an energy resolved picture of dipole active inelastic transitions during tunneling. Our STM light emission (STM-LE) experiments aim to get closer insights into the nature of these effects. In our study on field emission resonances (FER) on a metal surface we demonstrate the observation of direct optical electron transitions. A second study deals with the activation of inelastic transitions inside a single molecular wire and their effects on the STM-LE spectra.

O 60.68 Wed 17:30 P4

Leakage radiation microscopy of surface plasmons — •Jörg Schmauder, Michael Lutz, Stephen Riedel, Paul Leiderer, Elke Scheer, and Johannes Boneberg — Universität Konstanz

We excite surface plasmons on metal layers (Ag, Au) using an ATR (attenuated total reflection) setup in Kretschmann-configuration with a laserdiode at the wavelenght of 980 nm. A small fraction of the surface plasmons is scattered at the surface into the half space above the prism. The natural roughness of the metal film is sufficient for this scattering process.

We observe the light emitted from the scattered surface plasmons by optical microscopy in dark field mode (leakage radiation microscopy). We report on the decay of the surface plasmons as well as on interference patterns around step structures and optical elements like mirrors, curved mirrors and diffractive gratings.

O 60.69 Wed 17:30 P4

Calculation of the Equilibrium Electron Density of Plasmonic Nanostructures — •Timo Köllner, Kurt Busch, and Jens Niegemann — Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany

The hydrodynamic description of plasmonic devices allows the modeling of the nonlocal and nonlinear response of such structures to optical excitation. However, in order to properly conduct numerical calculations of the full hydrodynamic model, one first needs to find the equilibrium electron density of the system. In particular, the behaviour of the density at the surface of a metallic object is suspected to have a significant influence.

Here, we present an efficient and accurate finite-element approach to calculate the equilibrium electron density distribution and the electrostatic fields at the edge of the positively charged jellium background.

O 60.70 Wed 17:30 P4

Kerr-microscopy of magnetic nanostructures — •Christian Dicken[1,2], Klas Lindfors[1,2], Mario Hentschel[1,2], and Markus Lippitz[1,2] — [1]Max-Planck-Institute for Solid State Research, Stuttgart — [2]4th Physics Institute, University of Stuttgart

Merging the fields of micromagnetism and plasmonics promises many new applications in both industry and science. As a first step towards experiments on micromagnetic particles, we use a combination of Sagnac interferometry and an improved sample design to measure the magnetization of isolated nickel-gold particle systems. With the present technique, we were able to observe the Kerr rotation of particles smaller than 90nm in diameter with an SNR of 28. We will show a model that describes the size dependence of the signal and allows us to adapt our sample design for even better performance.

O 60.71 Wed 17:30 P4

Development of a Raman Correlation Spectroscopy Experiment — •Aude Barbara[1,2], Tomas Lopez-Rios[1], Pascal Quémerais[1,3], Martin Helfrich[2], and Lukas Eng[2] — [1]Institut Néel, CNRS-UJF, Grenoble, France — [2]IAPP, TU Dresden, Germany — [3]MPI-PKS, Dresden, Germany

We develop a Raman Correlation Spectroscopy (RCS) experiment. Analogous to Fluorescent Correlation Spectroscopy, we measure the time-dependence of Raman band intensities of particles in solution. The main advantages of Raman spectroscopy is its direct chemical selectivity and its non-dependence to the wavelength while its biggest drawback its cross-section that may be up to 10^{14} times smaller than that of the fluorescence. However, adding metallic colloids may significantly enhance the Raman signal. Taking advantage of this SERS (Surface Enhanced Raman Scattering) effect has two goals: (i) increase the sensibility of the RCS experiments and (ii) establish a direct link between the Raman exaltation and the size of the metallic colloids which can be simultaneously measured. More insight into the SERS mechanism could thus be obtained. We present the preliminary experiments that aim at demonstrating the capabilities of the set-up to perform reliable time-dependent and particle sizing measurements. Experiments done with fluorescent and Raman light on toy-system will also be presented.

O 60.72 Wed 17:30 P4

Surface plasmon polariton induced electronic transport through metallic nanostructures — •Daniel Benner, Matthias Bädicker, Johann Berres, Reimar Waitz, Johannes Boneberg, Paul Leiderer, and Elke Scheer — Universität Konstanz, Fachbereich Physik

We investigate the influence of pulsed and cw laser light onto the electronic transport through a metallic nanoconstriction. Light-matter interaction, in particular when the matter is in the nanometer scale, is an important and steadily growing field of research due to possible applications in opto-nanoelectronics. We use lithographically fabricated Mechanically Controllable Break-junctions (MCBJs) operated at ambient conditions for fabricating atomic-size contacts and atomically-sharp tips of gold. Detailed analysis of light-induced conductance changes has shown photo-assisted transport due to the excitation of high-energetic quasiparticles [1] and collective effects such as surface plasmon excitation. Also optical near fields due to antenna effects as well as thermal expansion contribute to the signal [2, 3, and 4]. We optimize the plasmon-induced effect for the development of optoelectronic devices by studying systematically the effects on different wavelengths, position of the laser spot, and geometries (e.g. design of the nanocontacts and polarization of the laser light). [1]J.K. Viljas et al., Phys. Rev. B 75, 075406 (2007) [2]D. Guhr et al., Phys. Rev. Lett. 99, 086801 (2007) [3]D. Guhr et al., J. of Microscopy 229, 407 (2008) [4]N. Ittah et al., Nano Lett. 9, 4 (2009)

O 60.73 Wed 17:30 P4

Gold nanocones for Raman-based biosensing — •Christian Schäfer, Katharina Broch, Yuliya Fulmes, Dominik Gollmer, Frank Schreiber, Dieter Kern, and Monika Fleischer — Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

Raman spectroscopy is a powerful tool for detection and analysis of biomolecules because it delivers a specific fingerprint of the tested molecule. In order to develop a highly sensitive biosensor the small cross section of Raman scattering has to be increased. This is usually done by rough metallic surfaces or nanoparticles and their strong plasmon induced near-field. We use gold nanocones, with sharp tips of less than 10 nanometers in diameter [1], for surface enhanced Raman spectroscopy (SERS). The nanocones, which are fabricated by e-beam lithography and Argon ion-milling, have a well-defined plasmon resonance frequency which can be tuned through the size of the cones. Therefore they can be optimized for the applied laser frequency. The Raman enhancement by the cones is demonstrated by the measurement of thin pentacene films on arrays of different-sized gold nanocones.

[1] M. Fleischer et al., Appl. Phys. Lett. 93, 111114 (2008)

O 60.74 Wed 17:30 P4

Parallel methods for the fabrication of gold nanocones — •Andreas Horrer, Christian Schäfer, Yuliya Fulmes, Dominik Gollmer, Monika Fleischer, and Dieter Kern — Institut für Angewandte Physik, Eberhard Karls Universität Tübingen, Auf der Morgenstelle 10, D-72076 Tübingen

When interacting with an electromagnetic field, metallic nanoparticles create a local field enhancement caused by excitation of localized surface plasmons. The resonance frequency depends on the shape, the size and the material of the nanoparticle and its dielectric environment. At the tip of a nanocone the field enhancement is particularly strong. A large array of identical nanocones could be used for biosensing. The fabrication of such large arrays in reasonable time requires parallel methods. Nanosphere lithography is a low cost technique which utilizes highly ordered self-assembled hexagonally close-packed layers of colloids. Different processes were developed using double or monolayers of polystyrene beads. They either directly act as an etch mask, or as a mask for the deposition of an aluminium oxide etch mask for an underlying gold layer, from which the cones are formed in an argon ion milling step.

O 60.75 Wed 17:30 P4

Coupled exciton-plasmon modes in metal-dye hybrid systems — •Sabine Auer, David Leipold, and Erich Runge — Technische Universität Ilmenau, 98693 Ilmenau, Germany

At nano-structured metal surfaces, visible light can be localized to spatial regions well below the diffraction limit by the excitation of surface plasmon polaritons (SPPs). A major challenge for future devices employing SPPs is the fact that SPPs can only travel for very short ranges since they are strongly damped by Ohmic losses in the metal. One idea to overcome this problem is to compensate the damping by coupling of the SPPs to active media (e.g., dyes [1] or quantum wells [2]).

We present calculation results for the coupling of quantum mechanical excitations in a j-aggregated dye with the SPP excitation at a metal grating [1]. The strong coupling (energy transfer) of the SPP and the dye resonance manifests itself as avoided crossing in the dispersion relation. At resonance, the coupled eigenmodes show excitonic as well as plasmonic features.

The good agreement of the calculation with the experiment confirms that our description can be used in future work on the design of devices with SPPs coupled to gain media.

[1] P. Vasa, et al., “Ultrafast control of strong coupling in metal-molecular aggregate hybrid nanostructures”, *ACS Nano*, accepted. [2] P. Vasa, et al., “Coherent exciton–surface-plasmon-polariton interaction in hybrid metal-semiconductor nanostructures”, Phys. Rev. Lett. **110**, 116801 (2008).

O 60.76 Wed 17:30 P4

Low dimensional plasmons in Ag-nanowires grown on Si (557) — •Ulrich Krieg, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover, Germany

A quasi 1-dimensional system was prepared by adsorption of about 1 monolayer Ag on Si(557) at 550° via self assembly. The morphology and metallicity of these uniaxially grown nanowires were studied by the combination of using low electron energy diffraction and high resolution electron energy loss spectroscopy in one instrument (ELS-LEED) . The clean Si(557) surface consists of a periodic sequence of (111) mini-terraces (3 nm width), separated by (112) facets. After adsorption of Ag LEED reveals the same spot splitting along the [$\bar{1}\bar{1}2$] direction, i.e. the initial alternating facet structure is conserved upon adsorption. A streaky $\sqrt{3} \times \sqrt{3}R30°$ reconstruction suggests further the formation of nanowires along the [$1\bar{1}0$] direction. An alternating contrast seen by STM with spatial separations similar to those seen on Si(557) indeed confirms the growth of separated nanowires. These findings are fully supported by angle resolved EELS measurements. While along the wires a dispersion of a sheet plasmon has been found, across the wires only a non-dispersing state at around 450 meV has been identified. The localized peak, which is apparent also in the direction along the wires, can be reasonably explained assuming metallic wires with finite width of around 2.5 nm. Similar results were obtained recently for DySi$_2$2 wires grown on vicinal Si(111) substrates (PRB 81 (2010) 165407)

O 60.77 Wed 17:30 P4

Plasmon propagation in structural and dieletric controlled gold films probed by phase-resolved PEEM — •Christoph Lemke[1], Till Leissner[1], Christian Schneider[2], Martin Aeschlimann[2], and Michael Bauer[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel — [2]Fachbereich Physik, Technische Universität Kaiserslautern

In a phase-resolved photoemission electron microscopy experiment, the near field associated with propagating surface plasmon polaritons (SPP) can be locally sensed via interference with the excitation laser field [1]. Here we apply this technique to monitor and analyze SPP propagation in gold films where the plasmonic response is controlled by structural design via e-beam lithography as well as by dielectric loading. Phase resolved simulations based on Huygens principle allow us to reconstruct SPP properties such as group velocity, damping, direction of propagation.

[1] A. Kubo, N. Pontius, and H. Petek, Nano Lett. 7, (2007) 470

O 60.78 Wed 17:30 P4

Plasmonic Nanocones — •Dominik Gollmer, Christian Schäfer, Yuliya Fulmes, Andreas Horrer, Dieter Kern, and Monika Fleischer — Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

Through external electromagnetic excitation, plasmons can be generated in metallic nanostructures. The resulting enhanced electromagnetic near-field can be used for applications, e. g. near-field imaging or surface enhanced Raman spectroscopy (SERS). The plasmon resonance of nanostructures depends on their geometry and composition [1]. We fabricate well-defined metallic nanocones, with tip radii of less than 10 nm [2]. The cones are fabricated using e-beam lithography, defined aluminium oxide masks and Ar ion-milling. The resonance frequency of these cones can be tuned by variation of material or size. The shift of the plasmon frequency when the height of Au cones is varied is shown in dark field spectra. Both an accurate fabrication process and the tunability of the plasmon resonance are fundamental requirements for applications.

[1] H. Kuwata et al. ; Appl. Phys. Lett. 83 (2003); 4625

[2] M. Fleischer at al.; Nanotechnology 21 (2010); 065301

O 60.79 Wed 17:30 P4

Tuning resonant infrared antennas with phase change materials — •Kathrin Schönauer[1], Jens Richter[1], Xinghui Yin[2], Jón Mattis Hoffmann[1], and Thomas Taubner[1,2] — [1]1st Institute of Physics, RWTH Aachen University, Sommerfeldstraße 14, 52074 Aachen, Germany — [2]Fraunhofer Institute for Laser Technology, Steinbachstraße 15, 52074 Aachen, Germany

In the field of active plasmonics one recent interest lies in tunable resonances, e.g. for the use as optical switches [1]. Tuning of resonances of metallic nanostructures can be done by changing their dielectric environment. Phase change materials show a change of their refractive index between amorphous and crystalline phase. Especially in the mid-infrared spectral region some of these materials show the advantage of having low losses.

Thin films of phase change materials, e.g. Ge$_2$Sb$_2$Te$_5$, are deposited by sputtering onto Si-substrates. On top of these films nanostructures are prepared by nanosphere lithography. We use Fourier-Transform Infrared Microscopy for measuring the resonance frequency of these infrared antennas.

A future application of these systems could be their use as tunable sensors for enhanced infrared spectroscopy [2-3].

[1] Z. L. Sámson et al., APL 96, 143105 (2010)

[2] R. Adato et al., PNAS, 106, 19227 (2009)

[3] F. Neubrech et al., PRL 101, 157403 (2008)

O 60.80 Wed 17:30 P4

Time-Resolved Near-Field Microscopy of Acoustic Vibrations — •Matthias Brandstetter[1,2], Ralf Vogelgesang[1], and Markus Lippitz[1,2] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]4th Physics Institute, University of Stuttgart,70550 Stuttgart, Germany

The localized surface plasmon resonance (LSPR) of a metal nanoparticle depends directly on the geometry and the dielectric constant of the nanoobject. The resonance is influenced by the electron density which can be modified locally by acoustic oscillations of the nanostructure. The optical near-field thus contains information on the structure's acoustic oscillation pattern. The combination of an apertureless scanning near-field optical microscope (aSNOM) and ultrafast pump-probe spectroscopy gives an instrument to detect the temporal and spatial dependence of the LSPR. We present our implementation of a pump-probe aSNOM which at the end will allow us to map out nanoscale mechanical oscillation patterns. We show numerical simulation of the field changes caused by local plasma frequency changes, nanoacoustical modes as well as first experimental results.

O 60.81 Wed 17:30 P4

Imprinting the optical near field of single and monolayered micro spheres into phase-change films — •Paul Kühler[1], Jan Siegel[2], Javier García de Abajo[2], Andreas Kolloch[1], Philipp Leiprecht[1], Johannes Boneberg[1], and Paul Leiderer[1] — [1]Fachbereich Physik, Universität Konstanz — [2]Instituto de Optica, CSIC, Madrid

Control over the optical near-field is a crucial prerequisite for several applications of light at the nanoscale, such as material processing, microscopy and biosensing. We present a method that allows for directly imaging the near-field distribution of nanostructures. Our test systems were scattering dielectric micro spheres on a planar substrate. Irradiation with short, infrared laser pulses were performed on particles on a thin, chalcogenide film, which is modified depending on the local fluence and therefore records the scattering field distribution. Single particles as well as monolayers of these particles were used as target. Investigating the single particle patterns with optical microscopy, we demonstrate the influence of polarization and angle of incidence of the incident beam as well as the particle size on the imprints. Due to the monotonicity over a large fluence range of the chalcogenide film's response to irradiation, the experimental results could be shown to be in quantitative agreement with a model based on a rigorous solution of Maxwell's equations. In case of monolayers, high-resolution scanning electron measurements reveal modifications in the chalcogenide film with lateral dimensions down to 1/16 of the irradiation wavelength.

O 60.82 Wed 17:30 P4

Fabrication and application of core-shell nanorod structures — •Vera Hoffmann[1], René Kullock[1], Mathias Böhm[1], Gunther Scheunert[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Physik/Photophysik, TU Dresden, Dresden, Germany — [2]Department of Physics and Astronomy, Queen's University Belfast, Belfast, UK

The fabrication of nanorod arrays made of a single material such as gold, silver, cobalt and others is already an established technique. However, nanorods made of material combinations have hardly been exploited so far, and may lead to novel physical properties of the array. In this study, we present how gold-nickel core-shell nanorod structures are fabricated: An anodised aluminium oxide matrix containing gold nanorods is partly etched to obtain an air shell around the gold rods. Then the resulting gaps are filled with nickel in a subsequent electrodeposition step .

Nanorod arrays can be used for various sensor applications. For example, the interrod distance and the angle of incidence strongly influence the collective surface plasmon resonance (CSP) of the structure [1,2]. Thus, if the structure is prepared on a transparent flexible substrate, application of external mechanical stress affects the optical properties of the device, which can be used to detect strain on a local scale. Furthermore, the magnetic properties of nickel-gold nanorod arrays can be exploited for magnetic sensors with optical read-out.

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O 60.83 Wed 17:30 P4

Improving SHG Calculations with 3D Curved Elements in the Discontinuous Galerkin Method — •Andreas Hille, Rene Kullock, Alexander Haussmann, Stefan Grafström, and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, 01069 Dresden, Germany

The existence of optical second-harmonic generation (SHG) at metallic surfaces has been well known for a long time in experiment as well as in theory, where several electron gas models [1] exist. Further investigations have dealt with SHG at thin metallic films and nanoparticles, for which these models have been checked against experimental data. In order to apply the model not only to films or spheres but also to more complex structures such as nanorods, efficient and powerful numerical methods are needed.

One such method is the Discontinuous Galerkin method (DG) [2], which allows for explicit time stepping and finite-element-like meshing. We demonstrate here that, due to the nonlinear sensitivity of SHG signals, an accurate boundary description by means of curved elements is necessary in order to obtain reliable and non-erroneous results. Furthermore, we apply this DG method to metallic nanorods and show their usefulness as SHG antennas.

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O 60.84 Wed 17:30 P4

Dependence of the photochromic transformation of TiO$_x$- and ZrO$_x$-embedded Ag nanoparticles on the photon energy of the irradiating light — Hendrik Holzapfel[1], Alexander Sprafke[1], Florian Hallermann[1], •Nils Becker[1], Melanie Meixner[2], Matthias Wuttig[1], and Gero von Plessen[1] — [1]Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]present address: Fraunhofer Institute for Laser Technology ILT, 52074 Aachen, Germany

Photochromic materials change their color under irradiation with light. Uniform TiO$_x$- and ZrO$_x$-embedded Ag nanoparticles with photochromic properties can be fabricated through a combination of nanosphere lithography and electron-beam evaporation. In comparison to the dc-sputter deposition technique as employed in our previous work [1], the good reproducibility of this approach and the less inhomogeneously broadened plasmon line of the resulting samples allow us to analyze the photochromic transformation in a more quantitative way.

In this work, we investigate the dependence of the photochromic transformation of TiO$_x$- and ZrO$_x$-embedded Ag nanoparticles prepared by nanosphere lithography on the photon energy of the irradiating light. We find a photon energy below which no photochromism is observed, almost independently of the embedding medium. Furthermore, the photochromic effect increases with increasing photon energy.

[1] C. Dahmen et al., Appl. Phys. Lett. 88, 011923 (2006)

O 60.85 Wed 17:30 P4

Calculation of up-conversion signal of Er^{3+} ions near gold nanospheres — •Florian Hallermann[1], Stefan Fischer[2], Jan Christoph Goldschmidt[2], and Gero von Plessen[1] — [1]Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]Fraunhofer Institute for Solar Energy Systems, Heidenhofstr. 2, 79110 Freiburg, Germany

In conventional silicon solar cells, photons with energies below the silicon band gap (1.12 eV) do not contribute to current generation. The near-infrared part of the solar spectrum could possibly be exploited by use of up-conversion processes. For example, electrons could be excited from the ground state to a final state via intermediate states through sequential absorption of infrared photons. Such electrons subsequently relax from the final state by emitting photons whose energy is high enough to be absorbed in the silicon.

In this work, we show on the basis of model calculations how the up-conversion signal of Er^{3+} ions can be enhanced using spherical gold nanoparticles. In the vicinity of the nanoparticles, the excitation rate of the ions is changed due to the near-field of the particles. These changes are computed using Mie theory and a rate equation system. In addition, also the relaxation times of all involved excited states of the ions are changed by the presence of metal nanoparticles. This is caused by a near-field induced energy transfer from the ions to the nanoparticles, which offer additional radiative and nonradiative decay channels. Here, we semi-analytically calculate the effects that these changes have on the up-conversion signal.

O 60.86 Wed 17:30 P4

Near-and farfield investigations of individual sub-nanometre plasmonic gap resonances — •Florian Schertz[1], Reza Mohammadi[2], Marcus Schmelzeisen[2], Hans-Joachim Elmers[1], Gerd Schönhense[1], and Max Kreiter[2] — [1]Inst. f. Physik, J. Gutenberg-Universität, Mainz — [2]MPI f. Polymerforschung, Mainz

An increasing interest evolved on the mutual interaction of distinct plasmonic resonances during the last years, due to the extremely enhanced and localized electromagnetic fields that are provoked. Prominent examples are nanoparticle (NP) dimers with an ultrasmall gap between them or NPs close to metallic films, the latter can be manufactured with reproducible sub-nm gaps. These coupled plasmons supporting systems act as optical antennae, as they efficiently convert free-propagating radiation into localized electromagnetic energy. Hence, understanding the optical near-field (NF) and far-field (FF) properties is essential for a full understanding of nano-antennae and for application-oriented optimization. We present NF- and FF-spectra and corresponding SEM images of the same individual gap-resonance supporting Au NPs on a Au film with a gap of 0.8nm. Dark-field confocal microscopy is used for detection of the FF response, photoemission electron microscopy for the NF characteristics. Beside the well-known FF gap-resonances, additional dark-mode resonances were observed exclusively in the NF, depending strongly on the NP properties. The experimental findings are analyzed and systematized concerning their correlation to FIT-simulations of the optical NF and FF. Funded by DFG EL172-16.

O 60.87 Wed 17:30 P4

Plasmonic Collimation of near-IR Laser Diodes — •Xinghui Yin[1,2], Thomas Taubner[2,3], and Peter Loosen[1,2] — [1]Institute for Technology of Optical Systems, RWTH Aachen University, Steinbachstr. 15, 52074 Aachen — [2]Fraunhofer Institute for Laser Technology ILT, Steinbachstr. 15, 52074 Aachen — [3]I. Institute of Physics (IA), RWTH Aachen University, Sommerfeldstr. 14, 52074 Aachen

Laser diodes are compact and versatile components for numerous applications. However, they show a strongly asymmetric beam-profile in the far-field due to the confined dimensions of their emitting area (ca. 1 μm × 5 μm). Currently, high-index cylindric lenses are employed to reduce the beam divergence. This is a nonmonolithic, costly approach as lenses have to be manually adjusted.

We investigate beam collimation in one direction by effectively enlarging the emitting area. To do so, we use a plasmonic structure consisting of a slit and a grating structured in a gold layer directly on top of the laser facet. Previous work done by Ebbesen et al [1] confirm the beaming properties of such structures. Capasso et al [2] successfully combined plasmonic collimators and Quantum Cascade Lasers at wavelengths of $\lambda = 9.8$ μm. We optimize the structure parameters for near-infrared wavelengths ($\lambda = 960$ nm). Using the obtained parameters, we fabricate the plasmonic collimator and characterize it.

[1] Ebbesen et al., Beaming Light from a subwavelength Aperture, 2002, Vol 297, Science

[2] Capasso et al., Nature Photonics, 2008

O 60.88 Wed 17:30 P4

Probing subwavelength plasmonic components from the far field — •Jing Wen[1,2], Arian Kriesch[1,2,3], Daniel Ploss[1,2,3], Peter Banzer[1,2], and Ulf Peschel[1,2] — [1]MPI für die Physik des Lichts, Erlangen, Germany — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [3]Erlangen Graduate School in Advanced Optical Technologies (SAOT)

Optical antennas connected to waveguides with subwavelength width enable the investigation of different nanoplasmonic components. An high-NA focal scanning setup exploits the distinctive spectral and polarization selectivity of these antennas. A clever combination of several antennas for receiving and emitting light in mutually orthogonal configurations allows unprecedented signal-to-noise ratio in probing different waveguide configurations. We report the first experimental characterization of an optical antenna connected to a nanoplasmonic gap waveguide. A strongly confined bound mode can not leak to the far field unless it is scattered out at an antenna or a waveguide end. Far-field measurements of the light emitted from those waveguide ends or extra antennas are performed in crossed polarization and enable the detection of extremely weak signals. To allow for highly efficient crossed polarization detection, a 90° waveguide bend is used. Our method allows for the probing nano-structures that were previously only accessible by Scanning Near-field Optical Microscopy, and we therefore circumvent the intrinsic disadvantages of near-field microscopy such as high losses and elaborate operation. Instead of intruding the near field directly, we focus the far field to the nanoscale and vice versa.

O 60.89 Wed 17:30 P4

Plasmonic antennas and wireless interconnects on a subwavelength scale — •Daniel Ploss[1,2,3], Arian Kriesch[1,2,3], Jing Wen[1,2], and Ulf Peschel[1,2] — [1]MPI für die Physik des Lichts, Erlangen, Germany — [2]Friedrich-Alexander-Universtität Erlangen-Nürnberg, Erlangen, Germany — [3]Erlangen Graduate School in Advanced Optical Technologies (SAOT)

Wireless transfer of electromagnetic radiation requires antennas with well-designed directivity and high efficiency. In optics those antennas offer particularly interesting applications in the intermediate domain between the far- and near- field; integrating wireless transfer channels with highly confined plasmonic circuitry can significantly decrease losses, thus avoiding the major disadvantage of nanoplasmonics. We report on optical antennas loaded with nanostructures under investigation and which are optimized for low reflection at the connection. Different types of antennas were designed and simulated with Finite Elements Methods (FEM), and their estimated performance finally compared with experimental results. A concept for engineering exceptionally high directionality are Yagi-Uda antennas, well known from the radio-frequency range. We intend to use them as wireless interconnects between highly packed, plasmonic waveguide structures. Hence, carefully designed antennas can not only be used to transfer the far field to the near field, but also for optimizing the arrangement of waveguide structures and for allowing more efficient, less lossy configurations.

O 60.90 Wed 17:30 P4

Towards the realization of an efficient nanoantenna — •Reto Giannini[1], Patrick Leidenberger[2], Christian Hafner[2], and Jörg F. Löffler[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — [2]Laboratory for Electromagnetic Fields and Microwave Electronics, ETH Zurich, 8092 Zurich, Switzerland

Different aspects of nanoantennas, such as radiation pattern or wavelength-dependent near-field enhancement, are being heavily discussed in recent years. Many simulation-based contributions concentrate either on the general usability of simulation methods or use such methods to verify experimental data. Especially in systems that are more complex to realize, estimations concerning performance and its reproducibility are needed before the development of the production process starts. In this study, we present a series of FEM-based simulations carried out using JCMsuite on a nanoantenna consisting of two stacked nanodiscs. The goal was to realize a geometry that delivers first and second order plasmon resonance at the later excitation and emission wavelength of the activated nanoantenna as well as estimations concerning design stability. Besides the most important geometry parameters, such as height, diameter or gap, production-based parameters (diminution of the antenna or round corners) as well as the influence of a later integration (excitation and emission) are considered. The results of the simulations are compared with actual experiments on nanoantennas, produced using guidelines obtained from the simulation studies.

O 60.91 Wed 17:30 P4

Structural changes of percolated metal films by laser irradiation — Christian Maasem, •Daniela Schneevoigt, Florian Hallermann, and Gero von Plessen — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

In semi-continuous, percolated metal films, both localised and propagating surface-plasmon modes can be excited by light irradiation over a wide spectral range. This can lead to strong optical field enhancements which are confined to 'hot spots' of a few nanometers in size.

In this work, we show that percolated silver films on glass substrates change their structure upon irradiation with focussed laser light. The irradiated areas exhibit more light scattering and higher light transmission than non-irradiated areas. This could point towards an aggregation of the films to larger structures and thus towards a reduction of the coverage of the substrate surface. Even after an additional coating with SiO_2, changes of the structure of the silver films occur already at low laser intensities.

In contrast, no changes are observed when irradiating percolated gold films. Thus, it can be assumed that the restructuring of the film material is not purely a thermal effect.

O 60.92 Wed 17:30 P4

Investigations on laser-beam immobilised gold nanoparticles — •Falko Brögger[1], Ninet Babajani[2], Malte Linn[1], and Gero von Plessen[1] — [1]Institute of Physics (1A), RWTH Aachen University, 52056 Aachen, Germany — [2]FZ Jülich, Inst. of Solid State Research (IFF-6), 52428 Jülich, Germany

The plasmon lines of chemically synthesized noble-metal nanoparticles of nearly spherical shape and approximately uniform size exhibit surprisingly large particle-to-particle variations of their resonance peak positions and line widths. The reasons for these spectral variations are still unknown. Possible explanations include faceting of the nominally spherical particles, charges and chemical effects within the suspension, and interactions with the substrate.

In this work, single gold nanoparticles suspended in an aqueous environment are trapped by an optical tweezer, and their light-scattering spectra, which are free of substrate effects, are measured. Each of the trapped nanoparticles is subsequently deposited onto a substrate using the optical tweezer and its spectrum is measured again. A comparison of the single-particle spectra shows that the particle-to-particle plasmon line variations in the aqueous suspension and the substrate-induced line changes do not seem to be correlated. Remarkably, additional line changes are observed upon drying the sample surface and covering it again with water.

O 60.93 Wed 17:30 P4

Second Harmonic Generation and Two Photon Photoemission from Cs on Cu(111) — •Mariusz Pazgan, Cheng-Tien Chiang, Aimo Winkelmann, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle (Saale), Germany

We report on a combined study of nonlinear-optical Second Harmonic Generation (SHG) and Two-Photon Photoemission (2PPE) from the system of Cs on Cu(111). The SHG and photoemission signals were simultaneously measured during real time deposition of Cs atoms on Cu(111) surface. Clear resonances in 2PPE and SHG were observed in measurements at 140K and 300K. We interpreted our results by optical transitions between the occupied Cu(111) Shockley surface state band and the unoccupied Cs anti-bonding state at the photon energy of 3.07eV used in the experiment.

O 60.94 Wed 17:30 P4

Investigation of spin-polarized electron transmission through Co/C/Co tunnel junctions — •Felix Huerkamp, Bernd Stärk, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster, Germany

We investigate transmission properties of electrons at the interfaces of Co/C/Co metal-semiconductor hybrid systems within an ab-initio approach. The considered open system is a tunnel junction consisting of three parts: the left and right semi-infinite cobalt leads, as well as the scattering region built by N layers of carbon atoms. We employ spin-polarized density-functional theory within the generalized gradient approximation to calculate the spin-polarized transmission. To this end, we use a Greens function technique which is based on the representation of the wave functions by Gaussian orbitals. This enables us to treat the scattering problem as a localized perturbation of a Co crystal. In a first step, we calculate self-consistently the potential in the region of the C layers and the neighboring Co layers. Then we construct the exact self-energies from the potential of bulk Co. Finally, we evaluate the transmission coefficient T(E) calculating the Greens function in the subspace of the perturbation. We have investigated junctions of hexagonal Co with C layers grown in (111) direction, as well as junctions of fcc Co with C layers oriented in (001) direction. The results for the transmission are discussed as a function of the number of C layers in the scattering region.

O 60.95 Wed 17:30 P4

Electronic States of Polar and Non-polar Surfaces within the Quasiparticle Approach — •Abderrezak Belabbes and Friedhelm Bechstedt — Institut für Festköpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany

DFT provides an incorrect description of the band gap and excited states of InN. The correction of this error is of considerable importance in understanding the surface physics and semiconducting properties of InN. The purpose of this work is to reevaluate the quasiparticle band structure using the novel LDA-1/2 method for the surfaces states of InN. We restrict ourselves to a discussion of the electronic structure of the clean polar and non-polar surfaces. Our calculations allow us to explain the n-type conductivity of polar InN surfaces and the pinning of the Fermi level. The electronic structure of non-polar InN surfaces is found to be very different from that of the polar surface. It shows a semiconduting behavior, but with surfaces states that energetically overlap with bulk states. Therefore, these findings suggest an absence of electron accumulation on the non-polar InN surfaces. Our results agree with the previous calculations by C. G. Van de Walle and experimental observations by Wu et al, who provided evidence for an unpinned Fermi level at non-polar surfaces. The results have been obtained with low computational effort, similarly to standard LDA calculations, much in contrast to the GW quasiparticle approach.

O 60.96 Wed 17:30 P4

Defects in amorphous silica : from density functional to many-body perturbation theory — •David Waroquiers[1,2], Matteo Giantomassi[1,2], Martin Stankovski[1,2], Gian-Marco Rignanese[1,2], and Xavier Gonze[1,2] — [1]Université Catholique de Louvain IMCN-NAPS, Louvain-la-Neuve, Belgique — [2]European Theoretical Spectroscopy Facility (ETSF)

Amorphous silica is of particular technology interest for its electronic and optical properties. It is commonly used in a lot of devices such as optical fibers, lenses, filters, gate dielectrics in MOS transistors, ... In the present work, we investigate the effect of hydrogen on the properties of amorphous silica.

Accurate electronic structure is obtained using many-body perturbation theories such as GW approximation. Till recently, this method could only be applied to small systems because of its large computational cost. New theoretical and algorithmic developments in the version 6 of ABINIT [1] (extrapolar method, band parallelism and projector-augmented wave formalism) now enable us to perform GW calculations in large supercells with a reasonable cost in CPU time.

We report results obtained for several hydrogen-containing silica cells of 72 atoms. The electronic structure has been computed using many-body perturbation theory in its GW approximation. Formation energies are calculated at the DFT and GW level [2]. Some preliminary results on the optical properties are also presented.

[1] X. Gonze et al., Comput. Phys. Comm. 180, 2582 (2009).

[2] P. Rinke et al., Phys. Rev. Lett. 102, 026402 (2009).

O 60.97 Wed 17:30 P4

H-Adsorption and surface resonances on Pd and Pt — •Alexander Menzel[1], Peter Amann[1], Michael Cordin[1], Erminald Bertel[1], Josef Redinger[2], Sebastian Stolwijk[3], Karen Zumbrägel[3], and Markus Donath[3] — [1]Inst. f. Phys. Chemie, Univ. Innsbruck, Austria. — [2]Dep. of Appl. Physics, Techn. Univ. Wien, Austria. — [3]Physikal. Institut, Univ. Münster, Germany

In this contribution, the influence of Hydrogen adsorption on the isoelectronic surfaces Pt(110) and Pd(110) is observed with ARPES (in some cases spin resolved) and compared with DFT-calculations. A strong surface resonance at $\overline{S}$ can be identified experimentally in ARPES by backfolding due to adsorbate-induced changes of surface-symmetry. Whereas Hydrogen adsorption induces no energetic shift of the surface resonance at $\overline{S}$ in Pt(110), a downward shift on Pd(110) is observed. This difference is related to the different adsorption sites for hydrogen on both surfaces and compares favourably with DFT calculations [2]. Interestingly, upon hydrogen adsorption a pairing-row reconstruction on Pd(110) develops together with a satellite peak of the $\overline{S}$ resonance. The band dispersion of this satellite is parallel to the dispersion of the main resonance, but is shifted to lower energies by roughly 400meV. The spectra resemble Ni(110), however, a spin polarization could not be detected. Possible origins of the satellite peak are discussed.

References: [1] M. Minca, S. Penner, E. Dona, A. Menzel, E. Bertel, V. Brouet and J. Redinger, New J. Phys. 9, 386 (2007). [2] W. Dong, V. Ledentu, Ph. Sautet, A. Eichler, J. Hafner, Surf. Sci. 411, 123 (1998).

O 60.98 Wed 17:30 P4

Field Emission Resonances on the Quasi One-Dimensional Si(111)5x2-Au Reconstruction — •Stefan Polei, Ingo Barke, Kristian Sell, Viola von Oeynhausen, and Karl-Heinz Meiwes-Broer — Institut für Physik, Universität Rostock, D-18051, Rostock, Germany

Scanning tunnelling spectroscopy measurements of field emission resonances (FER) have shown to be a suitable tool to investigate local work function variations particularly on metal surfaces [1]. About FER on semiconductors or nanostructured surfaces less literature can be found. In this contribution we compare FER on different regions of a Si(111)7x7 substrate which is partially covered by the quasi one-dimensional Si(111)5x2-Au structure. Across a transition between Si(111)7x7 and Si(111)5x2-Au a shift of the FER peak positions is found which can be attributed to changes of the local work function. At increased spatial resolution dI/dV maps reveal a periodic shift of the higher order FER in the direction perpendicular to the chains of Si(111)5x2-Au. This effect appears on a length scale of less than one nanometer and is caused by surface-potential variations. Model calculations are shown to quantify their amplitude.

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O 60.99 Wed 17:30 P4

Energy-filtered PEEM at ferroelectric nanostructures: Fingerprints of the ferroelectric polarization in the electronic structure of PbZr$_{0.52}$Ti$_{0.48}$O$_3$ — •Ingo P. Krug[1], Nick Barrett[2], Astrid Besmehn[4], Alessio Morelli[3], Ayan Roy Chaudhuri[3], Ionela Vrejoiu[3], Marten Patt[1], Olivier Renault[5], Fausto Sirotti[6], and Claus M. Schneider[1] — [1]IFF-9, Forschungszentrum Jülich GmbH, Jülich, GERMANY — [2]DSM/IRAMIS/SPCSI, C.E.A. Saclay, Gif-sur-Yvette, FRANCE — [3]MPI für Mikrostrukturphysik, Halle, GERMANY — [4]ZCH, Forschungszentrum Jülich GmbH, Jülich, GERMANY — [5]LETI group, MINATEC, C.E.A. Grenoble, Grenoble, FRANCE — [6]TEMPO beamline, Synchrotron SOLEIL, Gif-sur-Yvette, FRANCE

Ferroelectrics are promising materials for nanoelectronic devices. Their versatility offers a widespread range of applications, for example, non-volatile memory-cells, controllable surface catalysts, or energy harvesting devices. The key to improved functionality is to understand the interrelations between electronic structure and ferroelectricity. Many ferroelectrics are thought to exhibit a combined structural and electronic reconstruction upon ferroelectric ordering. While the structural aspects can easily be investigated by diffraction, determining the electronic structure by photoemission is often challenging due to the insulating nature of this material class. Nevertheless, as we show for the case of PbZr$_{0.52}$Ti$_{0.48}$O$_3$ (PZT), spectromicroscopic studies in these materials are rewarding: Energy-filtered PEEM by a NanoESCA microscope reveals polarization effects in core-levels and the valence-band.

O 60.100 Wed 17:30 P4

Development of an impurity-embedding code based on the Korringa-Kohn-Rostoker (KKR) Green function method — •David Bauer, Phivos Mavropoulos, Rudolf Zeller, and Stefan Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We present a new implementation of the KKR Green function method for performing electronic structure calculations based on the density functional theory of impurity atoms embedded in a periodic host.

Our code is able to treat impurity atoms positioned unrelated to the host sites. This became possible by a two step approach: For large deviations of the impurity from the host position a virtual atom method is used where the host Green function is expanded around the new impurity position. Then, small displacements are treated as described in [1].

In addition, we include in our code a recently developed accurate method to directly solve the coupled Lippmann-Schwinger equations for non-spherical potentials via systems of linear equations obtained by Chebyshev expansions for radial variables. This is especially important for the irregular solutions when spin-orbit coupling is included in the presence of a magnetic field, since then, the effective potential close to the origin is not necessarily spherical. Further, the code has been parallelized in energies, which enables us to use typically 100 processors with an almost linear speedup.

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Rev. B **55**, 4157 (1997).

O 60.101 Wed 17:30 P4

Angle-resolved photoelectron spectroscopy of strained $SrRuO_3$ thin films — •Arndt Quer[1], Erik Kröger[1], Matthias Kalläne[1], Adrian Petraru[2], Rohit Soni[2], Hermann Kohlstedt[2], Lutz Kipp[1], and Kai Rossnagel[1] — [1]Institute of Experimental and Applied Physics, University of Kiel, 24098 Kiel, Germany — [2]Department of Nanoelectronics, Technical Faculty, University of Kiel, 24143 Kiel, Germany

The magnetoelectric effect in composites based on oxides and in particular the coupling mechanism between the electric and magnetic order parameters have recently attracted much attention in basic research. By combining different piezoelectric and magnetostrictive substances it is possible to optimize the magnetoelectric properties of the composite, for example, with regard to technological applications such as ultra-sensitive magnetic sensors. Due to its adequate electrical conductivity in combination with lattice-strain induced changes of the magnetic moment, ferromagnetic $SrRuO_3$ is a good test candidate for the magnetostrictive component of the magnetoelectric composite. Our goal here was to study the magnetostrictive behavior by analyzing the electronic structure of $SrRuO_3$ thin films in different strain-states. To this end, we prepared pulsed-laser-deposition grown $SrRuO_3$ films on different oxide substrates. The samples were annealed by O_2 under various conditions, resulting in atomically clean and mostly defect-free surfaces. The samples were studied by low-energy electron diffraction and angle-resolved photoelectron spectroscopy. This work was supported by the DFG through SFB 855.

O 60.102 Wed 17:30 P4

Theoretical approach to adatom structures on semiconductor surfaces: Ab-initio studies and explicit many-body extensions. — •Sergej Schuwalow and Frank Lechermann — I. Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Deutschland

Single adatoms, dimers and general quasi-twodimensional adsorbate arrays on semiconductor surfaces exhibit a great variety of interesting effects, while having the advantage of being directly accessible via surface-sensitive experimental probe techniques. The reduced dimensionality and the coupling to the substrate can produce, e.g., peculiar magnetic effects and also correlation effects may become important due to strong electron localization at the adatom sites.

Within this work, we investigate the electronic structure of submonolayer surface systems, namely the Sn/Si(111) and the Sn/Ge(111) alpha surfaces [1], as well as single magnetic adatoms (Fe,Co,Ni) on the InSb(110) substrate [2] by density-functional theory (DFT) and, where appropriate, its combination with explicit many-body methods. Our main focus lies on determining the structural, bonding and magnetic properties, and in case of the Sn submonolayer systems, the influence of a finite Hubbard U on the surface states.

[1] Sergej Schuwalow, Daniel Grieger, Frank Lechermann, Phys. Rev. B **82**, 035116 (2010)

[2] A. A. Khajetoorians, B. Chilian, J. Wiebe, S. Schuwalow, F. Lechermann and R. Wiesendanger, Nature **467**, 1084 (2010)

O 60.103 Wed 17:30 P4

The plasma treatment of Titanium in Oxygen, Nitrogen, Argon and air studied with MIES, UPS and XPS — •René Gustus[1], Sebastian Dahle[1], and Wolfgang Maus-Friedrichs[1,2] — [1]Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [2]Clausthaler Zentrum für Materialtechnik, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany

The treatment of Titanium with different kinds of plasma is commonly used for etching, oxidation, carbonization or nitriding. During some of these techniques, a lot of heat is carried into the material, whereas others operate at room temperature. All of the processes reported so far have in common that cover gas is needed. The gas is choosen in terms of application, thus Nitrogen-rich or Carbon-rich gases are utilized for hardening and pure Argon as inert gas. It is also reported that an Oxygen plasma can be used for the removal of a TiN film.

We investigated the reaction and etching rates of an Oxygen and a Nitrogen dielectric barrier discharge (DBD) plasma and opposed both in an air plasma. The etching depth and surface purgation in an air plasma is then compared to an Argon plasma, to determine the use of an air plasma for technical applications. For our studies, we employed Metastable Induced Electron Spectroscopy (MIES), Ultraviolet Photoelectron Spectroscopy (UPS), and X-ray Photoelectron Spectroscopy (XPS).

O 60.104 Wed 17:30 P4

An Overview of Methanol Reactions on Ru based Catalyst Surfaces under UHV Conditions — •Pawel Gazdzicki and Peter Jakob — Fachbereich Physik, Philipps-Universität Marburg, Deutschland

The conversion of methanol to CO_2 is of substantial importance referring to the direct methanol fuel cell where CO from methanol dehydrogenation is responsible for the poisoning of the electrodes. In this comprehensive study thermally induced reaction pathways ($T = 20 - 600$ K) of methanol on various Ru based catalysts (Ru(0001), (sub)monolayer Cu/Ru(0001), Cu(111)/Ru(0001), pseudomorphic Pt/Ru(0001) and Pt_xRu_{1-x}/Ru(0001) surface alloys) have been investigated in detail using Fourier transform infrared spectroscopy, temperature programmed desorption and photoelectron spectroscopy. Particular interest is devoted to the influence of preadsorbed oxygen on the formation and stability of the various reaction intermediates. Among the various stable surface species hydroxyl, formaldehyde, formate, methoxy and carbon monoxide have been identified. A reaction scheme is presented to illustrate trends.

O 60.105 Wed 17:30 P4

In-situ alkylation reaction of two ionic liquids studied by X-ray photoelectron spectroscopy (XPS) — •Inga Niedermaier[1], Claudia Kolbeck[1], Florian Maier[1], Nicola Taccardi[2], Peter Wasserscheid[2], and Hans-Peter Steinrück[1] — [1]Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen — [2]Lehrstuhl für Chemische Reaktionstechnik, Egerlandstr. 3, 91058 Erlangen

Ionic liquids (ILs) - salts with a melting temperature below 100 °C - have highly attracted attention due to their great potential in many fields, e.g. in catalysis or electrochemistry, and as a new class of tailored solvents. Due to their extremely low vapour pressure, ILs can be investigated with X-ray photoelectron spectroscopy (XPS) under ultra-high vacuum conditions allowing for in-situ studies of reactions in the near-surface region.

For the first time, an in-situ alkylation could be directly monitored by XPS in a 1:1 mixture of the two ILs $[C_8C_1Im][Cl(CH_2)_3SO_3]$ (IL 1) and $[(Me_2N(CH_2)_3)C_1Im][Tf_2N]$ (IL 2). In this thermally activated reaction, the amine group of the $[(Me_2N(CH_2)_3)C_1Im]^+$ cation (2) reacts quantitatively with the $[Cl(CH_2)_3SO_3]^-$ anion (1), producing an ammonium group in a new cation and a free chloride anion. Cl 2p spectra directly reflect the transformation of the covalently bound chlorine of (1) into the chloride anion. Additionally, angle resolved XPS (ARXPS) provides information on surface enrichment and orientation effects of the pure ILs and in the binary mixture before and after alkylation. - This work was supported by the DFG through SPP 1191 and the Cluster of Excellence 'Engineering of Advanced Materials'.

O 60.106 Wed 17:30 P4

Investigations of different techniques for oxygen termination of ultrananocrystalline diamond films — •Alexandra Voss, Hermann Koch, Cyril Popov, and Johann Peter Reithmaier — Universität Kassel, Institut für Nanotechnologie und Analytik, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

Due to the high electrochemical potential window and high chemical stability, combined with a number of superior physical properties, all types of diamond films are ideal candidates for platforms for biosensors and DNA-chips. In almost all cases, after growth the surfaces of these films are hydrogen terminated and require photo-, plasma-, electro- or thermochemical processes to change the termination or to attach desired surface functionalities. In the current work we present the results for the surface modification of ultrananocrystalline diamond/amorphous carbon (UNCD/a-C) composite films by two different methods for oxygen termination, a O_2-plasma process and a UV/ozone treatment. The surfaces emerging from both modification ways were characterized by contact angle (CA) measurements, SEM, XPS, ToF-SIMS and STM, and their longtime stability with respect to different storage conditions was observed. In addition, the rate of the modification was determined with time dependent experiments to achieve highly hydrophilic surfaces (CA below 10°). The modification of the UNCD/a-C films increases their versatility for tailoring the surface properties for applications in biosensors, which requires a variety of functionalities in order to immobilize biomolecules.

O 60.107 Wed 17:30 P4

Conductivity of nano-porous Titania (TiO_2) during UV-illumination — •Thomas Kriesche[1] and Thomas Bürgi[2] — [1]Phys.-Chem.-Institut, Im Neuenheimer Feld 253, 69120 Uni Heidelberg — [2]Faculté des Sciences, Séction de Chimie, Département de Chimie Physique, Quai Ernest-Ansermet 30, CH-1211 Genève 4

The photocatalytic property of TiO_2 is used in many applications as solar cells for the production of hydrogen and electric energy, degradation of harmful substances, corrosion-protective coating. It is also investigated for energy storage (solar-to-fuel). Absorbed UV-light creates electrons and holes in the semiconductor, which recombine or can do reduction respectively oxidation on surface adsorbed molecules. The change of the conductivity during UV-irradiation reveals fundamental information about processes in nano-porous TiO_2 layers. Time resolved measurements offer the possibility to combine information from other methods like infrared spectroscopy, especially ATR-FTIR in MIR range. Data from scanning-electron-microscopy is used to show the porous structures. The conductivity is measured on top of a TiO_2 pill via a four point method in an Argon or Nitrogen atmosphere. It is possible to change the temperature and the humidity. For UV irradiation a Xenon lamp or 350nm diodes are in use with $\sim 0,5-1mW/cm^2$. The received data should be a step to describe the electron behavior of nano-porous TiO_2 under UV-irradiation.

O 60.108 Wed 17:30 P4

Spectroscopic Identification of initial decomposition mechanism of Prenal on a Platinum Model Catalyst — •Jan Haubrich[1], David Loffreda[2], Francoise Delbecq[2], Philippe Sautet[2], Yvette Jugnet[3], Conrad Becker[4], and Klaus Wandelt[1] — [1]Inst. für Phys. und Theo. Chemie, Uni. Bonn — [2]Lab. de Chimie, Ecole Normale Supérieure de Lyon — [3]Inst. de Rech. sur la Catalyse, Villeurbanne — [4]CINAM, Aix-Marseille Uni.

The prediction of reaction mechanisms consisting of complex networks of elementary steps and the identification of corresponding intermediates are major challenges in multifunctional catalysis and surface chemistry. We demonstrate that this difficulty can be overcome by tracking the temperature dependent formation of the intermediates and identifying the decomposition pathways in the case prenal, an α,β-unsaturated aldehyde, on the Pt(111) model catalyst surface by combining vibrational spectroscopy, temperature-programmed reaction spectroscopy and DFT analysis. Desorption states of H_2 (280 K, 410 K and 473 K) and CO (414 K) suggest that the loss of H and the CO functions are among the first elementary steps. HREELS performed after annealing to specific temperatures results in spectra which can be assigned to several subsequently formed surface intermediates with the help of complementary theoretical vibrational analysis. The most likely reaction pathway obtained from DFT for intial decomposition occurs from the strongly bonded prenal adsorption structures via an dehydro-η^3-triσ(CCC)-H1 intermediate to the η^1-isobutylidyne species at high temperatures.

O 60.109 Wed 17:30 P4

Monitoring and adjusting the temperature of ultra-thin metal catalysts *in situ* — •Ievgen Nedrygailov, Kevin Stella, Cordelia Soostmeyer, Eckart Hasselbrink, and Detlef Diesing — Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany

Despite the widespread usage of metal thin films in surface science experiments, the *in situ* measurement of the thin film temperature using traditional methods remains challenging. To address this problem the technique of adjusting and measuring the temperature of metal thin films by passing an electric current through them is proposed. The current flowing directly through the thin film serves for both: Joule heating of the thin film and monitoring the temperature using the temperature dependence of the thin film resistance. Direct heating is used to clean the platinum thin films (15-20 nm) on top of the silicon based electronic devices under ultra high vacuum conditions. Temperature programmed desorption of water and CO molecules from the polycrystalline platinum surface of the devices is studied to characterize the chemical state of the device surface.

O 60.110 Wed 17:30 P4

Photoinduced CO oxidation by association with defect-bound atomic oxygen on thin MgO films — •Philipp Giese, Harald Kirsch, Christian Frischkorn, and Martin Wolf — Fritz-Haber-Institut, Abt. Physikalische Chemie, Faradayweg 4-6, 14195 Berlin

As a prototype system for chemistry of defect-bound atomic oxygen on MgO, the CO oxidation has been studied. Atomic oxygen species were generated by photoinduced N_2O dissociation on thin MgO films grown on Ag(100). CO oxidation was studied as a function of photon exposure and initial CO coverage. The reaction products were studied by temperature programmed desorption spectroscopy (TPD). Carbon monoxide was co-adsorbed on films with atomic oxygen (10^{13} atoms/cm^2) at 20 K. If the coadsorbate is irradiated with UV light (5 eV), a CO_2 desorption peak at about 300 K appears, accompanied by a depletion of the atomic oxygen. The amount of CO oxidation increases with photon exposure and stops when the atomic oxygen is completely depleted. However, this process does not happen by irradiation of CO without previous atomic oxygen preparation, thus a direct reaction between the adsorbed CO molecules can be excluded. In addition, without UV excitation of the coadsorbate no reaction occurs either, revealing that the activation barrier for the CO oxidation on MgO surfaces is too high for a thermally activated reaction.

O 60.111 Wed 17:30 P4

Selforganization in ultrathin, K-promoted V-oxide layers on Rh(111) during the O2+H2 reaction. — •Martin Hesse, Fernando Sotoca Usina, and Ronald Imbihl — Institut für Physikalische Chemie und Elektrochemie, Leibniz-Universität Hannover, Callinstr. 3 - 3a, D-30167 Hannover, Germany

Alkali metals (AM's) promoted V-oxides play an important role as catalysts in a number of industrial partial oxidation reactions. As catalytic model system we studied the behaviour of K-promoted ultrathin V-oxide films (0.25 ML of V) on Rh(111) in the O2+H2 reaction using photoemission electron microscopy (PEEM) as spatially resolving method. With LEED, ordered phases of the ternary system V+K-O were detected. Similar to the unpromoted system stationary patterns develop under reaction conditions formed by stripes of V+O+K surrounded by bare Rh(111) surface. In addition, we observe also dynamic chemical wave patterns leading to K redistribution and enrichment of K at interfaces. The main effect of the addition of the AM is that it makes the VOx system very dynamic as evidenced by violent chemical turbulence. Tentatively, the stationary patterns were explained as being a consequence of reactive phase separation.

O 60.112 Wed 17:30 P4

Chemical trends in the metal-substrate interaction for adsorbed Pt atoms — •Chong Gao and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, D-89069 Ulm, Germany

Catalysts typically consist of small metal particles deposited on a oxide substrate. The interaction of the support with the metal particles can play quite a significant role for the catalytic activity of the particles. Using density functional theory, we have addressed the catalytic activity of small supported Pt clusters with up to 6 atoms. As the support, we considered Au, Ru, Si and TiO_2 substrates in order to derive chemical trends from metals to semiconductors and oxides. The electronic structure of the adsorbed Pt atoms and calculated CO adsorption energies on these metal-support systems are used as a probe of the chemical reactivity. The results are compared to recent results of the local reactivity of surface alloy systems [1,2]. In general, we find a strong anti-correlation between the binding energies of the Pt clusters on the substrates and the CO adsorption energies on the metal clusters.

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O 60.113 Wed 17:30 P4

Cluster chemistry in the gas phase: a new approach for laser spectroscopy — •Kathrin Lange, Bradley Robert Visser, Martin Tschurl, Ulrich Kaspar Heiz, and Ulrich Boesl-von Grafenstein — Lichtenbergstr. 4, 85748 Garching

The characterization and determination of organic molecules which exist as enantiomers or diastereomers are today of crucial importance especially for the pharmaceutical industry. It has been shown that chiral metal clusters are able to catalyse one form of the enantiomer or diastereomer [1].

The aim of the present work is to build a new setup to produce chiral metal clusters and to implement the idea of separating enantiomers by laser spectroscopy.

The chiral metal clusters will be produced by a laser vaporisation cluster source [2] and reacted with target organic species in the gas phase.

In this work we will describe the setup of our apparatus and a number of laser spectroscopy techniques (REMPI, CD Spectroscopy) in detail. These techniques will be used to induce photochemical processes in the metal cluster and molecule complexes to achieve enantiomeric or diastereomeric sensitive separation and detection [3].

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O 60.114 Wed 17:30 P4

Experimental setup of a time-of-flight mass spectrometer for reaction product detection in heterogeneous catalysis — •Andreas Winbauer, Martin Tschurl, Josef Kiermaier, and Ulrich Kaspar Heiz — Lichtenbergstraße 4, 85748 Garching

Mass spectrometry is a very powerful analytical tool for the study of heterogeneous catalysis. It's often used to study reaction processes by analyzing the reaction products, both in a qualitative and in a quantitative way.

Often mass spectrometers work by using electron impact ionization, where a discrimination between isomers is difficult to achieve. Their fragmentation patterns must differ to a large extent.

A powerful and soft method for selective ionization is REMPI (Resonant Enhanced Multiphoton Ionization). In this technique a laser of specific wavelength is employed to ionize only one isomer through resonant intermediate states. Other isomers cannot be ionized as they are non resonant at the energy used.

For the study of catalytic reactions on metal clusters supported on single crystal surfaces under UHV conditions a new experimental setup was built. For the spectroscopic studies custom ion optics were designed to incorporate the crystal support and enable future desorption-ionization studies.

In this work we will present our experimental setup, in which we combine time of flight mass spectrometry with resonance enhanced multiphoton ionization. Furthermore we will show first experimental results and possible applications for our setup.

O 60.115 Wed 17:30 P4

First-Principles Calculations of Hydrogen Generation Due to Water Splitting on Polar GaN Surface — •Po-Tuan Chen — Physics Department, Osnabrueck, Germany

We present the chemical reactions leading to hydrogen gas generation via water splitting on polar GaN surfaces, which can be a significant source of renewable energy. To build an understanding at the atomic level of the activations afforded by the GaN (0001) and (000-1) surfaces, we determine the reaction mechanism of hydrogen generation on the polar faces using density functional theory calculations. The calculation results show that the first H splitting from water can occur with ground-state electronic structures; the barriers of H2O splitting are 0.10 and 0.34 eV on the Ga-face and the N-face, respectively. However, the second H splitting requires huge energies of 1.42 and 1.73 eV, respectively, on the Ga-face and the N-face. Although the polar GaN surface can catalyze the first hydrogen splitting from water, we suggest that photoexcitation should be necessary for the second splitting.

O 60.116 Wed 17:30 P4

In-situ spectroscopic investigation of adsorption and reaction of pyridine molecules on Pt surfaces — •Claudia Wöckel[1], Kristina Fischer[1], Andre Dorsch[1], Sandra Wickert[1], Regine Streber[2], Hans-Peter Steinrück[2], and Reinhard Denecke[1] — [1]Wilhelm-Ostwald-Institut, Universität Leipzig, Linnestr. 2, 04103 Leipzig, Germany — [2]Physikalische Chemie II, Department Chemie, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Using high-resolution and time-dependent XPS adsorption and reaction processes can be followed in-situ. We are applying this method to pyridine molecules adsorbed on Pt. Using a regularly stepped Pt(355) and a Pt(111) surface, C 1s and N 1s core level data are recorded during adsorption at various temperatures. As additional parameter, the free Pt terrace width is varied by deposition of Ag atoms on the surface, forming rows along the step edges at 300 K. Temperature-programmed XPS allows to follow the thermal reaction of the adsorbed species. The experiments have been performed at BESSY II in Berlin.

In line with literature reports about a temperature- and coverage-dependent reorientation from flat to upright[1], we observe changes in the core level binding energies and intensities during the uptake. Upon heating the strong N 1s feature observed at 200K is transformed into a contribution at higher binding energy. This is accompanied by respective changes in the C 1s data, suggesting again temperature- and coverage-dependent changes, here towards α -pyridyl. Supported by BMBF (05 ES3XBA/5).

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O 60.117 Wed 17:30 P4

Solar2Fuel: XPS and TPD characterization of functionalized TiO_2 surfaces for photocatalytic reduction of CO_2 — •Florian Staier, Michael Grunze, and Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, INF 253, 69120 Heidelberg

The handling of CO_2 produced by industrial installations and power plants has become a very important environmental issue nowadays because of it's generally accepted impact on the green house effect. In this context, a storage of CO_2 or its conversation to fuel or useful chemicals are highly desirable. Along these lines, the solar2fuel project, funded by BMBF, aims on photocatalytic conversion of CO_2 to methanol with a sufficient quantum efficiency which can justify and make rentable an industrial realization of the process. As the primary catalytic system TiO_2 nanoparticle powder coatings are used. These particles are doped with metals to enhance their catalytic activity and functionalized with specially designed dyes which promote photocatalytic reaction and move the absorption spectrum from UV (characteristic of TiO_2) to the visible range. We present first results on characterization of these catalytic systems by several complimentary techniques as well as on temperature-programmed-desorption of CO_2 and methanol from these functionalized surfaces.

O 60.118 Wed 17:30 P4

Gold-containing model catalysts studied with in-situ XPS — •Martina Pistor, Karifala Dumbuya, Ole Lytken, Lorenz Ringel, Jörg Michael Gottfried, and Hans-Peter Steinrück — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II

The noble metal gold, if supported as nanoparticles on oxides such as TiO_2, is a promising catalyst for many oxidation reactions. Up to now, it is still debated why gold, which is not active as a bulk material, becomes active in the dispersed state (with optimum particle sizes 2-5 nm). Explanations include quantum size effects, low-coordinated gold atoms, the substrate/gold perimeter interface and anionic as well as cationic gold species. Using in-situ X-ray photoelectron spectroscopy (XPS), we have studied various gold-based powder catalysts and model catalysts, both in the presence of CO, O_2 and propene and under ultra-high vacuum conditions. The studied systems include gold nanoparticles supported on TiO_2(110) and titania nanoparticles supported on Au(111) as well as reference powder catalysts. Depending on the experimental conditions, especially the oxygen partial pressure, the intrinsic catalytic activity of the system is superimposed by X-ray-induced effects such as the formation of gold oxide. On the basis of these beam damage effects, we will discuss possible limitations of in-situ XPS. This work is supported by the DFG through grant GO 1812/1 and by the Cluster of Excellence "Engineering of Advanced Materials" granted to the Universität Erlangen-Nürnberg.

O 60.119 Wed 17:30 P4

Investigation of new Catalysts for PEM Fuel Cells — •Roy Mbua[1], Ulricke Kramm[2], Klaus Mueller[1], Matthias Richter[1], Karsten Henkel[1], Ioanna Paloumpa[1], and Dieter Schmeisser[1] — [1]Brandenburgische Technische Universitaet Cottbus, Angewandte Physik/Sensorik, K. - Wachsmann-Allee 1, 03046 Cottbus — [2]Helmholtz-Zentrum für Materialien und Energie, Berlin

Increasing green house emissions amplify global warming concerns worldwide. Fuel cells, based on polymer electrolyte membranes (PEM) are part of the solution to this issue. We aim at developing and testing new catalysts for fuel cells. Platinum catalysts perform best in PEM fuel cells to date but they are very expensive. For fuel cells to be perfectly applicable and economically affordable, an alternative catalyst with similar or even greater efficiency should be developed.

Metal phthalocyanines are known to be good oxygen reduction catalysts and are associated with high electron transfer properties. We investigated Cobalt Phthalocyanine in its pure state mixed with Carbon Black (CoPc:Carbon Black=1:9) untreated and also after a treatment in N2 at several temperatures, up to 1000°C for 30 minutes.

Results of XPS and EDX analyses reveal that the treatment at higher temperatures causes a rearrangement in the chemical states of Co, N and C atoms. Furthermore, results of cycling voltammetry (CV) analysis reveal that CoPc treated in N2 at 800°C exhibited a higher current density, in conclusion, a higher catalytic activity than the untreated CoPc.

O 60.120 Wed 17:30 P4

Methanol synthesis over binary Cu/ZnO surfaces: exploration of energy surfaces for determining adsorption sites for CO_2 — •luis martínez suárez[1], johannes frenzel[1], bernd meyer[2], and dominik marx[1] — [1]Ruhr University Bochum, Theoretical Chemistry, Bochum, Germany — [2]Interdisziplinäres Centrum für Molekulare Materialien (ICMM) and ComputerChemieCentrum (CCC), Department Chemie und Pharmazie, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Methanol is synthesized from syngas over Cu/ZnO in a heterogeneous catalytic process with CO_2 as carbon source. Atomistic insight into the strong metal substrate interaction (SMSI) effect in Cu/ZnO catalysts has been obtained in a static picture. Calculations of surface phase diagrams by *ab initio*-thermodynamics determined realistic structures of a small Cu_8 cluster on $ZnO(000\bar{1})$ in a hydrogen atmosphere with temperature and pressure conditions as required in the industrial process. These structures are stabilized by the interplay of structural changes as a result of redox properties of the syngas with realistic saturation of the catalyst surface by hydrogen interacting with defect sites. Herein the global energy landscape of the CO_2 reactant over several thermodynamically relevant catalyst surface structures is explored with spatial resolution employing density functional theory. After having identified all possible adsorption sites on the complex Cu/ZnO surfaces the adsorption modes of the complexes are refined investigating their individual structures.

O 60.121 Wed 17:30 P4

Ceria promoted CO oxidation on Pt(111): Oxygen-spillover and active border concept — Stefan Becker[1], •Kathleen Müller[1], Rafal Wróbel[1,2], and Helmut Weiss[1] — [1]Otto-von-Guericke-University Magdeburg, Institute of Chemistry, Universitätsplatz 2, D-39106 Magdeburg, Germany — [2]West Pomeranian University of Technology, Institute of Chemical and Environmental Engineering, Pulaskiego 10, 70-322 Szczecin, Poland

The influence of CeO_x nanoformations on the heterogeneously catalysed CO oxidation above the bistable region was investigated. A well-defined CeO_x/Pt(111) model catalytic system with homogeneous 2D islands has been produced by evaporating Ce on Pt(111) in oxygen ($5\cdot10^{-8}$ mbar). The clean Pt(111) surface was characterised by XPS, LEED and STM and the inverted model catalysts CeO_x/Pt(111) by XPS, STM and CO titration. The temperature and pressure dependency of the reaction rate was analysed via mass spectrometry. An enhanced reactivity was observed for a surface covered with CeO_x islands as compared to clean Pt(111). The CeO_x leads to a change in the adsorption characteristics for oxygen as well as for carbon monoxide (promotional effects). An active border concept for oxygen and carbon monoxide and a spillover mechanism for oxygen are suggested.

O 60.122 Wed 17:30 P4

Hydrogen adsorption on $RuO_2(110)$ — •Bianca Eifert[1], Christian Heiliger[1], Jan Philipp Hofmann[2], Herbert Over[2], and Ari Paavo Seitsonen[3] — [1]Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany — [2]Physikalisch-Chemisches Institut, Justus Liebig University Giessen, D-35392, Germany — [3]Physikalisch-Chemisches Institut, University of Zurich, CH-8057, Switzerland

Complementary to experimental work, density functional theory calculations are utilized to gain a deeper insight into the adsorption and insertion behavior of hydrogen and water species on the $RuO_2(110)$ surface at an atomic level. This is important for an improved understanding of RuO_2 as a model and real catalyst system in reactions spanning from oxide-catalyzed dehydrogenation to a wide range of electrochemical reactions.

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O 60.123 Wed 17:30 P4

Spectroscopic and microscopic characterization of potential catalysts for the hydrogenation of CO2 — •David Hoffmannbeck, Matthias Richter, Matthias Städter, Ioanna Paloumpa, Karsten Henkel, and Dieter Schmeisser — BTU-Cottbus, LS Angewandte Physik II - Sensorik K.-Wachsmann-Allee 1, D-03046 Cottbus

The reduction of CO2 emissions is a general demand of the society in order to avoid irreversible climate changes. We are investigating potential catalysts for the hydrogenation of CO2 in particular for its application in the so called oxyfuel combustion process.

In order to understand the catalytic behavior of the investigated materials we use the techniques X-Ray Photoemission (XPS) and -absorption (XAS) Spectroscopy as well as X-Ray Diffraction (XRD) and Scanning Electron Microscopy (SEM). The prospective of our work is to figure out the electronic and structural properties of the material and to optimize proper catalysts or design new ones for best catalytic activity. Beside the spectro-microscopic investigations the catalysts are tested under Sabatier reaction conditions in terms of activity, stability and sensitivity against poisoning. In our preliminary work we constructed a Sabatier reactor system with analytical parts based on infrared absorption and mass spectroscopy modules. First spectroscopic and catalytic results achieved on a commercially available Ru/Al2O3 catalyst will be presented.

O 60.124 Wed 17:30 P4

Reduction of Thin NiO Films by Carbon Monoxide — •Oliver Höfert[1], Wei Zhao[1], Karin Gotterbarm[1], Andreas Bayer[1], Junfa Zhu[2], Christian Papp[1], and Hans-Peter Steinrück[1] — [1]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen — [2]National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei 230029, People's Republic of China

NiO is an important material in heterogeneous photocatalysis for degradation of azodyes [1] or water splitting [2]. We studied the reactivity of different thin NiO films on Pd(100) towards CO by in situ XPS applying synchrotron radiation at BESSY II. Our data shows that closed and well ordered NiO films with less than 2 ML are indeed reduced to metallic Ni by exposure to CO above 400 K. The reduction of NiO by CO is chemically reversible as was shown by subsequent reoxidation of the metallic Ni by O_2. The influence of Pd to the reaction could be excluded. Our kinetic investigations revealed a coupling of diffusion and reaction in the reduction process. For both mechanisms we determined the activation energy. Additionally, the reoxidized films showed a different behaviour and could not be fully reduced due to structural changes.

This work was supported by BMBF (05 ES3XBA/5) and the DFG through the Cluster of Excellence "Engineering of Advanced Materials".

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O 60.125 Wed 17:30 P4

Nucleation, growth and thermal behaviour of Au and Cu-clusters on ZnO — •Dietmar Rother, Martin Kroll, and Ulrich Köhler — Institut für Experimentalphysik IV / AG Oberflächenphysik, Ruhr-Universität Bochum

The growth of Au and Cu on $ZnO(10\bar{1}0)$ single crystal surfaces was studied as a first step to understand complex catalytically active systems, often consisting of small metal clusters on metal oxide surfaces. Thermal evolution of Au and Cu clusters on $ZnO(10\bar{1}0)$ was studied in-situ with STM at elevated temperature. Au and Cu were deposited using MBE sources at room temperature. On the mixed terminated $ZnO(10\bar{1}0)$ surface separated Cu clusters are formed at room temperature. A partial entrenching of Cu into the ZnO substrate at elevated temperature of $T > 670$K was found and points to a reaction of the Cu-clusters with the ZnO support. Au on ZnO shows a different behaviour: Annealing RT-deposited Au-clusters to comparable temperatures shows no reaction of Au-Clusters with the ZnO-substrate. After the initial coarsening, Au on ZnO shows no changes while scanning insitu at elevated temperature up to 770K on a time scale of hours. The minimum cluster density is already reached at 420K. The behaviour on $ZnO(10\bar{1}0)$ is compared to other ZnO surfaces and to $TiO_2(110)$.

O 60.126 Wed 17:30 P4

CO oxidation reaction on thin mesoporous Au/TiO_2 layers — •Matthias Roos[1], Dominique Böcking[2], Kwabena Offeh Gyimah[1], Gabriela Kucerova[1], Joachim Bansmann[1], Nicola Hüsing[2,3], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069, Germany — [2]Institut für Anorganische Chemie II, Ulm University, D-89069, Germany — [3]Abteilung Materialchemie, Universität Salzburg, A-5020, Austria

The catalytic properties of thin homogeneous layers of mesoporous Au/TiO_2 [1] deposited onto silicon substrates to study the CO oxidation reaction was investigated. The mesoporous TiO_2 layers are fabricated using a sol-gel process followed by the precipitation-deposition of Au nanoparticles. The measurements on the catalytic activity were performed in a vacuum system using a quadrupole mass spectrometer which allows to collect the reaction gases very close to a specific region on the surface [2]. Using this setup, the activation energy and the reaction orders of CO and O_2 were measured and compared to respective measurements on planar Au/TiO_2(110) model catalysts and standard Au/TiO2 powder catalysts. Furthermore, the catalytic stability and the deactivation behaviour of the mesoporous Au/TiO_2 films was studied. To test the accessibility by reaction gases of deeper lying regions within the catalytically active films, the thickness of the TiO_2 layers was varied for different measurements.

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O 60.127 Wed 17:30 P4

HR-EELS studies on zinc oxide powders samples — •Sebastian Frey, Martin Kroll, Dietmar Rother, and Ulrich Köhler — Ruhr-Universität Bochum, Deutschland

Zinc oxide powders are an important catalyst for a number of organic reactions, e.g. the synthesis of methanol. Corresponding surface science studies, on the other hand, mainly deal with single crystalline surfaces. Since this situation is quite different from a real catalyst, this work concentrates on the vibrational spectroscopy analysis of ZnO powder samples using high resolution electron energy loss spectroscopy (HR-EELS) to deliver supplementary information to the existing single crystal studies. At first we present different approaches to fix the ZnO powder on a gold substrate for vacuum treatment including XRD and SEM-analysis. Finally, the results of our HR-EELS measurements of the ZnO powder samples exposed to different organic molecules like methanol and formic acid are displayed in comparison to the (0001), (000-1) and (10-10) single crystal surfaces.

O 61: Invited Talk (Qikun Xue)

Time: Thursday 10:15–11:00 Location: TRE Phy

Invited Talk O 61.1 Thu 10:15 TRE Phy
Novel properties of topological insulator thin films of Bi2Te3 and Bi2Se3 prepared by molecular beam epitaxy — •Qikun Xue — Physics Department, Tsinghua University, Beijing100084, China

We have grown topological insulator thin films of Bi2Te3 and Bi2Se3 on Si(111) and 6H-SiC(0001) substrates by using state-of-art molecular beam epitaxy (MBE). We studied nontrivial surface states and their thickness-dependence of the films by in situ angle resolved photoemission spectroscopy (ARPES) and scanning tunneling microscopy/spectroscopy (STM/STS). By direct imaging standing waves associated with magnetic and nonmagnetic impurities and steps on Bi2Te3 and Bi2Se3 (111) surfaces, we show that the topological states have a surface nature and are protected by the time reversal symmetry. We demonstrated the high mobility of the Bi2Se3 films by direct observation of Landau quantization. We also studied the growth of superconducting and magnetic thin films on Bi2Te3 and Bi2Se3. Implication on probing Majorana fermions and topological magneto-electric effect will be discussed.

O 62: [DS] Organic Electronics and Photovoltaics I (jointly with CPP, HL, and O)

Time: Thursday 10:15–11:45 Location: GER 38

O 62.1 Thu 10:15 GER 38
Structuring of Organic Conductors by Laser Ablation — •Alexander Esser, Moritz Schaefer, Jens Holtkamp, and Arnold Gillner — Fraunhofer ILT, Steinbachstraße 15, 52074 Aachen

PEDOT:PSS is a transparent organic polymer with a sheet resistivity of about 200ohm/sq. These attributes make it an ideal candidate for substituting ITO in organic LEDs and organic photovoltaic cells: making them fully organic, flexible, lightweight and cheap to produce. Organic thin-film photovoltaics are a low cost alternative to state of the art silicon and other inorganic semiconductor-based solar cells. OLEDs can be made more flexible without the use of transparent conducting oxides.

We present structuring of organic conductors by laser ablation from spin coated films of PEDOT:PSS. We have investigated ablation characteristics of PEDOT:PSS depending on laser wavelength in the deep UV and required fluence. The smallest structuring resolution by UV laser patterning has been found.

In further measurements we have determined the conductivity depending on layer thickness and structure size. Especially the influence of laser radiation on conductivity and electrical properties in the vicinity of the ablated area has been studied. Therefor we have performed AFM measurements as well as four-point probing.

O 62.2 Thu 10:30 GER 38
Investigation of the origin of the memory effect in devices based on C_{60} — •Philipp Sebastian, Alexander Zakhidov, Björn Lüssem, and Karl Leo — Institut für Angewandte Photophysik, George-Bähr-Straße 1, 01069 Dresden, Germany

Besides their application in organic solar cells and organic light emitting diodes, organic semiconductors also show much potential in the field of flexible and lightweight electronics, such as organic memory. In particular, the development of organic memory devices has turned out to be challenging. So far, many different approaches for organic memory devices have been reported in literature [1].

In this contribution, we report on an organic memory device comprising SiO_2 layer on top of a indium tin (ITO) ground contact, followed by electron accepting C_{60} layer, a n-doped (Cs) 4,7-diphenyl-1,10-phenanthroline (BPhen) layer and an Al top electrode. IV measurements reveal a reproducible hysteresis of our devices with a maximum ON-OFF ratio of about one order of magnitude. The memory devices also demonstrate a remarkable switching cycle durability of more than 10^4 successfully applied write read erase read cycles, whereas the ON-OFF ratio remains constant at about 10. Retention times of several weeks underline a reasonable non-volatility. Further, the memory mechanism has been investigated by impedance spectroscopy. A hysteresis in capacitance-voltage measurements expresses the accumulation of electrons in the C_{60} and at the interface to the SiO_2 layer.

[1] J. Scott, L. Bozano, Advanced Materials 19, 1452 (2007)

O 62.3 Thu 10:45 GER 38
Growth and morphology of aluminium contacts on P3HT films — •Gunar Kaune[1,2], Robert Meier[1], Ezzeldin Metwalli[1], Volker Körstgens[1], Kai Schlage[3], Sebastien Couet[3], Stephan V. Roth[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Straße 1, 85747 Garching — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Fachgruppe Photovoltaik, Von-Danckelmann-Platz 3, 06120 Halle — [3]HASYLAB at DESY, Notkestraße 85, 22603 Hamburg

The characteristics of organic electronic devices are strongly influenced by the type and structure of the metal electrodes needed to inject or extract charge carriers. Therefore understanding of the metal growth process and its relation to the interactions at the metal-organic interface are necessary. We investigate the growth of an aluminium layer on the surface of a P3HT thin film by in-situ application of grazing incidence small-angle X-ray scattering (GISAXS). By subsequent modelling of the scattering data the structural parameters of the growing film are extracted and a growth process is found, which proceeds two-dimensional by stacking single atomic layers on top each other. This process results in a homogeneous film with a large contact area to the polymer and is explained by a strong chemical interaction between aluminium and P3HT, which suppresses clustering of the metal on the polymer surface. The diffusion of single aluminium atoms into the P3HT and the formation of an intermixing layer is revealed by X-ray reflectivity measurements.

O 62.4 Thu 11:00 GER 38

Effect of high-k substrates on the photocurrent of organic semiconductors: Tailoring the Coulomb interaction — •Miriam Engel[1], Doru C. Lupascu[2], Niels Benson[1], and Roland Schmechel[1] — [1]Nanostrukturtechnik, Universität Duisburg-Essen, 47057 Duisburg — [2]Institut für Materialwissenschaft, Universität Duisburg-Essen, 45117 Essen

A major difficulty for organic photovoltaic cells is the dissociation of excitons into free charge-carriers. This is caused by high exciton binding energies, due to the low permittivity of the organic material. There are approaches to use acceptor-donator systems in the form of bulk-heterojunctions, which leads to successful exciton dissociations per volume. However, re-trapping may occur even after efficient charge-carrier separation due to Coulomb interaction (CI). Our aim is to use inorganic high-k materials to increase the exciton dissociation and to lower CI. In our proof of principle experiments devices are based on substrates with different permittivities. Pentacene is deposited as the active organic layer on them. Silver electrodes are used as top-contacts. For the electrical characterization we performed I(V) measurements in the dark and under illumination. Because of the known influence of the pentacene morphology on the mobility of the charge-carriers, we corrected the current under illumination by the dark current to obtain the pure contribution from the photo-effect. We obtained an improvement of the photocurrent using high-k substrates. The final goal is to transfer the layered system into an organic-inorganic composite system with high-k nanoparticles embedded in a photoactive organic matrix.

O 62.5 Thu 11:15 GER 38

Organic pin-Diodes with Adjustable Current-Voltage Performance Applicable at Ultra-High-Frequencies — •Hans Kleemann, Christoph Schünemann, Paul Pahner, Alexander A. Zakhidov, Björn Lüssem, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Straße 1, 01069 Dresden, Germany

Organic diodes have been intensively studied during the past years and great progress has been achieved in the field of organic light-emitting diodes (OLEDs) and organic solar cells (OSC). Moreover, the development of other organic devices like thin film transistors, vertical transistors, memory arrays, and high-frequency diodes which are required for an electronic circuitry will allow the design and integration of complete organic electronics. In this contribution we present organic *pin*-diodes with adjustable forward and reverse current-voltage performance applicable in the ultra-high-frequency region. Key parameters to design these diodes are the doping concentration, the intrinsic interlayer thickness and the material properties. In this way the reversible backward breakdown can be shifted from $-3V$ to more than $-20V$ independently of the forward performance [1]. Due to the high rectification ratio (10^5) and since the diodes contain high mobility materials like pentacene and C_{60} we present high-frequency properties of these pin-diodes above 13.56MHz required for RFID-tags.

[1] H. Kleemann et al., Organic Zener Diodes: Tunneling across the Gap in Organic Semiconductor Materials, Nano Letters 2010, published online.

O 62.6 Thu 11:30 GER 38

Photoinduced degradation process of Fir6 emitter molecules: a laser desorption/ionization time-of-flight mass spectrometry investigation — •Ines Rabelo de Moraes[1], Ruben Seifert[1,2], Sebastian Scholz[1,3], Björn Lüssem[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, 01062 Dresden, Germany — [2]Von Ardenne Anlagentechnik GmbH, Plattleite 19/29, 01324 Dresden, Germany — [3]Fraunhofer-Institut für Keramische Technologien und Systeme, Winterbergstraße 28, 01277 Dresden, Germany

Phosphorescent Organic Light Emitting diodes (OLEDs) have attracted much interest for their potential application in the field of full color displays and as next generation of lighting sources. One of the major problems related to the OLED technology is the short lifetime of the blue phosphorescent emitters. For improving the lifetime of the OLEDs a deep understanding of the intrinsic chemical degradation is required. Our work is focused on the photoinduced degradation process of single layer of the Fir6 molecule used as blue phosphorescent emitter by laser desorption/ionization time-of-flight mass spectrometry (LDI-TOF-MS). The LDI-TOF spectra collected at the laser intensity of 114 μJ/pulse indicate that the Fir6 molecule dissociates into [Ir(F2ppy)2]+ and [Fir6-(pyrazole)1]+. The reaction between the Fir6 fragments and the Fir6 molecule itself resulting in the formation of [Fir6+(pyrazole)1]+, and [Fir6-(pyrazole)1+Ir(F2ppy)2]+ could be observed as well. Additionally, the degradation processes of full processed OLEDs based on Fir6 emitter will be presented.

O 63: [MA] Surface magnetism III

Time: Thursday 11:00–13:00 Location: HSZ 103

O 63.1 Thu 11:00 HSZ 103

Spin reorientation related changes of the electronic structure in ultrathin Fe/Mo(110) films — •Torsten Methfessel and Hans-Joachim Elmers — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudingerweg 7, D-55099 Mainz

The magnetic easy axis in ultrathin Fe/Mo(110) films changes from a perpendicular easy axis at low temperatures to an in-plane easy axis at hight temperatures at the transition point around 13 K. We investigated this spin reorientation (SRT) using spin-resolved scanning tunneling microscopy (STM) and spectroscopy (STS). Magnetic domain patterns remain stable near the SRT. We measured domain wall widths versus temperature resulting in a measurement for the temperature dependent anisotropy. The electronic structure of the mono (ML) and double layer (DL) Fe/Mo(110) shows a variation with the reorientation of the magnetic easy axis. The spin averaged tunneling conductivity of the DL Fe shows a distinct increase with rising temperature clearly below the transition temperature which can be attributed to a magnetization along a magnetic hard axis. The SRT of Fe/Mo(110) can be identified as a discontinuous reorientation transition, revealing two simultaneous minima of the free energy in a certain temperature range.

O 63.2 Thu 11:15 HSZ 103

Uniaxial anisotropy in Fe/GaAs(001): oriented bonds versus magneto-elastic interaction. — •Günther Bayreuther[1,2], Jörg Premper[1], Matthias Sperl[2], Dirk Sander[1], and Jürgen Kirschner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]Inst. für Experimentelle und Angewandte Physik, Universität Regensburg, Regensburg, Germany

Ultrathin Fe films epitaxially grown on GaAs(001), in addition to their thickness-dependent cubic anisotropy, show a pronounced in-plane uniaxial magnetic anisotropy with the easy axis along [110], controversially attributed either to oriented interface bonds or to a magneto-elastic interaction. In order to check the relevance of magneto-elastic contributions we performed MOKE and magneto-elastic stress measurements on MBE-grown Fe(001) and $Fe_{32}Co_{68}$(001) films on GaAs(001). The uniaxial anisotropy constant K_U has the same sign for Fe and $Fe_{32}Co_{68}$. The magneto-elastic coupling coefficients B_2 of the films were measured using a cantilever method [1] and resulted to be of opposite sign for Fe and $Fe_{32}Co_{68}$ films, respectively. As all the films are under compressive strain with a lattice misfit of -1.16 % for Fe and -0.41 % for $Fe_{32}Co_{68}$ the magneto-elastic anisotropy contribution to K_U is expected to be of opposite sign for both materials, based on the respective values of B_2. The observed identical sign of K_U in both cases means that a magneto-elastic interaction is not the main origin of the uniaxial magnetic anisotropy in ultrathin Fe(001) films on GaAs(001).

[1] D. Sander, Rep. Prog. Phys. 62, 809 (1999)

O 63.3 Thu 11:30 HSZ 103

Influence of the growth temperature on the electronic structure of ultrathin cobalt films studied by spin-resolved photoemission — •Cheng-Tien Chiang, Aimo Winkelmann, Martin Ellguth, Ahmet Akin Ünal, Christian Tusche, and Jürgen

Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120, Halle (Saale), Germany

We investigate the electronic structure of ultrathin cobalt films grown on Cu(001) by spin-resolved one- and two-photon photoemission (1PPE and 2PPE). A majority quantum well state located at 2.1 eV above the Fermi level and a minority surface resonance state at 0.4 eV below the Fermi level are identified in 6 monolayer thick cobalt films. The photoemission features of the quantum well state and the surface resonance state are strongly suppressed for cobalt films grown at 170 K as compared to films grown at 330 K. 2PPE through the quantum well state increases the photoelectron spin-polarization by about 10%, and in 1PPE a sign reversal of the spin-polarization is observed from the surface resonance state. These observations are applied for electronic state sensitive imaging of magnetic domains in energy- and spin-resolved photoelectron emission microscopy (PEEM).

O 63.4 Thu 11:45 HSZ 103

NiO thickness and temperature dependent coercivity of Fe layers grown on NiO/Ag (100) — •Anita Dhaka, Dirk Sander, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 061120 Halle (Germany)

We have performed temperature dependent magneto-optical kerr effect (MOKE) measurements in the longitudinal geometry to investigate the coercivity of 6 monolayers (ML) Fe on NiO deposited on Ag (100). MOKE indicates that the coercivity of Fe on NiO strongly depends on the thickness of NiO, and this effect is temperature dependent. We find that the coercivity of 6 ML films deposited on 20 ML NiO of H_c=142 mT at 300 K,which increases to 172 mT at 150 K. For 40 ML NiO, the coercivity is 148 mT at 300 K, and 284 mT at 150 K. 6 ML Fe on Ag (100) show a constant H_c of 9±3 mT from 150 K to 470 K. The change of coercivity with temperature is reversible up to T=470 K. At higher temperature intermixing is found by Auger elctron dpectroscopy, and the magnetic behavior is no longer reversible upon cooling. No increase of coercivity is observed for Fe films on 20 ML and 40 ML NiO at 470 K. Temperature dependence of the coercivity is ascribed to presence of antiferromagnetic NiO, and our data indicate a Neel temperature of 20 ML NiO of approximately 470 K [1]. Financial support by SFB 762 is gratefully acknowledged. [1] D. Alders, L. H. Tjeng, F. C. Voogt, T. Hibma, G. A. Sawatzky, C. T. Chen, J. Vogel, M. Sacchi, S. Iacobucci, Phys. Rev. B **57**, 11623, (1998).

O 63.5 Thu 12:00 HSZ 103

Antiferromagnetic Mn chains on Ni(110) — •Simon Holzberger, Tobias Schuh, and Wulf Wulfhekel — Physikalisches Institut, Karlsruher Institut für Technologie, Germany

A novel even-odd effect has recently been predicted for atomic manganese chains supported by a ferromagnetic substrate [1]. While odd chains possess a net spin that aligns according to the coupling to the substrate resulting in a collinear spin state, even chains display a non-collinear state. To investigate atomic chains experimentally, low-temperature spin-polarized scanning tunneling microscopy (Sp-STM) was used. To favor the growth of linear chains, a ferromagnetic Ni(110) surface was chosen as substrate. While self assembly of chains by thermal diffusion always led to intermixing with the substrate, pure manganese chains could be created by atomic manipulation. The electronic structure of the chains was investigated by scanning tunneling spectroscopy revealing a strong dependence on the length of the chain. This is explained within the model of an unoccupied quasi atomic state in single manganese adatoms. Sp-STM confirmed the predicted collinear antiferromagnetic ground state for linear trimers. In contrast to the calculations, however, there was no indication of an antiferromagnetic or non-collinear spin structure for even-numbered chains. This observation is explained by the degeneracy of the antiferromagnetic ground state highlighting the quantum nature of the magnetic state.
[1] S. Lounis *et al.*, Phys. Rev. Lett. **101**, 107204 (2008)

O 63.6 Thu 12:15 HSZ 103

Spinresolved UPS: Study of the O p(1x1) phase on Fe(100) Using a Novel Multichannel Spinpolarimeter — •Michaela Hahn, Bernd Petereit, Martin Jourdan, Hans-Joachim Elmers, and Gerd Schönhense — Institut für Physik, Staudinger Weg 7, 55128 Mainz

A novel type of multichannel spindetector has been implemented recently, with strongly improved efficiency as compared to modern state-of-the-art single channel spin analysers. By the usage of parallel multichannel detection, it is possible to reduce the measuring time by orders of magnitude [1]. The sample systems Fe/MgO and O/Fe/MgO have been studied as a first application exploiting the detector's efficiency. Epitaxial iron layers were evaporated onto MgO(100) single crystals, oxygen was dosed in small steps.

The O p(1x1) phase on Fe(100) is of particular interest, as for example described in [2]. It is formed at a dosage of 6L oxygen on the clean Fe(100) surface. Due to additional FeO-bands in the surface layer, the spin asymmetry close to the Fermi edge is expected to exhibit new features as compared to clean iron. Our spectra show a strong quenching of the minority peak very close to E_F with increasing oxygen dosage. Furthermore, new features occur in the majority bandstructure.

Funded by Stiftung Rheinland-Pfalz für Innovation (project 886) and DFG (Scho 341/9-1)

[1] M. Hahn et al., this conference

[2] A. Tange et al., Phys. Rev. B 81, 195410 (2010)

O 63.7 Thu 12:30 HSZ 103

Magnetic Properties of Fe-Co alloy films on Ir(001) — •Rantej Bali, Marek Przybylski, and Jürgen Kirschner — Max Planck Institut für Mikrostruktur Physik, Halle, Germany 06120

We report on the magnetic behavior of $\mathrm{Fe}_{1-x}\mathrm{Co}_x$ alloy films grown on the Ir(001) surface. A variety of properties are observed depending on the Co content and film thickness. The first 4 monolayers (ML) of Fe (x = 0) do not exhibit magnetic hysteresis hinting to the existence of an antiferromagnetic phase, since thicker films are ferromagnetic. Ferromagnetism in the first 4 ML begins to be observed above x = 0.25 and further increase in Co content causes the easy axis to be perpendicular to the film plane [1]. For 10 ML thickness, this perpendicular anisotropy remains larger than the shape anisotropy at least up to the x = 0.6 composition. The increase and decay of the perpendicular anisotropy are observed through spin reorientation transitions that occur between the out-of-plane and in-plane magnetization directions of the film.

The differences in magnetic ordering such as the occurrence of antiferromagnetic and ferromagnetic phases and in-plane and perpendicular easy axes can be caused by the combination of strain induced modification of the electronic structure and the composition dependent adjustment of the Fermi energy.

[1] F. Yildiz *et al.*, J. Appl. Phys. 105, 07E129 (2009).

O 63.8 Thu 12:45 HSZ 103

Qualitative extraction of spin polarization on a single magnetic nanostructure — •Hirofumi Oka, Pavel Ignatiev, Sebastian Wedekind, Guillemin Rodary, Larissa Niebergall, Valeri Stepanyuk, Dirk Sander, and Jürgen Kirschner — Max-Planck-Institute of Microstructure Physics, Weinberg 2, D-06120, Halle, Germany

We present a qualitative extraction of spin polarization on single Co nanoislands using SP-STM. We use low-temperature STM in magnetic fields to manipulate parallel (P) and anti-parallel (AP) states of the magnetization orientation between a Co island on Cu(111) and a magnetic tip [1]. We measure the differential conductance (dI/dV) on the same island in both states as a function of energy, and obtain the asymmetry of the dI/dV, $(dI/dV_{AP} - dI/dV_P)/(dI/dV_{AP} + dI/dV_P)$, which is related to the spin polarization of a sample [2]. We find that the sign and magnitude of the dI/dV asymmetry strongly depend on energy. In conjunction with ab initio calculations, we demonstrate that the dI/dV asymmetry obtained by our method is proportional to the spin-polarization of the sample [3]. We find in the theoretical results a minimum and a maximum spin-polarizations on a Co film at energies of −0.25 and +0.15 eV, respectively, which agrees with the energy dependence of the dI/dV asymmetry.

[1] G. Rodary *et al.*, JJAP 47, 9013 (2008). [2] D. Wortmann *et al.*, PRL 86, 4132 (2001). [3] H. Oka *et al.*, Science 327, 843 (2010).

*Present address (G.R.): Laboratoire de Photonique et Nanostructures, CNRS UPR20, 91460 Marcoussis, France.

O 64: Focussed session: Theory and computation of electronic structure: new frontiers V (jointly with HL, DS)

Time: Thursday 11:15–13:00 Location: TRE Phy

Topical Talk O 64.1 Thu 11:15 TRE Phy

Electronic excitations in thin-film materials for solar cells: beyond standard density functional theory — •Silvana Botti — LSI, École Polytechnique, CNRS, CEA-DSM, Palaiseau, France — LPMCN, Université Claude Bernard Lyon 1, CNRS, Villeurbanne, France — European Theoretical Spectroscopy Facility

$Cu(In,Ga)(Se,S)_2$ (CIGS) thin-film solar cells have emerged as a technology that can challenge the current hegemony of silicon solar panels. CIGS conserve to a very high degree their electronic properties in a large non-stoichiometric range and are remarkably insensitive to radiation damage or impurities. Kesterites $Cu_2ZnSe(S,Se)_4$ have very similar electronic properties. Unlike CIGS, they are composed of abundant, non-toxic, less expensive chemical elements.

The origin of the exceptional electronic properties of these complex materials is still not completely understood, despite the large amount of experimental and theoretical work dedicated to that purpose. In particular, standard density functional theory (DFT) yields band structures in quantitative and qualitative disagreement with experiments. This is a serious problem when it comes to designing new materials for more efficient photovoltaic energy conversion.

I will discuss which theoretical approaches beyond standard DFT are reliable at a reasonable computational cost, together with the new physical insight that they allow to obtain.

O 64.2 Thu 11:45 TRE Phy

What is the G^0W^0 band gap of ZnO? — Martin Stankovski[1], •Gabriel Antonius[2,1], David Waroquiers[1], Anna Miglio[1], Hemant Dixit[3], Patrick Rinke[4], Hong Jiang[4], Matteo Giantomassi[1], Xavier Gonze[1], Michel Côté[2], and Gian-Marco Rignanese[1] — [1]IMCN-NAPS, Université catholique de Louvain,B-1348 Louvain-la-Neuve, Belgium — [2]Département de physique, Université de Montréal , Montréal, Canada — [3]CMT-EMAT, Departement Fysica, Universiteit Antwerpen, Groenenborgerlaan 171, B-2020, Antwerpen, Belgium — [4]Fritz-Haber-Institut, Berlin-Dahlem, Germany

Zinc oxide is known to be a challenging system for G^0W^0 calculations. Its theoretical description has been widely discussed recently, and authors do not agree on the value of the band gap one should obtain from the G^0W^0 method. In an attempt to clarify the situation, we study the accuracy and the convergence properties of many schemes or approximations used at each level of the calculation, and show how different procedures may lead to very different conclusions. We first invest the sensitivity of the final band gap on the initial exchange-correlation potential used to generate the Kohn-Sham structure. We then study the behaviour of various plasmon pole models used to reproduce the dynamical properties of the dielectric matrix and discuss their validity for this particular system. Finally, the pseudopotential approach is compared to the PAW formalism, equivalent to an all-electrons calculation.

O 64.3 Thu 12:00 TRE Phy

Global exploration of the energy landscape of solids on the ab initio level — •Klaus Doll[1,2], Aniket Kulkarni[1], Dejan Zagorac[1], J. Christian Schön[1], and Martin Jansen[1] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart — [2]Institut für Math. Phys., TU Braunschweig, D-38106 Braunschweig

In the first step of rational synthesis planning, one needs to identify targets, i.e. (meta)stable crystal structures [1]. Simulated annealing has been shown to be one possibility to explore the respective energy landscape [2]. Our approach consists of a global search for structure candidates based on (up to very recently) empirical potentials, and subsequently a high accuracy local optimization. In order to overcome the limitation of employing potentials, ab initio energies are now used in all the stages [3-7].

After LiF [4] and BN [5], GeF_2 has been studied as an example of a system with stereochemically active lone pairs. Chain-like structures have been found. Further examples include CaC_2 with newly predicted structures at zero pressure as well as at high pressure [6], and PbS [7].

[1] M. Jansen, Angew. Chem. Int. Ed. 41, 3746 (2002); [2] J. C. Schön and M. Jansen, Angew. Chem. Int. Ed. 35, 1286, (1996); [3] J. C. Schön, K. Doll, M. Jansen, Phys. Status Solidi (b) 247, 23 (2010); [4] K. Doll, J. C. Schön, M. Jansen, Phys. Chem. Chem. Phys. 9, 6128 (2007); [5] K. Doll, J. C. Schön, M. Jansen, Phys. Rev. B 78, 144110 (2008); [6] A. Kulkarni, K. Doll, J. C. Schön, M. Jansen, J. Phys. Chem. B 114, 15573 (2010); [7] D. Zagorac, K. Doll, J. C. Schön, M. Jansen, in preparation

O 64.4 Thu 12:15 TRE Phy

Ab initio calculations of electronic excitations: Collapsing spectral sums — •Arjan Berger[1,2], Lucia Reining[1,2], and Francesco Sottile[1,2] — [1]Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF)

We present a method for the evaluation of electronic excitations of advanced materials by reformulating spectral sum-over-states expressions such that only occupied states appear. All empty states are accounted for by one effective energy. Thus we keep the simplicity and precision of the sum-over-states approach while speeding up calculations by more than an order of magnitude. We demonstrate its power by applying it to the GW method, where a huge summation over empty states appears twice (screening and self-energy). We show the precision bulk silicon and argon. We then use it to determine the band structure and optical spectrum of the technologically important oxide SnO2. We will also show how our approach can be used to develop exchange-correlation kernels for time-dependent density-functional theory that are both accurate and computationally efficient.

O 64.5 Thu 12:30 TRE Phy

Oxides – a challenge for (theoretical) spectroscopy — •Patrick Rinke[1], Hong Jiang[1], Matthias Scheffler[1], Andreas Greuling[2], Michael Rohlfing[2], Anderson Janotti[3], Emmanouil Kioupakis[3], and Chris G. Van de Walle[3] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Universität Osnabrück, Osnabrück — [3]University of California at Santa Barbara, CA

Oxides are of tremendous technological importance, yet challenging materials to characterize. In many cases the agreement between experimental and theoretical spectroscopy observed for other material classes has not been attained. We use rutile TiO_2 as an example to illustrate some of the problems. Many-body perturbation theory in the G_0W_0 approach based on density-functional theory in the local-density approximation gives a fundamental band gap of 3.3 eV in seemingly good agreement with the 3.3±0.5 eV measured in direct and inverse photoemission [1]. However, the lowest exciton computed in Bethe-Salpeter calculations for the optical spectrum is found at an energy of 3.21 eV, while optical experiments only give 3.03 eV [2]. Polaronic effects, i.e. the renormalization of the band edges due to electron-phonon coupling, reduce the band gap, but it remains a challenge to include the ionic contribution to the dielectric function, which can be substantial in oxides, in the G_0W_0 calculations and to incorporate both effects consistently into Bethe-Salpeter calculations. Another aspect to consider is the role of electron correlations. [1] Y. Tezuka *et al.*, J. Phys. Soc. Jpn.**63**, 347 (1994). [2] J. Pascual *et al.*, Phys. Rev. B **18**, 5606 (1978).

O 64.6 Thu 12:45 TRE Phy

The surprising accuracy of semilocal functionals within density functional theory (DFT): A study of systems involving point defects — •Rampi Ramprasad[1], Patrick Rinke[2], and Matthias Scheffler[2] — [1]University of Connecticut, Storrs, USA; Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Fritz-Haber-Institut der MPG, Berlin, Germany

The use of screened nonlocal exchange functionals within hybrid DFT computations is becoming practical, providing improved electronic structure descriptions [1]. However, the appropriate amount of nonlocal exchange (α) and the extent of screening (ω) to be used are still being explored. Here, we will focus on two properties relevant for systems containing point defects: charge transition levels and defect formation energies. By making the α and ω as variables, it will be shown that semilocal treatments of the exchange interaction for defects in Si and ZrO_2 yield charge transition levels that are quantitatively competitive with more involved nonlocal treatments, extending notions presented recently [2]. This implies that the difference in formation energies of neutral and charged defects remains a constant, although the formation energy itself may vary with the type of treatment. We have identified correlations between defect formation energies and features of the electronic structure of the defect-free parent material, allowing for extrapolations of the formation energy to the "correct" values.

[1] A. V. Krukau, et al, J. Chem. Phys. 125, 224106 (2006). [2] H. Komsa, et al, Phys. Rev. B 81, 205118 (2010).

O 65: Metal substrates: Adsorption of organic / bio molecules VII

Time: Thursday 11:15–13:00 Location: PHY C213

O 65.1 Thu 11:15 PHY C213

Coverage dependent isomerisation behaviour of tetra-*tert*-butyl-imine on Au(111) — •Felix Leyssner, Matthias Koch, Stephan Meyer, and Petra Tegeder — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, D-14195 Berlin

High resolution electron energy loss spectroscopy (HREELS) is employed to analyze thermally activated changes in the geometrical structure of the photochromic molecular switch 3,3',5,5'-tetra-*tert*-butyl-imine (TBI) adsorbed on Au(111). Measurements have been performed for two coverage regimes: The monolayer and the bilayer regime. For both coverages all molecules are found in the *trans* state after deposition at sample temperatures of T=210K, but conformational changes upon heating are observed, which are assigned to a *trans* to *cis*-isomerization. When heating the sample to T=440K two different conformations are observed depending on the initial coverage. Annealing of a monolayer leads to an increasing number of *cis* isomers, pointing towards an inverted thermal isomerisation behaviour of TBI, since the *trans*-isomer is the more stable compound in solution. Whereas for a bilayer the temperature induced isomerization of the TBI can be monitored as well, but desorption of the second layer at T=440K leads to the formation of a *trans*-monolayer. The fact that different molecular configurations are found for equal coverages annealed at the same temperature is highly surprising and shows that collective effects may govern the switching properties of molecular switches on surfaces.

O 65.2 Thu 11:30 PHY C213

Switching behavior of double-decker single molecule magnets on a metal surface — •yingshuang fu[1], joerg schwoebel[1], andrew dillulo[2], germar hoffmann[1], jens brede[1], svetlana klyatskaya[3], mario ruben[3,4], and roland wiesendanger[1] — [1]University of Hamburg, Hamburg, Germany — [2]Ohio University, Athens, USA — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany — [4]Université de Strasbourg, Strasbourg, France

Single molecule magnets (SMM) are most promising materials for spin based molecular electronics. Due to their large magnetic anisotropy stabilized by inside chemical bonds, SMM can potentially be used for information storage at the single molecule level. For applications, it is of importance to adsorb the SMM onto surfaces and to study their subsequent conformational, electronic and magnetic properties.

We have investigated the adsorption behavior of Tb and Dy based double-decker SMM on an Ir(111) surface with low temperature scanning tunneling microscopy and spectroscopy. It is found that Tb double-decker molecules bind tightly to the Ir(111) surface. By resonantly injecting tunneling electrons into its LUMO or HOMO state, the Tb double-decker molecule can be switched from a four-lobed structure to an eight-lobed structure. After switching, energy positions of the HOMO and LUMO states both shift closer to the Fermi level. Dy double-decker molecules also exhibit the same switching properties on the Ir(111) surface. The switching behavior of the molecules is tentatively attributed to a conformational change of the double-decker molecular frame.

O 65.3 Thu 11:45 PHY C213

Simulation of vibrational spectra of self-assembled monolayers on metal surfaces — •Katrin Tonigold and Axel Gross — Institute for Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

Vibrational spectroscopy is a common and valuable experimental tool to analyze the chemical composition as well as the orientation of self-assembled monolayers (SAMs) on metal surfaces [1]. The simulation of such vibrational spectra might be helpful for the analysis of experimental spectra and further information might be gained by the theoretical insight in the vibrations occuring at the surface.

In this study vibrational spectra of thiolate-based SAMs on Au(111) have been simulated by means of DFT-GGA-calculations employing two different methods: a harmonic approach using finite differences is compared to an approach using *ab initio* molecular dynamics simulations showing the influence of temperature and anharmonicity. The impact of different conformers and coverages on vibrational spectra has been considered. Furthermore, the influence of defects such as adatoms or vacancies in the gold surface on the structure of the SAMs and their vibrational spectra is discussed.

[1] Xia Stammer *et al.*, PCCP **12**, 6445-6454 (2010).

O 65.4 Thu 12:00 PHY C213

The effect of molecular vibration on the Resonant Auger Raman spectra of Sn-phthalocyanine thin films — Marc Haeming[1], Johannes Ziroff[1], Lothar Weinhardt[1], •Achim Schöll[1], and Friedrich Reinert[1,2] — [1]Universität Würzburg, Experimentelle Physik VII, D-97074 Würzburg — [2]KIT, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe

On the example of epitaxially grown layers of Tin-phthalocyanine (SnPc) as well as ultrathin SnPc layers adsorbed on a monolayer of PTCDA/Ag(111) we demonstrate the capabilities of Resonant Auger Raman Spectroscopy in analyzing the electron-vibration coupling in thin films of large organic molecules and at their interfaces. The constant initial state signal of particular SnPc levels is substantially enhanced by autoionization and participant decay of the core excited state. We show that the fine structure of the autoionization signal can differ significantly from that of the direct photoemission signal, which is related to electron-vibration coupling. Moreover, continuous modifications of the vibronic fine structure of the autoionization spectra are observed when tuning the excitation energy through an absorption resonance. By comparing SnPc in multilayer samples to SnPc on PTCDA we can demonstrate that these effects are obviously very sensitive to the molecular environment, even in case of weak, predominantly non-covalent interaction. Therefore Resonant Auger Raman Spectroscopy can provide new insight into electron-vibration coupling and into intermolecular interaction in films of organic molecules.

O 65.5 Thu 12:15 PHY C213

Systematic studies of bonding distances of diindenoperylene on noble metal surfaces — •Christoph Bürker[1], Alexander Gerlach[1], Takuya Hosokai[1], Jens Niederhausen[2], Blanka Detlefs[3], Norbert Koch[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [3]ESRF, 38043 Grenoble Cedex, France

The interaction of organic semiconducting molecules with different substrates is essential for the understanding of these systems and for possible applications in organic electronic devices. Diindenoperylene (DIP) is one promising semiconductor and has been studied widely in the recent years concerning its growth and ordering behavior on different substrates as well as electronic properties [1]. Despite these efforts the bonding distance d_0 and thus the coupling to the substrate is still an unknown key parameter of DIP adsorption.

Here we present a systematic study of d_0 of DIP on Cu(111), Ag(111) and Au(111) surfaces, determined by the X-ray standing wave (XSW) technique [2]. Different bonding distances for different substrates indicate a substrate dependent interaction strength. Our results are compared with the well-established bonding distances and interaction strength of PTCDA on the same noble metal surfaces. Interesting similarities as well as differences between the two molecules are discussed.

[1] A. C. Dürr et al., Phys. Rev. B **68**, 115428 (2003)

[2] A. Gerlach et al., Phys. Rev. B **71**, 205425 (2005)

O 65.6 Thu 12:30 PHY C213

Transfer of chirality from individual helicene derivatives into 2D supramolecular structures on Cu(111) — •Meike Stöhr[1], Serpil Boz[2], Michael Schär[3], Francois Diederich[3], Manh-Thuong Nguyen[4], Daniele Passerone[4], and Thomas Jung[5]

— [1]University of Groningen, Netherlands — [2]University of Basel, Switzerland — [3]ETH Zürich, Switzerland — [4]EMPA, Switzerland — [5]Paul-Scherrer-Institute, Switzerland

The investigation of chiral phenomena in two dimensions has increased over the last two decades substantially. Both chiral recognition and transfer of chirality are two aspects amongst others which spurred fundamental research in this area. With STM, insight into the processes on the (sub)molecular scale can be gained. In addition, information on intermolecular and molecule substrate interactions, which govern the 2D assembly structure and thus, also determine how chiral recognition and transfer of chirality are expressed, are obtained. We investigated the adsorption of a helicene derivative featuring two cyano groups which are in opposition to each other on Cu(111) with UHV-STM. Through the functional cyano groups, the guided arrangement in 2D supramolecular structures is enabled. For the adsorption of both the racemic mixture and the enantiopure forms, a transfer of chirality into well-ordered structures is observed. The adsorption of one enantiomer results in structures which are mirror images of those obtained after deposition of the opposite enantiomer. By combining STM experiments with DFT calculations, the intermolecular interactions stabilizing the observed self-organized structures were elucidated.

O 65.7 Thu 12:45 PHY C213

Precursors for sergeant-and-soldiers experiments: dimethyl succinic acid on Cu(110) — •Chrysanthi Karageorgaki, Christian Roth, Manfred Parschau, and Karl-Heinz Ernst — EMPA, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland

In order to better understand chiral recognition at the molecular level, we are currently studying interactions between different chiral butanedioc acids, like tartaric acid (TA), malic acid (MA) and 2,3-dimethyl succinic acid (DMSU) as well as achiral analogues like succinic acid (SU), meso-TA and meso-DMSU on metal surfaces. This led to first a observation of chiral amplification 2D crystals via the so-called "sergeant-and soldiers effect" [1]. In order to discriminate if through-substrate or lateral hydrogen bonding dominates the chiral recognition at surfaces, we currently synthesize chiral DMSU, i.e., replacing the hydroxyl groups of TA by methyl. Here we present LEED, XPS, TPD and RAIRS results of achiral meso-DMSU (HOOC-CH(CH$_3$)-CH(CH$_3$)-COOH) on Cu(110). Besides coverage-dependent "surface-explosion" decomposition chemistry and ordered C$_2$-symmetric structures, DMSU spontaneously undergoes symmetry breaking, observed as superposition of mirror domains in LEED, which makes this system indeed interesting for doping experiments with chiral DMSU.

[1] M. Parschau, S. Romer, K.-H. Ernst, J. Am. Chem. Soc. 2004, 126, 15398.

O 66: Plasmonics and Nanooptics VI

Time: Thursday 11:15–13:00 Location: WIL A317

O 66.1 Thu 11:15 WIL A317

Nano-plasmonics with single epitaxial quantum dots — •Markus Pfeiffer[1,2], Klas Lindfors[1,2], Christian Wolpert[1,2], Paola Atkinson[3], Armando Rastelli[3], Oliver G. Schmidt[3], Harald Giessen[2], and Markus Lippitz[1,2] — [1]Max Planck Institute for Solid State Research — [2]4. Physikalisches Intitut, Universität Stuttgart — [3]Institute for Integrative Nanosciences Dresden

Plasmon resonant metal structures are a particularly interesting choice to alter the emission properties of single quantum emitters since the electromagnetic field can be significantly modified close to the metal surface. This offers exciting possibilities in both fundamental light-matter studies as well as in applications.

We have experimentally investigated the influence of gold nanostructures on the photoluminescence properties of individual semiconductor quantum dots (QDs). The quantum dots are epitaxially grown GaAs/AlGaAs QDs which are buried a few nanometers beneath the semiconductor surface. The position of these emitters can be determined with high precision from a characteristic feature in the surface topography above each dot.

We have studied the enhancement of the excitation rate of single quantum dots using spherical gold nanoparticles. We observe enhancement factors up to 8 on resonance. We furthermore demonstrate significant differences between the enhancement spectrum and the far-field scattering spectrum of the antennas. We have also taken first steps towards incorporating single QDs in integrated plasmonic circuits.

O 66.2 Thu 11:30 WIL A317

Extraordinary Kerr effect in the transmission through ferromagnetic-plasmonic hybrid nanostructures — •M Pohl[1], V Belotelov[2], I Akimov[1,3], V Kotov[2,4], S Kasture[5], A Vengurlekar[5], A Gopal[5], D Yakovlev[3], A Zvezdin[2], and M Bayer[1] — [1]Experimentelle Physik E2, TU Dortmund, Germany — [2]A.M. Prokhorov General Physics Institute, Moscow, Russia — [3]A.F. Ioffe Physical-Technical Institute, St. Petersburg, Russia — [4]V.A. Kotelnikov Institute of Radio Engineering and Electronics, Moscow, Russia — [5]Tata Institute of Fundamental Research, Mumbai, India

The transverse magneto-optical Kerr effect (TMOKE) has been studied on a new magneto-optical heterostructure. The sample, consisting of a periodically nanostructured gold film on top of a ferromagnetic dielectric bismuth-iron-garnet film, allows the measurement of the TMOKE in transmission geometry via extraordinary optical transmission (EOT). It is shown that the effect is enhanced by up to three orders of magnitude exclusively near surface plasmon polariton resonances. The TMOKE signal is highly sensitive to the angle of light incidence, its polarization and the applied magnetic field strengths. Moreover, it changes sign for SPPs traveling in opposite directions. Thus, TMOKE can become an important tool for the complete characterization of plasmonic nanostructures. Additionally, the effect can be controlled by fields on the order of 100 Oe, which is very promising for ultra high sensitive devices and optical data processing.

O 66.3 Thu 11:45 WIL A317

Distinguishing between ultrafast optical harmonic generation and multi-photon-induced luminescence from ZnO thin films by interferometric frequency-resolved autocorrelation microscopy — •Slawa Schmidt[1], Manfred Mascheck[1], Martin Silies[1], Takashi Yatsui[2], Kokoro Kitamura[2], Motoichi Ohtsu[2], and Christoph Lienau[2] — [1]Carl-von-Ossietzky-Universität, Oldenburg — [2]University of Tokyo

The nonlinear optical properties of a thin ZnO film are studied using interferometric frequency-resolved autocorrelation (IFRAC) microscopy. By exciting the film with 6-fs, below-bandgap laser pulses at 800nm focused to a spot size of $1\,\mu$m two emission bands in the blue and blue-green spectral region with distinctly different coherence properties can be detected. We show that an analysis of the wavelength-dependence of the interference fringes in the IFRAC signal allows for an unambiguous assignment of these bands as coherent second harmonic emission and incoherent, multiphoton-induced photoluminescence, respectively. More generally our analysis shows that IFRAC allows for a complete characterization of the coherence properties of the nonlinear optical emission from nanostructures in a single-beam experiment. Since this technique combines a very high temporal and spatial resolution we anticipate broad applications in nonlinear nano-optics.

O 66.4 Thu 12:00 WIL A317

Nanooptical control of hot-spot field superenhancement and long-lived coherences on a corrugated silver surface — Martin Aeschlimann[1], Tobias Brixner[2], Stefan Cunovic[3], Alexander Fischer[1], Christian Kramer[2], Pascal Melchior[1], Walter Pfeiffer[3], Christian Schneider[1], •Christian Strüber[3], Philip Tuchscherer[2], and Dmitri V. Voronine[3,4] — [1]TU Kaiserslautern, Germany — [2]Universität Würzburg, Germany — [3]Universität Bielefeld, Germany — [4]Texas A&M University, College Station, USA

Hot-spots on deterministically or randomly structured metal surfaces enable ultra-sensitive optical spectroscopy by increasing the optical signals. For example, Raman signals from molecules placed on Ag surfaces may be enhanced dramatically and single molecule sensitivity is reached. Here we combine photoemission photoelectron microscopy (PEEM) and polarization pulse shaping to investigate the multiphoton photoemission from hot-spots on a corrugated silver surface. The hot-spot related multiphoton photoemission is enhanced and manipulated with high contrast. Adaptive optimization reproducibly yield long complex pulse shapes for various optimization goals. This and results from pre-determined few-parameter control scans indicate the presence of long-lived coherences. The existence of such resonances with coherence lifetimes in the order of 100fs is proven in time-resolved local coherent spectroscopy. The high resolution of PEEM allows spatial mapping of these resonances across the surface. Spectral correlations between neighboring hot-spots indicate that weakly localized plasmon polariton states are responsible for the hot-spot emission.

O 66.5 Thu 12:15 WIL A317

Hotspot related plasmon assisted multiphoton photocurrents in metal-insulator-metal junctions — •Dominik Differt[1], Detlef Diesing[2], and Walter Pfeiffer[1] — [1]Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — [2]Universität Duisburg-Essen, Universitätsstr. 5, 45117 Essen, Germany

Scanning photocurrent microscopy of metal-insulator-metal junctions (MIM) is used to investigate the mechanisms of femtosecond multiphoton photocurrent injection at liquid nitrogen temperature. The locally induced multiphoton photocurrent in a Ag-TaO-Ta MIM junction is measured in a scanning microscope cryostat under focused illumination (5μm focus diameter, 800nm, 30fs, 80MHz repetition rate). The intensity dependence reveals a mixture of two-photon and three-photon processes that are responsible for the photocurrent. Its lateral variation shows hotspot-like behaviour with significant magnitude variations on a 100 to 200nm length scale. Assuming an injection current duration of 40fs the peak injection current density of about 10^4 A cm^{-2} is estimated - 10^6 times higher than that for 400nm continuous wave illumination slightly below the damage threshold. The simultaneously measured extinction of the incident radiation reveals a 20 to 30% increased absorption at the hotspots. We attribute the local photocurrent enhancement to the defect-assisted excitation of surface plasmon polaritons at the silver electrode leading to an enhanced local excitation.

O 66.6 Thu 12:30 WIL A317

Controlling two-photon excited luminescence in gold nanostructures with polarization pulse shaping — •Giovanni Piredda[1], Zhimin Shi[2], Caroline Gollub[3], Regina de Vivie-Riedle[1], and Achim Hartschuh[1] — [1]Physikalische Chemie, Department Chemie und Biochemie, Ludwig-Maximilians-Universität München — [2]The Institute of Optics, University of Rochester, Rochester, NY 14620, USA — [3]Institute for Materials Science, TU Dresden

Ultrafast nanooptics is an emerging field that combines the concepts and tools of ultrafast spectroscopy and coherent control with those of near-field optics [1]. A simple demonstration of coherent control is the ability to maximize the yield of nonlinear optical processes; we choose for our demonstration two-photon excited luminescence from gold nanostructures [2]. We compare optimization results in different nanostructures showing that the pulse characteristics that result in the highest luminescence yield depend on the single structure; control has therefore a local character. We also provide numerical simulations to support our experimental findings [3].

[1] M.I. Stockman, S.V. Faleev, and D.J. Bergman; Phys. Rev. Lett., 88, 067402 (2002).

[2] M.R. Beversluis, A. Bouhelier, and L. Novotny; Phys. Rev. B 68, 115433 (2003).

[3] G. Piredda, C. Gollub, R. de Vivie-Riedle, and A. Hartschuh; Appl. Phys. B-Lasers O., 100, 195 (2010).

O 66.7 Thu 12:45 WIL A317

Investigation of polarization effects in reconstruction of highly focused vector beams using the knife-edge method — •Christian Huber[1,2], Pavel Marchenko[1,2], Sergejus Orlovas[1,2], Peter Banzer[1,2], Ulf Peschel[2], and Gerd Leuchs[1,2] — [1]Max Planck Institute for the Science of Light, Günther-Scharowsky-Str. 1, D-91058 Erlangen — [2]Institute of Optics, Information and Photonics, University Erlangen-Nuremberg, Staudtstr. 7/B2, D-91052 Erlangen

For experiments with highly focused vector beams the focal field distribution has to be known. The knife-edge method can be used to reconstruct the intensity distribution of the electric field in the focal plane of a high NA objective. For that purpose, a thin knife-edge fabricated on a photodiode is moved through the focal spot while the photocurrent is recorded. To calculate the beam profile by inverse Radon transform the measurements have to be performed for different angels from 0 to 180 degrees of the edge relative to the beam. As demonstrated previously [1] the focal spot can be experimentally characterized at a wavelength of 633 nm using a special mixture of Zink and Gold as knife-edge material. However for pure materials the reconstructed field distribution is modified by polarization dependent effects. To investigate these effects in detail we performed measurements for different edge materials, edge thicknesses and for different wavelengths. According to our experimental and theoretical results the observed polarization dependency for pure materials is caused by effects such as the excitation of plasmonic modes. [1] R. Dorn et al., Opt., 50 (12), 1917-1926 (2003)

O 67: Graphene IV

Time: Thursday 11:15–13:00 Location: WIL B321

O 67.1 Thu 11:15 WIL B321

Electronic properties and localization of Fe atoms on bilayer graphene on Ru(0001) — Thomas Eelbo, Mike Gyamfi, •Marta Waśniowska, and Roland Wiesendanger — Institute of Applied Physics, University Hamburg, Jungiusstr. 11, 20355 Hamburg

We have investigated the electronic properties and a localization of iron adatoms and clusters on monolayer and bilayer graphene on Ru(0001). The epitaxial monolayer graphene (MLG) on Ru(0001) displays a Moiré pattern revealing a strong electronic coupling with the substrate [1], but the second layer (BLG) reveals properties of uncoupled graphene with a Dirac point at -0.5 eV [2]. In order to provide insights into the electronic properties of single Fe adatoms on graphene on Ru(0001) we performed scanning tunneling microscopy/spectrocopy at 5 K. We find that Fe adatoms are weakly attached to MLG and form clusters. However, when atoms are adsorbed on BLG, they are attracted by point defects and strained regions of graphene. Scanning tunneling spectroscopy measurements show that adatoms adsorbed on defect sites reveal the existence of a resonance state at +0.5 eV for single adatoms on BLG, which is also observed for single Fe atoms on Ru(0001).

[1] S. Marchini *et al.*, *Phys. Rev. B* **76**, 075429 (2007)

[2] P. Sutter *et al.*, *NanoLett.* **9**, 2654 (2009)

O 67.2 Thu 11:30 WIL B321

Nucleation behavior of Pt clusters on monolayer graphene supported by Ru(0001) — •Christoph U. Lorenz[1], Albert K. Engstfeld[1], Harry E. Hoster[1,2], and R. Jürgen Behm[1] — [1]Ulm University, Institute of Surface Chemistry and Catalysis, 89069 Ulm, Germany — [2]Current address: Technische Universität München, Centre for Electromobility, 50 Nanyang Drive, Singapore 637553

The Moiré-type nm-scale patterns of graphene monolayers supported by metal single crystals were recently shown to allow facile fabrication of ordered arrays of virtually monodisperse metal nanoclusters by simple metal vapor deposition in UHV [1-3]. In this work we analyzed the nucleation behavior of Pt clusters on monolayer graphene supported by Ru(0001). The cluster size dependency on the deposition rate was determined by statistical evaluation of STM images. Furthermore we investigated the ripening behavior of the Pt clusters at elevated temperatures. The results of these experiments lead us to the proposal of mobile Pt oligomers during the initial nucleation process on the monolayer graphene films.

[1] A.T. N'Diaye et al., New J. Phys. 11, 2009, 103045.

[2] Yi Pan et al., Appl. Phys. Lett. 95, 2009, 093106.

[3] K. Donner and P. Jakob, J. Chem. Phys. 131, 2009, 164701.

O 67.3 Thu 11:45 WIL B321

Nucleation and growth of magnetic nanoclusters on graphene moiré on Rh(111) — •Philipp Leicht[1], Muriel Sicot[1], Samuel Bouvron[1], Ole Zander[1], Thomas Tietze[2], Eberhard Goering[2], Yuriy Dedkov[3], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz — [2]Max-Planck-Institut für Metallforschung, Stuttgart — [3]Fritz-Haber-Institut der Max-Planck Gesellschaft, Berlin

Magnetic nanoclusters with narrow size distributions are of key importance in modern nanotechnology. The bottom-up fabrication of self-organized nanoclusters on graphene moiré templates has been shown recently [1,2] and suggests a viable way to applications such as data storage. In this work, we use a graphene moiré grown on Rh(111) as a template. Submonolayers of ferromagnetic metals including Ni, Fe and Co are deposited on the graphene moiré template at room temperature and at low temperature around 150 K and are investigated by scanning tunneling microscopy and by x-ray magnetic circular dichroism (XMCD). Deposition at room temperature shows significant differences in the growth mode for Ni compared to Fe and Co. Whereas Ni preferentially forms flat triangles with alignment to the moiré structure of the graphene template, the growth of Fe clusters shows only little faceting. Deposition at low temperatures yields smaller clusters with hemispherical shape and a narrow size distribution. XMCD measurements on the Ni clusters are currently in progress to study their magnetic behavior. References: [1] A. T. N'Diaye et al, Phys. Rev. Lett. 97, 215501 (2006) [2] M. Sicot et al, Appl. Phys. Lett. 96, 093115 (2010)

O 67.4 Thu 12:00 WIL B321

Highly Anisotropic Dirac cones in epitaxial Graphene modulated by an island superlattice — •Markus Etzkorn[1], Stefano Rusponi[1], Marco Papagno[2], Paolo Moras[2], Sergio Vlaic[1], Polina M. Sheverdyaeva[2,3], Daniela Pacile[4], Harald Brune[1], and Carlo Carbone[2] — [1]Institute of Condensed Matter Physics, Ecole Polytechnique Fédérale de Lausanne, Switzerland — [2]Istituto di Struttura della Materia-Consiglio Nazionale delle Ricerche, Trieste, Italy — [3]Sinctrotrone Trieste, Trieste, Italy — [4]Istitut. Naz. di Fisica Nucleare and Dip. di Fisica Universit'a della Calabria, Cosenza, Italy

We present angle-resolved photoemission spectroscopy measurements of Graphene (G) on Ir(111) perturbed by self-assembled Ir clusters. While G/Ir(111) exhibits a sixfold symmetric band structure, the cluster superlattice induces a threefold symmetry with a strong renormalization of the electron group velocity close to the Dirac point giving rise to highly anisotropic Dirac cones. For the region up to 0.5 eV below E_F a tight binding model of free standing G predicts an asymmetry of $\frac{v_{\Gamma K}-v_{p\Gamma K}}{v_{p\Gamma K}} = 5\%$. For G/Ir(111) we measure a value of $\frac{v_{\Gamma K}-v_{p\Gamma K}}{v_{p\Gamma K}} = 16 \pm 2\%$ indicating that the periodically modulated interaction between the G and the Ir-substrate already alters the band structure. This effect significantly increases for the case of the Ir superlattice on G/Ir(111) where we find $\frac{v_{\Gamma K}-v_{p\Gamma K}}{v_{p\Gamma K}} = 70 \pm 5\%$. We further observe an influence of the cluster superlattice on the electronic gaps in the graphene band structure.

O 67.5 Thu 12:15 WIL B321

DFT and Photoemission Study of Water and Ammonia Adsorbed on Graphene/Ni(111) — •Stefan Böttcher[1,2], Martin Weser[1], Karsten Horn[1], Yuriy Dedkov[1], Elena Voloshina[2], and Beate Paulus[2] — [1]Fritz-Haber Institut der Max-Planck Gesellschaft, Berlin, Germany — [2]Freie Universität Berlin, Berlin, Germany

In order to use graphene in "real-world" application, the influence of ambient conditions has to be examined. We investigate the interaction of small molecules, H_2O and NH_3, with graphene/Ni(111) as model for ambient environment. We compare our results obtained with spectroscopical methods (ARPES and NEXAFS) and their comparison with DFT calculations. The live-PES measurements were performed in order to study the growth mode and the amount of adsorbed molecules. For NEXAFS and ARPES experiments we have prepared a reproducible amount of less than one molecular layer of water or ammonia on the graphene/Ni(111) interface. The inert properties of graphene/Ni(111) are confirmed, but we found a weak interaction of the physisorbed molecules with the graphene/Ni(111) system. The DFT calculations with GGA-PBE and PBE-D2 functionals were performed for several system geometries, which are based on the NEXAFS data. From the combination of ARPES and NEXAFS we can compare the experimentally and theoretically obtained electronic structures, to assign possible origins for the obtained interactions.

O 67.6 Thu 12:30 WIL B321

Structural and Electronic Properties of Graphene - Nanographene Systems — •Stefan Eilers[1], Stefan Machulik[1], W Ted Masselink[1], Klaus Müllen[2], and Jürgen P Rabe[1] — [1]Institute of Physics, Humboldt-Universität zu Berlin, Germany — [2]Max Planck Institute for Polymer Research, Mainz, Germany

Graphene, because of its unique combination of electronic, optical and mechanical properties, is an attractive electrode for functional molecules. On the other hand, nanographenes can be synthesised with various functionalities, which could find use in applications for future molecular and organic electronics. But can a functional system of graphene and nanographenes be realised? We show that nanographenes can self-assemble on exfoliated monolayer and bilayer graphene to form functional highly ordered molecular layers with defined orientations and electronic properties, largely independent of surface roughness and local environment. We present scanning tunnelling microscopy data at the solid-liquid interface for graphene and nanographene as well as tunnelling spectroscopy data. Graphene as electrode and substrate for aligned layers of functional molecules on insulating wafers offers a wide range of potential applications and the aggregation of functional molecules from solution supplies a basis for future cost-effective production of devices.

O 67.7 Thu 12:45 WIL B321

Fabrication of metal patterns on freestanding graphenoid nanomembranes — •Andre Beyer, Andrey Turchanin, Christoph T. Nottbohm, Nils Mellech, Mark Schnietz, and Armin Gölzhäuser — Fakultät für Physik, Universität Bielefeld, Universtätsstr. 25, 33615 Bielefeld

Metallic patterns on freestanding ultrathin supports are desirable for many applications in modern optics or nanomechanics. The authors present four fabrication paths to create gold patterns that are supported by 1 nm thick freestanding graphenoid nanomembranes from self-assembled monolayers. Two fabrication schemes apply resist based lithographic processes to define gold structures on nanosheets. The gold/nanomembrane hybrids are then released from their substrates to form a freestanding structure. In two further fabrication schemes, the direct metal deposition of metal onto a freestanding graphenoid is performed. All four schemes are capable of producing gold patterns on two-dimensional nanomaterials, thus resembling new paths for the routine fabrication of free-floating metallic structures.

O 68: Polymeric biomolecular films

Time: Thursday 11:15–13:00 Location: WIL B122

O 68.1 Thu 11:15 WIL B122

Dynamic photothermal laser manipulation of surface-grafted thermoresponsive polymer brushes — •Crispin Amiri Naini, Steffen Franzka, Sven Frost, Mathias Ulbricht, and Nils Hartmann — Fakultät für Chemie, CeNIDE, NETZ, Universität Duisburg-Essen, Universitätsstr. 5, 45141 Essen, Germany

Stimuli-responsive polymers have become a versatile material in designing smart functional devices, e. g. as adaptive microoptics, microfluidic chips, membranes and sensors. Controlled reaction schemes allow one to build up surface-grafted polymer brush films with thicknesses from the submicron down to the sub-100 nm range [1]. This opens up an avenue towards highly integrated device structures with unprecedented functionalities. In order to stimulate miniaturized polymeric components, e. g. for valving, suitable techniques are required. Here, we demonstrate a facile noncontact laser technique for switching of surface-grafted poly-n-isopropylacrylamide brushes at the water/substrate interface. A modulated beam of a microfocused laser at a wavelength of 532 nm is used to heat the substrate surface and locally trigger swelling and deswelling of the polymer film. Switching on length scales from millimeters down to a few microns is feasible at very low laser power densities. Also, in conjunction with masks, parallel switching at distinct surface areas can be carried out. Prospects in micro- and nanofluidic applications, e. g. in designing freely configurable device structures, are discussed.

[1] M. Mathieu, A. Friebe, S. Franzka, M. Ulbricht, N. Hartmann,

Langmuir 25 (2009) 12393.

O 68.2 Thu 11:30 WIL B122

Synthesis of 2D COFs through exfoliation and coalesence of nano-crystalls — •Jürgen F. Dienstmaier[1], Wolfgang M. Heckl[2,3], and Markus Lackinger[1,2] — [1]Ludwig-Maximilians-University and Center for NanoScience (CeNS) — [2]Deutsches Museum — [3]Department of Physics, TUM School of Education, Technical University Munich

Self-condensation of Benzene-1,4-diboronic acid can yield highly crystalline Covalent Organic Frameworks (COF). In the COF-1 structure, monomers are covalently interlinked into two-dimensional sheets which are then stacked along the c-axis. These sheets are comprised of a hexagonal alternating arrangement of phenyl and boroxine rings and are an ideal model structure for 2D COF variants. In this contribution we demonstrate a new approach to first synthesize nanocrystalls of COF-1. The product of this synthesis was independently characterized by PXRD, TGA, IR-, and Raman-spectroscopy. After exfoliation, two-dimensional nanocrystalline flakes, whose structure correspond to a single layer of COF-1, are dispersed in solvent and deposited onto a substrate. STM imaging under ambient conditions reveals full monolayer coverage of nanocrystalline COF flakes with well ordered internal structure. Tempering of these highly polycrystalline structures results in ripening and increasing domain size.

O 68.3 Thu 11:45 WIL B122

Contact energy landscapes by means of mobile nanoparticles — •Ute Queitsch[1], Anja Blüher[1], Alfred Hucht[2], Berndt Rellinghaus[3], Ludwig Schultz[3], and Michael Mertig[1] — [1]TU Dresden, Phys. Chem. Measurement & Sensor Technol, D-01062 Dresden, Germany — [2]Univ. Duisburg-Essen, Fac. Phys, D-47048, Duisburg, Germany — [3]IFW Dresden, P.O. Box 270116 D-01171, Germany

The key to successful applications of nanoparticles is their organization at the nanoscale, i.e. the creation of defined nanostructures of particles with controlled morphology in highly ordered arrays. Gas phase preparation has proven to allow for the preparation of nanoparticles of various materials with narrow size distribution. A regular arrangement of the particles can be accomplished by self organization on bacterial S-layer templates [1]. There the main driving force to achieve particle ordering, is the reduction of the surface free energy of the particles by maximizing the contact area between particles and the S-layer surface [2]. The effective contact energy can be quantitatively determined by simulations on the density-dependent particle distribution on the S-layer. Therefore a simple model on the particle diffusion on S-layers including the deposition, diffusion and agglomeration of the particles within the periodic surface potential of the protein template is developed. By means of the presented method for the first time a quantification of the templating effect of S-layer templates is realized.

[1] U.Queitsch et al., Appl. Phys. Lett. 90, 113114 (2007)

[2] U.Queitsch et al., J. Phys. Chem. C., 113, 24, 10471 (2009)

O 68.4 Thu 12:00 WIL B122

NEXAFS of azobenzene-based molecular photoswitches — •Eric Ludwig[1], Sonja Kuhn[1], Thomas Strunskus[2], Alexei Nefedov[3], Ulrich Jung[1], Jens Kubitschke[4], Rainer Herges[4], Christof Wöll[3], Olaf Magnussen[1], Lutz Kipp[1], and Kai Rossnagel[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel — [2]Institut für Materialwissenschaft, Universität Kiel, D-24098 Kiel — [3]Institut für Funktionelle Grenzflächen, Karlsruher Institut für Technologie, D-76344 Eggenstein-Leopoldshafen — [4]Otto-Diels-Institut für Organische Chemie, Universität Kiel, D-24098 Kiel

The adsorption behavior of azobenzene-based molecular switches was investigated by NEXAFS. We deposited pure azobenzene on weakly interacting surfaces of layered compounds. Furthermore, we report results of photoswitches employing molecular platforms based on the triazatriangulenium (TATA) ion with functional groups attached to the central carbon atom which form self-assembled monolayers on Au(111) surfaces. This "platform approach" enforces equal spacing of the molecules as well as decoupling of the functional group from the substrate. NEXAFS measurements were performed at BESSY (beamline HE-SGM) utilizing a Prevac endstation.

Results on azobenzene indicate flat-lying molecules when preparing monolayer systems and a non-planar configuration within multilayer systems. Data on Azo-TATA molecules corroborate successful and non-destructive sample preparation. This work was supported by the DFG through SFB 677.

O 68.5 Thu 12:15 WIL B122

Polariton effect in α-Sexithiophene films revealed by reflectance difference spectroscopy — •Günther Weidlinger, Lidong Sun, and Peter Zeppenfeld — Institute of Experimental Physics, Johannes Kepler University Linz, Altenberger Straße 69, A-4040 Linz, Austria

α-Sexithiophene (α-6T) films consisting of either flat-lying or standing molecules were prepared on clean and carbon-terminated Ag(110) surfaces, respectively, using organic molecular beam epitaxy. The optical properties of the α-6T films were investigated by reflectance difference spectroscopy (RDS). For films composed of flat lying molecules the higher Davydov component derived from the intramolecular HOMO-LUMO transition is located at 2.6 eV, whereas for standing α-6T molecules the transition is shifted to 3.5 eV. This observation can be explained by the so-called polariton effect, i.e., the interaction between photons and excitons [1]. The energetic position of the higher Davydov component thus becomes a function of the angle between the α-6T molecular axis in the films and the propogation direction of the light. This result demonstrates that crystalline orientation and thus the excitonic optical properties of organic thin films can be controlled by the substrate and thin film preparation. Furthermore, RDS is shown to be a sensitive method not only for the determination of the in-plane alignment of organic molecules, but also for their out-of-plane orientation.

[1] G. Weiser and S. Möller, Organic Electronics 5 (2004) 91-97

O 68.6 Thu 12:30 WIL B122

Vibrational spectroscopy of organic monolayers by sum-frequency generation — •Jan Weber, Raissa Mongo, Thorsten Balgar, and Eckart Hasselbrink — Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany

Organic monolayers display an interesting field of surface science because of their diverse characteristics. Prominent examples are siloxanes on silica surfaces which are stable under ambient conditions. These self-assembled monolayers have been of interest since the 1980's yet the mechanisms of ordering, degredation or adsorption of other molecules is not fully understood on the molecular scale. In this context we analyze Octadecyltrichlorosilane (OTS) and Aminopropylmethoxysilane (APS) with regard to orientationally ordering and thermally induced degradation mechanisms.

The experiments are carried out via sum-frequency generation (SFG) spectroscopy by using a picosecond laser system, which provides visible light as well as tunable infrared light. SFG spectroscopy is a convenient method because it provides a very high surface sensitivity for the analysis.

O 68.7 Thu 12:45 WIL B122

The effect of chain-length on the branching of irradiation-induced processes in alkanethiolate molecular films — •Frederick Chesneau, Hicham Hamoudi, and Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany

The effect of X-ray and low-energy (50 eV) electron irradiation on short-chain alkanethiolate (AT) self-assembled monolayers (SAMs) on Au(111) was studied by synchrotron-based high-resolution X-ray photoelectron spectroscopy and infrared reflection absorption spectroscopy. As a test system, a SAM of hexanethiolate (C6) was used. An analogous long-chain film, dodecanethiolate (C12) SAM, was taken as reference. Whereas both C6 and C12 films exhibited a full range of irradiation-induced reactions characteristic of AT SAMs on coinage metal substrates, the branching of the reactions in these two systems was distinctly different. Whereas in the case of C12/Au, the dominant processes were decomposition of the alkyl chains and capture of the released alkylsulfide moieties in the aliphatic matrix, desorption of the complete molecular species emerging after the cleavage of the thiolate-gold bond prevailed in the case of C6/Au. A tentative explanation for this behavior will be proposed.

O 69: Electronic structure I

Time: Thursday 11:15–13:15 Location: WIL C107

O 69.1 Thu 11:15 WIL C107

Structural/electronic interplay in tunable dislocation networks — •Frederik Schiller[1], Zakaria Abd-el-Fattah[1], Manfred Matena[2], Javier Cordon[3], and Enrique Ortega[1,2,3] — [1]Centro de Fisica de Materiales (CFM-CSIC), Materials Physics Center (MPC), San Sebastian, Spain — [2]Donostia International Physics Center, San Sebastian, Spain — [3]Dpto. Fisica Aplicada, Universidad del Pais Vasco, San Sebastian, Spain

Moiré and strain dislocation networks arise when a monolayer or two of one material grows on a substrate with the same crystal symmetry but different atomic lattice constant. Beyond their use as growth templates, such metallic superlattices may be used as model two-dimensional metallic superstructures at which surface states scatter, thereby leading to two-dimensional superlattice band folding and gap opening. The Ag monolayer on Cu(111) system, with its characteristic free-electron-like surface state, is a prototype scenario. At low temperature, it forms a perfect coincidence lattice (Moiré), which transforms into a hexagonal array of triangular dislocations by annealing above 300 K. Such structural transition is accompanied by a deep surface state transformation, i.e., from a parabolic band in the Moiré structure to a superlattice-folded and gapped two-dimensional band structure in the dislocation network. The latter features a full 25 meV gap that can be brought below the Fermi level by lowering the temperature or by gold doping, thereby making the noble metal surface effectively semiconducting.

O 69.2 Thu 11:30 WIL C107

Localized gap states in cobalt/nickel mixed oxides — •Stephan Schmidt and Dieter Schmeisser — Brandenburg University of Technology Cottbus, Konrad-Wachsmann-Allee 17, 03046 Cottbus

Replacing Co by large amounts of Ni is considered to reduce costs in Li-Ion-Batteries while maintaining their performance. We investigate the electronic structure of Co/Ni compounds because of their direct impact on battery operation. Thin Co/Ni oxide films on metal substrates were prepared by dropping/spin-coating from nitrate solutions followed by subsequent annealing in air and UHV. The following Co to Ni ratios have been investigated: 50/50, 40/60, 30/70, and 20/80. The results are compared with the pure Co-oxide and magnetron sputtered $LiCoO_2$ reference samples. Spectroscopic measurements on these samples were carried out at the U49/2 beamline at BESSYII, Berlin. XPS of the transition metal (TM) 2p states reveals the existence of charge transfer ground states and different oxidation states. NEXAFS at the Co L_3, Ni L_3 and O K edges reflects the density of unoccupied states while resonant PES at these edges provides the related partial density of states (pDOS). Therefore, these techniques can be used in order to distinguish between the different contributions of TM3d and O2p states in the valence band region. We find sharp localized features at the valence band edge and at the O K and Co L_3 absorption edges that are discussed to originate from the strong hybridization between metal and oxygen states in that region.

O 69.3 Thu 11:45 WIL C107

Surface electronic structure of clean and oxidized Fe and O/Fe films on Pd(001) — •Christian Eibl, Anke B. Schmidt, and Markus Donath — Westfälische Wilhelms-Universität Münster

Spin-polarization detectors based on exchange interaction have attracted great attention due to their rather high figure of merit and Sherman function compared with spin-orbit-interaction based detectors. Especially oxidized iron films are already in use [1,2].

Here we report on spin-resolved inverse photoemission and target current spectroscopy measurements on Fe(001) and differently prepared O/Fe(001) films. A Pd(001) crystal is used as substrate for film growth. The aim is to understand in detail the influence of oxygen on the Fe(001) surface electronic structure and thereby to improve the spin-detector efficiency in view of Sherman function and stability.

[1] A. Winkelmann *et al.*, Rev. Sci. Instrum. **79**, 083303 (2008)

[2] T. Okuda *et al.*, Rev. Sci. Instrum. **79**, 123117 (2008)

O 69.4 Thu 12:00 WIL C107

Photoelectron momentum mapping over the whole hemisphere: Experiment and theory for Cu(111), Ag(111), and Cu(001) — •Aimo Winkelmann, Christian Tusche, Martin Ellguth, A. Akin Ünal, Jürgen Henk, and Jürgen Kirschner — MPI für Mikrostrukturphysik, Halle (Saale), Germany

Knowledge of the detailed electronic structure in the entire Brillouin zone and in the whole valence-band regime is a prerequisite for understanding new effects at surfaces. This information is obtained with unprecedented efficiency by an energy- and momentum-resolving photoelectron emission microscope (momentum microscope) that detects constant-energy intensity distributions of electrons emitted into the full hemisphere.

The complete valence-band structure which is accessible by unpolarized He I radiation was mapped for the paradigmatic systems Cu(111), Ag(111), and Cu(001) using the momentum microscope.

The measurements provide simultaneous access to extended parts of the photoelectron momentum space beyond high-symmetry regions and, thus, serve as a testing ground for theoretical photoemission from bulk and surface states. For example, agreement of the experimental and theoretical intensity distributions in the entire phase space is obtained only by improving the treatment of the *d*-bands which are unsatisfactorily described within the local density approximation.

O 69.5 Thu 12:15 WIL C107

Circular Dichroism in the Angular Distribution in Surface Alloys — •Carola Strasser, Isabella Gierz, Hadj-Mohamed Benia, Klaus Kern, and Christian R. Ast — MPI für Festkörperforschung, Stuttgart

Circular dichroism in the angular distribution (CDAD) refers to the difference of the measured photocurrent for right and left circularly polarized light. To observe this effect either the target has to be chiral or the experimental geometry has a defined handedness. The CDAD signal is dependent on the geometry of the setup, the orbital composition of the initial state and the relative phases of the partial waves in the final state.

Different surface alloys on Ag(111) and also graphene have been investigated with circularly polarized light and the CDAD signal has been measured. We compare the experimental data for the different systems to the theoretical description of CDAD by Schönhense [1] and estimate the orbital composition of the initial state.

[1] G. Schönhense, Phys. Scr., **T31**, 255, (1990)

O 69.6 Thu 12:30 WIL C107

Interplay between morphology and electronic structure of ultrathin Ni films on W(110) — •Henry Wortelen[1], Sebastian Stolwijk[1], Anke B. Schmidt[1], Kristian Döbrich[2], Martin Weinelt[2,3], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster — [2]Max-Born-Institut, 12489 Berlin — [3]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin

For Ni, a prototype band ferromagnet, measurements of the electronic structure at the phase transition suffer from dominant temperature-induced linewidth broadening. This hampers the interpretation of experimental results. An effective way to overcome this problem is to lower the Curie temperature by going from bulk samples to ultrathin films.

In this contribution, we present morphological and electronic structural changes of ultrathin Ni films grown on a W(110) substrate, as the film thickness is reduced from 10 to 1 monolayer. A combined study with scanning tunneling microscopy, low-energy electron diffraction and (inverse) photoemission shows the close relation between film thickness, quality and electronic structure. Particular attention is given to crystal-induced and image-potential surface states due to their surface sensitivity.

O 69.7 Thu 12:45 WIL C107

A Non-destructive Technique of Investigating Bulk Electronic Properties and Buried Interfaces — •Mihaela Gorgoi, Franz Schäfers, and Alexander Föhlisch — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, BESSY II, Albert-Einstein-Str. 15, 12489 Berlin, Germany

In the past couple of years hard x-ray high kinetic energy photoelectron spectroscopy (HAXPES) has lead to a break-through in the field of photoemission due to its non destructive way of investigating the bulk electronic properties of materials and in particular buried interfaces. In the present contribution we will report recent experiments performed at the hard x-ray HIgh Kinetic Energy (HIKE) photoelectron spectroscopy facility [1] at the Berliner synchrotron light source BESSY II of the HZB. The facility successfully combines the bending magnet source of the KMC-1 beamline [2] with a new generation electron spectrometer optimized for high kinetic energy electrons. Several topics will be detailed such as the recoil effect of high energy photoelectrons from light elements and the interface electronic properties in organic and inorganic thin films and multilayers with emphasis on the performance and abilities of the technique. [1] M. Gorgoi, S. Svensson, F. Schäfers, G. Öhrwall, M. Mertin, P. Bressler, O. Karis, H. Siegbahn, A. Sandell, H. Rensmo, W. Doherty, C. Jung, W. Braun, W. Eberhardt, Nucl. Instrum. Methods Phys. Res. A 601 (2009) 48. [2] F. Schäfers, M. Mertin, M. Gorgoi, Rev. Sci. Instrum. 78 (2007) 123102.

O 69.8 Thu 13:00 WIL C107

The electronic structure and Fermi surface of Ru(0001) and Ru(10$\bar{1}$0) surfaces measured with high resolution angle-resolved photoemission spectroscopy — •Thanh-Nam Nguyen[1], Mattia Mulazzi[1], Sina Gusenleitner[1], Marius Ernst[1], Holger Schwab[1], Dirk Ehm[3], and Friedrich Reinert[1,2] — [1]Experimentelle Physik 7, University of Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruhe Institute of Technology, Germany — [3]Carl Zeiss SMT AG, Rudolf-Eber-Str. 2, 73447 Oberkochen, Germany

Single-crystalline Ru surfaces are model systems for the capping of optical elements in extreme ultraviolet (EUV) lithography setups. The momentum-resolved electronic structure of these surfaces yields important information on their chemical and catalytic properties. The Fermi surface and the band structure of two ruthenium surfaces Ru(0001) and, for the first time, Ru(10$\bar{1}$0) were investigated by high-resolution angle-resolved photoemission spectroscopy (ARPES). The experimental results, though consistent with previous data, show several new features that could not be previously observed by the limited energy and angular resolution. The present results provide detailed information about the momentum-resolved electronic structure of Ruthenium that constitutes a reference to understand its chemical and catalytic properties.

O 70: Gerhard Ertl Young Investigator Award

Time: Thursday 11:15–13:45 Location: WIL C307

O 70.1 Thu 11:15 WIL C307

A chemical switch for molecular spins undergoing exchange coupling with magnetic substrate — Chriatian Wäckerlin[1], Dorota Chylarecka[1], Armin Kleibert[2], Kathrin Müller[1], Cristian Iacovita[3], Frithjof Nolting[2], Thomas A. Jung[1], and •Nirmalya Ballav[1] — [1]Laboratory for Micro and Nanotechnology, Paul Scherrer Institut, 5232 Villigen, Switzerland — [2]Swiss Light Source, Paul Scherrer Institut, 5232 Villigen, Switzerland — [3]Department of Physics, University of Basel, 4056 Basel, Switzerland

The regulation of oxygen affinity in hemoglobin by the iron-porphyrin moiety as shown in nature has been used as a designed concept to perform the switching event of single molecular spins on the surface. This degree of control is achieved upon modifying the coordination sphere of the metal ion of a cobalt(II)tetraphenylporphyrin (CoTPP) molecule ferromagnetically coupled to a nickel (Ni) thin film substrate by the nitric oxide (NO) functioning as an axial ligand. On NO addition, coordination sphere of the Co-ion is modified and a NO-CoTPP nitrosyl complex is formed, which corresponds to an off-state of the Co spin. Thermal dissociation of NO from the nitrosyl complex restores the on-state of the Co spin. The NO-induced reversible off-on switching of surface adsorbed molecular spins observed here is attributed to a spin-trans effect. Use of external stimuli to control single molecular spins at magnetic-interfaces is of potential interest for spintronics and quantum information.

O 70.2 Thu 11:45 WIL C307

Manipulation of the spin structure of metallic QWS and topological insulators. — •Hugo Dil[1,2], Fabian Meier[1,2], Bartosz Slomski[1,2], and Juerg Osterwalder[1] — [1]Physik-Institut, Universitat Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland — [2]Swiss Light Source, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland

The electronic structure of non-magnetic low-dimensional materials can acquire a spin structure due to the breaking of the inversion symmetry at the surface or interface. This so-called Rashba effect is a prime candidate for the manipulation of the electron spin without using any magnetic fields. This is crucial for the emerging field of spintronics, where the spin of the electron instead of its charge is used to transport or store information. Spin and angle resolved photoemission is currently one of the main experimental methods to measure the spin resolved electronic structure, which contains all the relevant information for spintronics [1]. Here it will be shown how the knowledge obtained from model Rashba systems can be applied to increasingly complex systems and result in the possibility to manipulate the spin structure of ultrathin Pb films [1] and topological insulators [3].

[1] For a review see: J. Hugo Dil, J. Phys.: Condens. Matter 21 403001 (2009). [2] H. Dil et al. Phys. Rev. Lett. 101, 266802 (2008). [3] D. Hsieh et al. Nature 460, 1101 (2009).

O 70.3 Thu 12:15 WIL C307

Substrate-Induced Mechanical Transformations in Graphene Films: A Basic Surface Science Approach Towards Controlled Nanoscale Engineering — •Nicola Ferralis — University of California, Berkeley, CA 94720, USA

Compared to research into graphene's remarkable electronic properties, much less is known about how its mechanical and elastic properties are affected by the presence of a supporting substrate. Yet, the response of graphene films to mechanical stimuli is an important fundamental surface science and nanotechnology topic, with potentially far reaching applications in high performance linear and nonlinear electronic, photonic, electrochemical and electromechanical elements. Here, the results of direct investigations of graphene's elastic and mechanical properties at the graphene-substrate interface are presented. Substrate-induced strain in epitaxial graphene grown on SiC surfaces is found to be related to the large difference in the linear expansion coefficient of graphene and the substrate. Furthermore, the amount of strain induced by the substrate is found to be tunable, through optimized graphene growth conditions, from strain-free to up to 0.1%. A comprehensive description of the temperature dependent evolution of the graphene Raman spectra is used to determine and quantify the strength of the graphene-substrate pinning. Through a comprehensive modeling of the interaction of interatomic potentials, it is found that the degree of pinning is substrate-dependent. While graphene on SiC shows a high degree of pinning, graphene grown on metal surfaces behaves as freestanding graphene.

O 70.4 Thu 12:45 WIL C307

Measuring Nanosecond Spin Dynamics at the Atomic Scale — •Sebastian Loth — IBM Research - Almaden, San Jose, CA, USA

Transition metal atoms that were placed on a monolayer-thin film of copper nitride (Cu_2N) on Cu (100) exhibit unusually large magnetic anisotropy that enables long electron spin lifetimes. The magnetic atoms exhibit discrete spin states that can be probed by inelastic electron tunneling spectroscopy (IETS). We make use of a quantized analogue of spin-momentum transfer to interact with the local spin. A large spin-polarized tunnel current pumps the spin of the magnetic atoms into highly excited states allowing us to quantify the lifetimes of different spin excitations.

Direct access to the dynamical evolution of magnetic atoms in the time domain can be obtained by combining spin-polarized scanning tunneling microscopy (SP-STM) with an all-electronic pump-probe measurement scheme: a continuous train of fast voltage pulses is applied to the tunnel junction where a pump pulse excites the magnetic atom and a time-delayed weaker probe pulse monitors the post-excitation dynamics with nanosecond precision. We find that the spin relaxation time of a Fe atom on Cu_2N can be increased beyond 200 ns by placing a Cu atom adjacent to it. This enables studies of quantum tunneling of magnetization that occurs in these dimers.

The ability to probe individual nanostructures with atomic spatial and nanosecond temporal resolution opens a new avenue to explore spin dynamics and other dynamical phenomena on the intrinsic length scale of the underlying interactions.

O 70.5 Thu 13:15 WIL C307

Towards accurate modeling of van der Waals interactions for surfaces and interfaces — •Alexandre Tkatchenko — Fritz-Haber-Institut der MPG, Berlin, Germany

Density-functional theory (DFT) is the method of choice for the modeling of properties and functions of surfaces and interfaces, typically yielding reasonable trends for strong chemical bonding. In the quest for a predictive method for interface modeling, the most pressing issue is thus an accurate description of the long-range van der Waals (vdW) interactions [1,2]. We have recently developed a set of efficient methods for an accurate description of intermolecular vdW interactions in DFT and MP2 theories [2,3]. When applied to the adsorption of nitrogen on graphite, our methods yield quantitative agreement with all experimentally measured data. Our PBE+vdW method also leads to accurate adsorption geometries for complex switches on metallic surfaces [4], as well as for the isophorone/Pd(111) system, where a balanced description of both the chemisorbed and the physisorbed state is essential. Despite these successes, the adsorption energies for molecules on metallic surfaces are systematically too large. The inclusion of screening effects inside the bulk by approximate methods leads to an improved agreement with experimental desorption enthalpies. The comparison of our theory with the non-local vdW-DF functional [1] and the many-body EX+cRPA method will be discussed. [1] M. Dion *et al.*, PRL 92, 246401 (2004); [2] A. Tkatchenko and M. Scheffler, PRL 102, 073005 (2009); [3] A. Tkatchenko *et al.*, JCP 131, 094106 (2009); [4] G. Mercurio *et al.*, PRL 104, 036102 (2010).

O 71: [DS] Organic Electronics and Photovoltaics II (jointly with CPP, HL, and O)

Time: Thursday 12:00–13:00 Location: GER 38

O 71.1 Thu 12:00 GER 38

Improving the performance of phosphorescent light-emitting electrochemical cells without sacrificing stability — •Sebastian Meier[1,2], Wiebke Sarfert[2], David Hartmann[2], and Albrecht Winnacker[1] — [1]University of Erlangen-Nuremberg, Department of Materials Science, Chair VI: Materials for Electronics and Energy Technology, Martensstr. 7, 91058 Erlangen, Germany — [2]Siemens AG, Corporate Technology, GTF ORE, Günther-Scharowsky-Str. 1, 91058 Erlangen, Germany

Within the past few years a novel class of solution-processable solid-state organic light-emitting devices referred to as light-emitting electrochemical cells (LECs) has attracted considerable interest. Key feature of these devices is the existence of mobile ions within the active layer, which enable in-situ electrochemical doping with subsequent formation of a light-emitting p-n-junction. Due to their simple architecture and the use of air-stable electrodes LECs are regarded as an attractive approach for flexible large area lighting applications.

To compete with state of the art lighting technologies, however, the overall device performance of LECs has to be improved. For this purpose, an optimization of the device configuration and processing conditions as well as the use of a proper driving mode can be helpful. We show that the performance can be significantly enhanced due to modifications in the stack configuration (e.g. interfaces, layer thickness, cathode), processing conditions and by an adequate mode of operation without any losses in the device stability.

O 71.2 Thu 12:15 GER 38

OLEDs under high current densities – transient electroluminescence turn-on dynamics and singlet-triplet quenching — •Daniel Kasemann, Hartmut Fröb, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany

Organic solid state lasers have been intensively studied during the last decade due to the promising combination of versatile organic materials with the advantages of solid state emitters. Even though various optically pumped devices comprising different resonator types and material combinations have been shown, direct electrical pumping has not been achieved yet. The high excitation density needed in the active layer to achieve inversion is easily created by pulsed optical pumping, but additional losses prevent the excitation to reach the critical point when driven electrically.

To estimate the dimensions of these additional losses, we investigate full pin-OLEDs comprising the singlet emitter system DCM doped into Alq3 under high current densities. With the OLED active area reduced to $100x100\mu m^2$, these devices sustain current densities in the order of kA/cm^2 in pulsed operation. The results of time resolved electroluminescence (EL) measurements as well as power dependent emission spectra give promising insight into the behaviour of OLEDs under these extreme excitation conditions. Intense EL transient turn-on peaks on the nanosecond time scale can be explained by modelling the singlet and triplet population taking into account singlet-triplet and triplet-triplet quenching in the emission layer.

O 71.3 Thu 12:30 GER 38

Investigation of the chemical and electronic structure of F_{16}CoPc from Monolayer to thick films by photoemission spectroscopy — •M. Grobosch and M. Knupfer — IFW Dresden, D-01069 Dresden, Germany

We have grown F_{16}CoPc with different film thickness under ultra high vacuum conditions on polycrystalline Au surfaces. By means of combined X-ray and ultraviolet photoemission spectroscopy (XPS, UPS) we have investigated the chemical and electronic structure of the F_{16}CoPc films. Within the first monolayers we could identify a charge transfer from the substrate on the F_{16}CoPc molecules. Our results indicate a clear difference in the valence band spectra for submonolayer thin and several nm thick F_{16}CoPc films. Furthermore, for F_{16}CoPc the ionization potential can be changed by the fluorination of the molecules from 4.8 eV for CoPc to 6.5 eV for F_{16}CoPc. The investigated heterointerface CoPc/F_{16}CoPc can be characterized as free from chemical reactions.

O 71.4 Thu 12:45 GER 38

Influence of sample geometry and contact metal on the characterictics of organic field-effect transistors — •Dominik Klaus, Christopher Keil, Jan Hartel, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de

Thin films of $F_{16}PcCu$ were prepared by physical vapor deposition on μ-structured electrode arrays of different contact metals. I/V-measurements of structures with various channel lengths showed a nonlinear injection of charge carriers for low Source-Drain-Voltages V_{DS}. Such behavior was especially found for μ-structures of small channel length indicating an influence of the contact behavior at the interface between metal electrode and organic semiconductor channel. A model was developed based on different aspects of an injection barrier, channel resistance and a parameter characterizing the geometry of the conducting channel which were separately used in the literature before. The model was used to determine the charge carrier mobility also for low values of V_{DS} and consistent values with those from typically evaluated large V_{DS} in the saturation regime were obtained. Implications for technical applicability of such transistors and general validity of such model are discussed.

O 72: Invited Talk (Andreas Stierle)

Time: Thursday 14:00–14:45 Location: TRE Phy

Invited Talk O 72.1 Thu 14:00 TRE Phy
In-situ Study of Nanoparticle Shape Changes under Reaction Conditions — •Andreas Stierle — AG Festkörperphysik / Grenzflächen, Universität Siegen, Walter-Flex-Str. 3, D-57072 Siegen, Germany

In the last decades, the adsorption of gas molecules on late 4d transition metal single crystal surfaces and nanoparticles was investigated at pressures close to ultrahigh vacuum employing standard surface science techniques. In practical applications as heterogeneous catalysts or gas sensors these materials are however operating at ambient pressures which makes an extrapolation from low pressure results very often difficult. During my talk I will demonstrate, that surface sensitive x-ray diffraction represents a very powerful tool allowing *in-situ* monitoring of surfaces and nanoparticles under ambient pressure reaction conditions providing novel insight into structure / reactivity relationships. From the quantitative analysis of the x-ray diffraction data, an atomic scale picture of surfaces and nanoparticles under reaction conditions can be drawn, which I will elucidate for the interaction of O_2 and CO with Pd single crystal and vicinal surfaces, as well as supported Pd nanoparticles on MgO(100) and Al_2O_3(0001).

O 73: [DS] Organic Electronics and Photovoltaics III (jointly with CPP, HL, and O)

Time: Thursday 14:00–16:00 Location: GER 38

O 73.1 Thu 14:00 GER 38
Influence of the thickness dependent structural order on the electrical potential distribution in the channel of OFET's — Richa Sharma, Benedikt Gburek, •Torsten Balster, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen

Soluble organic semiconductors often exhibit a charge carrier dependent mobility and energetic disorder, which typically vary with layer thickness. In this study, organic field effect transistors (OFET) with different thicknesses of regio-regular P3HT as semiconductor and PMMA as gate-insulator on PET foils are investigated and analyzed statistically.

The mobility, which is very low for layers up to 10 nm, increases with the thickness over two orders of magnitude and saturates after 30 nm. This behavior is analyzed according to the Vissenberg-Matters model (VM) of the charge carrier density dependent mobility $\mu = \mu_0((V_{GS} - V_{th})/V_{aa})^{\gamma}$, where the disorder parameter γ decreases from 1.7 to 0.8 over the examined thicknesses proving the higher energetic disorder for thinner films. Increasing domain sizes in phase contrast AFM pictures confirm these findings.

The potential distribution within the channel, which has been measured by additional sense electrodes, is used to determine the potential steps at source and drain contact applying the VM model. The influence of the disorder parameter on the potential distribution is elucidated.

O 73.2 Thu 14:15 GER 38
Local analysis on organic field effect transistors — •Harald Graaf[1], Franziska Lüttich[1], Daniel Lehmann[2], Dietrich R.T. Zahn[2], and Christian von Borczyskowski[1] — [1]Optische Spektroskopie und Molekülphysik, Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz — [2]Halbleiterphysik, Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

Within the last decade the interest on organic electronics increased tremendously and reaches even industrial applications. Nevertheless, there are still a lot of open questions concerning e.g. the charge transport in the organic materials especially on a local scale. Here the focus is on the influence of trap states at interfaces and within the bulk provided e.g. by grain boundaries. By the combination of diverse measurement techniques a deeper insight and a better understanding of the local properties of the materials can be obtained.

We will present recent results on organic materials gained by electrical DC-measurements, Kelvin probe force microscopy on operating devices, optical and topographical investigations. By the results one obtain on the one hand information about the orientation and the coupling of the chromophoric systems (which is responsible also for the charge transport) within the film. On the other hand the electrical and electronical characterizations permit insight in the properties especially at the relevant interfaces (electrode/semiconductor and semiconductor/isolator) and on the local transport characteristics of the charges.

O 73.3 Thu 14:30 GER 38
Dynamics of optically induced instabilities in P3HT field-effect transistors — •Lorenz Kehrer, Christian Melzer, and Heinz von Seggern — Electronic Materials Department, Institute of Materials Science, TU Darmstadt, Petersenstr. 23, 64287 Darmstadt

The development of stable printed organic electronic circuits for everyday use remains a great challenge. Under ambient conditions electrical instabilities may be driven by external influences such as gases, humidity or light. Here, we report on a light induced instability of state of the art poly(3-hexylthiophene) field-effect transistors under ambient atmosphere. By illuminating p-type, top-gate poly(3-hexylthiophene) field-effect transistors in depletion mode with visible light a substantial shift of the threshold-voltage and an increase in the off-current by three orders of magnitudes has been observed. Both phenomena, the threshold-voltage shift and the increase of the off-current, require the presence of oxygen and are persistent for days at room temperature. The origin of this long lasting instability is attributed to traps which are induced in the semiconductor by oxygen incorporation and subsequent optical filling of these traps by electrons. This charge trapping shifts the threshold voltage and increases the doping level. The temporal evolution of the optically induced changes in the OFET characteristics under different thermal conditions will be highlighted. Such an instability is crucial for logic elements where OFETs are normally hold in the off-state, thus in depletion. Under these operational conditions light induces the aforementioned change in the OFET characteristics affecting the functionality of the employed logic circuit substantially.

O 73.4 Thu 14:45 GER 38
Towards a biosensing device based on pentacene transistors — •Martin Göllner, Martin Huth, and Bert Nickel — Department für Physik und CeNS, Ludwig-Maximilians-Universität, Geschwister-Scholl-Platz 1, 80539 München, Deutschland

Organic semiconductors can be processed on flexible, biocompatible plastic substrates and offer a soft and non-toxic ambience to living cells (e.g. neurons). Therefore organic thin film transistors (OTFTs) are considered as promising candidates for the next generation of biosensing devices. However, most high mobility organic semiconductors have a limited lifetime in physiological aqueous conditions. For a stable device operation it is necessary to suppress redox reactions with the electrolyte and so called leakage currents.

For this purpose we recently used a thin alkane layer to passivate a pentacene thin film transistor, enabling the operation in an aquatic environment for many hours [1]. A transducer based on a capped OTFT should be sensitive to subtle changes of the charges at the interface to the electrolyte. Ongoing measurements indicate that it is possible to change the source-drain current of the transistor by changing the electrochemical potential of the electrolyte by a few mV. This suggests that the device should also be sensitive to the adsorption of charged molecules and the activity of cells. The sensing mechanism is discussed.

[1] M. Göllner, M. Huth, B. Nickel, Advanced Materials 22, 4350-4354 (2010)

O 73.5 Thu 15:00 GER 38
Electronic properties of spiro-compounds: A combined photoelectron spectroscopy and energy-loss spectroscopy study — •B. Mahns[1], M. Grobosch[1], T. Saragi[2], J. Salbeck[2], and M. Knupfer[1] — [1]IFW Dresden, Helmhotzstrasse 20, 01069 Dresden,

Germany — [2]Macromolecular Chemistry and Molecular Materials, Institute of Chemistry, Department of Science and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany

The electronic properties of three different spiro-compounds have been investigated using a combination of photoelectron spectroscopy and electron energy-loss spectroscopy. The compounds are characterized by parts with different electron affinity, and we demonstrate their variation in ionization potential and optical gap. Moreover, our data give a measure of the occupied density of states as well as the dielectric properties in a wide energy range.

O 73.6 Thu 15:15 GER 38

Spatially resolved photoresponse of pentacene thin film transistors: slow component by trap release — •Christian Westermeier, Matthias Fiebig, and Bert Nickel — Department für Physik und CeNS, Ludwig-Maximilians-Universität München

Organic thin film transistors (OTFTs) have witnessed continuous improvement over the past years and become suited for widespread application. Small organic molecules, such as pentacene, are often used for OTFTs, since their ordered thin-film structures result in high charge carrier mobilities. Although pentacene has attracted high interest of research, the electronic transport and photoresponse mechanisms and their relation to the morphology and trap densities of the polycrystalline film are not well understood.

We perform spatially and time resolved photoresponse measurements of pentacene TFTs using a laser scanning setup for local illumination with varying laser frequencies and a photon energy of 1.96 eV. The excitation corresponds to the upper Davydov component of the S_1 state of pentacene. Besides the absorption in the 50 nm pentacene film, a significant fraction of the laser light is absorbed in the Si wafer upon reflection. Since the excitons in pentacene decay mostly radiationless, both contributions result in local heating. We argue that heat assisted detrapping results in the release of holes from trap states, thus the effective charge carrier mobility increases locally. These bolometric effects are associated with a slow contribution to the photoresponse on a millisecond timescale and with an inhomogeneous structure presumably corresponding to the trap density distribution in pentacene.

O 73.7 Thu 15:30 GER 38

Contact properties of organic PCBM field effect transistors analyzed by combined photoemission spectroscopy and electrical measurements — •M. Grobosch[1], I. Hörselmann[2], J. Bartsch[2], S. Scheinert[2], M. Knupfer[1], and G. Paasch[1] — [1]IFW Dresden, D-01069 Dresden, Germany — [2]Technical University Ilmenau, D-98684 Ilmenau, Germany

Source/drain contacts in OFETs based on a solution prepared modified PCBM were characterized by combined X-ray and ultra violet photoemission spectroscopy (XPS, UPS) and electrical measurements of the OFET. Thereby the sample preparation for the different measuring principles has been realized in parallel, differing only in the layer thickness of the polymer. By means of UPS a reduced work function could be demonstrated for differently prepared, sputtered, and as-received Au and Al contacts in agreement with previous publications [1]. On top of the Al contacts a natural AlO_x layer could be identified. For both the PCBM/Au and PCBM/Al systems from UPS a hole injection barrier of 1.8 eV has been determined. Considering the gap of 2.0 eV [2] the electron injection barrier would be the same of 0.2 eV. In contrast to these identical barriers as following from UPS, the OFET currents with Au and Al contacts differ by more than two orders of magnitude. A possible origin of this striking discrepancacy will be presented. [1] M. Grobosch et al., Adv. Mater. 19 (2007) 754. [2] Z.-L. Guan et al., Organic Electronics 11 (2010) 1779.

O 73.8 Thu 15:45 GER 38

Dye directed changes in ZnO matrices in organic/inorganic photovoltaic systems — •Harald Graaf[1], Franziska Lüttich[1], Mirko Kehr[1], Christian Dunkel[2], and Torsten Oekermann[2] — [1]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz — [2]Institut für Physikalische Chemie und Elektrochemie, Leibniz Universität Hannover, 30167 Hannover

Dye-sensitized photovoltaic cells with zinc oxide (ZnO) as the inorganic semiconductor and organic dye molecules as the sensitizer are well-known devices with high efficiency. Such cells are prepared by electrochemical deposition of an aqueous zinc salt solution including dye molecules. After deposition the dye is desorbed to obtain a porous ZnO network followed by re-adsorption of the dye as a sensitizer. The dye molecules influence the crystal orientation of the ZnO as they tend to physisorb on different crystal surfaces.

We will present recent results on as-deposited and desorbed dye/ZnO films obtained by different analytic methods: X-ray investigations, Scanning Electron Microscopy, Atomic and Kelvin probe force microscopy and optical spectroscopy. This allows a deep insight into the dye/semiconductor system, which is necessary to improve the efficiency of such devices. Here the focus is on crystal orientation, morphology and work function of the ZnO matrix. Also the arrangement of the dye molecules in as well as on top of the as-deposited films and the band edge of the zinc oxide is accessible.

O 74: Focussed session: Theory and computation of electronic structure: new frontiers VI (jointly with HL, DS)

Time: Thursday 15:00–16:30 Location: TRE Phy

O 74.1 Thu 15:00 TRE Phy

Excited States from *GW*: the role of self-consistency — •Fabio Caruso[1], Xinguo Ren[1], Patrick Rinke[1], Angel Rubio[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut, Faradayweg 4-6, Berlin, Germany — [2]Universidad del Pais Vasco, San Sebastian, Spain

The GW approximation offers an accurate framework to study *ab-initio* electronic excitations in molecules and solids. However, due to its numerical cost, GW is mostly introduced perturbatively following a density-functional theory (DFT) calculation (G_0W_0). We have implemented a fully self-consistent GW scheme based on the iterative solution of Dyson's equation in the all-electron localized basis set code FHI-*aims* [*http://www.fhi-berlin.mpg.de/aims*]. The self-consistent treatment corrects several pathologies of the G_0W_0 scheme, such as the violation of particle number conservation and the dependence on the starting point. Our self-consistent GW total energies are in good agreement with available literature values [Stan *et al*, JCP **130**, 114105 (2009)]. From the GW spectral function we extracted the ionization energies of a set of small molecules. The values are close to experimental results, but exhibit a slight tendency to underestimate. Building on this we apply self-consistent GW to charge-transfer systems. At large separation between the molecular fragments time-dependent DFT in (semi-)local approximations underestimates the charge-transfer energy. This error can be traced back to the wrong description of the HOMO-LUMO gap and its evolution with intermolecular distance. This error is capture by GW as it properly accounts for the difference between the donor ionization potential and acceptor electron affinity.

O 74.2 Thu 15:15 TRE Phy

Electronic excitations from a perturbative LDA+GdW approach — •Michael Rohlfing — Fachbereich Physik, Universität Osnabrück, Germany

We discuss an efficient approach to excited electronic states within ab-initio many-body perturbation theory (MBPT). Quasiparticle corrections to density-functional theory result from the difference between metallic and non-metallic dielectric screening. They are evaluated as a small perturbation to the DFT-LDA band structure, rather than fully calculating the self energy and evaluating its difference from the exchange-correlation potential. The dielectric screening is desribed by a model, which applies to bulk crystals, as well as, to systems of reduced dimension, like molecules, surfaces, interfaces, and more. The approach also describes electron-hole interaction. The resulting electronic and optical spectra are slightly less accurate but much faster to calculate than a full MBPT calculation. We discuss results for bulk silicon and argon, for the Si(111)-(2×1) surface, the SiH_4 molecule, an argon-aluminum interface, and liquid argon.

[1] M. Rohlfing, Phys. Rev. B 82, 205127 (2010).

O 74.3 Thu 15:30 TRE Phy

First-principles study (GW+PAW) on new phosphors for white LED — •Bruno Bertrand[1,2], Masayoshi Mikami[3], Martin Stankovski[1], and Xavier Gonze[1] — [1]European theoretical spectroscopy facility (ETSF), Université Catholique de Louvain, Louvain-la-Neuve, Belgium — [2]CERDECAM, Institut Supérieur Industriel ECAM, Bruxelles, Belgium — [3]Mitsubishi Chemical Group Science and Technology (S&T) Research Center, Inc., Yokohama, Japan

White-LEDs will be one of the major actor involved in the future generations of eco-friendly light sources. For novel types of white LEDs, an optimal combination of two green- and red-emitting phosphors absorbing partly the blue light from the InGaN LED is mandatory to obtain a white light source by post recombination of the light.

We have theoretically studied two oxynitride phosphors, one is an efficient green phosphor $Ba_3Si_6O_{12}N_2$:Eu developed at the Mitsubishi Chemical Group (S&T) Research Center, and the other is a bluish-green phosphor $Ba_3Si_6O_9N_4$:Eu that exhibits little luminescence at room temperature. Our results rely on many body perturbation approach (GW+PAW) applied to the two hosts : $Ba_3Si_6O_{12}N_2$ and $Ba_3Si_6O_9N_4$. The calculation shows a slightly narrower energy gap for $Ba_3Si_6O_9N_4$, that is 0.33 eV. Yet such a result provides keys to understand the thermal quenching mechanism, by comparing materials with a similar chemical composition, but different thermal behaviour. Then a deeper analysis with Eu-doped models sheds new light onto the relationship between emission/excitation colors from the Europium luminescent centers, and the properties of their complex ligands.

O 74.4 Thu 15:45 TRE Phy

First principle calculation on the Fermi contact shift of lithium ion in paramagnetic battery materials — •Yuesheng Zhang[1], Florent Boucher[1], Aurore Castets[2], Dany Carlier[2], and Michel Ménétrier[2] — [1]IMN, Nantes, France — [2]ICMCB, Pessac, France

Solid state NMR in materials for lithium-ion batteries is considerably developing. In paramagnetic materials, the NMR shift of lithium is mainly contributed by the Fermi contact that can be qualitatively interpreted using chemical intuition and the concept of delocalization or polarization mechanisms. In this paper, with accurate first principle methods implemented into WIEN2k, we have obtained the spin density at the nucleus of lithium ions, and then calculated the contact shifts of lithium in several selected transition metal oxides or phosphates. The results show that the calculated values are sensitive to the exchange/correlation potential used in calculation. GGA or LDA generally overestimate the shifts, the calculated values being always shifted along positive direction comparing to the experimental ones. Adding orbital potential "U" or exact exchange on transitional metal ions can improve the results, but still some differences are found with experiments for some cases. The best agreement can be obtained when partial exact exchange potential is applied to both transitional metal and oxygen ions. This means that appropriate exchange correlation potential for transitional metals and oxygen ions is really crucial to calculate the contact shift of lithium ions. This work is funded by Agence Nationale de la Recherche (ANR-09-BLAN-0186-01)

O 74.5 Thu 16:00 TRE Phy

First-principle approach to the temperature dependence of electronic energies. — Paul Boulanger[1,2], Michel Cote[2], and •Xavier Gonze[1] — [1]ETSF / IMCN, Université Catholique de Louvain, 1 Place Croix du Sud, B-1348 Louvain-la-Neuve, Belgium — [2]Département de physique, Université de Montréal, C.P. 6128, succ. Centre-ville, Montréal (Québec) H3C 3J7, Canada

The energy bands of semiconductors exhibit significant shifts with temperature, due to electron-phonon interactions. In search of an efficient first-principle approach to this effect, we have found that formulas derived by Allen, Heine and Cardona in a semi-empirical context cannot be transposed to Density-Functional Theory or to Many-Body Perturbation Theory without critical reexamination. For these theories, the correct formulation includes a extra term, the non-site-diagonal Debye-Waller term, which is dependent on second-order derivatives of the self-consistent electron-lattice potential with respects to atomic displacements. We have studied the importance of this extra term for diatomic molecules and found that it partially cancels the standard Debye-Waller and Fan terms leading a decrease by 52% for H2, 10% for N2 and 37% for LiF. For CO it adds about 15% to the temperature dependence. The lack of this term might explain the discrepancy found between previous theory and experiment for solids. Furthermore, the slow convergence of the sum-over-states approach of Allen-Heine-Cardona approach can be avoided in a new formalism proposed here, based on Density-Functional Perturbation Theory, leading to a dramatic decrease of calculation times.

O 74.6 Thu 16:15 TRE Phy

Quasiparticle calculations of core levels — •Arno Schindlmayr and Dominik Biffart — Department Physik, Universität Paderborn, 33095 Paderborn, Germany

Electrons that occupy core orbitals are tightly bound to the atomic nucleus and do not participate in chemical bonding. Nevertheless, their binding energies are sensitive to the chemical environment, because the redistribution of the valence electrons due to bond formation strongly influences the interaction with the nucleus. For this reason, core-level spectroscopy is an important tool to clarify the atomic structure of materials, such as the geometry of surfaces, interfaces or defects, which can be used even when direct imaging techniques are not applicable. Theoretical calculations of core levels are typically based on density-functional theory. Although these often show the correct trends, they are plagued by the well known deficiencies of common exchange-correlation functionals as well as technical difficulties, especially in the prevalent pseudopotential approximation. As an alternative, we employ many-body perturbation theory, where the quasiparticle correction to the Kohn-Sham eigenvalues provides a formally exact description of dynamical screening around the core hole in the final state. Our implementation is based on the full-potential linearized augmented-plane-wave (FLAPW) method and employs the *GW* approximation for the electronic self-energy. The calculated core levels of selected systems, such as silicon in various crystalline materials with differing local environments, are in very good quantitative agreement with experimental data from X-ray photoemission measurements.

O 75: Metal substrates: Adsorption of organic / bio molecules VIII

Time: Thursday 15:00–17:00 Location: PHY C213

O 75.1 Thu 15:00 PHY C213

Self-assembled structures of a molecular switch on Ag(111) — •Konrad Boom[1], Andreas Schaate[2], Boris Ufer[2], Peter Behrens[2], Jörg Henzl[1], and Karina Morgenstern[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, ATMOS, Appelstraße 2, 30167 Hannover — [2]Leibniz Universität Hannover, Institut für Anorganische Chemie, AK Festkörper- und Materialchmie, Callinstraße 9, 30167 Hannover

Molecular switches are a potential answer to meet future requirements of electronics. We investigated one possible molecule, p-hydroxy-azobenzene, on Ag(111) with a low-temperature STM. A coverage of 0.6 ML was deposited at a sample temperature of 213-233K. With these parameters p-hydroxy-azobenzene self-assembles into islands with varying local densities. In some areas the molecules build regular, symmetric, and reoccurring structures. These structures are classified depending on density and regularity. For special structures the molecules have different apparent heights. In some of the structures, it is possible to induce isomerisation of single molecules. The main requirement for that is enough space around the switching molecule. In this presentation we show the classification of the structures and give some examples for likely bindings in prominent structures. Possible origins of the apparent height difference will be discussed.

O 75.2 Thu 15:15 PHY C213

Reversible switching of ex-situ surface mounted molecular switches probed by laser-based photoemission. — •Nils Heinemann[1], Jan Grunau[1], Till Leissner[1], Sonja Kuhn[1], Dordaneh Zargarani[2], Ulrich Jung[1], Oleksiy Andreev[1], Rainer Herges[2], Olaf Magnussen[1], and Michael Bauer[1] — [1]Inst. f. Exp. u. Angew. Phys., Uni Kiel — [2]Inst. f. Org. Chem., Uni Kiel

Molecular electronics hold the potential as boom town of nanotechnology. The controlled manipulation of molecular switches adsorbed on surfaces is a key prerequisite to advance into more sophisticated applications. In this contribution we will present a photoemission study of the molecular switch 3-(4-(4-Hexylphenylazo)-phenoxy)-propan-1-thiol adsorbed on Au(111) single crystal (**1**/Au).

This molecule undergoes trans-cis isomerisation upon absorption of UV light (365 nm), the back-isomerisation is induced by absorption of blue light (440 nm) or thermal activation. With regard of application, we chose an ex-situ preparation for the experiments, i. e. deposition from solution. The switching behavior of these samples was investigated with photoemission spectroscopy under UHV conditions, using the forth harmonic laser light of a tuneable 80 MHz fs-laser system.

In our study we were able to follow the reversible switching between the trans- and the cis-isomere of **1**/Au, induced by photo-thermal and photo-photo stimulation. The quantitative analysis of our data show that only a minor fraction of the adsorbed molecules undergo a switching indicating the potential relevance of substrate and/or film defects in this process.

O 75.3 Thu 15:30 PHY C213

Isomerization Dynamics of Adsorbed Molecular Switches: A ΔSCF Density-Functional Theory Study — •Reinhard J. Maurer and Karsten Reuter — Department Chemie, Technische Universität München

Stabilizing molecules at solid surfaces and switching them reversibly between defined states would be a key component of a future molecular nanotechnology. Adsorption at metal surfaces is of particular interest as it could lead to novel functionality in form of isomerization mechanisms not present in gas-phase or solution. Recent experiments indeed suggest such a photo-induced mechanism for tetra-tert-butyl functionalized azobenzene (TBA) at Au(111) [1], involving electron transfer from the molecule to a photo-excited hole in the metal *d*-band.

Addressing this suggestion with first-principles modeling requires a numerically highly efficient approach to make the calculations of photo-excited molecular motion at the extended surface tractable. To this end we explore a density-functional theory based Delta self-consistent field approach and assess its reliability for a test set of small, related molecules against higher-level theory. Obtaining encouraging results we proceed to a discussion of azobenzene and TBA in excited states corresponding to the suggested hole-mechanism. [1] S. Hagen *et al.*, J. Chem. Phys. **129**, 164102 (2008).

O 75.4 Thu 15:45 PHY C213

Coverage and temperature driven isomerization of TBI on Au(111) — •Cornelius Gahl[1], Daniel Brete[1], Robert Carley[1], Roland Schmidt[1], Erik R. McNellis[2], Karsten Reuter[2,3], Petra Tegeder[4], Johannes Mielke[2], Leonhard Grill[2], and Martin Weinelt[1,4] — [1]Max-Born-Institut, Max-Born-Str. 2a, 12489 Berlin — [2]Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin — [3]Technische Universität München, Lichtenbergstr. 4, 85747 Garching — [4]Freie Universität Berlin, Arnimallee 14, 14195 Berlin

Tetra-*tert*-butyl azobenzene (TBA) is one of the few examples of molecular switches which have been successfully photoisomerized after adsorption on a metal surface. We have now studied the corresponding imine, N-(3,5-di-*tert*-butylbenzylidene)-3,5-di-*tert*-butylaniline, referred to as TBI, by core-level spectroscopy, STM and dispersion corrected DFT . Although isomerization of TBI/Au(111) could not be optically induced, the molecules can run through a complete thermally driven isomerisation cycle. At 210 K TBI adsorbs in *trans*-conformation. Upon annealing to 320 K a bilayer of *trans*-TBI is transformed into a densely packed *cis*-monolayer. Further heating to 420 K results in desorption of half of the molecules leaving a close-packed *trans*-monolayer. Experiment and theory result in a consistent picture of the molecular adsorption geometry for both isomers as well as the lateral layer structures. The isomerization reaction is governed by the activation energy as well as the interplay of adsorption energies (*cis* $<$ *trans*) and maximal monolayer coverage (*cis* $>$ *trans*).

O 75.5 Thu 16:00 PHY C213

Intramolecular proton transfer: surface-confined porphyrins as four-level conductance switches — •Knud Seufert, Wili Auwärter, Felix Bischoff, David Écija, Saranyan Vijayaraghavan, and Johannes V. Barth — Physik Department E20, TUM, Germany

Free-base porphyrins accommodate two protons bound at opposing nitrogen positions in the macrocycle. The saddle-shape deformation of 2H-TPP anchored on a Ag(111) surface leads to two different configurations for every molecule, represented by a 90° rotation of the hydrogen pair. By using a low-temperature STM to apply a tunneling current, we induce a proton transfer and thus can switch the 2H-TPP reversibly between these two configurations. Controlled voltage pulses lead to a single or double deprotonation of the macrocycle resulting in 1H-TPP or TPP species. In the first case, the remaining hydrogen has four possible positions that can be clearly identified in high-resolution STM images. Again, a tunneling current applied at a bias voltage above a given threshold induces the transfer of the proton between the different nitrogens. This switching process can be directly monitored by recording I(t) traces. We present a statistical analysis of the proton transfer rate as a function of bias voltage and current. The linear current dependence of the switching events for both the 2H-TPPs and the 1H-TPPs points to a single electron process, where twice as many electrons are necessary for the case of two protons. This is related to a transition state represented by two hydrogens in a cis-like configuration that can relax either into the initial state or the rotated configuration.

O 75.6 Thu 16:15 PHY C213

Switching and electron transport through Sn-Phthalocyanin — •Yongfeng Wang[1], Jörg Kröger[2], and Richard Berndt[1] — [1]IEAP, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Technische Universität Ilmenau, 98684 Ilmenau

SnPc exhibits two configurations (SnPc-up and SnPc-down) upon adsorption on Ag(111). A localized but irreversible conformational switching from up to down state was obtained on the bare Ag(111) surface. From the second layer, local and reversible switching was achieved via resonant electron or hole injection into molecular orbitals.

SnPc molecules adsorbed on Ag(111) were contacted with the tip of a STM. Orders-of-magnitude variations of the single-molecule junction conductance were achieved by controllably dehydrogenating the molecule and by modifying the atomic structure of the surface electrode. Nonequilibrium Green's function calculations reproduce the trend of the conductance and visualize the current flow through the junction, which is guided through molecule-electrode chemical bonds.

O 75.7 Thu 16:30 PHY C213

Molecular switching analyzed with sub-molecular precision: CuPc on Cu(111) — •Johannes Schaffert[1], Maren Cottin[1], Andreas Sonntag[1], Hatice Karacuban[1], Nicolás Lorente[2], Christian Bobisch[1], and Rolf Möller[1] — [1]Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Centro de Investigación en Nanociencia y Nanotecnología, Campus de la Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain

The current fluctuations in Scanning Tunneling Microscopy and Spectroscopy have been analyzed in real time using special analogue electronics. This type of Scanning Action Microscopy technique allows to map topography and switching processes simultaneously. For the Cu-Phthalocyanine (CuPc) molecule on Cu(111), switching between two states is observed. The switching frequency, the switching amplitude and the ratio between the residence times in the observed states can be studied with Angstrom spacial resolution. Spectroscopic data obtained at 7K yields information about the involved electronic states. Based on the experimental data as well as DFT calculations a model will be presented. The CuPc molecule switches between different adsorption configurations, which are attributed to different angles of molecular rotation on the Cu(111) surface.

O 75.8 Thu 16:45 PHY C213

Electronic Structure of a Spiropyran Derived Molecular Switch in Direct Contact with the Au(111) Surface — •Christopher Bronner, Gunnar Schulze, Katharina J. Franke, José Ignacio Pascual, and Petra Tegeder — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany

As nanometer scale phenomena advance into the grasp of technological application, the potential building blocks of molecular electronics and sensorics are studied in detail. Surface-bound molecular switches are of particular interest, since the functionality of the substrate/adsorbate system can be switched by an external stimulus.

We present combined two-photon photoemission (2PPE) and scanning tunneling spectroscopy (STS) investigations of a nitro-spiropyran derivative's occupied and unoccupied electronic states at the Au(111) surface in both its open and closed form. Both forms exhibit significant differences in the electronic structure which allows following a potential ring-opening/closure reaction. Resonant electron tunneling from the STM tip into the LUMO of the adsorbate molecule induced ring-opening, while the corresponding photon driven process via transfer of electrons from the substrate to the adsorbate turned out to be inefficient. The loss of the molecule's functionality is attributed to a strong electronic coupling between adsorbate and metallic substrate and accordingly to short lifetimes of molecular excited states.

O 76: Plasmonics and Nanooptics VII

Time: Thursday 15:00–16:15 Location: WIL A317

O 76.1 Thu 15:00 WIL A317

Optical and electronic properties of Ag clusters on SiO_2 — •Sabrina Hoffmann[1], Kamil Latussek[1], Stefanie Duffe[1], Christian Sternemann[1], Ralph Wagner[2], and Heinz Hövel[1] — [1]TU Dortmund, Experimentelle Physik I, Otto-Hahn-Str. 4, 44221 Dortmund, Germany — [2]BU Wuppertal, Fachbereich C - Fachgruppe Physik - Materialwissenschaften, Gaußstraße 20, 42097 Wuppertal, Germany

Clusters assembled materials are of great impact for future applications in science and nanotechnology. In particular, advances in metal cluster-beam technology allow experiments on free and supported or embedded clusters resembling nanostructures in realistic, technical relevant environments. Optical properties of noble metal clusters and nanostructures such as their UV-VIS absorption band alter significantly with size, shape and interparticle spacing as well as with the properties of the local environment. The plasmon resonance of Ag clusters on SiO_2 before and after exposure to air is examined using optical spectroscopy [1]. Then the same clusters are examined with XANES at the Ag L_3 edge. With this method changes in the uDOS of clusters can be investigated which occur either due to the cluster size or a change in their chemical environment. After exposing the Ag clusters to H_2S the plasmon resonance disappears and the XANES spectra show that the clusters are transformed to silver sulfide.

[1] U. Kreibig et al., Optical Investigations of Surfaces and Interfaces of Metal Clusters, In: Advances in Metal and Semiconductor Clusters Vol. 4, (ed. M.A. Duncan), JAI press Inc., 345 (1998).

O 76.2 Thu 15:15 WIL A317

Quantifying Chirality in 2D and 3D Metallic Metamaterials — •Martin Schäferling, Daniel Drégely, Thomas Weiss, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

Chirality on the nanoscale is an emerging field for metamaterials. Circular dichroism in metallic spirals can exceed the best liquid crystals or helical molecules by many orders of magnitude. Broadband quarter-wave plates can be assembled by 3D spirals that are fabricated by direct laser writing [1]. Bichiral metallic photonic crystals exhibit phases and optical properties that are unattainable in nature [2,3].

In this contribution, we investigate numerically various planar and three-dimensional metallic metamaterials with respect to their degrees of circular dichroism and optical chirality. The latter is a measure for the local chirality of electromagnetic fields [4]. Chiral metamaterials can lead to local superchiral fields, which exhibit extremely high optical chirality. We discuss the structural, spectral and spatial dependence of these values. This provides a comparison of the chiroptical properties of different practical geometries.

[1] J. K. Gansel et al., Science **325**, 1513 (2009).
[2] M. Thiel et al., Adv. Mat. **21**, 4680 (2009).
[3] A. Radke, P. V. Braun, and H. Giessen, to be published.
[4] Y. Tang and A. E. Cohen, Phys. Rev. Lett. **104**, 163901 (2010).

O 76.3 Thu 15:30 WIL A317

Weak localization of light in ZnO nanorods in space and time — •Manfred Mascheck[1], Slawa Schmidt[1], Martin Silies[1], David Leipold[2], Erich Runge[2], Takashi Yatsui[3], Kokoro Kitamura[3], Motoichi Ohtsu[3], and Christoph Lienau[1] — [1]Carl von Ossietzky Universität Oldenburg — [2]Technische Universität Ilmenau — [3]University of Tokyo

An array of ZnO nanorods is used to directly visualize the weak localization of light in both space and time. Ultrashort laser pulses from a Ti:Sapphire oscillator with a pulse duration of 6 fs are focused to their diffraction-limit of $1\,\mu m^2$ onto the ZnO nanorod array using an all-reflective Cassegrain objective. The generated SH emission is collected in reflection geometry and detected as a function of the lateral position of the laser focus. Pronounced intensity fluctuations on a sub-μm scale due to the multiple random scattering inside the nanoneedle array are taken as the spatial hallmark of weak the localization of light. By varying the delay between the phase-stabilized pair of laser pulses from a dispersion-balanced Michelson interferometer, interferometric frequency-resolved autocorrelation (IFRAC) traces are measured. By analyzing these traces in the frequency domain, the dephasing time and therewith the temporal evolution of the electric field within the ZnO array could be deduced.

O 76.4 Thu 15:45 WIL A317

Octave-wide Photonic Band Gap in Three-Dimensional Plasmonic Bragg Structures — •Richard Taubert and Harald Giessen — University of Stuttgart, 4th Physics Institute and Research Center SCoPE, Pfaffenwaldring 57, 70550 Stuttgart

We investigate radiative coupling of particle plasmons in various three-dimensional, stacked geometries of plasmonic oscillators. The arrays of gold nanowires with fixed dimensions and lateral periodicity are stacked on top of each other, separated by a dielectric spacer layer. The vertical distance as well as the number of layers is varied.

The dependence of the optical spectra on spacing distance is investigated in a system consisting of two layers. We show that the coupled system exhibits a superradiant mode when the vertical distance of the oscillators matches half their emission wavelength. This means that the Bragg criterion for the particle plasmonic resonance wavelength is fulfilled.

Upon increase of the number of radiatively coupled oscillators, the spectral width of the superradiant mode increases alongside with a change of the spectral shape from Lorentzian to stop-gap like. Eventually the superradiant mode evolves into a very broad photonic band gap which spans almost over one octave.

By changing the dimensions of the gold nanowires, keeping their aspect ratio constant, the oscillator strength is modified, and therefore the radiative damping rate can be tuned. This allows for a convenient tailoring of very broad photonic band gaps.

O 76.5 Thu 16:00 WIL A317

Palladium-based perfect plasmonic absorber in the visible and its application to hydrogen sensing — •Andreas Tittl[1], Patrick Mai[1], Richard Taubert[1], Thomas Weiss[1], Na Liu[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany — [2]Department of Chemistry, University of California, Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California, 94720, USA

We report on the first experimental realization of a palladium-based perfect plasmonic absorber at visible wavelengths and its application to hydrogen sensing.

Our design utilizes palladium wires on top of a MgF_2 spacer layer on a 200 nm thick gold mirror and exhibits an absorbance $> 99\%$ at the given design wavelength in the red part of the visible spectrum.

Exposure to hydrogen causes a change in the complex refractive index of palladium, resulting in reduced absorption and hence enhanced reflection at the interrogation wavelength[1]. Our sensor has a very fast reaction time of less than 1 second, a recovery time of about 10 seconds, and a lower detection limit of less than 0.5% hydrogen in air.

This pronounced response and background-free operation should enable extremely sensitive optical gas detection schemes down to the ppm range in the future.

[1] N. Liu, et al., Nano Lett. **10**, 2342 (2010)

O 77: Graphene V

Time: Thursday 15:00–17:00 Location: WIL B321

O 77.1 Thu 15:00 WIL B321

Large area quasi-free standing two to four layer graphene on SiC(0001) — •Camilla Coletti[1], Stiven Forti[1], Konstantin V. Emtsev[1], Kevin M. Daniels[2], Biplob K. Daas[2], MVS Chandrashekhar[2], Alexei A. Zakharov[3], and Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [2]University of South Carolina, 301 S. Main St, Columbia, SC 29208, USA — [3]MAX-lab, Lund University, Lund, S-22100, Sweden

Graphene epitaxially grown on SiC substrates is an appealing candidate for a wide variety of electronic applications, provided that large area, charge neutral layers can be produced. We have recently reported that hydrogen intercalation can be used to obtain technologically promising undoped quasi-free standing monolayer graphene [1]. In this work we demonstrate that by intercalating hydrogen we can also obtain large-area undoped quasi-free standing bi-, tri- and tetralayer graphene on SiC(0001). LEEM analysis shows that the thickness of the quasi-free standing graphene is homogenous on a scale of tens of micrometers. High resolution ARPES provides evidence that intercalated graphene can reach, upon UHV annealing, charge neutrality within a few meV. Furthermore, this work devotes particular attention to the electronic and structural properties of quasi-free standing trilayer graphene. A combined evaluation of ARPES and LEEM data allows us to shine light on the trilayer stacking sequence, whose determination and control are necessary for advances in graphene-based electronics. [1] C.Riedl et al., Phys. Rev. Lett. 103, 246804 (2009)

O 77.2 Thu 15:15 WIL B321

Intercalation of ferromagnetic metals underneath graphene on Rh(111) — •Mikhail Fonin[1], Philipp Leicht[1], Muriel Sicot[1], and Yuriy S. Dedkov[2] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin

Structure and electronic properties of atomically sharp interfaces between graphene and transition metal surfaces are both of fundamental and technological interest in view of possible device applications. Insertion of other metals between graphene and TM surface (intercalation) can be used to controllably modify the electronic or even magnetic properties of the graphene/metal interfaces.

Here, we present a systematic scanning tunneling microscopy (STM) study of the intercalation process of ferromagnetic metals (Fe, Co, Ni) underneath graphene monolayer on the Rh(111) surface. Ferromagnetic metals were shown to be intercalated effectively at temperatures starting about 300 K yielding single monoatomically thin epitaxial islands underneath the graphene film. Atomically-resolved imaging of the graphene surface after intercalation shows no considerable changes of the moiré structure on top of intercalated metal islands. The strongly bound areas of the moiré structure were found to suppress the lateral growth of metallic islands. We show that in the temperature range of 300-600 K the intercalation process involves diffusion through defects in the graphene layer such as domain boundaries or point defects.

O 77.3 Thu 15:30 WIL B321

Electronic and Magnetic Properties of the graphene/Fe/Ni(111) System: XMCD and ARPES studies — •Martin Weser[1], Elena Voloshina[2], Karsten Horn[1], and Yuriy Dedkov[1] — [1]Fritz-Haber Institut der Max-Planck Gesellschaft, 14195 Berlin, Germany — [2]Institut für Chemie und Biochemie, Freie Universität Berlin, 14195 Berlin, Germany

In our latest works we have demonstrated by means of XMCD and spin-resolved PES that the net magnetic moment of about 0.05-0.1 μ_B per carbon atom is induced in the graphene layer via its contact with ferromagnetic Ni(111) substrate. The magnetic properties of the graphene layer in this system are expected to be improved via intercalation of thin Fe layers underneath graphene on Ni(111) due to the larger magnetic moment of an Fe atom. Here we present studies of the electronic and magnetic properties of the graphene/Fe/Ni(111) intercalation-like system by means of PES, XAS, and XMCD at the Ni, Fe $L_{2,3}$ and C K absorption edges. The presented results reveals an induced magnetic moment of the carbon atoms in the graphene layer aligned parallel to the Ni $3d$ and Fe $3d$ magnetization. It is found that intercalation of Fe changes drastically the magnetic response from the graphene layer. Obtained experimental results are compared with DFT calculations and magnetic moment of carbon atoms in the graphene layer is estimated before and after Fe intercalation in the graphene/Ni(111) system.

O 77.4 Thu 15:45 WIL B321

Effect of the graphene moiré on Ir(111) on intercalated Eu patterns — •Daniel F. Förster[1], Stefan Schumacher[1], Tim Wehling[3], Marin Petrović[4], Iva Šrut[4], Marko Kralj[4], Petar Pervan[4], Carsten Busse[1], Achim Rosch[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [2]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [3]I. Institut für Theoretische Phsik, Universität Hamburg, Jungiusstr. 9, 20355 Hamburg — [4]Institut za fiziku, Bijenicka 46, HR-10000 Zagreb

The electronic properties of graphene on a given substrate may be tailored by adsorption or intercalation.

We have grown Eu on graphene on Ir(111) between 45 K and 720 K with deposited amounts Θ in the monolayer regime. STM and LEED measurements, supported by DFT calculations, were used to determine the structure. Upon adsorption at 720 K Eu intercalates through point defects in the graphene. It forms intercalated line (small Θ) and line+island (larger Θ) patterns. Surprisingly, the line and island widths and spacings are integer units of the moiré cell dimensions. Depending on Θ the intercalated layer forms a $p(2\times2)$ or a $(\sqrt{3}\times\sqrt{3})R30°$ superstructure with respect to the graphene lattice. As these structures are commensurate the moiré of graphene on Ir(111) is preserved. The intercalation patterns may be understood as a combined effect of the inhomogenous binding of graphene to Ir(111) within the moiré unit cell and of the elastic energy changes in graphene associated with intercalation.

O 77.5 Thu 16:00 WIL B321

Doping of epitaxial graphene on Ir(111) — •Iva Šrut[1], Marin Petrović[1], Petar Pervan[1], Milorad Milun[1], Daniel Förster[2], Carsten Busse[2], Thomas Michely[2], and Marko Kralj[1] — [1]Institut za fiziku, Bijenička 46, 10000 Zagreb, Croatia — [2]II. Physikalisches Institut, Zülpicher Str. 77, 50937 Köln, Germany

Graphene's remarkable electronic properties give rise to great expectations of this new material for future electronic devices and spintronic applications. For such purposes a manipulation of its electronic band structure is desired. We have shown that it is possible to engineer the electronic structure of graphene by fine-tuning the Dirac cone of the epitaxial graphene on Ir(111). We had intercalated several different materials, which led to the n-type doping of graphene: Cs, Li, Eu, and their combination. Doping with a specific material leads to different fine effects, such as: (a) gradual or stepwise doping, (b) apparent gap opening at the Dirac point and (c) group velocity changes. We study these effects through direct comparison of the band structure measured by angle resolved photoemission spectroscopy (ARPES).

O 77.6 Thu 16:15 WIL B321

Epitaxial graphene on Ir(111): How it forms mountains and how it gets a Rashba surface state out into the fresh air — •Andrei Varykhalov — Helmholtz-Zentrum Berlin, 12489 Berlin

A new phase of epitaxial graphene on Ir(111) is discovered. It occurs as a periodic array of pyramids with giant height corrugation of 3.5Å, is free of carbide, and can be easily recognized by its unique LEED pattern. The corrugation is 10× larger than for the known Moiré-type phases of graphene/Ir [1] which suggests that a novel formation mechanism is at work. STM, XPS, ARPES, as well as LEED simulations of pyramid-shaped graphene and Moiré-type control samples indicate that the pyramids occur by relief of lateral strain from a chiral dislocation network which renders them a prospective playground for quasi-Landau quantization of Dirac fermions in giant pseudomagnetic fields [2]. The bare Ir(111) harbors fascinating electronic and spin properties as well. By spin-ARPES we reveal a previously unobserved giant (α_R of the order of 10^{-10} eVm) Rashba-type spin splitting of a prominent Ir surface state. It will be shown that this spin-orbit split surface state is not affected when Ir(111) is epitaxially covered with graphene. Moreover, it will be demonstrated that graphene itself protects the Ir surface so efficiently that the surface state remains stable in ambient atmosphere. This behavior is explained based on topological properties of this surface state.

[1] A. T. N'Diaye et al., Phys. Rev. Lett. **97**, 215501 (2006) and refs. therein; [2] F. Guinea et al., Nat. Phys. **6**, 30 (2010); N. Levy et al., Science **329**, 544 (2010).

O 77.7 Thu 16:30 WIL B321

Mobility of molecular liquid layers confined between graphene and mica — •Martin Dorn, Nikolai Severin, Philipp Lange, Patrick Amsalem, Norbert Koch, and Jürgen P. Rabe — Humboldt-Universität zu Berlin, Department of Physics, Germany

Properties of water confined to a nano-scale are of scientific and technological interest ranging from lubrication to protein folding. Water has been demonstrated to remain liquid at room temperature when confined to different geometries ranging from confinement between two flat walls to nanopores. Recently crystalline molecular layers of water on mica surfaces have been reported, based on the visualization of graphene conforming to their surface [1]. We argue that the stable graphene topography may be caused by entrapped contaminations at the graphene-mica interface and not by the crystallinity of water. We find that contamination-free graphenes deposited on mica surfaces exhibit an atomically flat topography in the entire area independently on the ambient humidity during preparation. From this we conclude a substantial mobility of the water layer confined at the graphene-mica interface. Based on these and further experiments with confined molecular layers of other contaminated liquids we propose a model for the stabilization of the graphene topography on the liquid molecular films.

[1] K. Xu, P. Cao, J.R. Heath, *Science* 329 (2010) 1188.

O 77.8 Thu 16:45 WIL B321

Novel routes towards the chemical functionalization of graphenoid and graphene: Janus nanomembranes — Zhikun Zheng[1], Christoph Nottbohm[1], •Andrey Turchanin[1], Heiko Muzik[1], André Beyer[1], Mike Heilemann[1], Markus Sauer[2], and Armin Gölzhäuser[1] — [1]Fakultät für Physik, Universität Bielefeld — [2]Biotechnology & Biophysics, Julius-Maximilians-University Würzburg

The chemical functionalization of graphene is essential for the use in molecular sensors or nanoelectromechanical components. However, a functionalization is difficult to achieve for graphene single crystals due to their chemical inertness. Here we present a route towards the chemical functionalization of graphenoid carbon nanomembranes fabricated from self-assembled monolayers. These 1 nm thick membranes possess amino functionalities on their top sides and thiol functionalities on their bottom sides. It is demonstrated how such two-dimensional (2D) "Janus membranes" can be used for the selective immobilizations of functional molecules. As a proof of concept, we functionalized both sides with different fluorescent dyes. The functionalization is observed by X-ray photoelectron spectroscopy and fluorescence resonant energy transfer. The potential of Janus nanomembranes as a 2D-platform for the chemical functionalization of graphene is discussed.

Z. Zheng, C.T. Nottbohm, A. Turchanin, H. Muzik, A. Beyer, M. Heilemann, M. Sauer, A. Gölzhäuser, Angew. Chem. Int. Ed. 49 (2010) 8493-8497

O 78: Surface chemical reactions

Time: Thursday 15:00–16:15 Location: WIL B122

O 78.1 Thu 15:00 WIL B122

Investigations on induced dissociation of Dicobaltoctacarbonyl — •Johannes Schwenk, Evgenia Begun, Fabrizio Porrati, Roland Sachser, and Michael Huth — Physikalisches Institut, Goethe-Universität, D-60438 Frankfurt am Main, Germany

Dicobaltoctacarbonyl ($Co_2(CO)_8$) is used as a precursor gas for focused electron beam induced deposition (FEBID) performed in a scanning electron mikroscope. In order to understand the processes which lead to the dissociation of the precursor we performed in situ electrical conductivity measurements during the FEBID process and right after it. In particular, the influence of the composition of the residual gas in the vacuum chamber on a possible autocatalysis of the $Co_2(CO)_8 \rightarrow$ Co reaction was studied. We observed an enhanced spontaneous dissociation of $Co_2(CO)_8$ on thermal silicondioxide surfaces after using a plasma downstream asher. For a characterisation of the obtained films we performed an X-ray diffraction analysis and made temperature-dependent conductivity and magnetotransport measurements.

O 78.2 Thu 15:15 WIL B122

Reversible bond formation in an atom-molecule complex as a molecular switch — •Fabian Mohn[1], Jascha Repp[2,1], Leo Gross[1], Gerhard Meyer[1], Matthew S. Dyer[3], and Mats Persson[3,4] — [1]IBM Research – Zurich, 8803 Rüschlikon, Switzerland — [2]Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [3]Surface Science Research Centre, Department of Chemistry, University of Liverpool, Liverpool, L69 3BX, UK — [4]Department of Applied Physics, Chalmers University of Technology, SE-412 96, Göteborg, Sweden

We report on the formation of a metal-molecule complex that can be used as a molecular switch. Using a cryogenic scanning tunneling microscope, a covalent bond was formed reversibly between a gold atom and a perylene-3,4,9,10-tetracarboxylic dianhydride molecule supported by a thin insulating film. Atomic force microscopy molecular imaging [Gross et al., *Science* **325**, 1110 (2009)] was employed to determine precisely the atomic structure of the complex, and the experimental results were corroborated by density functional theory calculations. The switching between the bonded and the nonbonded state of the complex was found to be accompanied by a considerable change in the tunneling current and could be reliably controlled by locally applying voltage pulses of according polarity. A new mechanism of bond formation, which involves different charge states of the metal-molecule complex, was identified as the reason for the enhanced reliability compared to bond activation by inelastic electron tunneling.

O 78.3 Thu 15:30 WIL B122

Photoinduced generation of defect bound atomic oxygen by N_2O dissociation on thin MgO films — •Philipp Giese, Harald Kirsch, Christian Frischkorn, and Martin Wolf — Fritz-Haber-Institut, Abt. Physikalische Chemie, Faradayweg 4-6, 14195 Berlin

Photoinduced dissociation of N_2O adsorbed on thin MgO films (4 - 30 monolayers) grown on Ag(100) has been studied with temperature programmed desorption spectroscopy (TPD). After irradiation with 248 nm light from a KrF laser four processes can be identified by postirradiation TPD: Depletion of the initial N_2O coverage, generation of molecular nitrogen desorbing at 55 K, tightly bound atomic oxygen desorbing associatively at 550 K and a shift of the N_2O and N_2 desorption peaks towards higher temperatures. Analysis of the reaction yield as a function of photon exposure confirms a defect driven reaction. However, since the amount of generated atomic oxygen exceeds the amount of generated nitrogen significantly, a second reaction channel with a high nitrogen desorption cross section needs to be incorporated. Our results are interpreted as a reaction mediated by electron hole pair generation at edges of the MgO film followed by electron trapping at defects leading to the N_2O dissociation. This interpretation is corroborated by a saturation of the oxygen generation with increasing N_2O adsorption on edges.

O 78.4 Thu 15:45 WIL B122

Electronic energy dissipation of vibrationally excited HCl/Al(111): model study and *ab initio* results — •Michael Grotemeyer and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel, Germany

Molecular dynamics simulations based on time-dependent density functional theory have revealed an unexpected scaling of the dissipated energy with the mass of the nuclei in case of highly vibrationally excited HCl molecules in front of an Al(111) surface. The energy transfer from the molecular vibrations into electron-hole pair excitations is traced back to a molecular orbital which is unoccupied in the equilibrium geometry and which periodically shifts towards the Fermi level of the metal when the molecule vibrates. We suggest a simple one-dimensional tight binding model, which is capable of explaining our observations from the *ab initio* simulations. Our approach is similar in spirit to a recent (three-dimensional) model studied by Mizielinski and Bird [1]. Both the TDDFT simulations as well as the one-dimensional tight-binding model yield electron-hole pair excitation spectra that differ distinctly from a simple exponential decay. The dissipation mechanism essentially occurs independent of the orientation of the molecule with respect to the metal surface.

[1] M. S. Mizielinski, D.M. Bird, J. Chem. Phys, **132**, 184704 (2010)

O 78.5 Thu 16:00 WIL B122

Theoretical elucidation of the competitive electro-oxidation mechanisms of Formic Acid on Pt(111) — •Wang Gao, John A. Keith, Josef Anton, and Timo Jacob — Institut für Elektrochemie, Universität Ulm, Albert-Einstein-Allee 47, D-89069 Ulm, Germany

The mechanisms of formic acid (HCOOH) oxidation on Pt(111) under electrochemical conditions have been studied using density functional theory, itself an very important reaction in energy conversion. Compared with the analogous gas-phase reaction,[1] HCOOH oxidation at a water-covered surface behaves substantially differently than those in gas phase or using a solvation model involving only a few water molecules. Using these models, we evaluated the detailed reaction process, including energies and geometric structures of intermediates and transition states under the influence of different solvation models and electrode potentials. Our calculations indicate that this potential-dependent electrochemical oxidation proceeds via a multi-path mechanism (involving both the adsorbed HCOOH and HCOO intermediates), a result succinctly rationalizing conflicting experimental observations. Moreover, this study highlights how subtle changes in electrochemical reaction environments can influence (electro-) catalysis.[2] The results provide a conceptual basis to better interpret the complicated reaction kinetics of HCOOH electro-oxidation.

[1] W. Gao, J. A. Keith, J. Anton, T. Jacob, *Dalton Trans.*, **39**, 8450 (2010).

[2] W. Gao, J. A. Keith, J. Anton, T. Jacob, *J. Am. Chem. Soc.*, in press

O 79: Electronic structure II

Time: Thursday 15:00–17:00 Location: WIL C107

O 79.1 Thu 15:00 WIL C107

Towards a molecular understanding of cation-anion interactions in ionic liquids — •Till Cremer[1], Claudia Kolbeck[1], Florian Maier[1], Natalia Paape[2], Peter Schulz[2], René Wölfel[2], Peter Wasserscheid[2], Kevin Lovelock[3], Jens Thar[4], Henry Weber[4], Barbara Kirchner[4], and Hans-Peter Steinrück[1] — [1]Physikalische Chemie II, FAU Erlangen, D — [2]Chemische Reaktionstechnik, FAU Erlangen, D — [3]School of Chemistry, University of Nottingham, UK — [4]Ostwald Institut, University of Leipzig, D

Ionic liquids (ILs), organic salts with melting points below 100°C, are a new class of materials labelled ”designer solvents” for the exciting prospect of tailoring their physical properties by combining an appropriate choice of cation and anion. Regarding the enormous number of possible ion combinations, reliable prediction concepts based on the chemical nature of the IL compounds are needed. In order to estimate the deviation from a simplified superposition of individual anion- and cation-related properties, one has to understand the complex nature of interactions between IL ions, namely coulombic, hydrogen-bond-type and dispersive forces. In this combined XPS, NMR and DFT study[1], interionic interactions in ten different imidazolium-based ILs are examined. In particular, first direct experimental and theoretical evidence for anion-cation charge transfer phenomena in ionic liquids is found. This work was supported by the DFG through SPP1191 ”Ionic Liquids” and the Cluster of Excellence ”Engineering of Advanced Materials”.

[1] T. Cremer et al., Chem. Eur. J. 2010, 16, 9018

O 79.2 Thu 15:15 WIL C107

Lattice-strain induced changes in the electronic structure of SrRuO$_3$ investigated by angle-resolved photoelectron spectroscopy — •Erik Kröger[1], Matthias Kalläne[1], Arndt Quer[1], Adrian Petraru[2], Rohit Soni[2], Hermann Kohlstedt[2], Lutz Kipp[1], and Kai Rossnagel[1] — [1]Institute of Experimental and Applied Physics, University of Kiel, 24098 Kiel, Germany — [2]Department of Nanoelectronics, Technical Faculty, University of Kiel, 24143 Kiel, Germany

Changes of magnetic and electrical properties associated with atomic rearrangements, such as magnetostriction and piezoelectricity, have attracted much attention in basic research due to the possibility of novel applications. Especially transition metal oxides with perovskite crystal structure exhibit multiple electronic correlations that are linked to the crystal lattice. Ferromagnetic SrRuO$_3$, for example, shows lattice-strain induced changes in the magnetic moment. In order to investigate the origin of this behavior we studied the electronic structure of SrRuO$_3$ in different strain states by angle-resolved photoelectron spectroscopy. The SrRuO$_3$ samples were grown by pulsed laser deposition and were measured in different strain-states of the order of -1% to +1%. Experiments were performed at BL7 of the Advanced Light Source (Berkeley). This work was supported by the DFG through SFB 855 ”Magnetoelectric Composite Materials — Biomagnetic Interfaces of the Future”.

O 79.3 Thu 15:30 WIL C107

Fermi Surface Mapping and Heavy Hermion Behaviour in ARPES on CePt$_5$ and CeAg$_5$ Surface Alloys — •Holger Schwab[1], Markus Klein[1], Andreas Nuber[1], Johannes Ziroff[1], H. Hayashi[2], Jian Jiang[2], Kenya Shimada[3], Mattia Mulazzi[1], F.F. Assaad[4], and Friedrich Reinert[1] — [1]Universität Würzburg, Experimentelle Physik VII, Am Hubland, D-97074 Würzburg, Germany — [2]Graduate School of Science, Hiroshima University, Higashi-Hiroshima 739-8526, Japan — [3]Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan — [4]Universität Würzburg, Institut für Theoretische Physik und Astrophysik, Am Hubland, D-97074 Würzburg, Germany

Using high-resolution angle-resolved photoemission we studied ordered Cerium surface alloys on Pt(111) and Ag(111) surfaces. We present light polarization dependent bandstructure and Fermi surfaces for several photon energies including Ce 4d-4f resonant photoemission. In the CePt$_5$ surface alloy, we show the temperature dependence of the Cerium 4f electron spectral weight near the Fermi level. There we observed the opening of a hybridisation gap between the flat 4f Cerium band and one strongly dispersing Pt conduction band that has a strong temperature dependence. The comparison to LDA+DMFT calculations based on an NCA solver shows the on-set of the coherent heavy fermion state at low temperature below the Kondo temperature of the material.

O 79.4 Thu 15:45 WIL C107

Electronic structure of RScO$_3$ from x-ray spectroscopies and first–principles calculations — •Christine Derks[1], Karsten Kuepper[2], Andree Postnikov[3], Reinhard Uecker[4], and Manfred Neumann[1] — [1]Department of Physics, University of Osnabrück, D-49069 Osnabrück — [2]Department of Solidstate Physics, University of Ulm, D-89069 Ulm — [3]Laboratoire de Physique des Milieux Denses, Universite Paul Verlaine, F-57078 Metz — [4]Institute for Crystal Growth, D-12489 Berlin

Perovskites of the type RScO$_3$, where R represents a trivalent rare-earth metal, are *high k* materials and belong to the best available thin film substrates for the epitaxial growth of high quality thin films. This allows a so called strain tailoring of ferroelectric, ferromagnetic, or multiferroic perovskite thin films by choosing different RScO$_3$.

With respect to these interesting properties there is up to now only rare knowledge available about the electronic structure of RScO$_3$. In a previous work we have already published a work on the electronic structure of SmScO$_3$, GdScO$_3$, and DyScO$_3$ [1]. As far as we know, it is the only work combining XPS, XES and XAS with ab initio electronic structure calculations. We are extending these successful investigations to single crystalline PrScO$_3$, NdScO$_3$, EuScO$_3$ and TbScO$_3$. A complete electronic structure was obtained and the band gaps could be deduced for all these rare-earth scandates. All the results were found to be in good agreement with LDA+U calculations.

[1] M. Raekers et al., Phys. Rev. B79 125114 (2009)

O 79.5 Thu 16:00 WIL C107

localized vs. delocalized character of charge carriers in LaAlO3/SrTiO3 heterostructure — •kejin zhou[1], milan radovic[2,1], justine schlappa[1], vladimir strocov[1], ruggero frison[1], joel mesot[1,2], luc patthey[1], and thorsten schmitt[1] — [1]Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [2]Laboratory for synchrotron and neutron spectroscopy, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland

Oxide heterostructures have been attracting great attention due to extraordinary phenomena occurring at the interface and their potential application for device design. A particularly fascinating system is the two-dimensional conductive interface between the band insulators $LaAlO_3$ (LAO) and $SrTiO_3$ (STO), which can be even driven to magnetic and superconducting phases at low temperatures. Resonant inelastic x-ray scattering at Ti L-edges is particularly suitable to address the electronic structure of its interface since the Ti^{3+} states clearly display strong dd excitations while Ti^{4+} states exhibit only elastic emission in the low energy loss regime. Our studies on LAO/STO superlattices prepared by pulsed laser deposition unambiguously reveal the presence of both localized and delocalized Ti 3d carriers generated during the building of the LAO/STO interfaces. Systematic studies on samples before and after annealing under O_2 atmosphere and high temperature show that the dual character carriers can be either induced by electron transfer due to the polar-discontinuity or by oxygen vacancies defects. Oxygen vacancies and electronic reconstruction are equivalent in balancing the built-up electric potential.

O 79.6 Thu 16:15 WIL C107

Band Structure of ZrS_xSe_{2-x} by ARPES — •Mohamed Moustafa, Alexander Paulheim, Christoph Janowitz, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany

The valence band structure of mixed samples of ZrS_x Se_{2-x} single crystals, where x varies from 0 to 2, has been studied by means of high-resolution angle-resolved photoelectron spectroscopy (ARPES) using synchrotron radiation. The crystals were found to be extrinsic n-type semiconductors with indirect bandgap. The composition dependence of the band structure is presented and discussed. A characteristic splitting of the chalcogen p-derived valence bands at the symmetric point A is observed. The size of the splitting shows to increases almost linearly as progressing from ZrS_2 to $ZrSe_2$ reaching 320 meV. Further, the energy gap values are estimated from the valence band maximum to the observed emission close to the conduction band minimum. The gaps are found to vary from 1.78 eV to 1.16 eV for ZrS_2 to $ZrSe_2$, respectively, and are compared to our previously reported optical values [1].

[1] M. Moustafa, Th. Zandt, C. Janowitz, and R. Manzke, Phy. Rev. B 80, 035206 (2009).

O 79.7 Thu 16:30 WIL C107

Energetics and dynamics of hot electrons at GaP and InP surfaces — •Philipp Sippel, Robert Schütz, Klaus Schwarzburg, Thomas Hannappel, and Rainer Eichberger — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

The surface electronic structure and dynamics of hot electrons was investigated for InP(100) and GaP(100) samples with time-resolved 2PPE (TR-2PPE). The In- and Ga-rich grown surfaces were prepared via metal organic chemical vapour deposition, exhibiting (2x4) reconstruction checked by in-situ reflectance anisotropy spectroscopy. The samples were transferred to the experimental setup with a contamination-free UHV commuting system. TR-2PPE spectroscopy was used, applying laser pulses of 40fs duration. The technique allowed for detection of surface states for this GaP(100) reconstruction and a comparison with the similar surface electronic structure of InP(100) was made. For InP, the dynamics of unoccupied surface states was studied, varying excitation energies. Using 4.66eV pump-photons, we excited hot electron bulk states and observed subsequent filling of surface states by scattering of electrons. Furthermore, we excited electrons from the valence band to bulk levels that were isoenergetic with the well known C2 surface state. This energy also corresponds to a potential excitation scheme, involving a direct optical transition from an occupied surface state (V1) to C2. Since we could not observe a noticable magnification of the surface state peak in the photoelectron spectra, we assume that this resonant transition is not allowed.

O 79.8 Thu 16:45 WIL C107

Unveiling a two-dimensional electron gas with universal subbands at the surface of $SrTiO_3$ — •Olivier Copie[1,2], Andrés Felipe Santander-Syro[3], Takeshi Kondo[4], Marcelo Rozenberg[5], and Agnès Barthélémy[2] — [1]Universität Würzburg, Experimentelle Physik VII, 97074 Würzburg, Germany — [2]Unité Mixte de Physique CNRS/Thales, 1 Av. A. Fresnel 91767 Palaiseau, France. — [3]CSNSM, Université Paris-Sud and CNRS/IN2P3 Bâtiments 104 et 108, 91405 Orsay, France. — [4]Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, IA 50011. — [5]Laboratoire de Physique des Solides, Université Paris-Sud, Bâtiments 510, 91405 Orsay, France.

We present our angle-resolved photoemission spectroscopy (ARPES) results showing that there is a highly metallic universal two-dimensional electron gas (2DEG) at the vacuum-cleaved surface of $SrTiO_3$, independent of bulk carrier densities. Our data unveil a remarkable electronic structure consisting on multiple subbands of heavy and light electrons. The similarity of this 2DEG with those reported in $SrTiO_3$-based heterostructures suggests that different forms of electron confinement at the surface of $SrTiO_3$ lead to essentially the same 2DEG.

O 80: Epitaxy and growth: Metals and semiconductors I

Time: Thursday 15:00–17:00 Location: WIL C307

O 80.1 Thu 15:00 WIL C307

Strain aspects of the atomic structure of the InAs wetting layer grown on GaAs(001)-c(4×4) — •Christopher Prohl, Jan Grabowski, Britta Höpfner, Mario Dähne, and Holger Eisele — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin

InAs/GaAs is the model system for III-V-semiconductor quantum dots and is also a well-known example for the Stranski-Krastanow growth mode in epitaxy. As shown before by scanning tunneling microscopy (STM) investigations of molecular beam epitaxy (MBE) grown samples, the InAs wetting layer evolution on GaAs(001)-c(4×4) can be separated into three phases before quantum dot occurrence: signatures of InAs on GaAs-c(4×4) for low coverages, an $In_{2/3}Ga_{1/3}As$-(4×3) reconstructed monolayer at about 0.67 ML, and different InAs-(2×4) reconstructions forming on top of the latter. In this talk, a closer look at the surface strain of the identified atomic surface structures will be taken. The strain situation of the different growth regimes will be discussed in detail. For this purpose, mainly the bond lengths defining the stress situation will be considered.

The authors thank K. Jacobi and the MPG for providing the experimental set-up. This work was supported by project Da 408/12 of the DFG.

O 80.2 Thu 15:15 WIL C307

Anion-enhanced self-diffusion on Au(100) — •Mostafa Mesgar, Payam Kaghazchi, and Timo Jacob — Institut für Elektrochemie, Universitüt Ulm, Albert-Einstein-Allee 47, 89069 Ulm

Surface phenomena, such as thin film growth, corrosion and crystal growth, are determined by the diffusion of atoms on surfaces. Although several experimental and theoretical studies already focused on the adatom diffusion, much less is known about how possible co-adsorbates might influence diffusion barriers or even migration mechanisms, which could lead to modifications in the surface morphology. Performing large-scale density functional theory (DFT) studies we have investigated the anion-modified self-diffusion on Au(100). We investigated the adsorption and various migration mechanisms of Au atoms on clean [1] and Cl-covered Au(100) with and without surface defects (e.g. steps, kinks, or vacancies). Our studies indicate that in both systems (i.e. clean and Cl-covered) the exchange mechanism, is the most favorable mechanism. Further, we find that for all diffusion processes the presence of co-adsorbed Cl decreases the diffusion barriers, which should result in faster Ostwald ripening. Based on our DFT results the next aim will be to generate a reactive forcefield for Au-Au and Au-Cl interactions,[2] which coupled with kinetic Monte-Carlo will allow for large-scale simulations, providing macroscopic quantities (e.g.

diffusion coefficients) readily comparable to experiments.

1. K. Pötting, W. Schmickler, T. Jacob, *Chem. Phys. Chem.*, **11**, 1395 (2010). 2. D. Fantauzzi, J. A. Keith, A. C. T. van Duin, T. Jacob, *Phys. Rev. B*, **81**, 235404 (2010).

O 80.3 Thu 15:30 WIL C307

Growth of atomically flat Zn films on ZnO(0001) surface — •Hao Zheng, Natalia Schneider, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Transition metal/oxide heterostructures have been investigated as model catalyst. Owing to the largely different surface energies of these materials, three-dimensional metal islands usually form on oxide surfaces. On semiconductors, flat metal films are obtained by a two-step growth method involving low temperature deposition followed by room temperature annealing. Up to now, there are no reports of similar results on oxide surfaces. Here we present scanning tunnelling microscopy data from atomically flat Zn films on ZnO(0001) obtained by a simple one step growth. Subtle variations of the apparent height of the Zn surface are observed, which resemble structures observed from the ZnO(0001) surface underneath. This observation is discussed in terms of tunnelling to quantum well resonances of the Zn films. Support by the DFG via SFB 855 is acknowledged.

O 80.4 Thu 15:45 WIL C307

The Interaction of Copper with a Rhenium$(10\bar{1}0)$ **Surface** — •Daniel Przyrembel and Klaus Christmann — Institut für Chemie und Biochemie, Freie Universität Berlin

Ultrathin Cu films have been deposited in UHV on a Re$(10\bar{1}0)$ surface between 650 K and 800 K and studied by means of MEED, LEED and TPD. Two desorption states are observed between 1000 K and 1180 K. The low temperature α state exhibits zeroth order desorption kinetics, the high temperature β state shows first-order desorption for low Cu coverages shifting to zeroth order with increasing coverage. *In-situ* observation of the MEED (0,0) beam intensity during Cu deposition shows only one maximum that coincides with the saturation of the β TPD peak and a LEED (1×1) structure. No other LEED structures were observed in the investigated coverage range in contrast to the behaviour of Au and Ag [1,2]. Linear superposition of the LEED I,V curves from the clean Re surface and the closed Cu layer reproduces the respective I,V curves for all Cu coverages in that range. Together with the data for Au and Ag on Re$(10\bar{1}0)$ and for Au, Ag and Cu on Re(0001) [3] these findings suggest: (i) On Re$(10\bar{1}0)$ Cu grows in a Stranski-Krastanov mode. (ii) The closed Cu layer is a *bilayer* with two atoms per unit mesh. (iii) The bilayer is formed from two-dimensional islands with local (1×1) structure that show a temperature dependent phase transition towards a two-dimensional lattice gas.

[1] C. Pauls and K. Christmann, J. Phys.: Condens. Matter **21** (2009) 134012; [2] A. Vollmer, Ph.D. thesis, FU-Berlin (1999); [3] R. Wagner, D. Schlatterbeck, K. Christmann, Surf. Sci. **440** (1999) 231-251.

O 80.5 Thu 16:00 WIL C307

Initial stages of the ion-beam assisted epitaxial GaN film growth on 6H-SiC(0001) — •Lena Neumann[1], Jürgen Gerlach[1], Thomas Höche[1], and Bernd Rauschenbach[1,2] — [1]Leibniz Institute of Surface Modification (IOM), D-04318 Leipzig, Germany — [2]University Leipzig, Institute of Experimental Physics II, D-04103 Leipzig, Germany

The influence of the nitrogen ion-to-gallium atom flux ratio (I/A ratio) on the early stages of gallium nitride (GaN) nucleation and thin film growth directly on super-polished 6H-SiC(0001) substrates is studied. Ultrathin GaN films below 15 nm were formed using the ion-beam assisted molecular-beam epitaxy (IBA-MBE) technique. The deposition process was performed at a constant substrate temperature by evaporation of gallium using a conventional effusion cell and irradiation with hyperthermal nitrogen ions from a constricted glow-discharge ion source. The nitrogen ion flux was kept constant and the selection of different I/A flux ratios was done by varying the Ga flux. The GaN growth was determined by in situ reflection high energy electron diffraction and scanning tunneling microscopy measurements. The film microstructure was investigated by transmission electron microscopy. A strong dependence of the resulting film morphology and topography as a function of the Ga deposition rate could be observed. A three-dimensional island growth mode is favoured at I/A ratio >1. At higher Ga deposition rates (I/A ratio <1) the formation of islands developed through early coalescence into two-dimensional growth with the coalescence thickness being about 12 to 30 monolayers of GaN.

O 80.6 Thu 16:15 WIL C307

AES/LEED/I(V) LEED investigation of ultrathin Pb and In layers deposited on Ni(001) and Ni(111) faces — •Katarzyna Miśków and Aleksander Krupski — Institut of Experimental Physic, University of Wrocław, Wrocław, Poland

Properties of ultrathin indium and lead layers deposited on Ni(001) and Ni(111) faces at temperature between T = 150 K and T = 950 K and coverage up to 6 ML have been studied by AES-t, LEED and I(V) LEED. For In/Ni(111), Frank-van den Merwe and Stranski-Krastanov type of growth is observed for temperature below and above 450 K, respectively. In case of In/Ni(001), below T < 600 K it seems that Volumer-Weber or Simultanoeous Multilayers type of growth plus Simultanous Multilayers type of growth. For the adsorption of Pb on Ni(001) only Volumer-Weber type of growth is observed. Two different indium structures have been found for (001) and (111) faces of nickel. For In/Ni(001) the p(2x2) structure has been observed for temperature between 600 K and 950 K. At about 950 K, reconstruction of the p(2x2) structure to c(2x2) one takes place. In case of In/Ni(111) the p(2x2) structure has also been observed, but for temperature between 450 K and 850 K. At about 900 K reconstruction of the p(2x2) structure to the p(3x3)R30 one is observed. In case of Pb/Ni(001) only the c(2x2) structure has been observed. Indium makes surface alloy on both nickel crystal faces upon annealing while for lead, only desorption process is observed. The atomic structure and relaxation of the clean Ni(111) surface were investigated with the use of experimental I(V) LEED profiles and theoretical TensErLEED calculations.

O 80.7 Thu 16:30 WIL C307

Epitaxial growth of Group IV materials by Chemical Vapor Deposition for Germanium Metal Oxide Semiconductor devices — •Benjamin Vincent, Roger Loo, and Matty Caymax — imec, Kapeldreef 75, B-3001 Leuven, Belgium

Over the past 5-10 years, germanium has attracted a lot of interest to replace Silicon as a high carrier mobility material in future p-Metal Oxide Semiconductors transistors. This paper reviews developments of epitaxial Group IV materials (silicon, germanium, tin and alloys) by means of Reduced Pressure Chemical Vapor Deposition for use as Channel, Gate stack and Source/Drain in high performance Germanium transistors. We will first describe Germanium growth on standard Silicon wafers. Selective epitaxial growth within Shallow Trench Isolation structures allows seamless integration of Germanium channels in Si platform with a significant defect reduction down to levels required for state-of-the-art VLSI technology. Next we will focus on the most successful passivation approach for Germanium MOS interfaces by means of ultrathin epitaxial Si capping layers. This moves the problem of gate stack formation from a germanium surface to a silicon surface. We will discuss novel extremely low temperature CVD processes involving innovative precursors, and impacts of point defects, strain relaxation and Silicon-Germanium intermixing on Germanium device performance. Finally, the implementation of Germanium-Tin alloys in embedded Source/Drain regions in Germanium transistors will be proposed as an innovative architecture to implement strain in Germanium channels.

O 80.8 Thu 16:45 WIL C307

Ab-initio study on the temperature dependence of adsorbate-induced segregation in C/$\mathbf{Pt_{25}Rh_{75}(100)}$ — •Tobias C. Kerscher and Stefan Müller — Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungswerkstoffe, Denickestr. 15, 21073 Hamburg, Germany

Understanding the adsorbate-induced segregation of alloy surfaces is essential for catalytic surfaces. An interesting example is the C/$Pt_{25}Rh_{75}$(100) system: In comparison to the clean surface [1,2], even a small amount of carbon impurities leads to a considerable decrease in the Pt concentration of the top layer [1]. Previously, our first principles study of the coupled surface–adsorbate system was restricted to $T = 0$ K, where density functional theory shows that this change in segregation is driven by the antagonism between the segregation energies of Pt and Rh, and their binding energies to C. Now, we use an ab-initio-based cluster expansion in the framework of the UNCLE code [3] to investigate the $T > 0$ K temperature behaviour of the system by means of Monte Carlo simulations. We discuss the substitutional ordering of both the carbon adsorbate layer and the four topmost surface layers of $Pt_{25}Rh_{75}$(100) as a function of temperature and concentration. Our predictions are compared to experimental data in a quantitative manner.

Supported by Deutsche Forschungsgemeinschaft.

[1] E. Platzgummer *et al.*, Surf. Sci. **419** (1999), 236.

[2] P. Welker *et al.*, J. Phys.: Condens. Matter **22** (2010), 384203.

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

O 81: [MA] Surface magnetism IV

Time: Thursday 15:15–17:15 Location: HSZ 103

O 81.1 Thu 15:15 HSZ 103

SP-STM study on bulk nickel (111) surface — •Liudmila Dzemiantsova, André Kubetzka, Kirsten von Bergmann, and Roland Wiesendanger — Institut für Angewandte Physik, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg

It has been recently reported that ferromagnetic materials, in particular nickel, can be used as ideal substrates for a high quality graphene formation [1, 2]. Despite the fact that nickel is a good source of spin-polarized electrons, there remains a lack of information about spinpolarized scanning tunneling microscopy (SP-STM) investigations of its surfaces [3, 4].

In our study we used SP-STM to explore the domain structure of a bulk nickel crystal (111) surface on a large scale. We showed that domains can easily be shifted at low magnetic fields or by the stray field of the magnetically coated tip. The strongest magnetic signal was achieved at energies below the Fermi level. This result is in contrast to previous theoretical expectations [3].

[1] A. Varykhalov et al., Phys. Rev. B., 80, 035437 (2009)

[2] Yu.S. Dedkov et al., App. Phys. Lett., 92, 052506 (2008)

[3] K-F. Braun et al., Phys. Rev. B, 77, 245429 (2008)

[4] Y. Nishimura et al., Phys. Rev. B, 79, 245402 (2009)

O 81.2 Thu 15:30 HSZ 103

Orientation-dependent Kondo resonance of the Ni_2(hfaa)$_4$(bpm) and Mn_2(hfaa)$_4$(bpm) single molecular magnets — •Lei Zhang[1], Michael Schackert[1], Toshio Miyamachi[1], Toyokazu Yamada[1], Frank Schramm[2], Mario Ruben[2], and Wulf Wulfhekel[1] — [1]Physikalisches Institut, Karlsruhe Institut of Technology, Germany — [2]Institut of Nanotechnology, Karlsruhe Institut of Technology, Germany

Single molecular magnets (SMM) attract much interest due to their potential applications in spintronics. We investigated metal organic molecules based on (hfaa)$_4$(bpm) containing two $3d$ ions (Ni or Mn) using low temperature scanning tunneling microscopy (STM) at 1 K in ultra-high vacuum. In the bulk, the two metallic ions couple antiferromagnetically leading to an $S = 0$ ground state [1,2].

The Ni_2 and Mn_2 molecules were sublimed onto atomically clean Cu(100) surfaces resulting in two different absorptions configurations. Scanning tunneling spectroscopy (STS) with a high energy resolution of 0.3 meV showed a strong Kondo resonance on the position of the metal ions inside the molecules indicating that the hybridization of the local spins with the substrate is more efficient than their antiferromagnetic coupling. The Fano resonance showed a pronounced dependence on the adsorption geometry indicating different Kondo temperatures and q-parameters. This is explained by a adsorption dependent hybridization between SMM and the substrate.

[1] G. Brewer *et al.*, Inorg. Chem. **24**, 4580-4584 (1985)

[2] M. Barquín *et al.*, Transition Metal Chemistry **24**, 546-552 (1999)

O 81.3 Thu 15:45 HSZ 103

Search for homochiral magnetic structures along the step edge of Pt(664) — •Benedikt Schweflinghaus, Bernd Zimmermann, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Co chains at the step edge of Pt(997) is historically the prime example of a one-dimensional metallic magnet. A series of experimental and theoretical studies uncovered and explained the magnetic properties of this novel magnet. We re-investigate this type of system in the light of the recently discovered Dzyaloshinskii-Moriya interaction (DMI) of ultrathin films causing spin-orbit driven homochiral magnetic structures. The question arises whether the DMI in the Co chain at the Pt edge is strong enough to drive a spin-spiral state of one handedness.

In this contribution we investigate this point applying the material specific density functional theory by means of the Full-Potential Linearized Augmented Plane-Wave (FLAPW) method as implemented in the FLEUR code [1] to a variety of transition-metal (TM) chains on Pt(664). We compare TM chains to the previous analysis of the magnetic anisotropy energy (MAE) for Co chains on Pt(664) [2]. Via a micromagnetic model that includes the MAE, as well as the spin stiffness and the Dzyaloshinskii vector we investigate the possible magnetic phases. While in the Co chain it appears that the ground state is collinear, yet in other TM chains non-collinear states may be possible.

[1] http://www.flapw.de

[2] S. Baud *et al.*, Physical Review B **73**, 104427 (2006)

O 81.4 Thu 16:00 HSZ 103

Magnetism of Cobalt-coordination nodes in 2D supramolecular networks — •Uta Schlickum[1], Willi Auwärter[2], Markus Etzkorn[1], Stefano Rusponi[1], Pardeep Thakur[3], Knud Seufert[2], Svetlana Klyatskaya[4], Mario Ruben[4], Johannes V. Barth[2], and Harald Brune[1] — [1]Institute of Condensed Matter Physics, Ecole Polytechnique Fédérale de Lausanne, Switzerland — [2]Physik Department E20, Technische Universität München, Germany — [3]European Synchrotron Radiation Facility, Grenoble, France — [4]Institut für Nanotechnologie, Karlsruher Institut für Technologie, Germany

Supramocular engineering on crystalline surfaces offers the possibility to fabricate networks with embedded metal centers having specific physicochemical properties. Here we report on the magnetic nature of individual Co atoms in 2D architectures providing different coordination environments probed with X-ray magnetic circular dichroism. Changing the coordination symmetry using related functional organic ligands strongly influences the magnetic characteristics of the metal center. While Co atoms with threefold coordination to carbonitriles show large magnetic moments, these vanish in the case of fourfold coordination to pyrrole ligands in a Co-porphyrin. Further modification of the magnetic properties by site-selective decoration of the individual Co centers by small Fe clusters will be discussed.

O 81.5 Thu 16:15 HSZ 103

Charge-transfer correlation effects on the spin state of magnetic molecules at a metal interface — •Sebastian Stepanow[1], Piter Miedema[2], Aitor Mugarza[1], Gustavo Ceballos[1], Paolo Moras[3], Julio Cezar[4], Carlo Carbone[3], Frank de Groot[2], and Pietro Gambardella[1] — [1]ICN Barcelona — [2]U Utrecht — [3]CNR Trieste — [4]ESRF Grenoble

We investigate the hierarchy of local correlation and hybridization effects in metal-organic molecules adsorbed on metals. Using x-ray magnetic circular dichroism and ligand field multiplet calculations, we demonstrate that the $3d$ electronic ground state of monolayer metal-phthalocyanine (CoPc, FePc) on Au(111) is given by the coherent superposition of two charge states, $d^nE + d^{n+1}$, where E represents a substrate electron bound to the central metal ion and d^n the many-body ionic orbital configuration of the unperturbed molecule. These results differ from previous models of hybrid metal-organic systems, and provide a consistent description of their magnetic properties in terms of spin and orbital multiplicity.

O 81.6 Thu 16:30 HSZ 103

Adsorbate-Dependent Changes in the Surface Magnetization of TiO_2 terminated $SrTiO_3$ Surface from *Ab-Initio* Calculations — •Waheed A. Adeagbo, Guntram Fischer, and Wolfram Hergert — University of Halle, Halle, Germany

Motivated by a recent experiment by Khalid *et al.* [1], in which the surface magnetization of STO was increased (weakened) after ultrasonic cleaning in ethanol (acetone), we have studied the magnetic moment formation of the TiO_2 terminated STO surface.

For this we have considered the perfect surface as well as one containing an O vacancy or a Ti vacancy. Both of the latter are found to be magnetic, whereas the perfect surface is non-magnetic. Furthermore, we have investigated how the adsorption of the ethanol or acetone influences the results calculated above. We find that the two adsorbates affect the magnetization of the Ti vacancy differently.

Our results are compared to the experimental ones. The calculated observed effects are robust with respect to LDA+U correlation corrections applied to the Ti 3*d* orbitals.

[1] M. Khalid et al., *Phys. Rev. B* **81**, 214414 (2010)

O 81.7 Thu 16:45 HSZ 103

Chiral spin-structure of biatomic Fe chains on Ir(001) — •Yuriy Mokrousov[1], Matthias Menzel[2], Robert Wieser[2], Kirsten von Bergmann[2], Elena Vedmedenko[2], André Kubetzka[2], Roland Wiesendanger[2], Stefan Blügel[1], and Stefan Heinze[3] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institut für Angewandte Physik, Universität Hamburg, 20355 Hamburg, Germany — [3]Institut für Theoretische Physik und Astrophysik, Universität zu Kiel, 24098 Kiel, Germany

We investigate from *ab initio* the magnetism of biatomic Fe chains, which form due to self-organization on the (5×1)-reconstructed Ir(001) surface [1]. Using the `FLEUR` code [2], we calculate the magnetic anisotropy and exchange energies with different exchange-correlation functionals, and find very small Heisenberg exchange interactions along the chain of the order of 10 meV/Fe-atom. Upon including spin-orbit coupling we obtain the contribution from the Dzyaloshinskii-Moriya interaction and find that it leads to a 120° spin-spiral ground state of the Fe chains with a unique rotational sense. The results of the Monte-Carlo simulations based on the parameters from *ab initio* are in a very good agreement to STM experiments on the system. We acknowledge funding under HGF-YIG Programme VH-NG-513.

[1] L. Hammer *et al.*, Phys. Rev. B **67**, 125422 (2003).
[2] www.flapw.de

O 81.8 Thu 17:00 HSZ 103

Dzyaloshinskii-Moriya interaction in 3*d*-5*d* zig-zag biatomic chains — V. Kashid[1], •B. Zimmermann[2], T. Schena[2], Ph. Mavropoulos[2], H. G. Salunke[3], V. Shah[4], Y. Mokrousov[2], and S. Blügel[2] — [1]Department of Physics, University of Pune, Pune 411 007, India — [2]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [3]Technical Physics Division, Bhabha Atomic Research Centre, Mumbai 400 085, India — [4]Interdisciplinary School of Scientific Computing, University of Pune, Pune 411 007, India

We investigate from first principles the influence of the antisymmetric Dzyaloshinskii-Moriya interaction (DMI) on the magnetic properties of free-standing zig-zag biatomic chains consisting of 3*d* (Fe, Co) and 5*d* (Ir, Pt, Au) transition-metal atoms. Using the `FLEUR` code [1], we perform self-consistent spin-spiral calculations while treating the spin-orbit interaction within first-order perturbation theory [2]. In this way we can extract the strength of DMI and analyze it in terms of the electronic structure of the chains. Moreover, within a simple tight-binding model we are able to grasp main features of the DMI in these systems and characterize them in terms of symmetry, band-filling and spin-spiral vector.
We acknowledge funding under HGF-YIG Programme VH-NG-513.

[1] www.flapw.de
[2] M. Heide, G. Bihlmayer, S. Blügel, Physica B **404**, 2678 (2009)

O 82: [MA] Graphene (jointly with DY, DS, HL, O, TT)

Time: Thursday 15:15–17:00 Location: HSZ 401

O 82.1 Thu 15:15 HSZ 401

Tunable edge magnetism in graphene — •Manuel J. Schmidt[1], Daniel Loss[1], David J. Luitz[2], and Fakher F. Assaad[2] — [1]Universität Basel, Switzerland — [2]Universität Würzburg, Germany

Edge states with nearly zero energy that are exponentially localized at zigzag edges of graphene ribbons, in combination with electron-electron interactions give rise to edge magnetism. We show how the characteristic momentum-dependence of the transverse wave function of the edge states may be exploited in order to manipulate the edge state bandwidth [1]. This allows to tune graphene edges from the usual edge magnetism regime, over a regime of itinerant one-dimensional ferromagnetism, down to the non-magnetic Luttinger liquid regime. As an example we discuss graphene/graphane interfaces for which we propose an experimental setting in which the bandwidth may be tuned in situ by means of electrostatic gates [2]. We introduce an effective one-dimensional model for the edge states, on the basis of which we investigate the tunability of edge magnetism. Our analysis uses essentially three techniques: by a mean-field treatment of the effective interaction, the phase diagram is established. Quantum fluctuations, which may not be neglected in one dimension, are taken into account on the basis of a bosonization technique. Finally, these analytical calculations are complemented by an exact diagonalization analysis of the effective edge state model.

[1] M.J. Schmidt and D. Loss, Phys. Rev. B 81, 165439 (2010).
[2] M.J. Schmidt and D. Loss, Phys. Rev. B 82, 085422 (2010).

O 82.2 Thu 15:30 HSZ 401

Ballistic transport at room temperature in micrometer size multigraphene — •Srujana Dusari[1], José Luis Barzola Quiquia[1], Pablo Esquinazi[1], and Nicolas Garcia[2] — [1]Division of Superconductivity and Magnetism, Universität Leipzig, Faculty of Physics and Earth Sciences, Institute for Experimental Physics II, Linnéstr. 5, 04103 Leipzig, Germany — [2]Laboratorio de Física de Sistemas Pequeños y Nanotecnología, Consejo Superior de Investigaciones Científicas, Serrano 144, E-28006 Madrid, Spain

As an emergent material for electronic applications, graphite and graphene and their electrical transport properties have become a subject of intense focus. By performing transport measurements through micro and submicro constrictions in ~10 nm thick graphite samples, we observe drastic increase in the resistance decreasing the constriction width. Our experimental observations indicate that electrons behave ballistically even at room temperature and with mean free path of the order of microns. The values obtained for the mobility (~10^7 cm^2 v^-1 s^-1) and density of the electrons (~10^8 cm^-2) indicates that the graphene layers inside graphite are of higher quality than single ones. The decrease of magneto resistance with decreasing constriction width also indicates that the carrier mean free path is larger than few microns at room temperature.

O 82.3 Thu 15:45 HSZ 401

Long spin relaxation times in bilayer graphene — •Frank Volmer[1,2], Tsung-Yeh Yang[1,2], Jayakumar Balakrishnan[3], Ahmet Avsar[3], Manu Jaiswal[3], Julia Samm[1,2], Syed Rizwan Ali[1,2], Alexandre Felix Pachoud[3,4], Ming-Gang Zeng[3,5], Mihaita Popinciuc[1,2], Barbaros Özyilmaz[3,4,5], Gernot Güntherodt[1,2], and Bernd Beschoten[1,2] — [1]II. Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]JARA: Fundamentals of Future Information Technology, 52074 Aachen, Germany — [3]Department of Physics, National University of Singapore, 117542 Singapore — [4]NUS Graduate School for Integrative Sciences and Engineering (NGS), Centre for Life Sciences (CeLS), 117456 Singapore — [5]Nanocore, National University of Singapore, 117576 Singapore

The demonstration of micrometer long spin relaxation lengths in graphene at room temperature has made this material a promising candidate for spintronic applications. We investigated the spin transport in the non-local spin valve geometry in bilayer graphene using MgO barriers for spin injection. We demonstrate that the dominant spin relaxation mechanism in bilayer graphene is of the D'yakonov-Perel' type. In this case the spin dephasing time scales inversely with the charge carrier mobility. At room temperature spin dephasing times of up to 2 ns are measured in samples with the lowest mobility.

This work has been supported by DFG through FOR 912.

O 82.4 Thu 16:00 HSZ 401

The graphene Landau quartet unveiled — •Sander Otte[1,2,3], Young Jae Song[2,3], and Joseph Stroscio[2] — [1]Delft University of Technology, The Netherlands — [2]National Institute of Standards and Technology (NIST), USA — [3]Maryland NanoCenter, University of Maryland, USA

Some of the unique properties of graphene come to expression when its electrons are locked into Landau levels in an external magnetic field. Due to spin-degeneracy in combination with the two-atom unit cell of the hexagonal lattice (valley degeneracy), each Landau level is expected to host four electrons. We use a newly completed dilution refrigerator cooled STM system to study epitaxial graphene at 10 mK in magnetic fields up to 15 T. The unparalleled energy resolution of this instrument enables us to break the predicted fourfold Landau level degeneracy and to measure the sublevel splittings as a function of the magnetic field. Surprisingly large splittings are found for the valley states, which are not magnetic by nature. In addition, intriguing partial filling of the sublevels is observed, yielding access to promising electron correlation effects.

O 82.5 Thu 16:15 HSZ 401

Emergent magnetism of *5d* transition-metal adatoms on Graphene — •Hongbin Zhang[1], Cesar Lazo[2], Stefan Blügel[1], Stefan Heinze[2], and Yuriy Mokrousov[1] — [1]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institute of Theoretical Physics and Astrophysics, University of Kiel, 24098 Kiel, Germany

Owing to its peculiar electronic structure, graphene serves as a playground for many interesting physical properties and has drawn a lot of attention recently [1]. In this work, using the first principles FLAPW methods, we investigate the magnetism of 5*d* transition metal (TM) atoms from Hf to Pt deposited on graphene in different supercell geometries. By taking into account the effect of atomic relaxations, we find that most of the 5*d* TMs exhibit strong local magnetism when deposited on graphene. A combination of large spin moments with strong spin-orbit coupling in considered adatoms leads to gigantic values of the magnetic anisotropy energies, reaching values as large as 30 meV/atom. We also investigate the influence of external electric fields on the magnetic properties of 5*d* TM adatoms and discuss possible transport applications. We acknowledge funding under HGF-YIG Programme VH-NG-513.

[1] A. H. C. Neto, *et al.*, Rev. Mod. Phys. **81**, 109 (2009).

O 82.6 Thu 16:30 HSZ 401

Anisotropic magnetoresistance observed in graphite flakes — •Jose Barzola-Quiquia, Andreas Schadewitz, Winfried Böhlmann, and Pablo Esquinazi — Division of Superconductivity and Magnetism, University of Leipzig, D-04103 Leipzig, Germany

The possibility to have magnetic order at room temperature in a system without 3d metallic magnetic elements attracts the interest of the solid state physics community. Experimental evidence for the existence of ferromagnetism in virgin and proton-irradiated graphite samples was published based on SQUID [1] and XMCD [2] measurements. An alternative method to detect magnetic order is to measure the magnetoresistance (MR). The MR develops a characteristic butterfly loop when measured vs. magnetic field. In this work we have studied the magnetotransport properties of micrometer-size and ˜10 nm thick graphite flakes as a function of temperature, magnetic field applied in- and out-plane configurations. We investigated especially the MR as a function of the angle between current and applied field in order to study the anisotropic magnetoresistance (AMR). Virgin graphite flakes show a small AMR and flakes treated with H_2SO_4 show an increase in the AMR signal. The observed behavior provides evidence for intrinsic and induced ferromagnetism at the surface of graphite samples. This investigation also was complemented using SQUID magnetometry on graphite powder in virgin state and after treatment with H_2SO_4 resulting in a clear ferromagnetic signal. [1] P. Esquinazi et al., Phys. Rev. B 66, 024429 (2002), Phys. Rev Lett. 91, 227201 (2003). [2] H. Ohldag et al., Phys. Rev. Lett. 98, 187204 (2007).

O 82.7 Thu 16:45 HSZ 401

Magnetic clusters on graphene flakes — •Wolfgang Landgraf, Sam Shallcross, and Oleg Pankratov — Lehrstuhl fur Theoretische Festkorperphysik, Staudstr. 7-B2, 91058 Erlangen, Germany.

We present an investigation of the properties of magnetic ad-atoms and clusters on graphene flakes. We consider clusters of 1-7 atoms of metals from the 3d series assembled on graphene flakes composed of the order of 100 carbon atoms. All calculations are performed within the spin density functional theory formalism in the local density approximation. We elucidate the range of the magnetic interaction for pairs of magnetic ad-atoms on graphene flakes, as well as the equilibrium magnetic structure for various cluster types. By a comparison of such clusters on flakes with their counterparts on extended sheets, we are able to elucidate the role of the flake shape upon the magnetic interaction. In this way we determine the role of confinement on the magnetic interaction, and comment on the possibility of using flake shape as a design parameter of magnetic nanostructures on graphene flakes.

O 83: [MA] Focussed Session "X-ray absorption spectra - state of the art of theory and experiment" (jointly with DS, HL, MM, O)

Time: Thursday 15:15–19:00 Location: HSZ 403

Invited Talk O 83.1 Thu 15:15 HSZ 403

Simulations of X-ray Spectra using FEFF9 and OCEAN — •John Rehr — University of Washington, Seattle, WA, USA

There has been dramatic recent progress in the theory of x-ray spectra. This spectra probes excited state properties of a system, and thus requires theoretical treatments beyond the independent particle approximation. Here we discuss two complementary approaches based on the GW/BSE method. First is a real-space Green*s function approach, as implemented in the FEFF9 code [1]. FEFF9 has improved treatments of many-body effects and can also include LDA+U corrections. Second, is a new k-space approach implemented in the GW/BSE code OCEAN (Obtaining Core Excitation using ABINIT and NBSE)[2]. OCEAN also includes intra-atomic coulomb interactions and can also treat multiplet effects. FEFF9 and OCEAN have complementary spectral ranges. However, the combination is applicable from the UV-VIS to x-ray energies. These two approaches are illustrated with applications to several core-level specra including XAS and RIXS. This work is supported by US DOE Grant DE-FG03-97ER45623 and the CMCSN. [1]J. J. Rehr et al.,Comptes Rendus Physique 10,548 (2009). [2]J. Vinson et al., arXiv:1010.0025

Topical Talk O 83.2 Thu 15:45 HSZ 403

Polarisation dependent X-ray spectroscopy — •Andrei Rogalev, Fabrice Wilhelm, and Jose Goulon — European Synchrotron Radiation Facility (E.S.R.F.), 6 rue Jules Horowitz, 38000 Grenoble, France

In these recent years X-ray spectroscopies have been undergoing a continuous expansion, as illustrated by the discovery of a variety of new experimental techniques associated with the exploitation of the polarisation properties of synchrotron radiation. The detection of X-ray magnetic linear and circular dichroism in ferro-, ferri- and paramagnetic systems, the discovery of X-ray natural circular dichroism in gyrotropic single crystals as well as the observation of non-reciprocal X-ray linear dichroism and X-ray magneto-chiral dichroism in magnetoelectric systems are particularly interesting. In combination with sum rules these element and orbital selective spectroscopies have proved to be remarkable tools to study fundamental properties of magnetic matter via various order parameters, e.g., spin and orbital moments, electric dipole moment, orbital anapole etc. In this talk we report on advanced instrumentation developed at the ESRF beam line ID12 which is dedicated to polarization dependent x-ray spectroscopy at photon energies above 2keV. Several examples have been selected to illustrate the present performances of the beam line and to show the recent advances in the field.

Topical Talk O 83.3 Thu 16:15 HSZ 403

Theoretical description of X-ray absorption in correlated transition metal systems — •Hubert Ebert[1], Jan Minar[1], and Ondrej Sipr[2] — [1]Ludwig-Maximilians-Universität München, Department Chemie und Biochemie, Physikalische Chemie, Butenandtstraße 11, D-81377 München, Germany — [2]Institute of Physics AS CR, Prague, Czech Republic

During the last years, great progress has been made in dealing with correlation effects in solids. Among the various theoretical approaches available now, the LSDA+DMFT (local spin density approximation + dynamical mean field theory) plays a prominent role, as it accounts for dynamical correlations when dealing with the ground state. We present a description of x-ray absorption spectra based on combining the LSDA+DMFT and the multiple scattering formalism. Working with a fully relativistic formulation, this approach gives access to a corresponding treatment of x-ray magnetic circular dichroism (XMCD). By applying the XMCD sum rules, we can demonstrate that the enhancement of orbital magnetism in ferromagnetic 3d-transition metals, which results from using the LSDA+DMFT formalism instead of plain LSDA, is indeed reflected by the XMCD spectra. Comparing the LSDA+DMFT-based XAS and XMCD spectra with experiment, however, some discrepancies remain that are ascribed to dynamical effects connected with the absorption process itself. To account for these effects we extended the sketched approach by including the presence of a core hole within the XAS and XMCD calculations using various schemes.

15 min. break

Topical Talk O 83.4 Thu 17:00 HSZ 403

Paramagnetic molecules on metal surfaces: prototypes for spin-hybrid systems — •Heiko Wende — Faculty of Physics and CeNIDE, University of Duisburg-Essen, 47048 Duisburg, Germany

The fundamental understanding of the interaction of paramagnetic molecules with metal surfaces is crucial for the possible application of these spin-hybrid systems in molecular spintronics. We study the magnetic properties of Fe-porphyrin and Fe-phthalocyanine molecules with sub-monolayer coverages on Ni and Co films on Cu(100) with and without an intermediate layer of atomic oxygen. Dichroism in X-ray absorption spectra (XNLD and XMCD) at the respective absorption edges (Fe, Co and Ni $L_{2,3}$-edges, N and C K-edges) is investigated to identify the coupling of the molecules to the ferromagnetic layers, the orientation on the surfaces and the electronic structure. To determine the magnetic anisotropy of Fe- and Co-porphyrin molecules, the molecules were adsorbed on a non-magnetic substrate (Cu(100)). Therefore, angular-dependent XAS and XMCD spectra were measured at 5T and 8K. Calculated XAS spectra obtained from DFT and multiplet calculations using ligand field theory enable a solid interpretation of the experimental data. This work is done in collaboration with C. Weis, D. Klar, D. Bovenschen, M. Kaya, H.C. Herper, B. Krumme, A. Warland, C. Antoniak (Univ. Duisburg-Essen), M. Bernien, J. Miguel, M. Piantek, K. Baberschke, W. Kuch (FU Berlin), P. Srivastava (IIT Delhi), and B. Brena, Md. E. Ali, P.M. Panchmatia, P.M. Oppeneer, B. Sanyal, O. Eriksson (Uppsala Univ.). Supported by BMBF (05 ES3XBA/5), DFG (SFB 491 and SFB 658), STINT and ESRF(HE2700).

Invited Talk O 83.5 Thu 17:30 HSZ 403

Can Carbon Be Ferromagnetic? — •Hendrik Ohldag[1], Elke Arenholz[2], Pablo Esquinazi[3], Daniel Spemann[3], Annette Setzer[3], Martin Rothermel[3], and Tilman Butz[3] — [1]SLAC National Accelerator Center — [2]Lawrence Berkeley National Laboratory — [3]University Leipzig

The existence of long range magnetic order at room temperature in carbon based structures without magnetic elements is very unexpected. Theoretical results from different groups suggest that the existence of long range magnetic order in a graphite structure is possible, if one takes the effects of defects and/or the incorporation of hydrogen atoms into account. SQUID results provided first systematic hints for the existence of magnetic order at room temperature in virgin as well as irradiated graphite samples. We present a x-ray dichroism study of graphite surfaces [1] that addresses the origin and magnitude of ferromagnetism in metal-free carbon. Using element specific x-ray microscopy we can show that metallic impurities do not play a role in the ferromagnetism of carbon and that carbon can be ferromagnetic without ferromagnetic impurities. A detailed spectroscopic study shows that in addition to carbon pi-states, also hydrogen-mediated electronic states exhibit a net magnetization with magnetic remanence at room temperature. The observed magnetism is restricted to the top ~10 nm of the sample where the actual magnetization reaches a value similar to that of Nickel. [1] H. Ohldag et al., Phys. Rev. Lett. 98, 187204 (2007) and to appear in New. Jour. Phys. (2011).

O 83.6 Thu 18:00 HSZ 403

Investigation of strain and doping induced ferromagnetism in LaCoO$_3$ by x-ray absorption and magnetic circular dichroism — Michael Merz[1], Peter Nagel[1], Andrea Assmann[1,2], Stephan Uebe[1,2], Markus Wissinger[1,2], Hilbert von Löhneysen[1,3], Dirk Fuchs[1], and •Stefan Schuppler[1] — [1]Institut für Festkörperphysik, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [2]Fakultät für Physik, Karlsruhe Institute of Technology — [3]Physikalisches Institut, Karlsruhe Institute of Technology, 76031 Karlsruhe, Germany

Undoped bulk LaCoO$_3$ remains paramagnetic down to liquid He temperatures; it has been shown that upon cooling, the Co^{3+} ions undergo a spin-state transition to the $S = 0$ low-spin (LS) state. We explore two avenues for inducing ferromagnetism in this compound: (i) strain, applied by the lattice mismatch between a LaCoO$_3$ thin film and the substrate, and (ii) doping, both with electrons and holes. The spin-state structure of these systems can be studied in detail by near-edge x-ray absorption fine structure and by soft x-ray magnetic circular dichroism at the Co $L_{2,3}$ and the O K edges. It turns out that the mechanism responsible for ferromagnetism in each of the systems – strained undoped, electron doped, hole doped – is unique and distinctly different from the others, explaining the vastly differing transition temperatures. In all cases, a mix of Co spin states is realized, and thus their actual microscopic arrangement is a co-determining factor for magnetic parameters like the spin and orbital moments.

O 83.7 Thu 18:20 HSZ 403

Ab initio study of surface and interface effects on XANES and XMCD of Fe/BaTiO3 systems — •Stephan Borek[1], Angelika Chassé[1], Remya Kunjuveettil Govind[1], Vasili Hari Babu[2], Federica Bondino[3], Martin Trautmann[1], Marco Malvestuto[3], Karl-Michael Schindler[1], Reinhard Denecke[2], Igor Maznichenko[1], and Arthur Ernst[4] — [1]Institute of Physics, Martin-Luther-University Halle-Wittenberg, Germany — [2]Wilhelm-Ostwald Institute for Physical and Theoretical Chemistry, University Leipzig, Germany — [3]IOM CNR, Laboratorio Nazionale TASC, Area Science Park, Basovizza, Italy — [4]Max-Planck-Institut für Mikrostrukturphysik Halle

The aim of our work is the spectroscopic characterization of multiferroic heterostructures by means of x-ray absorption spectroscopy (XAS). Starting form first-principles calculations of bulk BaTiO$_3$ (BTO) the influence of surface and surface termination of BTO on x-ray absorption near edge structure (XANES) and x-ray magnetic circular dichroism (XMCD) is studied for different edges in BTO. In the case of iron layers on BTO, effects at the interface and of layer thickness on XANES and XMCD are considered by means of layer-resolved contributions within a multi-code approach. Calculations are shown in dependence on the direction of polarization of ferroelectric BTO (tetragonal phase). The calculated results are compared to experimental data.

O 83.8 Thu 18:40 HSZ 403

Co-doped ZnO epitaxial films: signs of phase separation by means of hard x-ray absorption spectroscopy — •Verena Ney, Shunagli Ye, Katharina Ollefs, Tom Kammermeier, and Andreas Ney — Fakultät für Physik and CeNIDE, Universität Duisburg-Essen, 47057 Duisburg, Germany

X-ray absorption spectroscopy (XAS) using linear and circular polarized light offers a powerful toolbox of element-specific structural, electronic, and magnetic probes that is especially well suited for studying Zn$_{1-x}$Co$_x$O (Co:ZnO) to unravel its intrinsic properties. We demonstrate that as long as phase separation or excessive defect formation is absent, Co:ZnO is paramagnetic [1]. We can establish quantitative thresholds based on four reliable quality indicators using XAS; samples which show ferromagnet-like behaviour fail to meet these quality indicators, and complementary experimental techniques indeed prove phase separation [2]. Careful analysis of XAS spectra is shown to provide valuable information of secondary phases in a highly sensitive, non-destructive manner.

[1] A. Ney et al., Phys. Rev. Lett. **100**, 157201 (2008).

[2] A. Ney et al., New J. Phys. **12**, 013020 (2010).

This work is supported by the DFG (Heisenberg-Programm) and the EU (MEXT-CT-2004-014195)

O 84: [DS] Organic Electronics and Photovoltaics IV (jointly with CPP, HL, and O)

Time: Thursday 16:15–17:45 Location: GER 38

O 84.1 Thu 16:15 GER 38

Energy level alignment at polymer/PCBM heterojunctions under operating conditions in an organic photovoltaic cell structure — •Johannes Frisch[1], Andreas Wilke[1], Patrick Amsalem[1], Jens Niederhausen[1], Antje Vollmer[2], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Brook-Taylor-Str. 6, D-12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie - Speicherring BESSY II, Berlin, Germany

For heterojunction organic photovoltaic cells (OPVCs) generally vacuum level alignment at the donor/acceptor interface is assumed. In contrast, it has been shown that interface dipoles might occur at organic/organic heterojunctions, which questions the assumption of vacuum level alignment at OPVC interfaces. Therefore, we investigated the energy level alignment at the poly(3-hexylthiophene)/1-(3-methoxycarbonyl)propyl-1-phenyl[6.6]C61 (P3HT:PCBM) heterojunctions with ultraviolet photoelectron spectroscopy (UPS). The valence band of P3HT shifted to higher binding energy by 0.45 eV after deposition of PCBM, while vacuum level alignment was found. This observation would imply an increase of the P3HT ionization energy upon interface formation, which is usually not considered in simple models. The observed phenomenon can be explained either by a structural rearrangement of the donor polymer layer upon acceptor deposition or by surface photovoltage effects that occur during photoemission, which charges the P3HT layer positively whereas negative charges are collected in the PCBM layer.

O 84.2 Thu 16:30 GER 38

New Imaging Approach for Organic Bulk Heterojunction Solar Cells Using Selective Dissolution — •Bettina Friedel, Bruno Ehrler, and Neil C. Greenham — University of Cambridge, Cavendish Laboratory, JJ Thomson Avenue, CB30HE Cambridge, United Kingdom

Morphology in organic photovoltaic devices is one of the most vital and most studied issues for optimum functionality, especially concerning bulk heterojunctions. However, it is always a challenge to control its microscopic structure towards improved exciton dissociation and charge transport. To get an insight into this microstructure usually a combination of various imaging techniques together with spectroscopic methods is used. Unfortunately imaging on all-organic structures is rather challenging since the high similarity of the carbon-based materials gives low contrasts and makes them hard to distinguish. We will present a new imaging approach for organic blends, based on a temperature controlled selective dissolution technique. We will demonstrate on two systems (polymer-polymer and polymer-PCBM) that this technique allows to selectively remove one of the components from a bulk heterojunction, leaving a scaffold of the other component, which can be easily characterized by high resolution imaging, due to the higher air-material contrast. Further the technique allows us to quantify the disordered fraction of semicrystalline components in a blend structure, which is valuable information for matters of charge transport. These new structural insights help understanding the changes in PV performance e.g. following thermal treatments or using solvent additives.

O 84.3 Thu 16:45 GER 38

improvement of the CdSe/P3HT solar cells efficiency due to surface modification of the CdSe nanoparticles by alkylamine treatments — •nikolay radychev, irina lokteva, holger borchert, joanna kolny-olesiak, and jürgen parisi — institute of physics, energy and semiconductor research laboratory, university of oldenburg,oldenburg,germany

Semiconductor quantum dots (QDs) continue to attract immense attention because of their size-dependent optical, physical, and chemical properties which causes them to be a promising material for hybrid solar cell applications. Meanwhile QDs in a polymer matrix have to be stabilized by organic ligands that show significant influence on the charge transport and charge separation processes. Surface modification procedures such as stabilizing ligand exchange or crosslinking the QDs can enhance the efficiency of the hybrid blends. In the present work, as-synthesized QDs, initially capped with oleic acid, were subjected to ligand exchange procedures with the intention to obtain nanoparticles capped by butylamine ligands. Detailed characterisations of the butylamine stabilized QDs based on thermogravimetric analysis, nuclear magnetic resonance and transmission electron microscopy are shown. Laboratory solar cells with blends of the butylamine capped CdSe QDs and poly-3-hexylthiophene (P3HT) as active layer were prepared and investigated by current-voltage and external quantum efficiency measurements. Energy conversion efficiency of about 2% was obtained. The fundamental reasons of the efficiency enhancement were analyzed

O 84.4 Thu 17:00 GER 38

Comparison of the operation of standard and inverted P3HT:PCBM solar cells — •Thomas J.K. Brenner, Yana Vaynzof, Zhe Li, Dinesh Kabra, Richard H. Friend, and Christopher R. McNeill — Cavendish Laboratory, Department of Physics, University of Cambridge, JJ Thomson Ave., Cambridge CB3 0HE, United Kingdom

Inverted organic solar cells have attracted recent attention due to their enhanced environmental stability compared to the standard device architecture. However to date inverted cells have shown poorer efficiencies compared to the standard geometry. To clarify the origin of this behaviour, we have investigated inverted (ITO/ZnO/P3HT:PCBM/ WO3/Ag) and regular (ITO/PEDOT:PSS/P3HT:PCBM/Al) P3HT:PCBM solar cells with different active layer thickness. Using white light bias external quantum efficiency and photocurrent transient measurements, we propose an explanation for the reduced performance of inverted cells. Whereas for inverted devices high EQEs of up to 68% are measured under low light intensities (3 mW/cm^2), EQE drops with increasing white light bias (up to 140 mW/cm^2) down to 20%. This drop is accompanied by a severe distortion of the spectra. For increased thickness (from 90 nm to 550 nm), the drop and shape change can be seen at lower intensities. For regular devices we also observe a drop in EQE, however they still resemble the absorption spectrum showing minor distortion. Unbalanced charge transport and/or unfavourable vertical phase separation in inverted devices are presented as likely causes of the observed behaviour.

O 84.5 Thu 17:15 GER 38

Organic Photovoltaic Cells with Pentacene Nanocolumn Arrays — •Shuwen Yu, Peter Schäfer, Jürgen P. Rabe, and Norbert Koch — Institut für Physik, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 6, 12489 Berlin, Germany

Highly ordered pentacene nanocolumn arrays were fabricated by glancing angle deposition (GLAD) on indium tin oxide (ITO) substrates. The nanocolumn diameter was set to 100-150 nm as revealed by scanning electron microscopy and atomic force microscopy. Interdigitated bulk heterojunction photovoltaic cells (OPVCs) were formed by spincoating [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) as the acceptor material onto the pentacene nanocolumn film. Bathocuproine (BCP) was deposited on top of PCBM as exciton blocking layer. The conversion efficiency of nanocolumn-based OPVCs was significantly higher compared to planar heterojunction OPVCs of the same materials. Further device performance improvement was achieved through employing a thin pentacene seed layer before GLAD, which promoted PCBM solution infiltration between pentacene nanocolumns.

O 84.6 Thu 17:30 GER 38

Performance and stability of P3HT/PCBM bulk heterojunction organic solar cells — •Nivedita Yumnam, Sidhant Bom, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Organic photovoltaic cells are promising candidates for large-area, low-cost production of solar cells. However, the low stability in conjunction with their medium performance is one of the major drawbacks in comparison to their inorganic counterparts. In this investigation environmental conditions for degradation of bulk heterojunction P3HT/PCBM solar cells are systematically analyzed over a period of one week. Devices were prepared by spin coating from different compositions of P3HT and PCBM in Chlorobenzene (C_6H_5Cl). Performance parameters, efficiency and I-V characteristics were determined in a N_2 glove box showing optimized efficiency for a 1:1 ratio. Degradation behavior in N_2 atmosphere, vacuum and solvent-enriched atmosphere (Chlorobenzene) showed best results for vacuum stored solar cells while for solvent-enriched atmosphere rapid degradation was observed. Remarkable degradation (open-circuit voltage and short-circuit current reduced to 90% and 60% after one week) was also found for N_2 atmosphere of the glove box used for the solar cell production. Residual solvent vapor left dispersed in the atmosphere of the glovebox after the spin coating process is identified as an important parameter of this degradation.

O 85: Electron and spin dynamics I

Time: Thursday 16:30–19:00 Location: WIL A317

O 85.1 Thu 16:30 WIL A317

Electron-phonon coupling in laser excited metals — •Isabel Klett, Benedikt Müller, and Bärbel Rethfeld — TU Kaiserslautern, Germany

Irradiation of metals with an ultrashort laser pulse leads to a hot electron gas while the lattice stays cold. The corresponding electron-phonon coupling has been calculated using a thermalized Fermi distribution function [1]. However, after laser excitation, the electrons cannot be assumed in equilibrium, due to their relaxation time of tens of femtoseconds. In order to allow a nonequilibrium distribution function, the Boltzmann equation is applied [2]. This model is extended by implementing the density of states of real metals into the Boltzmann collision terms. From the solution we extract the electron-phonon coupling in thermal nonequilibrium.

[1] Z. Lin, L. Zhigilei and V. Celli in Phys.Rev.B **77**, 075133 (2008)
[2] B. Rethfeld, A. Kaiser, M. Vicanek and G. Simon in Phys.Rev.B **65**, 214303 (2002)

O 85.2 Thu 16:45 WIL A317

Dangling-bond and image-potential states on Ge(100) — •Jens Kopprasch[1,2], Kristof Zielke[1,2], Cornelius Gahl[1], Christian Eickhoff[1], Jörg Schäfer[3], and Martin Weinelt[1,2] — [1]Max-Born-Institut, Max-Born-Straße 2a, 12489 Berlin, Germany — [2]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany — [3]Universität Würzburg, Fakultät für Physik und Astronomie, Am Hubland, 97074 Würzburg, Germany

Germanium is a material of growing interest in semiconductor industry debatted and used for solar cells, high-power transistors, infrared optics and x-ray detectors. Ge is an indirect semiconductor with a band gap of 0.67eV at 300K. The reconstruction of Ge(100) is comparable to the Si(100) surface. However, the surface electronic structure is still under debate.

In this talk we will present bichromatic 2PPE-measurements on Ge(100). We studied the photon-energy dependence of various transitions and identified the dangling-bond states D_{up} and D_{down} as well as the first image-potential state n=1. Besides the energetics the lifetime of these states have been investigated. Furthermore we discuss hot carrier dynamics in the conduction band and the concomitant surface recombination which proceed on a picosecond timescale.

O 85.3 Thu 17:00 WIL A317

Set in time of quasiparticle decay — •Yaroslav Pavlyukh[1], Angel Rubio[2], and Jamal Berakdar[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle — [2]Nano-Bio Spectroscopy Group and ETSF Scientific Development Centre, Dpto. Física de Materiales, Universidad del País Vasco, CFM- CSIC-UPV/EHU-MPC and DIPC, Av. Tolosa 72, E-20018 San Sebastián, Spain

The initial stages of the quasiparticle decay in a Fermi liquid are governed by a time-scale distinct from the scattering rates as derived from the Fermi golden rule approach. We show that the initial decay is non-exponential and that it is determined by the zeroth spectral moment of the electron self-energy. In contrast to the imaginary part of the on-shell self-energy yielding the exponential decay, the spectral moment does not depend on the artificially introduced broadening, and, thus, can be used to characterize even very small finite system with fragmented states. We performed exact and approximate configuration interaction calculations of the spectral moments of the electron self-energy and devised a numerically simple approach for computing the spreading of quasiparticle states even for very large systems.

O 85.4 Thu 17:15 WIL A317

Unoccupied dimer-bond state at Si(100) surfaces — •Thomas Fauster[1], Shin'ichiro Tanaka[2], Katsumi Tanumira[2], Christian Eickhoff[3], Martin Teichmann[3], and Martin Weinelt[3] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]The Institute of Scientific and Industrial Research, Osaka University, 8-1 Mihogaoka, Ibaraki, Osaka 567-0047, Japan — [3]Max-Born-Institut, Max-Born-Str. 2A, D-12489 Berlin, Germany

Two-photon photoemission from Si(100) shows a pronounced resonance for the occupied dangling-bond state D_{up} at photon energies around 2.95 eV. The polarization dependence indicates an intermediate state with a wave function oriented along the dimer axis. We assign this state to the antibonding dimer-bond orbital forming a surface resonance.

The interaction of the dimer-bond state with the bulk continuum leads to a Fano-like lineshape of the resonance curve. A two-dimensional Fano model including the interaction of the D_{up} state with bulk states can describe the data very well. The lifetime of the dimer-bond state is below 5 fs. The parameters for the D_{up} state are known from the description of the resonance curve observed for image-potential resonances.

O 85.5 Thu 17:30 WIL A317

Analysis of Si(001) 2PPE spectra obtained from *ab initio* simulations — •Henning Husser and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel, Germany

Two photon photoemission spectra have been calculated for the Si(001) surface by means of direct simulation of the time-dependent photocurrents. This work is motivated by experimental observations by Fauster *et al.* [1], Shudo and Munakata [2], and Kentsch *et al.* [3]. We present a series of spectra for both *s*- and *p*-polarized light and photon energies in the range of 2.8 – 4.8 eV. Time-dependent excitation spectra are derived approximately by projection of the time-dependent wavefunctions onto the Kohn-Sham eigenstates in order to investigate the dynamics of the photoemission process. The selection rules for the 2PPE process will be compared to the selection rules for 1PPE. In order to explore the possibility of surface resonances which might lead to an enhancement of the photoemission intensity in particular from the dangling bond state, we have calculated the projected density of states at the Si(001) surface in the energy range of the intermediate states.

[1] T. Fauster, S. Tanaka, K. Tanimura, Verhandl. DPG (VI) 45, 3/544 (2010). [2] K. Shudo and T. Munakata, Phys. Rev. B **63**, 125324 (2001). [3] C. Kentsch, M. Kutschera, M. Weinelt, Th. Fauster, M. Rohlfing, Phys. Rev. B **65**, 035323 (2002).

O 85.6 Thu 17:45 WIL A317

Dynamics of the intramolecular charge transfer in alkanethiolate self-assembled monolayers — Ping Kao[1], Stefan Neppl[2], Peter Feulner[2], David L. Allara[1], and •Michael Zharnikov[3] — [1]Departments of Chemistry and Material Science, Pennsylvania State University, University Park, PA 16802, USA — [2]Physik Departement E20, Technische Universität München, D-85747 Garching, Germany — [3]Angewandte Physikalische Chemie, Universität Heidelberg, D-69120 Heidelberg, Germany

Charge transport (CT) in individual molecules and their functional units is important for many frontier areas of modern science and technology. In particular, little is known about CT dynamics in self-assembled monolayers which are prototypes of future molecular electronics devices. By the example of alkanethiolate films on Au(111), we show that this phenomenon can be successfully addressed by resonant Auger spectroscopy, using the core hole clock method. The CT pathway was unambiguously defined by resonant excitation of the nitrile tailgroup attached to the alkyl backbone. The length of this backbone was varied to monitor the respective dependence of the CT time. Similar to the static conductance, this dependence was found to be coarsely described by an exponential function with an attenuation factor of 0.93 per a methylene unit. As a result, the CT time is quite long even for a short alkyl chain; e.g. ca. 100 fs for the chain of only four methylene units. In contrast, the CT time associated with the thiolate headgroup anchor was found to be less than 2.3 fs, suggesting an efficient interfacial coupling between the molecular backbone and substrate.

O 85.7 Thu 18:00 WIL A317

Electron Spin Dependent Transmission through Self-assembled Monolayers of dsDNA — •Matthias Kettner[1], Benjamin Göhler[1], Daniel Nürenberg[1], Volker Hamelbeck[1], Tal Markus[2], Zeev Vager[3], Georg F. Hanne[1], Ron Naaman[2], and Helmut Zacharias[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Münster, Germany — [2]Department of Chemical Physics, Weizmann Institute, Rehovot, Israel — [3]Department of Particle Physics, Weizmann Institute, Rehovot, Israel

Electron spin polarization has been measured for photoelectrons emitted from a gold substrate and transmitted through a self-assembled monolayers of chiral double-stranded DNA molecules. Electron spin polarization values of up to 60% are obtained independent of the polarization of the incident light. The measured electron spin polarization shows a dependence on the thickness of the layer, tested by varying the length of the oligomers. For surfaces covered with single-stranded DNA molecules, which do not form a well ordered layer, no significant spin polarization could be observed.

Samples are irradiated by either circularly or linearly polarized 213nm laser radiation, exciting photoelectrons within the gold substrate, not being sufficient to ionize adsorbed dsDNA molecules. Photoelectrons are analysed either by a time-of-flight detector or a small size conventional Mott polarimeter for spin analysis.

O 85.8 Thu 18:15 WIL A317

Time-resolved Fermi surface mapping and dynamics of the double-CDW transition in HoTe$_3$ — •L. Rettig[1,2], R. Cortes[1,3], J.-H. Chu[4], I.R. Fisher[4], F. Schmitt[4], P.S. Kirchmann[4], Z.-X. Shen[4], M. Wolf[3], and U. Bovensiepen[2] — [1]Fachb. Physik, Freie Univ. Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Fak. f. Physik, Univ. Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany — [3]Abt. Phys. Chemie, Fritz-Haber-Institut d. MPG, Faradayweg 4-6, 14195 Berlin, Germany — [4]Geballe Lab. f. Adv. Mat. and Dep. of Appl. Phys., Stanford Univ., CA 94305, USA

The family of rare earth tritellurides RTe$_3$ presents a textbook-like model system to study the effects of Fermi surface (FS) nesting driven charge density wave (CDW) formation in a low-dimensional electronic system. Depending on R, the system exhibits one or two successive CDW transitions. The collective excitations responsible for such phenomena can be investigated by time-resolved experiments. Employing fs time- and angle-resolved photoemission, the ultrafast melting of the CDW gapped state and the excitation of the amplitude mode could be demonstrated in the single-CDW compound TbTe$_3$. Using a novel position-sensitive Time-of-Flight spectrometer (pTOF) [2], we were now able to investigate the dynamics of both occupied and unoccupied electronic states over a contiguous area of the reciprocal space. Thus, we can follow the evolution of the FS after optical excitation with fs time resolution and observe the dynamics even of the smaller gap and its amplitude mode in the double-CDW compound HoTe$_3$.

[2] P. S. Kirchmann, et al., Appl. Phys. A 91, 211 (2008)

O 85.9 Thu 18:30 WIL A317

Electronic structure and electron dynamics on Si(001) studied by two-photon photoemission — •Christian Eickhoff[1,2] and Martin Weinelt[1,2] — [1]Max-Born-Institut, Max-Born-Straße 2a, 12489 Berlin, Germany — [2]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany

In this talk we will give an overview on the electron dynamics at the Si(001) surface. In the first part we will present new aspects regarding the electronic structure of the silicon surface. The temperature dependent changes in the binding energies of the dangling-bond surface states D_{up} and D_{down} and of the ionization energy will be discussed. In the second part we will highlight the rich variety of carrier dynamics in the conduction band which we access in a femtosecond pump-probe photoemission experiment using an electron analyzer with 2D-CCD-detector. Starting with the relaxation of photoinduced carriers in the Γ_{15}- and X_1-valley we followed the scattering pathway of carriers to the normally unoccupied surface state D_{down}; a process also known as surface recombination. Subsequent relaxation of the electrons in the dispersing branch of the dangling-bond band D_{down} by electron-phonon scattering is slowed down when reaching the band minimum. This is attributed to the blockade of optical phonon emission close to the D_{down} band bottom.

O 85.10 Thu 18:45 WIL A317

How to do time-resolved photoelectron spectroscopy at a free-electron laser — •Christian Sohrt[1], Stefan Hellmann[1], Martin Beye[2], Timm Rohwer[1], Martin Marcynski-Bühlow[1], Matthias Kalläne[1], Florian Sorgenfrei[3], Michael Bauer[1], Alexander Föhlisch[2], Wilfried Wurth[3], Lutz Kipp[1], and Kai Rossnagel[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24118 Kiel, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, 12489 Berlin, Germany. — [3]Institut für Experimentalphysik and Center for Free-Electron Laser Science, Universität Hamburg, 22761 Hamburg, Germany

The Free-Electron Laser in Hamburg (FLASH) generates highly brilliant, ultrashort, and coherent pulses in the soft X-ray regime enabling many fascinating experiments that are not possible at other sources. After various challenges concerning space-charge effects as well as timing, synchronization and data aquisition issues have recently been solved, optical pump-XUV probe photoelectron spectroscopy on solid surfaces is now possible. The wide probing photon energy range of up to 1000 eV should allow time-resolved core-level spectroscopy with time and energy resolutions of ~200 fs and ~100 meV, respectively. We performed a proof-of-principle experiment on the correlated layer compound 1T-TaS$_2$ [1] demonstrating that FLASH can indeed be used to investigate core-level dynamics at solid surfaces on the femtosecond time scale. This work is funded in part by the BMBF (FSP 301 FLASH).

[1] Hellmann *et al.*, PRL **105** 187401 (2010)

O 86: Heterogeneous catalysis I

Time: Thursday 16:30–19:30 Location: WIL B122

O 86.1 Thu 16:30 WIL B122

First-Principles kinetic Monte Carlo Simulations of Ammonia Oxidation at RuO$_2$(110): Selectivity vs. semi-local DFT — •Claudia Mangold[1] and Karsten Reuter[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Technische Universität München

Reaching a detailed mechanistic understanding of high selectivity in surface catalytic processes is one of the central goals in present-day catalysis research. The Surface Science approach to this problem focuses on the investigation of well-defined model systems that reduce the complexity but still capture the relevant aspects. In this respect, the almost 100% selectivity reported in detailed experiments for the oxidation of NH$_3$ to NO at RuO$_2$(110) [1] presents an ideal benchmark for a quantitative theoretical analysis. To this end we perform detailed kinetic Monte Carlo simulations based on kinetic parameters derived from density-functional theory (DFT). The obtained turnover frequency for molecular nitrogen is in rather good agreement with the experimental data. However, even with an extended set of elementary processes we are not able to reproduce the experimental findings for the production of NO and therewith the selectivity. The central quantities that decisively determine the latter are the binding energy of NO and the N diffusion barrier. Suspecting the approximate energetics obtained with the employed semi-local DFT functional as reason for the discrepancy, we recalculate the kinetic parameters with different functionals and discuss the resulting effects in the kMC simulations.

[1] Y. Wang *et al.*, J. Phys. Chem. B 109 (2005) 7883.

O 86.2 Thu 16:45 WIL B122

Au/TiO$_2$(110) model catalysts on stoichiometric supports: Size dependence of the Au nanoparticles and activation energy in the CO oxidation reaction — •Menhild Eyrich, Joachim Bansmann, and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, 89069 Ulm, Germany

Since the late 1980s numerous studies on Au nanoparticles on metal oxide supports were carried out. Due to the low conductivity of fully oxidized TiO$_2$(110) supports which hinders many surface science based methods such as STM, most investigations were carried out on reduced TiO$_2$(110) supports. The catalytic activity of planar Au/TiO$_2$(110) model catalysts depends, in analogy to the respective powder catalysts, strongly on the size of the Au nanoparticles and on the pretreatment of the catalyst or the catalyst support. Here, we report the experimental results from a study on fully oxidized planar Au/TiO$_2$ model catalysts with fully oxidized TiO$_2$(110) support materials performed at different Au coverages (i.e., different particle size) and different temperatures. The strong influence of the size of the Au nanoparticles on the catalytic activity was studied at different temperatures showing a less pronounced size dependence (but very high activity) at low temperatures (around room temperature). Then, the activation energy was determined for different particle sizes, in the size regime of the high catalytic activity (small Au nanoparticles) and for larger Au nanoparticles. The results will be compared to results for other (reduced) Au/TiO$_2$ model and for powder catalysts.

O 86.3 Thu 17:00 WIL B122

Role of Pt in SO_2 storage over ceria-based traps — Markus Happel[1], •Yaroslava Lykhach[1], Natalia Tsud[2], Tomáš Skála[3], Kevin C. Prince[3], Vladimír Matolín[2], and Jörg Libuda[1] — [1]Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, D-91058 Erlangen — [2]Department of Plasma and Surface Science, Charles University, CZ-18000 Prague 8 — [3]Sincrotrone Trieste, I-34012 Basovizza-Trieste

CeO_2 based materials are efficient SO_x traps that can be used in combination with three-way catalytic converters and NO_x storage and reduction catalysts. Pt significantly enhances the SO_x storage capability. However, the mechanism of this enhancement is not fully clear. In order to explore the role of Pt, we have studied the adsorption of SO_2 on single-crystal-based stoichiometric and reduced ceria films and on Pt/CeO_2(111) model catalysts. Reaction and decomposition of SO_2 were investigated by means of synchrotron radiation and resonant PES. We found that SO_3 is the major product of SO_2 reaction on the surfaces of both, stoichiometric and reduced ceria. On stoichiometric ceria, SO_3 decomposition occurs by desorption of SO_2. In contrast, we detect progressive decomposition of SO_3 to SO_x and S species on reduced ceria. This leads to partial reoxidation of ceria and formation of sulfides. On Pt/CeO_2, formation of SO_3 on the ceria surface is accompanied by partial decomposition of SO_2 to atomic sulfur on the Pt surface. Further decomposition of SO_3 proceeds via spillover of SO_x species to Pt followed by decomposition to atomic sulfur. Spillover of atomic sulfur from Pt to CeO_2 results in formation of cerium sulfides.

O 86.4 Thu 17:15 WIL B122

Size and Shape Changes of Pt Nanoparticles on α-Al_2O_3(0001) during CO Oxidation Reactions — •Uta Hejral[1], Richard van Rijn[2,3], Sander Roobol[2], Willem Onderwaater[2], Olivier Balmes[3], Helena Isern[3], Roberto Felici[3], Joost Frenken[2], and Andreas Stierle[1] — [1]University of Siegen, Walter-Flex-Str. 3, D-57072 Siegen, Germany — [2]Kamerlingh Onnes Laboratory, Leiden University, RA Leiden 2300, The Netherlands — [3]ESRF, Grenoble F-38043, France

Pt nanoparticles on aluminum oxide supports are widely used in heterogeneous catalysis and are applied successfully in reactions like the oxidation of hydrocarbons or CO. In order to achieve better catalyst efficiency, lifetime and selectivity it is important to understand catalytic processes on an atomic basis: the particle structure but also the interfacial region between particle and substrate is considered to be crucial for the catalytic properties.

To this end Pt nanoparticles were epitaxially grown on α-Al_2O_3(0001) substrates by means of physical vapour deposition at a substrate temperature of 500 °C. The particle size, shape and interfacial registry were studied in-situ during CO oxidation reactions (T=300 °C, p_{O2}=10 mbar, p_{CO}=10 mbar) by surface x-ray diffraction and x-ray reflectivity. The measurements were carried out at the ESRF ID03 beamline in a dedicated flow reactor supporting conditions from UHV to ambient pressures [1]. The x-ray investigations were completed by complementary atomic force microscopy studies.

[1] R. van Rijn, et al., *Rev. Sci. Instr.*, **81** (2010) 014101

O 86.5 Thu 17:30 WIL B122

Non-equilibrium surface pattern formation during catalytic reactions with nanoscale resolultion — •Jean-Sabin McEwen[1], Pierre Gaspard[1], Thierry Visart de Bocarmé[2], and Norbert Kruse[2] — [1]Center for Nonlinear Phenomena and Complex Systems, Université Libre de Bruxelles, Campus Plaine CP 231, 1050 Bruxelles, Belgium — [2]Chemical Physics of Materials, Université Libre de Bruxelles, Campus Plaine CP 243, 1050 Bruxelles, Belgium

Despite the large progress made in the recent years to provide a sound understanding of the oscillatory behavior of various catalytic surface reactions, there still are a number of questions apparently unsolved. One of these open questions concerns the gap between the choice of catalyst in surface science studies and those used in heterogeneous catalysis. Indeed, in surface science, oriented single crystals are mainly used while multi-facetted metal particles are present in catalysis. A field emitter tip on the other hand can be regarded as a good approximation of a nanometer-sized metal particle. Stunningly, a field emitter tip is also large enough to allow the emergence of regular oscillations from the molecular fluctuations. This is the case when a rhodium nanosized crystal is exposed to hydrogen and oxygen. Here, we show that the observed nonequilibrium oscillatory patterns find their origin in the different catalytic properties of all of the nanofacets that are simultaneously exposed at the tip's surface. These results suggest that the underlying surface anisotropy, rather than a standard reaction-diffusion mechanism, plays a major role in determining the self-organizational behavior of multifaceted nanostructured surfaces.

O 86.6 Thu 17:45 WIL B122

Molecular-level understanding of the water-gas-shift reaction on Rh(111) — •Matteo Maestri[1,3] and Karsten Reuter[2,3] — [1]Politecnico di Milano, Italy — [2]Technische Universität München, Germany — [3]Fritz-Haber-Institut der MPG, Berlin, Germany

The identification of the reaction mechanism is the center piece for the atomic-scale understanding of a catalytic process and requires the kinetic assessment of all potential steps at the surface. At this level, processes of technological interest involve a large number of potential reactions and, due to the huge computational costs, are still largely outside the capabilities of a full density-functional theory (DFT) analysis. To this end we propose a hierarchical approach for the identification of prevalent reaction mechanisms by efficiently combining DFT and semi-empirical methods [1]. The obtained computationally undemanding barrier estimates serve as initial approximate input for the identification of the prevalent paths that subsequently require refined kinetic parameters from explicit DFT calculations. As showcase we consider the water-gas-shift (WGS) and reverse reactions on Rh(111). Our results reveal that CO follows different chemical paths depending on the operating conditions. A carboxyl pathway is preferred for the consumption of CO, while its formation proceeds through the direct decomposition of carbon dioxide. These insights into the atomic-scale mechanism allow for a new understanding of the WGS system in full agreement with existing experimental evidence. [1] M.Maestri and K. Reuter, Angew. Chemie Int. Ed., 2010, in press.

O 86.7 Thu 18:00 WIL B122

Structure and stability of CH_3OH/Pt(111) under potential control — •Tanglaw Roman and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, D-89069 Ulm

The attention that has been given to fuel cell technology has increased interest in understanding the catalytic oxidation of methanol. Despite all the past efforts on this topic, the exact nature of this reaction is still a subject of debate. While theoretical descriptions of methanol electrooxidation have provided meaningful inputs into the discussions, studies up until now have been performed primarily for the solid/vacuum interface, i.e., no electrolyte and no external fields or excess charges were present. In light of the need to more realistically model the electrooxidation reaction, in this study we examine the structure and stability of methanol, as well as reaction intermediates in the oxidation process on Pt electrodes, for varying electrode potentials, but in the absence of water as a first step. In our model, a Gaussian-shaped counter electrode is used to complement the charged surface. Techniques in estimating the electrode potential corresponding to a certain charge of the counter electrode and steps to more realistically model the electrochemical solid-liquid interface are discussed.

O 86.8 Thu 18:15 WIL B122

The interaction of adsorbates on a roughened Cu(111) surface examined with HREELS and work function measurements — Heiner Maslosz, •Olaf Skibbe, and Annemarie Pucci

— Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, D-69120 Heidelberg

Rough an defect-rich surfaces play a key-role in heterogeneous catalysis as well as in surface enhancement effects (i.e. surface enhanced Raman scattering (SERS)). To contribute to a deeper understanding of the interactions at such surfaces, we performed vibrational spectroscopy (HREELS) and work function measurements of gases adsorbed on a Cu(111) surface which we roughened by evaporation of small amounts of copper at low temperatures. The examined gases are C_2H_4, O_2 and CO.

O 86.9 Thu 18:30 WIL B122

Investigation of the Ethylene Oxide Formation over Ag using $^{18}O_2$ — •Sebastian Böcklein, Manuel Joas, Christina Hettstedt, Sebastian Günther, and Joost Wintterlin — Ludwig-Maximilians-Universität, München, Germany

As part of an extensive surface science/catalysis project to investigate the reaction mechanism of the partial oxidation of ethylene to ethylene oxide (EtO) over Ag we have performed experiments in a model reactor. Experiments were performed with Ag-foils at pressures in the mbar range and by using $^{18}O_2$. The findings are in partial disagreement with the existing literature. The reaction probability to give EtO is extremely low, and proper product detection, and quantification are essential. In very careful experiments we have been able to unambiguously detect the product. By changing the reaction parameters we could also deactivate and reactivate the silver catalyst (by heating the catalyst up to 600°C in Ar) in a controlled way. There are strong hints of a bulk-dissolved oxygen species that desorbs during this procedure. Its role in the reaction was further investigated with $^{18}O_2$. Depending on whether $^{18}O_2$ was used in the high temperature/high pressure pretreatment with oxygen or in the reaction gas feed different isotope compositions were found in the EtO and in the total oxidation product (CO_2). The isotope used in the O_2 in the reaction feed is mainly found in the products but bulk-dissolved oxygen reacts too as well. The reaction is connected with transport processes of oxygen into and out of the Ag bulk. XPS investigations and sputter/heating experiments show large amounts of oxygen at the surface of the active Ag-foils.

O 86.10 Thu 18:45 WIL B122

Methane activation on palladium (-oxide) — •Anders Hellman[1], Adriana Trinchero[1], Henrik Grönbeck[1], Johan Gustafson[2], Edvin Lundgren[2], and Jesper Andersen[2] — [1]Applied Physics and Competence Centre of Catalysis, Chalmers University of technology, Göteborg, Sweden — [2]Division of synchrotron radiation research, Lund University, Sweden

The transition state and the activation energy of methane dissociation on several palladium and palladium oxide facets together with known surface oxides phase is investigated by density-functional theory calculations. Depending on the phase of the palladium there is a correlation between the activation energy and the final energy of the CH3+H product. The metal phase of palladium has a low activation energy, with a steep correlation to the final state. The palladium oxide and surface oxide have higher activation energies and a more moderate dependence on the final state. If the palladium oxide and surface oxide is reduced, i.e., a removal of an oxygen atom at the active site, another correlation appears that lie in between the metal and oxide phase.

Given the high activation energy of the two most stable palladium oxides, i.e., PdO(100) and PdO(101), the general belief that palladium oxide is a particularly active methane oxidation catalyst is challenged. Instead, our first-principles results suggest that the high activity of palladium can be explained by the appearances of high surface energy facets of the palladium oxide and/or as the occurrences of reduced palladium oxides as the temperature varies under the experiment.

O 86.11 Thu 19:00 WIL B122

Multi-lattice approach to first-principles kinetic Monte Carlo simulations: Application to catalytic CO oxidation at Pd(100) — •Max J. Hoffmann[1,2], Matthias Scheffler[1], and Karsten Reuter[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Technische Universität München

First-principles kinetic Monte Carlo (1p-kMC) simulations enable a quantitative microkinetic modeling of heterogeneous chemical reactions while accounting for the full spatial distributions at the surface. Application to reaction-induced surface morphological transitions is hitherto prevented by the inability to describe the system within prevalent fixed-lattice 1p-kMC and the excessive cost of off-lattice 1p-kMC variants.

To this end we develop a novel multi-lattice 1p-kMC approach and apply it as a case in point to the CO oxidation at Pd(100). In the catalytically active state this system is suspected to undergo transitions from the pristine metal surface to a PdO surface-oxide film. As a first step towards a comprehensive simulation we focus on the initial oxide destruction step induced by clustering of oxygen vacancies. First simulations confirm the stability of the oxide film at stoichiometric feed as predicted by preceding fixed-lattice 1p-kMC simulations [1]. [1] J. Rogal, K. Reuter, and M. Scheffler, Phys. Rev. Lett. **98**, 046101 (2007).

O 86.12 Thu 19:15 WIL B122

Pressure gap and electrode artefacts in the electrochemically induced oxygen spillover on Pt/YSZ electrodes — •Arafat Toghan[1], Liz Rösken[1], Michael Hävecker[2], Axel Knop-Gericke[2], and Ronald Imbihl[1] — [1]Institut für Physikalische Chemie und Elektrochemie, Leibniz-Universität Hannover, Callinstr. 3 - 3a, D-30167 Hannover, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

Mechanistically, the electrochemical promotion of catalytic reactions (EPOC) on Pt/YSZ (yttrium stabilized zirconia) catalysts has been shown to be due to the spillover of oxygen from the solid electrolyte onto the Pt surface. This spillover has been studied on Pt/YSZ catalysts with photoemission electron microscope (PEEM) and with a differentially pumped x-ray photoelectron spectrometer (XPS) allowing to conduct in situ studies up to 1 mbar. PEEM revealed that upon electrochemical pumping not only the expected darkening of the Pt electrodes can be observed which is due to spillover oxygen but that also bright spots develop. These bright spots were attributed to metallic zirconium formed as electrically disconnected parts of the Pt electrode assume a negative potential thus causing a local reduction of zirconia. With XPS the main goal was to study whether a second special spillove species develops upon electrochemical pumping at high pressure which is different from chemisorbed oxygen. This special spillover species has been postulated by Vayenas et al. and was supposedly responsible for the non-Faradaic nature of EPOC. Up to now even at p= 0.2 mbar only chemisorbed oxygen was detected.

O 87: Focussed session: Theory and computation of electronic structure: new frontiers VII (jointly with HL, DS)

Time: Thursday 17:15–19:15 Location: TRE Phy

Topical Talk O 87.1 Thu 17:15 TRE Phy

Continuum mechanics for quantum many-body systems: the anti-adiabatic approximation — •Giovanni Vignale[1], Xianlong Gao[2], Jianmin Tao[3], Stefano Pittalis[1], and Ilya Tokatly[4] — [1]Department of Physics, University of Missouri, Columbia, MO 65211, USA — [2]Department of Physics, Zhejiang Normal University, Jinhua, Zhejiang Province, 321004, China — [3]Department of Chemistry, Rice University, 6100 Main Street Houston, TX 77005, USA — [4]ETSF Scientific Development Centre, Dpto. Fisica de Materiales, Universidad del Pais Vasco, Centro de Fisica de Materiales CSIC-UPV/EHU-MPC, Av. Tolosa 72, E-20018 San Sebastian, Spain

Classical continuum mechanics is a theory of the dynamics of classical liquids and solids in which the state of the body is described by a small set of collective fields, such as the displacement field in elasticity theory; density, velocity, and temperature in hydrodynamics. A similar description is possible for quantum many-body systems. In this talk I show how the exact Heisenberg equation of motion for the current density of a many-body system can be closed by expressing the quantum stress tensor as a functional of the current density. I then introduce an "anti-adiabatic" approximation scheme for this functional. The anti-adiabatic scheme allows us to bypass the solution of the time-dependent Schroedinger equation, resulting in an equation of motion for the displacement field that requires only ground-state properties as an input. I illustrate the formalism by applying it to the calculation of excitation energies in a few model systems.

O 87.2 Thu 17:45 TRE Phy

Discontinuities of the Exchange-Correlation Kernel and Charge-Transfer Excitations in TDDFT

— •Maria Hellgren and Eberhard K.U. Gross — Max-Planck-Institute of Microstructure Physics, Weinberg 2, Halle, Germany

An intriguing consequence for density functional theory (DFT) arises when considering ensembles with densities integrating to fractional particle number. The total ground-state energy as a function of particle number consists of straight-line segments and, consequently, the corresponding exchange-correlation (XC) potential jumps discontinuously. This feature of the exact theory turns out to be a key property to incorporate in approximate functionals in order to obtain, e.g, accurate band-gaps of solids and correct molecular dissociation limits.

It has been demonstrated that the discontinuous nature of the static XC potential naturally carries over to the XC potential of time-dependent density functional theory (TDDFT) appearing in, e.g., time-resolved ionization processes. How the same property is reflected in the XC kernel, defined as the functional derivative of the XC potential with respect to the density, has, so far, not received any attention. The XC kernel is of fundamental importance in TDDFT as it gives access to the particle conserving excitation spectrum. In this work we have investigated the discontinuities of the XC kernel and found them to be crucial for the description of long-range charge-transfer excitations.

O 87.3 Thu 18:00 TRE Phy

Insights in the T-matrix formalism

— •Pina Romaniello[1,4], Friedhelm Bechstedt[2,4], and Lucia Reining[3,4] — [1]Université Paul Sabatier, Toulouse, France — [2]Friedrich-Schiller-Universitaet Jena, Jena, Germany — [3]École Polytechnique, Palaiseau, France — [4]European Theoretical Spectroscopy Facility

In many-body perturbation theory the self-energy $\Sigma = GW\Gamma$ plays a key role since it contains all the many body effects of the system. The exact self-energy is not known and approximations are needed. As first approximation one can neglect the vertex Γ and obtain the GW approximation. In some cases this is not sufficient, and one needs to go beyond this approximation. In this work we elucidate the concept of T-matrix [1] and its relation with Hedin's equations [2]. Starting from the exact definition of self-energy we illustrate several aspects of the T-matrix formalism: i) which approximations to the self-energy yield the T-matrix formulation, in comparison with those that, instead, yield GW and beyond; ii) the role of the particle-particle and electron-hole contributions to the T-matrix; iii) a screened version of the T-matrix; iv) an approximate vertex that produces the same self-energy as the screened T-matrix. Tests are done on the exactly solvable Hubbard molecule [3].

[1] L. P. Kadanoff and G. Baym, Quantum Statistical Mechanics, W. A. Benjamin, Inc. New York, (1962).

[2] L. Hedin, Phys. Rev. 139, A796 (1965).

[3] P. Romaniello, S. Guyot, and L. Reining, J. Chem. Phys. 131, 154111 (2009); P. Romaniello, F. Bechstedt, L. Reining, in preparation.

O 87.4 Thu 18:15 TRE Phy

Stochastic current DFT for periodic systems

— •Heiko Appel — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

Recently we have introduced stochastic current density functional theory (SCDFT) which is an approach that allows to describe decoherence and dissipation from first principles [1,2]. So far the method has been applied to finite systems only. In this talk I will present an extension of SCDFT to periodic systems. In particular I will discuss a scheme for the stochastic real-time propagation of the Kohn-Sham orbitals in extended systems and also address possible choices for the bath operators that appear in the SCDFT formalism. (Work supported in part by Lockheed Martin, DOE and MPG).

[1] Massimiliano Di Ventra and Roberto D'Agosta, Phys. Rev. Lett. 98, 226403 (2007).

[2] Heiko Appel and Massimiliano Di Ventra, Phys. Rev. B 80, 212303 (2009).

O 87.5 Thu 18:30 TRE Phy

Wave function based treatment of electronic correlation in solids

— •Andreas Grüneis[1], George H. Booth[2], James Spencer[3], Martijn Marsman[1], Ali Alavi[2], and Georg Kresse[1] — [1]University of Vienna, Faculty of Physics and Center for Computational Materials Science, Sensengasse 8/12, A-1090 Vienna, Austria — [2]University of Cambridge, Chemistry Department, Lensfield Road, Cambridge CB2 1EQ, U.K. — [3]Department of Physics and Thomas Young Centre, Imperial College London, Exhibition Road, London SW7 2AZ, U.K.

The use of wave function based methods to treat electronic correlation, such as Møller-Plesset perturbation theory, coupled-cluster theory, and full configuration interaction (CI) is common practice in the field of computational quantum chemistry. Due to the computational cost involved, however, these methods have rarely been applied to extended systems. We have implemented the second-order Møller-Plesset perturbation theory and coupled-cluster singles and doubles (CCSD) theory within the framework of the Projector-Augmented-Wave method, using periodic boundary conditions and a plane wave basis set in VASP.[1] Moreover, an interface between VASP and the full CI quantum Monte Carlo (FCIQMC) code presented in Ref.[2] has been developed. We have tested our implementations on small molecules and solids. We outline techniques that reduce the computational effort of CCSD and FCIQMC calculations, such as the use of natural orbitals and progressive downsampling. [1] A. Grüneis et al. JCP 133, 074107 (2010). [2] G. H. Booth et al. JCP 131, 054106 (2009).

O 87.6 Thu 18:45 TRE Phy

Finite temperature reduced density matrix functional theory (FT-RDMFT) A novel approach to the description of quantum systems in thermal equilibrium.

— •Tim Baldsiefen and E.K.U. Gross — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Despite the big success of DFT for the description of groundstate properties of quantum mechanical systems, the finite temperature extension FT-DFT showed only little success in a restricted field of research. We develop the theoretical foundation for an alternative description of equilibrium properties, by employing the one-reduced density matrix (1RDM) rather than the density as central variable. The zero-temperature version of this theory proved to be quite successful in the last years, allowing for the description of groundstate properties of a wide class of systems (e.g. small molecules [1] and solids [2]). This sparks the hope, that a description of finite temperature ensembles by means of the 1RDM will succeed on fields of research formerly inaccessible by FT-DFT.

In this framework of FT-RDMFT we are able to employ methods from many body perturbation theory to develop approximate free-energy functionals. An application to the groundstate of the electron gas shows, that FT-RDMFT is able to significantly improve the groundstate energy compared to a strictly perturbative treatment.

[1] N. N. Lathiotakis et al., Phys. Rev. A, 79, 040501 (2009)

[2] S. Sharma et al., Phys. Rev. B 78, 201103(R) (2008)

O 87.7 Thu 19:00 TRE Phy

Spin spirals in the uniform electron gas: Towards a new functional in SDFT

— •F. G. Eich[1,2] and E. K. U. Gross[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]Freie Universität Berlin, Berlin, Germany

Based on our studies of the spin-spiral state of the uniform electron gas [1], we present a novel exchange-correlation functional for Spin-Density-Functional Theory (SDFT).

Much like in the well known local-density approximation (LDA) the local exchange-correlation energy is approximated by the exchange-correlation energy of the uniform electron gas. In contrast to the standard LDA the state of the electron gas is not only specified by its density but furthermore by its spin magnetization and spin-spiral wave vector. We show that, in order to determine a local spin-spiral wave vector, gradients of the spin magnetization have to be included in the functional.

As a first step towards application for real materials we obtain the energy of the spin-spiral electron gas using the random-phase approximation.

[1] F.G. Eich, S. Kurth, C. R. Proetto, S. Sharma, and E. K. U. Gross, Phys. Rev. B 81, 024430 (2010)

O 88: Metal substrates: Adsorption of organic / bio molecules IX

Time: Thursday 17:15–19:30 Location: PHY C213

O 88.1 Thu 17:15 PHY C213

2D Nanoporous networks based on simultaneous expression of H-Bonds and Metal-Coordination — •Sushobhan Joshi[1], Saranyan Vijayaraghavan[1], David Ecija[1], Willi Auwärter[1], Knud Seufert[1], Claudia Aurisicchio[2], Davide Bonifazi[2], and Johannes V. Barth[1] — [1]Physik Department, E20 Technische Universität München,D-85748 Garching, Germany — [2]Department of chemistry, University of Namur,Namur B-500,Belgium

The control and understanding of self assembly protocols is a prerequisite to realize tailored stable molecular networks with novel functional properties. In particular, well defined metal surfaces have been employed as platforms to build highly regular 2D coordination networks, including porous patters suitable for hosting guest species. Here we present an STM study of supramolecular architechtures based on a de novo synthesised three fold symmetric molecule with 3 identical functional terminal pyridyl groups. they re instrumental for the development of porous networks stabilized by N..H hydrogen bonds and pyridyl Cu coordinations on Ag(111) and Cu(111) in UHV conditions. On Ag(111) a close packed layer is seen and subsequent Cu deposition essays three different coordinaiton strucutres. Two of the structures are based on both N...H Hydrogen bonds and Cu coordination and one is exclusively stabilized by Cu coordination. A glassy porous network was seen on Cu(111) substrate where the network topology is based again on both H-bonding and the linear pyridyl-Cu-pyridyl motifs.

O 88.2 Thu 17:30 PHY C213

Multi-component alternating nanostructures of functional organic molecules with adjustable feature size — •Dingyong Zhong, Lifeng Chi, and Harald Fuchs — Physikalisches Institut and Center for Nanotechnology (CeNTech), Universität Münster, Wilhelm-Klemm-Straβe 10, 48149 Münster, Germany

Since the diffusion length of excitons in organic semiconducting materials is typically in the range of ten(s) nanometers, segregation of different functional organic molecules in such length scales is of importance to promote electron-hole separation and therefore increasing the energy conversion efficiency of organic photovoltaic devices. Here we report a bottom-up strategy for fabricating multi-component alternating organic nanostructures based on the pre-template effect of vicinal surfaces. Two and three dimensional multi-component alternating nanostructures up to four components have been fabricated and analyzed by scanning tunneling microscopy. The feature size of the nanostructures is tunable from about ten to several tens nanometers by adjusting the processing temperatures.

O 88.3 Thu 17:45 PHY C213

Self-Assembly of Melem on Ag(111) - emergence of porous structures based on amino-heptazine hydrogen bonds — •Johanna Eichhorn[1], Stefan Schlögl[1], Bettina V. Lotsch[1], Wolfgang M. Heckl[2], and Markus Lackinger[1] — [1]Ludwig-Maximilians-University and Center for Nanoscience (CeNS), Munich, Germany — [2]Deutsches Museum, Munich, Germany

Supramolecular self-assembly has been proven to be a powerful bottom-up technique for surface functionalization. In particular, two-dimensional nanoporous networks have attracted broad interest. Depending on the molecular building blocks, size and shape of cavities can be tuned. Many porous structures are stabilized by intermolecular hydrogen bonds between carboxylic acids. Yet, on more reactive substrates, carboxylic acids often bind strongly to the surface which hampers network formation. Therefore, we investigate less reactive building blocks for nanoporous networks on more reactive surfaces. In this respect amino groups in combination with heterocycles offer a promising alternative.

We studied self-assembly of melem, a triply amine functionalized heptazine ring, on Ag(111) by means of UHV-STM. Three different polymorphs were observed, where two structures exhibit pores with a diameter of ˜1.5 nm. Each of those pores is bordered by six melem molecules interconnected by hydrogen bonds between amino groups and nitrogen in the heptazine ring. One of the porous structure exhibits two molecules per unit cell with a dimer as basic structural motif, while the densely packed polymorph exhibits only one molecule per unit cell.

O 88.4 Thu 18:00 PHY C213

Hierarchical interactions - network formation of organic molecules on graphene/Ru(0001) — •Michael Roos[1], Daniela Künzel[2], Harry E. Hoster[1,3], Axel Gross[2], and R. Jürgen Behm[1] — [1]Ulm University, Institute of Surface Chemistry and Catalysis, 89069 Ulm, Germany — [2]Ulm University, Institute of Theoretical Chemistry, 89069 Ulm, Germany — [3]Current address: Technische Universität München, Centre for Electromobility, 50 Nanyang Drive, Singapore 637553

Bis(terpyridine)derivatives (BTP) form highly ordered hydrogen-bonded 2D networks on solid surfaces. The hydrogen bond configurations and therefore the resulting structures are steered via the positions of the nitrogen atoms within the BTP molecules. On smooth surfaces such as graphite or metal single crystals, the molecule-substrate interactions play a secondary role for the structure formation, mainly by determining the rotational orientations of the ordered networks. In this contribution, we demonstrate that more pronounced template effects arise for substrates where the molecule-substrate interaction varies laterally at the nanometer scale. As an example, we will show the ordering behavior of BTP molecules on graphene monolayers grown on Ru(0001). Submolecularly resolved STM images show that the BTP molecules are confined to the valleys of the graphene. We will compare the resulting supramolecular assemblies with the ordered 2D networks formed by the same molecules on smooth substrates, and will discuss the effect of the template quantitatively by means of force field calculations and supporting thermal desorption experiments.

O 88.5 Thu 18:15 PHY C213

Temperature Induced Phase Transition of Pentacene Sub-Monolayers on Cu(110)-(2×1)O — •Johannes Gall, Michael Hohage, Lidong Sun, Daniel Queteschiner, Günther Weidlinger, Mariella Denk, and Peter Zeppenfeld — Institute of Experimental Physics, Johannes Kepler University, Linz, Austria.

A reversible temperature induced phase transition of pentacene submonolayer films on the Cu(110)-(2×1)O reconstructed substrate was observed by means of Reflectance Difference Spectroscopy (RDS). It is interpreted as a transition from a 2D condensed phase (stable at low temperatures) to a molecular 2D gas phase at high temperatures.

In the present study, we have performed Monte Carlo (MC) and Kinetic Monte Carlo (KMC) simulations in the framework of a rectangular two dimensional lattice-gas model with nearest neighbor interactions to reproduce the phase transition behavior.

From adsorption isotherm experiments of pentacene on Cu(110)-(2×1)O, the 2D-sublimation energy of pentacene was found to be 87 meV. In contrast, from simulations, the sum of the lateral molecule-molecule interaction energies of pentacene was determined to be 101 meV.

However, from the RD spectra and Scanning Tunneling Microscopy (STM) images evidence was found that the gas phase actually consists of pentacene dimers. Therefore, the influence of these dimers on the phase transition is dicussed.

O 88.6 Thu 18:30 PHY C213

Growth and thermal evolution of ultrathin NTCDA films on Ag(111) studied by FT-IRAS and TPD — •Carolin R. Braatz, Gregor Öhl, and Peter Jakob — Philipps-Universität Marburg

The growth and thermal evolution of ultrathin films of 1,4,5,8-naphthalene-tetracarboxylic dianhydride (NTCDA) adsorbed on Ag(111) was investigated by Fourier-transform infrared absorption spectroscopy (FT-IRAS) and thermal desorption. The films were grown by organic molecular beam deposition in an UHV environment and analyzed in situ. Results will be presented for coverages from the sub-monolayer to the lower multilayer regime and in a wide temperature range (20 - 500 K). Depending on growth conditions and annealing temperatures a variety of different phases could be identified from their characteristic vibrational signatures, allowing us to track related phase transformations in detail. Thereby, a parallel oriented metastable phase is observed prior to (crystalline) multilayer formation.

O 88.7 Thu 18:45 PHY C213

Face-dependent chemisorption bondlengths for the formate

species on copper. — •Dagmar Kreikemeyer-Lorenzo[1], Matt Bradley[2], Werner Unterberger[1], David Duncan[2], Tsenolo Lerotholi[2], Jim Robinson[2], and Phil Woodruff[2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Warwick, England

Chemisorption bondlengths of molecules at metal surfaces have been shown in the past to be dependent on the bond order or coordination number according to a Pauling-like relationship, independent of the crystal face. However, we report here the results of measurements that show a rather strong face-dependence. Specifically, we have investigated the adsorption of the formate species (HCOO), a surface intermediate of the catalytic decomposition of formic acid (HCOOH) on Cu (110) and Cu (111) using the well-established technique of scanned-energy mode photoelectron diffraction (PhD). By using the same technique to study the same adsorbate on the two different faces, we eliminate possible sources of systematic error. Formate is found to adopt the same local bridging geometry (with the O atoms in off-atom sites) on both surfaces, but the associated Cu-O bondlengths are found to be 1.99 Å on Cu(111) and 1.90 Å on Cu (110). The difference must be attributed to more open structure of the Cu(110) surface, on which the surface Cu atoms have lower coordination to the underlying bulk and are surrounded by a lower valence charge density due to Smoluchowski smoothing. Preliminary DFT calculations reproduce the effect qualitatively, but predict a significantly smaller bondlength difference.

O 88.8 Thu 19:00 PHY C213

K-resolved Inverse Photoemission on ultrathin PTCDA/ Ag(110) films — •Dirk Hauschild[1], Markus Scholz[1], Peter Puschnig[2], Achim Schöll[1], and Friedrich Reinert[1,3] — [1]Universität Würzburg, Experimentelle Physik VII, D-97074 Würzburg, Germany — [2]University of Leoben, Chair of Atomistic Modelling and Design of Materials, A-8700 Leoben, Austria — [3]Karlsruhe Institut für Technologie (KIT), Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe, Germany

The occupied valence regime of metal-organic interfaces has been intensively studied by e.g. angular resolved UV-photoelectron spectroscopy allowing direct identification of molecule-metal hybrid states due to interfacial interaction [1]. However, the unoccupied valence levels are much more complicated to access experimentally limiting the knowledge about the contribution of these orbitals on the interface bonding. K-resolved Inverse Photoelectron Spectroscopy (KRIPES) is a technique to study the unoccupied density of states of inorganic materials. We present the first KRIPES-measurement on an organic monolayer adsorbed on a metal surface and discuss the applicability of KRIPES on orbital tomography established for PES. The single-domain monolayer system PTCDA/Ag(110) shows two non-dispersing states. Comparison of the experimental variation of the KRIPES-spectra intensity and DFT calculation of the free PTCDA molecule identifies the first state as the LUMO+1. The origin of the second state is not clear yet but shows influences of LUMO+1 and LUMO+2.

[1] J. Ziroff *et. al.*, Phys. Rev. Lett., **104**, 233004 (2010)

O 88.9 Thu 19:15 PHY C213

Impact of spontaneous structural imperfection on the energy level alignment — •Takuya Hosokai[1], Hiroyuki Machida[2], Alexander Gerlach[1], Satoshi Kera[2], Nobuo Ueno[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Germany — [2]Graduate School of Advanced Integration Science, Chiba university, Japan

We report that structural imperfection in an organic layer affects the electronic structure to result in a serious band-bending in the organic layer and change in the energy level alignment (ELA). Ultraviolet photoelectron spectroscopy (UPS) and metastable atom electron spectroscopy (MAES) were adopted to investigate the thickness dependence of the valence electronic structure and molecular orientation of polar phthalocyanine molecules (chlorogallium phthalocyanine) in thin films grown on graphite. We observed a large band-bending-like shift of occupied molecular orbital bands towards the Fermi level and the vacuum level increases continuously for the as-grown film, whereas these phenomena were considerably less pronounced after annealing the film. High-resolution UPS and MAES measurements showed that structural defects, i.e. Cl-up molecules in bilayer domain boundaries, are the origin of the change in the ELA. Our results indicate that controlling the spontaneous structural imperfection is a key for the desired energy level alignment of polar organic thin films on this substrate.

O 89: Methods: other (experimental)

Time: Thursday 17:15–18:15 Location: WIL B321

O 89.1 Thu 17:15 WIL B321

Surface science in hell: understanding plasma-surface processes in a fusion reactor — •Gregory De Temmerman — FOM Institute for Plasma Physics Rijnhuizen, Association EURATOM-FOM, Trilateral Euregio Cluster, P.O. Box 1207, 3430 BE Nieuwegein, The Netherlands

In a fusion reactor, power from the core plasma is exhausted by the surrounding plasma-facing materials which are bombarded by high fluxes of energetic neutral and charged energetic particles. Study of the plasma-surface interface is very challenging as surface analysis techniques are often impossible to apply in-situ. Understanding of the plasma-surface processes is only possible by supporting experiments in large devices by dedicated small-scale experiments mimicking some specific conditions. 2 specific illustrations of this approach will be detailed. The systematic study of the co-deposition of beryllium with tritium using NRA, TDS, SEM and XPS allowed derivation of scaling laws able to reconcile discrepancies between different research groups and to identify the role of beryllium hydride formation as an important process. A novel experimental setup has been developed at FOM to study the response of a plasma-immersed surface to intense heat loads expected during plasma instabilities. Fast spectroscopic and infrared measurements allow in-situ diagnosing while high-resolution microscopy is routinely used to investigate the induced surface changes. An unexpected outcome of the system is its ability, by tuning the experimental conditions, to produce nano-particles with very narrow size distribution, bridging the gap with fundamental surface science.

O 89.2 Thu 17:30 WIL B321

Microcalorimetry Based on Thermally Induced Deformations of Ultra-thin Single Crystals — •Christian Punckt[1], Pablo Sanchez Bodega[2], and Harm Hinrich Rotermund[2] — [1]Dept. of Chem. and Biolog. Engineering, Princeton University, Princeton, NJ 08544 — [2]Dept. of Physics and Atmospheric Science, Dalhousie University, Halifax, NS B3H 3J5, Canada

We show that ultra-thin metal foils can be used to measure the heat of adsorption of molecular species with a sensitivity of a few nJ by monitoring their thermally induced mechanical deformation. A platinum foil with a thickness of 300 nm and 4 mm diameter has a heat capacity of 10 μJ/K. As carbon monoxide (CO) adsorbes on its surface, about 30 μJ of adsorption heat per monolayer are released. Therefore even the adsorption of fractions of a monolayer increases the foil temperature sufficiently, such that thermo-elastic stress leads to buckling of the foil. In order to detect this deformation, we set up an imaging interferometer capable of measuring deflections of a few tens of nanometers. We observe that adsorption of CO and oxygen causes a significant mechanical response of the Pt foil. Additionally, we can detect heat release during the oxidation of CO on the platinum catalyst. Fronts and pulses of deformation are found which we relate to reaction patterns on the catalyst surface. Our work provides a proof-of-concept for the direct measurement of adsorption heat based on a simple chemo-thermo-mechanical mechanism that operates in a wide temperature and pressure range. The system can be calibrated using continuous or pulsed laser light.

O 89.3 Thu 17:45 WIL B321

Surface stress and MOKE-measurements down to 30K — •Jörg Premper, Dirk Sander, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle

A new combined stress and magneto-optical Kerr-effect (MOKE) experiment under UHV conditions has been developed. The temperature range of an optical 2-beam-stress measurement [1] and for MOKE experiments in the longitudinal and polar geometry in fields of up to 0.7 T has been extended down to 30 K. A liquid helium cooled cryostat is used which allows an accurate control of the sample temperature in the range 30 – 300 K. First results for surface stress and MOKE measurements were performed for H-adsorption and Co-growth on Pt(111), respectively. The low temperature of 30 K is applied to study for the first time the Xe-induced surface stress change on Pt(111), where a compressive stress of -2.5 $\frac{N}{m}$ is observed after exposure of 10 L Xe. The results are discussed in view of previous work and new insights into inert gas induced surface stress changes.

[1] D. Sander, Zh. Tian, J. Kirschner: JPCM **21** (2009) 134015

O 89.4 Thu 18:00 WIL B321

Nanojoule adsorption calorimetry (NAC) and its application to metal/organic interfaces — •Hans-Jörg Drescher, Ole Lytken, Fabian Bebensee, Hans-Peter Steinrück, and J. Michael Gottfried — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II

NAC is a technique for measuring adsorption energies on single-crystals surfaces and other well defined substrates in ultrahigh vacuum. Unlike desorption-based methods such as TPD, it can be used for nonreversible adsorbate systems, in which the adsorbate or substrate decomposes before desorption occurs. Examples include large organic molecules on metal surfaces or metals on organic or polymer surfaces. Similar to previous adsorption calorimeters [1-3], NAC relies on the direct measurement of adsorption-induced temperature changes of thin substrates using pyroelectric detectors. In combination with pulsed molecular beam techniques and highly accurate flux, sticking probability and reflectivity measurements, this ensures outstanding sensitivity in the nanojoule and picomole regimes. This contribution covers design considerations for achieving high accuracies and the challenges arising therefrom. Novel methodical solutions for various classes of interfaces, e.g., metals on semiconducting polymers or π-conjugated organic molecules on metals will be presented. Support by the Alexander von Humboldt Foundation, the DAAD and the Universitätsbund Erlangen-Nürnberg e.V. is gratefully acknowledged. [1] S. Černy, Surf. Sci. Rep. 26 (1996) 1. [2] W. A. Brown et al., Chem. Rev. 98 (1998) 797. [3] O. Lytken et al., Chem. Soc. Rev. 37 (2008) 2172.

O 90: Electronic structure III

Time: Thursday 17:15–19:30 Location: WIL C107

O 90.1 Thu 17:15 WIL C107

Implementation of PAW method in localized-basis-set SIESTA code — •Tristana Sondon and Chu Chun Fu — SRMP - CEA - Saclay, 91191 Gif-sur-yvette Cedex, France

The Projector Augmented Wave Method (PAW)has been demonstrated to be a particularly efficient and accurate approach to perform electronic structure calculations. The main advantage of this method is that it has a computational cost similar to that of a pseudo-potential calculation while retaining the key physics of all electron methods, including the correct nodal behavior of the valence electron wave functions. The SIESTA code is an efficient DFT code that uses a linear combination of pseudo-atomic orbitals (LCAO) as a basis set, and in the present form of the code, the calculations are made within the formalism of Norm-Conserving Pseudo-Potentials of the Troullier-Martins type in their fully non-local form. The PAW method is already implemented in many plane-wave codes, by modifiying the previous available Ultra-Soft pseudo-potential scheme, but in our case, more significant changes to the code are required. The inclusion of PAW is expected to achieve a combination of the high accuracy of the PAW method with a more efficient LCAO basis set. The specific characteristics and main approximations of this implementation will be reported. In order to highlight the performance of PAW, we will show detailed comparison of point defects properties in Fe and Fe-Cr alloys predicted by various pseudo-potential aproaches, with the ones calculated with the PAW method for different type of basis sets (plane-waves and LCAO).

O 90.2 Thu 17:30 WIL C107

Bulk States Confinement as a Long Range Sensor for Impurities and a Quantum Information Transfer Channel — •Pavel Ignatiev, Oleg Brovko, and Valeriy Stepanyuk — Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

We show that confinement of bulk electrons can be observed at low-dimensional surface structures and can serve as a long range sensor for the magnetism and electronic properties of single impurities or as a quantum information transfer channel with large coherence lengths. Our ab-initio calculations reveal oscillations of electron density in magnetic chains on metallic surfaces and help to unambiguously identify the electrons involved as bulk electrons. We furthermore discuss a possibility to utilize bulk states confinement to transfer quantum information, encoded in an atom's species or spin, across distances of several nanometers with high efficiency.

O 90.3 Thu 17:45 WIL C107

Work-Function Modification beyond Pinning: When Do Molecular Dipoles Count? — •Oliver T. Hofmann, David A. Egger, Gerold M. Rangger, and Egbert Zojer — Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

Control over the work function (Φ) of metals can be exerted by creating a sheet of dipoles above the surface, e.g., via depositing strong electron donors or acceptors onto the surface. For systems with strong charge-transfer character, one observes pinning of the Fermi level at the molecular level that donates or accepts electrons; i.e., Φ of the combined system is almost independent on the underlying metal and only governed by properties of the adsorbate. At the same time, molecules with intrinsic dipoles are also well known to also modify Φ. This raises the question how these effects interfere in systems inducing charge transfer and simultaneously bearing a dipole. Using density functional theory, we find [1] that intrinsic molecular dipole moments are compensated by adjustments in the amount of the charge transferred, as long as they are located spatially between the metal and the region of the pinning level of the organic molecule. In this case, the intrinsic dipoles are essentially inconsequential for the net work function. In contrast, dipole moments located outside the immediate metal/molecule junction region leave the charge-transfer unscathed. Clever design of the molecules, therefore, allows going beyond Fermi level*pinning. Along these lines, we suggest strategies for work-function changes of unprecedented magnitude. [1] Hofmann et al.,Nano Lett.,2010,10(11),pp4369

O 90.4 Thu 18:00 WIL C107

From Molecule to Monolayer: Self-Induced Quantum-Confined Stark effect in Monolayers of Polar Molecules — •Ferdinand Rissner[1], David A. Egger[1], Amir Natan[2], Thomas Körzdörfer[3], Stephan Kümmel[3], Leeor Kronik[2], and Egbert Zojer[1] — [1]Institute of Solid State Physics, TU Graz, Graz, Austria — [2]Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth, Israel — [3]Physikalisches Institut, Universität Bayreuth, Bayreuth, Germany

Using density functional theory calculations, the electronic structure of the polar molecule terpyrimidinethiol is investigated in gas phase and in a 2D-periodic self-assembled monolayer (SAM). We find that hybrid functionals give qualitatively different results compared to a (semi-)-local description and rationalize this finding in terms of an orbital-dependent self-interaction error.

Upon self-assembly, we observe orbital energy shifts depending on the spatial structure of the orbital, which can render the ordering of the states a function of the SAM packing density. Related to this, the energy gap is modified and the symmetry of the frontier orbitals can change. Occupied and unoccupied frontier orbitals localize on opposite sides of the monolayer as known from the quantum-confined Stark effect. All this is caused by the internal electric field originating from the molecular dipole moments.

O 90.5 Thu 18:15 WIL C107

Local Electronic Structure and Surface Potential of Atomic Chains on Si(111)5x2-Au — •Ingo Barke, Stefan Polei, Kristian Sell, Viola von Oeynhausen, and Karl-Heinz Meiwes-Broer — Universität Rostock , Institut für Physik, Universitätsplatz 3, D-18051 Rostock

Quasi one-dimensional surface reconstructions are formed by various metals adsorbed on flat or vicinal Si(111). On Si(111)5x2-Au the spatially resolved density of states is measured by scanning tunneling spectroscopy. Spectral features are assigned to particular structural elements based on a recently proposed model [1]. In this contribution two key elements are discussed: (1) the Si honeycomb chain channel (HCC) with locally graphitic structure which is found on many chain systems, and (2) Si adatoms with an average coverage of 0.25 atom per 5x2 unit cell leading to pronounced bright protrusions in STM images. While the latter result in local electron doping, the HCC give rise to a pronounced corrugation of the surface potential perpendicular to the chains. These variations manifest themselves in energy modulations of unoccupied, image-state derived electron states.

[1] S. C. Erwin, I. Barke, and F. J. Himpsel, Phys. Rev. B 80, 155409 (2009).

O 90.6 Thu 18:30 WIL C107

Modification of field emission resonances by Cu and Cu/Ag islands on Ag(100) — •Christopher Zaum and Karina Morgenstern — Institut für Festkörperphysik, Abteilung ATMOS, Gottfried Wilhelm Leibniz Universität, Appelstr. 2, D-30167 Hannover, Germany

We deposited Cu islands containing 10 to 500 atoms on a clean Ag(100) surface at room temperature and investigated their electronic structure by STS spectroscopy with a low temperature scanning tunneling microscope. Islands containing less than 50 atoms per islands are pure Cu islands, while islands at sizes above 80 atoms per island are Cu/Ag alloy islands. STS measurements reveal that these two island types have a different impact on the field emission resonances (FERs) of the Ag(100) surface. While the observed modifications for large islands are marginal, noticeable shifts of the FERs occur for small islands. These different results in STS spectroscopy are discussed with respect to the different work functions of pure and alloyed islands. Such STS measurements could therefore be used to determine the composition of surface alloys with high spatial resolution.

O 90.7 Thu 18:45 WIL C107

Influence of Shake-Up Behaviour at Titanium Nitride Interfaces using AR-XPS — •Dominik Jaeger[1], Jörg Patscheider[1], and László Forró[2] — [1]Empa Dübendorf. Switzerland — [2]EPFL, IPMC/SB, Switzerland

Nanocomposites that consist of nanometric titanium nitride grains surrounded by an amorphous silicon nitride tissue phase, exhibit extraordinary properties such as hardness and high oxidation resistance. They originate from the interplay of grain size, nature of the tissue phase and the interface strength. In the ample literature on those nanocomposites an experimental description of their interface is largely missing. This study presents investigations on the interfaces of TiN in contact with different overlayers. Two dimensional layer system is used to probe the interfaces. Different overlayers are deposited on oxygen-free TiN by Unbalanced Magnetron Sputtering. These interfaces are investigated by Angle Resolved X-ray Photoelectron Spectroscopy (AR-XPS). To prevent contaminations at the interfaces, the samples have been transferred in situ between deposition and analysis. XPS spectra show for TiN a shake-up feature caused by extra-atomic relaxation processes. During this process electrons from the inner Ti2p shell are loosing energy due to inelastic scattering at higher occupied shells. This energy loss has been recorded for interfaces between TiN and Si3N4, Si, and AlN as overlayers. The shake-up intensities and energies provide information on the electronic states in the surrounding neighbourhood and thereby on the interfaces. The results will be discussed in terms of polarisation effects at these interfaces.

O 90.8 Thu 19:00 WIL C107

The role of diffraction in (e,2e) experiments — •Frank O. Schumann, Zheng Wei, Rajendra Dhaka, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany

We have performed an electron pair emission study from a Cu(100) surface excited by a primary electron beam covering the energy range 19-100 eV. In the sum energy spectra of coincident pairs we are able to identify distributions from the *d* states and the *sp* states. We notice a strong dependence of the relative contribution of these two spectral ranges as a function of the primary energy. The curve describing this behavior resembles the LEED I-V curve of the (0,0) beam. Extending the kinematical picture for the emergence of intensity peaks in LEED to electron pairs predicts intensity maxima in fair agreement with the experimental findings. Further, we studied the pair intensity as a function of the azimuthal orientation of the sample. From simple symmetry considerations we expect a variation of the coincidence intensity. We find an asymmetry up to 20 % when we compare sum energy spectra obtained along two different main symmetry directions. We are able to make contact to selection rules obtained for a (e,2e) process and identify the valence states involved. These results are a critical test of the validity of approximations made in the theoretical description.

O 90.9 Thu 19:15 WIL C107

Double photoemission illuminates the Auger process — •Zheng Wei, Grant van Riessen, Rajendra S. Dhaka, Carsten Winkler, Frank O. Schumann, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany

We performed a double photoemission (DPE) experiment on a Cu(001) surface at the BESSY-II storage ring. The energy of the linearly polarized photons was tuned to 125 eV. We are able to map out the photoelectron and Auger electron simultaneously in large energy space of 30 eV×30 eV [1]. Electron pairs emitted directly from the valence band are known to share continuously the available energy due to the fact that this process proceeds in a single-step [2]. Usually the emergence of an Auger electron is explained via a two-step process in which the relaxation leading to the Auger emission is preceded by the emission of a photo-electron. Our observation of a continuous energy sharing in the DPE intensity involving core electrons can only be explained within a single-step process.

[1] G. van Riessen, Z. Wei, R. S. Dhaka, C. Winkler, F. O. Schumann and J. Kirschner, J. Phys.:Condens. Matter **22**, 092201 (2010).
[2] F. O. Schumann, C. Winkler, J. Kirschner, Physica Status Solidi B **246**, 1483 (2009).

O 91: Epitaxy and growth: Oxides and insulators

Time: Thursday 17:15–19:30 Location: WIL C307

O 91.1 Thu 17:15 WIL C307

DFT study of structure and magnetism of CoO(111) bilayers on Ir(100) — Florian Mittendorfer[1], •Josef Redinger[1], Raimund Podloucky[2], and Michael Weinert[3] — [1]Inst. of Applied Physics, Vienna University of Technology, Vienna, Austria — [2]Inst. of Physical Chemistry, University of Vienna, Vienna, Austria — [3]Dept. of Physics, University of Wisconsin-Milwaukee, Milwaukee, USA

Experimentally, a hexagonal CoO(111) bilayer is formed on square fcc Ir(100) leading to a c(10x2) superstructure (9 CoO/10 Ir) with large lateral displacements and vertical buckling (5 high, 4 low) of the Co atoms [1]. The 4 O atoms above the Co atoms show a (111) NaCl-type arrangement, while the remaining 5 O atoms are found about 1Å lower, almost coplanar with Co, resembling a hexagonal BN-like arrangement. We have performed DFT calculations for the proposed c(10x2) structure and found the structure to be energetically stable and in good agreement with experimental LEED data, provided proper care is taken for the rather complex magnetic arrangement. The 5 high Co atoms couple anti-ferromagnetically (AF), while ferromagnetic (F) coupling is stabilized by the Ir substrate for the 4 low Co atoms. Considering a CoO registry shift on the Ir(100) substrate a new structure with similar energy emerges, but now with 5 high and 4 low Co/O atoms, resembling 9x2 CoO/Pd(100) [2]. The 5 low Co atoms close to Ir favor once more F-coupling, while the remaining 4 high Co couple AF to the former, abandoning an alternating AF-coupling along the high Co rows. [1] C. Ebensperger et al., Phys Rev. B81, 235405 (2010). [2] L. Gragnaniello et al., Surf. Sci. 604, 2002 (2010).

O 91.2 Thu 17:30 WIL C307

STM, LEED, and XPS study of ultrathin $BaTiO_3$ films on Pt(100): switching film orientation by controlling substrate reconstruction — •Hannes Beyer, Klaus Meinel, Stefan Förster, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

Ultrathin $BaTiO_3$ films have been prepared on Pt(100) using either reactive rf magnetron sputtering or MBE. For both cases the deposition has been performed at room temperature. The magnetron operates in an Ar/O_2 gas mixture at 3.6×10^{-3} mbar, whereas MBE is performed in an O_2-atmosphere of 1×10^{-6} mbar by reactive co-deposition of Ti and BaO. Long-range ordered films are achieved by post-annealing in O_2 at 950 K using both methods. XPS reveals bulk-like stoichiometry of the $BaTiO_3$ films. With STM smooth films with unit cell islands are observed for film thickness of 4 ML.

By either preserving or quenching of the quasi-hexagonal surface reconstruction of Pt(100), it is possible to control the $BaTiO_3$ orientation. The films grow by MBE epitaxially either in (111) or (100) orientation, respectively. In contrast, the sputter deposition of $BaTiO_3$ films results in an initially amorphous surface. Upon annealing of the $BaTiO_3$ film a brilliant $BaTiO_3$(100)-(1×1) pattern is observed independent of the prior substrate reconstruction for thicknesses above 2 ML.

O 91.3 Thu 17:45 WIL C307

Termination of the hexagonal ice (0001)-surface by admolecule structures

— •Anja Michl and Michel Bockstedte — Lehrstuhl Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr 7B2, 91058 Erlangen

Ice grown on metal substrates exhibits a wide range of structures including clusters of varying shape, amorphous and crystalline islands owing to the flexibility of the water bond network and the nature of the water-metal interaction. Focusing on crystalline ice, recent experiments (e.g. [1,2]) have shown that ice (0001)-surface areas are terminated by water admolecule structures rather than by the bi-layer. In particular detailed high-resolution STM-experiments [2] of ice islands grown on Cu(111) analyzed the arrangement of admolecules on top of the bi-layer. Here we address the interaction of admolecules on this surface that eventually leads to the observed admolecule structures theoretically with an *ab initio* method. We find that admolecules coalesce into a nominal (2x1) superstructure forming mutal hydrogen bonds. Furthermore hexagonal rows of admolecules can interact with additional admolecules. The energetics of such structures much depend on the arrangement of dangling OH-groups and the bonding of the row edge to the underneath bi-layer. Undercoordinated edge molecules are found to evolve to the top of the row to enhance their own coordination.

[1] Ph. Parent *et al.*, J. Chem. Phys. **117**, 10842 (2002).

[2] M. Mehlhorn and K. Morgenstern, Phys. Rev. Lett. **99**, 246101 (2007).

O 91.4 Thu 18:00 WIL C307

Strain-induced formation of mixed-oxide films

— •Xiang Shao[1], Niklas Nilius[1], Hans-Joachim Freund[1], Livia Giordano[2], and Gianfranco Pacchioni[2] — [1]Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany — [2]Università di Milano-Bicocca, Via R. Cozzi 53, 20125 Milano, Italy

By means of scanning tunneling microscopy, Auger spectroscopy and density functional theory, we have identified a new mechanism for strain relaxation in ultrathin oxide films grown on metal supports. Due to the considerable lattice mismatch of 8%, only disordered CaO films form on a Mo(001) substrate at low growth temperatures. However, annealing the system above 1000 K induces a phase transition, which becomes manifest in the occurrence of a sharp (2x2) LEED pattern and the formation of an atomically flat oxide surface. In the course of the transition, Mo from the substrate diffuses into the film and replaces 25% of the Ca ions. The resulting rocksalt-type Ca0.75Mo0.25O structure has a negligible lattice mismatch with the Mo(001) and is in perfect registry with the support. Apart from the strain release, the oxidation of Mo atoms provides a strong thermodynamic incentive for the phase transition. A similar behavior is not observed for MgO films grown on Mo(001), where the original lattice mismatch is smaller.

O 91.5 Thu 18:15 WIL C307

LEEM/LEED investigation of Fe3O4 thin film growth on a Pt(111) substrate

— •Thomas Schmidt, Alessandro Sala, Helder Marchetto, Shamil Shaikhutdinov, and Hans-Joachim Freund — Fritz-Haber-Institut, Abt. CP, 14195 Berlin

Iron oxide, widely used as a catalyst and as a support for catalytically active systems, has been intensively studied with various techniques [1]. However, controversies in the literature regarding the surface termination and structural inhomogeneities hinder the direct linking of surface electronic and structural properties to chemical properties. Our aim is therefore a comprehensive and consistent characterization of the Fe3O4 film growth on a Pt(111) substrate by using the SMART instrument, specially designed to obtain chemical and structural information with high lateral resolution. In particular, deviating from the optimum preparation conditions [2], the oxide thin film reveals defects like a coexistence of two different stoichiometric phases (Fe3O4 and FeO), a Moiré-like patterned morphology with a mesoscopic periodicity and a predominance of one of two possible rotational domains. In addition, a subsequent annealing at 900K changes significantly the IV-LEED spectra and SPA-LEED profiles, which corresponds to different atomic termination of the magnetite surface. [1] W. Weiss and W. Ranke, Prog. Surf. Sci. 70 (2002) 1-151 [2] Z.-H. Qin, M. Lewandowski, Y.-N. Sun, S. Shaikhutdinov, and H.-J. Freund, J. Phys. Chem. C 112 (2008) 10209-10213

O 91.6 Thu 18:30 WIL C307

Phonon dispersion of ultrathin NiO(100) films on Ag(100)

— •Sebastian Polzin, Krassimir L. Kostov, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Institute of Physics, Halle (Saale), Germany

HREELS is employed to characterize the growth and to measure the phonon dispersion of ultrathin NiO films on an Ag(100) surface. The films have been grown by reactive deposition of Ni in an O_2 atmosphere. The evolution of the spectra observed for different NiO film thickness between 0.5 and 15 ML will be compared to the dielectric response of an oxide film on a metal substrate. For an 15 ML thick NiO(100) film the phonon dispersion along the Γ-X direction has been determined. The data will be compared to NiO(100) single crystal data measured with HREELS [1] and HAS [2]. Due to the improved resolution two additional phonons have been detected which are visible in the entire surface Brillouin zone. In contrast to earlier work the dispersion of the Lucas mode (S_4) and a transverse optical mode (S_2) could be measured from the center to the X point at the zone boundary.

[1] Oshima C., Modern Phys. Lett. 5, (1991)

[2] Toennies J. P., et al., J. Electr. Spectr. Rel. Phen. 64/65, (1993)

O 91.7 Thu 18:45 WIL C307

Epitaxial Polar Europium Oxide on Ir(111)

— •Stefan Schumacher, Daniel F. Förster, Carsten Busse, and Thomas Michely — II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, D-50937 Köln

EuO is a ferromagnetic semiconductor with a Curie temperature of 69 K and a band gap of about 1.2 eV. We have grown submonolayer films of EuO by means of reactive molecular beam epitaxy on Ir(111). The initial growth shows atomically flat islands of polar EuO(111) as can be seen from scanning tunneling microscopy (STM) and low energy electron diffraction (LEED). Both in STM images and LEED we see a rotational mismatch of the dense-packed rows of EuO(111) and Ir(111) of up to about 5°.

Using dI/dz spectroscopy and analyzing the Gundlach oscillations in scanning tunneling spectra we find a strong increase of the work function for the first polar bilayer EuO compared to bare iridium. The work function increase also gives rise to a strong reduction of the apparent height of the EuO islands in STM images. We interpret the work function increase to result from the additional surface dipole created by the polar EuO(111) surface.

O 91.8 Thu 19:00 WIL C307

Photo electron spectroscopy study of the stoichiometric composition of ultrathin $La_{0.67}Sr_{0.33}MnO_3$ films

— •Åsmund Monsen[1], Fei Song[1], Justin Wells[1], Jos Boschker[2], Zheshen Li[3], Roland Mathieu[4], Matthias Hudl[4], Per Nordblad[4], Thomas Tybell[2], and Erik Wahlström[1] — [1]Dept. of Physics, NTNU, Norway — [2]Dept. of Electronics and Telecommunications, NTNU, Norway — [3]Institute for Storage ring facilities Aarhus, Denmark — [4]Dept. of Engineering Sciences, Uppsala University, Sweden

Ferromagnetic manganites, such as $La_{0.67}Sr_{0.33}MnO_3$ (LSMO), have for a long time been prime candidates for spintronic devices. However, tunneling junctions have yet to display high resistive switching states at room temperature, and reports indicate reduced magnetic properties in ultrathin single films. These observations point towards altered layers at the interfaces.

In order to elucidate the physics of the interface regions we have studied structurally and magnetically well characterized LSMO, grown by pulsed laser deposition, thin films utilizing synchrotron based angle and energy dependent photo electron spectroscopy. We will present an analysis of depth dependent stoichiometry in films ranging from 20 nm down to a few unit cells in thickness. We will especially focus on any changes between surface, film and interface stoichiometry. Changes in valance band electron structure and the effect of the annealing based cleaning procedures will also be assessed.

O 91.9 Thu 19:15 WIL C307

Electronic structure of the c(10x2) cobalt oxide phase on Ir(100): STM and DFT — •C. Tröppner[1], P. Weinhardt[1], M. Reuschl[1], T. Schmitt[1], F. Mittendorfer[2], J. Redinger[2], R. Podloucky[3], M. Weinert[4], L. Hammer[1], and M.A. Schneider[1] — [1]Lst. f. Festkörperphysik, U Erlangen — [2]Inst. of Applied Physics, TU Wien — [3]Inst. of Physical Chemistry, U Wien — [4]Dept. of Physics, University of Wisconsin-Milwaukee, Milwaukee, USA

We studied the electronic properties of the c(10x2) cobalt oxide bilayer on Ir(100) by low-temperature STM and STS in ultra-high vacuum and by DFT. The oxide films representing a bilayer of CoO(111) were produced by oxidation of cobalt deposited onto Ir(100)(1×1) at elevated temperatures. The DFT calculations were performed using the VASP package employing standard PBE as well as PBE+U to assess the importance of on-site correlations. A symmetric repeated 5 layer Ir slab setup separated by ≥ 16Å vacuum with a bilayer CoO on each side was used. The STS signal was calculated in the Tersoff-Hamann approximation. DFT reveals that STM mainly images the oxygen atoms. As a consequence the subtle modulation caused by the local interaction between the cobalt oxide bilayer and the Ir surface becomes obvious in STM. We also performed STS dI/dV mapping of the CoO films and identified signatures, which can be attributed to oxygen and cobalt features by comparison to the theoretical data. However, STS dI/dV spectra of the c(10x2) but also of other thin cobalt oxide phases on Ir(100) show "zero-bias anomalies" tentatively assigned to the Kondo effect that is not captured by the present state of the calculations.

O 92: General Meeting of the Surface Science Division

Time: Thursday 19:30–20:00 Location: TRE Phy

Report of the Chairman of the DPG Surface Science Division.

O 93: Post Deadline Session

Time: Thursday 20:00–21:00 Location: TRE Phy

Some contributed talks.

O 94: Invited Talk (Ralph Gebauer)

Time: Friday 10:15–11:00 Location: TRE Phy

Invited Talk O 94.1 Fri 10:15 TRE Phy

Computational study of optical and structural properties of an organic dye sensitized solar cell — •Ralph Gebauer[1] and Filippo De Angelis[2] — [1]The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy — [2]Istituto CNR di Scienze e Tecnologie Molecolari (ISTM), c/o Dipartimento di Chimica, Università di Perugia, Italy

Dye sensitized solar cells are intensely studied as possible low-cost alternatives to traditional silicon based photovoltaic devices. For further progress in this technology, a detailed understanding of the dye/semiconductor heterointerface and of the interactions of the dye molecules with the surrounding electrolyte is crucial.

In this talk, we will present *ab initio* molecular dynamics simulations of a dye sensitized semiconductor surface immersed in an explicit water environment. This simulation is complemented by time-dependent density functional theory computations of the optical properties of the whole system (surface + dye + solvent). This technique allows us to gain unprecedented insight into the excited states and the dynamics of the solvated system at room temperature.

We are able to reproduce the experimentally observed asymmetry of the absorption spectrum and provide an estimate of the effect of thermal fluctuations on the driving force for electron injection. Finally, we are able to provide a detailed picture of possible dye desorption dynamics in such systems.

O 95: [MA] Surface magnetism V

Time: Friday 10:15–10:45 Location: HSZ 04

Invited Talk O 95.1 Fri 10:15 HSZ 04

Spin-dependent quantum interference within a single magnetic nanostructure — •Dirk Sander[1], Hirofumi Oka[1], Pavel Ignatiev[1], Sebastian Wedekind[1], Guillemin Rodary[1,2], Larissa Niebergall[1], Valeri Stepanyuk[1], and Jürgen Kirschner[1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]now at: LPNS, CNRS UPR20, Marcoussis, France

We present results of a combined experimental and theoretical study of spin-polarized electron confinement on individual nm small Co islands on Cu(111) [1]. Spin-polarized low-temperature STM in magnetic fields is used [2] to identify and prepare parallel (P) and antiparallel (AP) states of the magnetization orientation between a Co island and the magnetic tip of the STM. We find a pronounced spatial modulation of the differential conductance within one island, which is ascribed to electron confinement. The modulation patterns for P and AP magnetization states differ. Maps of the asymmetry of the differential conductance show strong spatial variations, where the contrast depends on the gap voltage. These results are ascribed to a spatial modulation of the spin-polarization within the Co islands. In conjunction with theory we conclude that the modulation of the spin-polarization, and its variation with energy, can be described by the relative magnitudes of the spin-resolved density of states, where the spatial modulation is mainly due to electron confinement of majority electrons. [1] H. Oka, P. Ignatiev, S. Wedekind, G. Rodary, L. Niebergall, V. Stepanyuk, D. Sander, J. Kirschner, Science 327, 843 (2010). [2] G. Rodary, S. Wedekind, H. Oka, D. Sander, J. Kirschner, Appl. Phys. Lett. 95, 152513 (2009).

O 96: Focussed session: Theory and computation of electronic structure: new frontiers VIII (jointly with HL, DS)

Time: Friday 11:15–12:45 Location: TRE Phy

Topical Talk O 96.1 Fri 11:15 TRE Phy

Tunable bandgaps and excitons in doped semiconducting carbon nanotubes made possible by acoustic plasmons — •Catalin Spataru and Francois Leonard — Sandia National Laboratories, Livermore, California, USA

Doping of semiconductors is essential in modern electronic and photonic devices. While doping is well understood in bulk semiconductors, the advent of carbon nanotubes and nanowires for nanoelectronic and nanophotonic applications raises some key questions about the role and impact of doping at low dimensionality. Here we show that for semiconducting carbon nanotubes, bandgaps and exciton binding energies can be dramatically reduced upon experimentally relevant doping, and can be tuned gradually over a broad range of energies in contrast to higher dimensional systems. The later feature, made possible by a novel mechanism involving acoustic plasmons, establishes new paradigms for the understanding and design of nanoelectronic and nanophotonic devices.

O 96.2 Fri 11:45 TRE Phy

Electronic Excitations in Single-Wall Carbon Nanotubes: Building-Block Approach — •Ralf Hambach[1,2], Christine Giorgetti[1,2], Xochitl Lopez-Lozano[3], and Lucia Reining[1,2] — [1]LSI, Ecole Polytechnique, CNRS, CEA/DSM, Palaiseau, France — [2]European Theoretical Spectroscopy Facility — [3]University of Texas at San Antonio, United States

Parameter-free calculations of electron energy-loss spectra for low-dimensional systems like single-wall carbon nanotubes can become numerically very demanding or even unfeasible for large diameters.

We overcome this problem by means of a building-block approach: Combining effective-medium theory and ab-initio calculations we can describe the collective excitations in nanostructures (like carbon nanotubes) starting from the microscopic polarisability of their building blocks (bulk graphite). To this end, Maxwell's equations are solved using the full frequency- and momentum-dependent microscopic dielectric function $\epsilon(\mathbf{q},\mathbf{q}',\omega)$ of the bulk material. The latter is calculated from first principles within the random phase approximation [1].

Besides an important gain in calculation time this method allows us to analyse the loss spectra of nanostructures in terms of their normal-mode excitations. We apply the building-block approach to study angular-resolved loss spectra for graphene and single-wall carbon nanotubes and find a very good agreement with full ab-initio calculations of these systems and corresponding experiments.

[1] AbInit: www.abinit.org, DP-code: www.dp-code.org

O 96.3 Fri 12:00 TRE Phy

Functionalized Tips Leading to Atomic-Resolution Force Microscopy — •Nikolaj Moll, Leo Gross, Fabian Mohn, Alessandro Curioni, and Gerhard Meyer — IBM Research – Zürich, Säumerstrasse 4, CH-8803 Rüschlikon, Switzerland

Performing atomic force microscopy (AFM) with a molecule or an atom at the tip the resolution can be dramatically enhanced as the resolution crucially depends on the chemical nature of the tip termination. A pentacene molecule is imaged with atomic resolution with a tip functionalized with a CO molecule. The interactions between the CO tip and the pentacene are studied with first principles calculations. The different energy contributions are analyzed, and the Pauli energy is computed. The source of the high resolution is Pauli repulsion, whereas van-der-Waals and electrostatic interactions only add a diffuse attractive background. To validate the usefulness of AFM with functionalized tips the natural product cephalandole A is studied.The measurements together with first principle calculations demonstrate that the direct imaging of an organic compound with AFM facilitates the accurate determination of its chemical structure. The method might be developed further towards molecular imaging with chemical sensitivity, and could solve certain classes of natural product structures.

[1] Leo Gross, Fabian Mohn, Nikolaj Moll, Peter Liljeroth, and Gerhard Meyer, Science 325, 1110-1114 (2009).

[2] Leo Gross, Fabian Mohn, Nikolaj Moll, Gerhard Meyer, Rainer Ebel, Wael M. Abdel-Mageed, and Marcel Jaspars, Nat. Chem. 2, 821-825 (2010).

O 96.4 Fri 12:15 TRE Phy

Impact ionization rates from ab initio calculations — •Marton Voros[1], Dario Rocca[2], Gergely Zimanyi[3], Giulia Galli[2,3], and Adam Gali[1,4] — [1]Budapest University of Technology and Economics, Department of Atomic Physics — [2]UC Davis, Department of Chemistry — [3]UC Davis, Department of Physics — [4]Hungarian Academy of Sciences, Research Institute of Solid State Physics and Optics

Achieving multi exciton generation (MEG) in semiconducting nanocrystals may lead to overcome the well-known Shockley-Queisser limit when building semiconductor-based solar cells. A thourough, theoretical understanding of the experiments that reported MEG in e.g. Si and PbSe nanocrystals, is still missing and could significantly contribute to clarify the several controversial results in the field. Several theoretical and numerical studies have addressed the origin of the MEG formation, mostly supporting an impact ionization mechanism. However, impact ionization rates have only been evaluated for model nanocrystals by using empirical pseudopotentials fitted to bulk properties or by applying tight binding wavefunctions, and model dielectric functions to describe the screened Coulomb interaction. We present a full ab-initio scheme based on Density Functional Theory in a plane-wave pseudopotential implementation that includes static screening within the random-phase approximation. As a first application, we will discuss how impact ionization rates are affected by the size of small Si nanocrystals.

O 96.5 Fri 12:30 TRE Phy

Selective Excitation of Molecular Vibrations by Tunneling Electrons — •Jessica Walkenhorst[1], Marius Wanko[1], Alberto Castro[2], and Angel Rubio[1] — [1]Nano-Bio Spectroscopy group and ETSF Scientific Development Centre, Dpto. Física de Materiales, Universidad del País Vasco, Centro de Física de Materiales CSIC-UPV/EHU-MPC and DIPC, San Sebastián, Spain — [2]Institute for Biocomputation and Physics of Complex Systems (BIFI), University of Zaragoza, Spain

Tunneling electrons can be used to excite vibrations in molecules. By combining scanning electron microscopy (STM) with inelastic electron tunneling spectroscopy (IETS) one can obtain vibrational spectra of single molecules adsorbed on a surface. Interestingly in large molecules the vibrational spectrum depends on the impact point of the electrons on the molecular surface. Selective excitation of vibrational modes by the STM tip has been proposed to explain these experimental findings (the so-called 'excitation of local vibrations' model). Therefore, we want to simulate the dynamical response of Schiff base (CNH4+) to tunneling electrons. To this end, we perform molecular dynamics simulations based on time-dependent density functional theory (TDDFT). Vibrational spectra are then obtained by Fourier analysis of the velocity autocorrelation function. This way, we study the relative strength of the excited molecular vibrations in dependence on the impact point of the tunneling electrons. Finally, a comparison between numerical results and experimental findings is attempted and the validity of the 'excitation of local vibrations' model is discussed.

O 97: Heterogeneous catalysis II

Time: Friday 11:15–13:00 Location: PHY C213

O 97.1 Fri 11:15 PHY C213

Methanol synthesis on ZnO(000$\bar{1}$): Free energy landscapes, reaction pathways, and mechanistic insights. — •Johannes Frenzel[1], Janos Kiss[1], Nisanth Nair[2], Bernd Meyer[3], and Dominik Marx[1] — [1]LS Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, Germany — [2]Dep. of Chemistry, IIT, Kanapur, India — [3]ICMM and CCC, Universität Erlangen-Nürnberg, Germany

The interplay of physical and chemical processes in the heterogeneous catalytic synthesis of methanol on the ZnO(000$\bar{1}$) surface with oxygen vacancies is expected to give rise to a complex free energy landscape. A manifold of intermediate species and reaction pathways has been proposed over the years for the reduction of CO on this catalyst at high temperature and pressure conditions as required in the industrial process. In the present study, the underlying complex reaction network from CO to methanol is generated in the first place by using ab initio metadynamics for computational heterogeneous catalysis. After having synthesized the previously discussed intermediates in addition to finding novel species, mechanistic insights into this network of surface chemical reactions are obtained based on exploring the global free energy landscape, which is refined by investigating individual reaction pathways. Furthermore, the impact of homolytic adsorption and desorption of hydrogen at the required reducing gas phase conditions are probed by studying such processes using different charge states of the F–center.

O 97.2 Fri 11:30 PHY C213

charge localization dynamics induced by oxygen vacancies on the TiO2(110) Surface — •matteo farnesi camellone[1], piotr m. kowalski[2], and dominik marx[1] — [1]lehrstuhl für theoretische chemie, ruhr universität bochum, 44780 bochum, germany — [2]helmholtz centre potsdam, telegrafenberg, 14473 potsdam, germany

The dynamics of an F center created by an oxygen vacancy on the TiO2(110) rutile surface has been investigated using ab initio molecular dynamics (1). These simulations uncover a truly complex, time-dependent behavior of fluctuating electron localization topologies in the vicinity of the oxygen vacancy. Although the two excess electrons are found to populate preferentially the second subsurface layer, they occasionally visit surface sites and also the third subsurface layer. This dynamical behavior of the excess charge explains hitherto conflicting interpretations of both theoretical findings and experimental data.

(1) Phys. Rev. Lett. 105, 146405 (2010)

O 97.3 Fri 11:45 PHY C213

Oxygen vacancies in different charge states at the MgO(100) surface — •Norina A. Richter, Sergey V. Levchenko, and Matthias Scheffler — Fritz-Haber-Institut, Berlin (Germany)

Point defects can dramatically change the chemical properties of oxide surfaces. However, the concentration of the defects at realistic conditions is difficult to determine experimentally. In this work, we calculate electronic structure and formation energies of neutral and charged oxygen vacancies in the bulk and at the MgO(100) surface [1], and estimate their concentration and distribution at realistic temperatures and pressures using the *ab initio* atomistic thermodynamics approach [2]. We determine the stability of different charge states of the oxygen vacancy as a function of the Fermi level position within the band gap (simulating the global effect of doping). We also analyze how the proximity of a dopant providing localized acceptor states changes the vacancy formation energies (local effect of doping). We use the Li substitutional defect as a prototype of such a dopant. The effects of electron exchange and correlation on our results, in particular the self-interaction error and the band-gap problem, are discussed, based on comparison of LDA with the HSE06 functional with different values of the exchange screening parameter.

O 97.4 Fri 12:00 PHY C213

Exploring Morphology-Activity Relationships: Ab Initio Thermodynamics Wulff Construction of RuO$_2$ — •Jelena Jelic[1,2] and Karsten Reuter[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Technische Universität München

Systematic studies on polycrystalline powders are an appealing link between detailed Surface Science work on single crystals and the supported nanoparticles in real catalysis. On the other hand, the catalytic activity of the powder is sensitively influenced by the preparation procedure, with structure-morphology-activity relationships still only scarcely understood and controlled. A prominent example in this respect are the recently reported, largely different induction times for the CO oxidation over RuO$_2$ powder [1,2]. Suspecting differing calcination temperatures behind these findings we use *ab initio* thermodynamics for a Wulff construction of RuO$_2$ crystallites in contact with an oxygen gas-phase. Depending on the calcination temperature we indeed obtain distinctly different equilibrium shapes. Correlating the exposed facets with the reported activity data points to a prominent role of the hitherto not much studied (101) and (111) facets. [1] V. Narkhede, J. Assmann, and M. Muhler, Z. Phys. Chem. 219, 979 (2005); [2] D. Rosenthal *et al.*, Z. Phys. Chem. 223, 183 (2009).

O 97.5 Fri 12:15 PHY C213

Analysis of Silica-Supported Molybdena by X-ray Absorption Spectroscopy: theoretical cluster studies — •Chunsheng Guo and Klaus Hermann — Fritz-Haber-Institut der MPG, Faradayweg 4-6, D-14195 Berlin and Sfb 546, (Germany)

We have performed density-functional theory (DFT) calculations on oxygen core excitations in different molybdena-silica model clusters in order to analyze structural details of the molybdena species. Differently binding oxygen, characteristic for specific molybdena species and coordination of the corresponding molybdenum centers, tetrahedral, pentahedral, and octahedral, can be clearly distinguished in the theoretical spectra. Further, the oxygen of the silica support is found to contribute to the NEXAFS spectrum in an energy range well above that of the molybdena units. The theoretical results can be compared with X-ray absorption fine structure (NEXAFS) measurements near the O K-edge of molybdena model catalysts supported by SBA-15 silica. The experimental NEXAFS spectra exhibit a symmetric double-peak structure in the O 1s to Mo4d/O2p excitation range at 529 - 536 eV. The comparison with the present theoretical data gives clear indications that molybdena species with tetrahedral dioxo MoO_4 units, singly or doubly connected with the silica substrate, dominate the experimental spectrum. This is different from results for MoO_3 bulk material where octahedral MoO_6 units exist and lead to a strongly asymmetric peak structure in the O K-edge NEXAFS spectrum, in agreement with the theoretical result.

O 97.6 Fri 12:30 PHY C213

Selective Catalytic Reduction of NO with NH_3 at V_2O_5(010) and Silica supported Vanadium Oxide: DFT Studies. — •Mathis Gruber and Klaus Hermann — Fritz-Haber-Institut der MPG, Faradayweg 4-6, D-14195 Berlin and Sfb 546, (Germany)

The Selective Catalytic Reduction (SCR) of NO_x with NH_3 over vanadium based metal-oxide (VO_x) catalysts has been proven to be one of the most effective NO_x reduction processes. Details of the reaction mechanism are still under debate. Adsorption, (de)hydrogenation, reactions with NO, and surface water formation at the VO_x catalyst contribute elementary steps. These processes are examined in theoretical studies employing density-functional theory together with gradient corrected functionals. The VO_x substrate is modeled by clusters cut out from the clean V_2O_5(010) surface where peripheral oxygen bonds are saturated by hydrogen. Reduced surfaces are represented by introducing oxygen vacancies. In addition, silica supported vanadium oxide clusters are considered. NH_3 is found to interact with the clean V_2O_5(010) surface only in the presence of OH groups (Brønsted acid sites) where it can form a rather stable surface NH_4^+ species. Further, NH_3 can adsorb at vanadium centers of lower coordination at the reduced surface (Lewis acid sites). This leads to two different SCR reaction scenarios transferring NH_3 and NO to N_2 and H_2O which are discussed by corresponding reaction paths and intermediates.

O 97.7 Fri 12:45 PHY C213

Theoretical Investigations on the Structure of Copper Catalysts at Zinc Oxide Surfaces — •Björn Hiller and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44801 Bochum, Deutschland

The Cu@ZnO system is an important catalyst, e.g. in methanol synthesis. From experiments it is known that the structure of the copper particles strongly depends on the gas phase composition. In addition there is some evidence for strong interactions between the copper particles and the oxide support. To understand this system it is crucial to investigate the structure of the involved copper surfaces in different gaseous environments and the structure of the interface between the copper particles and the zinc oxide support.

Using density-functional theory we determine the relative stabilities of a variety of possible oxygen and hydrogen adsorbate phases on copper surfaces to predict the shape of copper clusters under catalytic conditions. Moreover some results concerning the structure of the interface between copper and zinc oxide are presented.

O 98: Graphene VI

Time: Friday 11:15–13:15 Location: WIL A317

O 98.1 Fri 11:15 WIL A317

Tuning the Kohn Anomaly in the Phonon Dispersion of Graphene by Interaction with the Substrate — •Ludger Wirtz and Adrien Allard — Institute for Electronics, Microelectronics, and Nanotechnology (IEMN), CNRS, Lille, France

The phonon dispersion of graphene displays two strong Kohn Anomalies (kinks) in the highest optical branch (HOB) at the high-symmetry points G and K. The slope of the HOB around K is a measure of the electron-phonon coupling (EPC) and determines the dispersion of the Raman D and 2D lines as a function of the laser energy [1]. We show that the EPC can be strongly modified both due to interaction with the substrate [2] (in particular, if the substrate is metallic) and due to doping [3]. For graphene grown on a Ni(111) surface, a total suppression of the Kohn anomaly occurs: the HOB around K becomes completely flat. This is due to the strong hybridization of the graphene pi-bands with the Nickel d-bands which lifts the linear crossing of the pi-bands at K. For other metallic substrates, where the distance between the graphene sheet and the substrate is larger, hybridization is much less pronounced and the Kohn anomaly is only weakly perturbed. From experimental phonon dispersions one can therefore draw conclusions about the interaction strength between graphene and its different substrates .

[1] S. Piscanec, M. Lazzeri, F. Mauri, A.C. Ferrari, and J. Robertson, PRL 93, 185503 (2004). [2] C. Attaccalite, L. Wirtz, M. Lazzeri, F. Mauri, and A. Rubio, Nano Lett. 10, 1172 (2010). [3] A. Allard and L. Wirtz, Nano Lett. 10, 4335 (2010)

O 98.2 Fri 11:30 WIL A317

Electronic and magnetic properties of the graphene/Fe/Ni(111) system: A theoretical study — •Elena Voloshina[1], Martin Weser[2], Karsten Horn[2], and Yuriy Dedkov[2] — [1]Institut für Chemie und Biochemie, Freie Universität Berlin, 14195 Berlin, Germany — [2]Fritz-Haber Institut der Max-Planck Gesellschaft, 14195 Berlin, Germany

Layers of graphene on ferromagnetic (FM) surfaces may provide an ideal spin filtering effect in FM/graphene/FM sandwich-like structures [1]. Prior to being able to implement graphene/FM system in any kind of spintronic unit, its electronic, magnetic, and interfacial properties have to be investigated. Related DFT studies of the graphene/Fe/Ni(111) trilayer system have been performed. We observed noticeable modifications of the graphene and substrate band structures in the system. Intercalation of iron underneath of graphene layer changes drastically the magnetic response from the graphene layer that is explained by the formation of the highly spin-polarized $3d$ quantum-well state in thin iron layer. Obtained results are compared with experimental data.

[1] V. M. Karpan et al., Phys. Rev. Lett. **99**, 176602 (2007).

O 98.3 Fri 11:45 WIL A317

Accurate adsorption energies of graphene/Ni(111) — •Florian Mittendorfer — TU Vienna, Vienna, Austria

Due to the exceptional transport properties of graphene, graphene-based materials offer a promising route for spintronics. Yet even a prototypical system for a spin-filtering device, the interface between a ferromagnetic surface and a graphene sheet, cannot be described consistently on the basis of density functional theory (DFT) calculations. Even advanced functionals, such as the van der Waals density functional (vdW-DF), vastly overestimate the metal-graphene distance for graphene/Ni(111) [1], and hence fail to predict the experimentally observed opening of a band gap at the Dirac point.

In a recent publication, we could demonstrate that the description of adsorption energies can be significantly improved using a many-electron approach, the random phase approximation (RPA) [2]. In this contribution, we present RPA calculations for the adsorption of graphene on Ni(111). Using this approach, we could not only predict the correct adsorption site and electronic structure of the adsorbed graphene, but also determine the adsorption energy of the system accurately. The RPA calculations allow to evaluate the non-local (van der Waals) contributions and consequently to assess the quality of computationally cheaper approaches.

[1] M. Vanin, J. J. Mortensen, A. K. Kelkkanen, et al., Phys. Rev. B 81, 081408(R) (2010)

[2] L. Schimka, J. Harl, A. Stroppa, et al., Nature Materials 9, 741 (2010)

O 98.4 Fri 12:00 WIL A317

Graphene on lattice-mismatched metal surfaces: STM and ARPES studies — •Hendrik Vita[1], Alexander Generalov[1], Martin Weser[1], Yuriy S Dedkov[1], Karsten Horn[1], Muriel Sicot[2], Philipp Leicht[2], Andreas Zusan[2], and Mikhail Fonin[2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin — [2]Universität Konstanz, Department of Physics, Universitätsstraße 10, D-78464 Konstanz

Since metal contacts to graphene are mandatory for potential electronic device applications of graphene, an investigation of graphene/metal interfaces is important. Here we study the electronic structure of graphene in a strongly bonded situation on Rh(111) and compare it to weakly bonded graphene/Ir(111). Angle-resolved photoemission maps of graphene/Ir(111), along the Γ-M-K-Γ direction, exhibit all features attributed to almost free-standing graphene (a Dirac cone with a linear dispersion of the π-band, weak p-doping). The graphene/Rh(111) system, on the other hand demonstrates strong hybridization between graphene band and the Rh 4d valence bands. This leads to pronounced corrugation of the graphene layer as revealed by STM, and a disappearance of the specific electronic band features of graphene. The deposition of thin ferromagnetic metal films on graphene/Ir(111) is also discussed.

O 98.5 Fri 12:15 WIL A317

Edge state on graphene probed by scanning tunneling spectroscopy — •Dinesh Subramaniam[1], Christian Pauly[1], Viktor Geringer[1], Rafael Reiter[2], Marco Pratzer[1], Marcus Liebmann[1], Yan Li[4], Carsten Busse[3], Riccardo Mazzarello[4], Florian Libisch[2], Thomas Michely[3], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B, RWTH Aachen University and JARA-FIT, Germany — [2]Institut für theoretische Physik, Technische Universität Wien, Austria — [3]II. Physikalisches Institut, Universität zu Köln, Germany — [4]Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany

Epitaxial graphene islands are prepared by ethylene deposition on Ir(111) at room temperature and subsequent annealing to 1050°C. The lateral dimension of the islands varies from 5 nm to 40 nm always showing zigzag edges. Atomic resolution STM images show singly saturated zigzag edges which are predicted to feature a spinpolarized state. Scanning tunneling spectroscopy (STS) measurements at the graphene edge partly show a pronounced peak at the Fermi level. Reference STS measurements on the iridium surface reveal a similar peak with lower intensity at the Fermi level, which could be identified as an iridium surface state. This suggests that the increase in intensity at the edge of the graphene is due to a coupling of the edge state to the iridium surface state which enhanced strongly the intensity of the peak. Recent DFT band structure calculation support this assumption. Spin-polarized STS has been performed using a bulk chrome tip in order to analyze the magnetic character of the edge state.

O 98.6 Fri 12:30 WIL A317

Scanning tunneling spectroscopy of confined states within graphene nanoislands — •Christian Pauly[1], Dinesh Subramaniam[1], Viktor Geringer[1], Rafael Reiter[2], Marco

Pratzer[1], Marcus Liebmann[1], Carsten Busse[3], Florian Libisch[2], Thomas Michely[3], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B, RWTH Aachen University and JARA-FIT, Germany — [2]Institut für theoretische Physik, Technische Universität Wien, Austria — [3]II. Physikalisches Institut, Universität zu Köln, Germany

Epitaxial graphene islands are prepared by ethylene deposition on Ir(111) at room temperature and subsequent annealing to 1050°C. The lateral dimension of the islands varies from 5 nm to 40 nm. Using scanning tunneling spectroscopy we were able to visualize confined states within the islands. The state energies and corresponding local density of states patterns are in good agreement with third nearest neighbor tight-binding calculations for graphene. However, we had to include the potential of the moiré structure as well as a strongly absorbing character of the edge states. The width of the confined state energy peaks has been used to determine the lifetime of the Dirac electrons, which is inversely proportional to energy.

O 98.7 Fri 12:45 WIL A317

Scanning Tunneling Microscopy of Graphene on a Boron Nitride Substrate — •Régis Decker[1,2], Yang Wang[1], Victor Brar[1,2], William Regan[1], Hsin-Zon Tsai[1], Qiong Wu[1], Alex Zettl[1,2], and Michael Crommie[1,2] — [1]University of California, Berkeley, 366 Le Conte Hall, Berkeley CA 94720 — [2]Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley CA 94720

Graphene placed on a boron nitride (BN) substrate has been shown to result in increased mobility and improved Quantum Hall measurements. It is therefore of great interest to understand how BN substrates differently influence graphene compared to more standard Silicon oxide substrates. I will present new scanning tunneling microscopy measurements of graphene placed on a BN substrate. Differences in the local behavior of graphene on a BN substrate versus a Silicon oxide substrate will be discussed.

O 98.8 Fri 13:00 WIL A317

Adhesion of graphene on hexagonal boron nitride substrates: First-principles investigation within the random phase approximation — •Burkhard Sachs[1], Tim Wehling[1], Mikhail Katsnelson[2], and Alexander Lichtenstein[1] — [1]1. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany — [2]Institute for Molecules and Materials, Radboud University Nijmegen, NL-6525 AJ Nijmegen, The Netherlands

Hexagonal boron nitride (h-BN) substrates in graphene devices promise enhanced electron mobilities and low carrier inhomogeneities [1]. The stability of such compounds originates from weak adhesive long-range forces. By applying the random phase approximation (RPA) within the adiabatic connection fluctuation-dissipation theory (ACFDT), we investigate the adsorption of graphene sheets on h-BN substrates from first-principles. In detail, we obtain adhesion energies for different crystallographic stacking configurations and compare the results to experiments. Analyzing the elastic properties of graphene and h-BN, we discuss possible mechanisms leading to stacking disorder.

[1] C.R. Dean et al., Nature Nanotechnology 5, 722-726 (2010)

O 99: Electron and spin dynamics II

Time: Friday 11:15–13:00 Location: WIL B321

O 99.1 Fri 11:15 WIL B321

Image-potential states on graphene on Ir(111) — •Daniel Niesner and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen, Germany

Graphene, a single layer of graphitic carbon, can be produced with high quality on different metal substrates by decomposition of hydrocarbons. On the hexagonal Ir(111) surface the growth of graphene is self-limiting to a single layer with pronounced Moiré superstructure.[1]

Image-potential states, which are unoccupied electronic surface states close to the vacuum level, were investigated by time- and angle-resolved two-photon photoelectron spectroscopy. Besides the work function of the material, binding energies and lifetimes of the lowest three image-potential states were determined. The dispersion and intensity distribution of the first two states will be presented.

[1]A. T. N'Diaye et al., Phys. Rev. Lett. **97**, 215501 (2006)

O 99.2 Fri 11:30 WIL B321

Time-resolved 2PPE Study of Image-Potential States on Helium Adlayers on Cu(111)/Ru(001) — •Nico Armbrust[1], Jens Güdde[1], Ulrich Höfer[1], Sarah Kossler[2], and Peter Feulner[2] — [1]Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg — [2]Physik-Department E20, TU München, D-85748 Garching

Image-potential states on thin He films on metal surfaces have attracted interest since their first observation on liquid He in the mid-seventies due to the possibility of preparing a dense two-dimensional electron gas. Because of the difficulties in combining UHV and cryogenic technology with two-photon photoemission spectroscopy (2PPE) image-potential states on well-defined He adlayers on single crystal surfaces have not been investigated systematically up to now. Here we present first results of a time-resolved two-photon photoemission study of the image-potential states on He/Cu(111). We used a specially designed lHe cryostat which made it possible to prepare He adlayers up to a thickness of 2 monolayers. These were deposited on a Cu(111) film which has been grown epitaxially on a Ru(001) substrate. The He adlayers lead to a decoupling of the image-potential states from the metal surface resulting in a reduction of the binding energy of up to 310 meV for the $n = 1$ state and only of about 15 meV for the $n = 2$ state. This goes along with a huge increase of the lifetime from 30 fs up to 350 fs for the $n = 1$ state and from 105 fs to 360 fs for the $n = 2$ state.

O 99.3 Fri 11:45 WIL B321

Spatially and momentum resolved electronic transport trough metal films using the Boltzmann Transport Equation — •Mourad El Kharrazi[1], Orkhan Osmani[1,2], Bärbel Rethfeld[2], and Marika Schleberger[1] — [1]University of Duisburg-Essen, Germany — [2]Technical University of Kaiserslautern, Germany

After the electronic excitation of a thin metal film, by e.g. laser or highly charged ion impact, the electronic system of the metal possesses high kinetic energy. Transport processes dissipate this excitation energy into the material. The hot electrons equilibrate at the same time to a new equilibrium distribution. These mechanisms can be described via a spatially and momentum resolved Boltzmann Transport Equation. We present results on both the transport inducing a momentum-dependent nonequilibrium distribution as well as the collisional processes of hot electrons.

O 99.4 Fri 12:00 WIL B321

Electron dynamics in the Rashba spin-orbit split Bi/Cu(111) quantum-well system — •Andreas Ruffing[1], Sebastian Jakobs[1], Indranil Sarkar[1], Mirko Cinchetti[1], Stefan Mathias[1,2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]JILA, University of Colorado and NIST, Colorado 80309 0440, USA

Metallic quantum wells (QW) have been studied extensively in the recent past motivated by their potential to tune condensed matter properties via control of the quantum mechanical boundary conditions in these low-dimensional systems. Additional to the tuneability of QW systems, they show interesting features in the electronic structure, such as avoided crossings, band gaps, spin-orbit splitting and modifications due to interaction with the substrate. All these features influence the decay dynamics of excited carriers. We investigated the quantum-well system of one monolayer Bi/Cu(111), which shows a giant spin-orbit splitting of its unoccupied quantum-well bands [1]. We use time- and angle resolved two-photon photoemission to explore the femtosecond electron dynamics in this peculiar two-dimensional band structure. The band structure dependence of the hot-electron lifetimes is discussed by means of femtosecond lifetime maps $\tau(\mathrm{E}, k_{||})$ with specific attention to a spin hot-spot at the Γ-Point of the Bi/Cu(111) quantum-well structure.

[1] S.Mathias et al., Phys. Rev. Lett. 104, 066802 (2010)

O 99.5 Fri 12:15 WIL B321

Two-photon photoemission study of ultrathin NiO(100) films on Ag(001) — •Mario Kiel, Klaus Duncker, Stephan Grosser, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

The electron dynamics within ultrathin transition metal oxide NiO films grown on a Ag(001) substrate have been investigated using time-resolved two-photon photoemission (2PPE) in combination with scanning tunneling microscopy and spectroscopy (STM, STS).

For sub-monolayer NiO coverages upward shifts of the well-known Ag(001) image potential states are observed. These are explained by the increase of the electrostatic potential close to the surface due to the local work function difference between Ag(001) and NiO islands.

Using two-color 2PPE an unoccupied Ni 3d state at 3.73 eV above the Fermi energy is identified for the NiO monolayer. This Ni 3d state is also observed as prominent feature in STS spectra for defect-free NiO monolayer islands. Time-resolved data reveal a short lifetime of approx. 35 fs for this state. Additionally a second unoccupied Ni 3d-derived state at 2.4 eV is identified in 2PPE as well as in STS spectra.

O 99.6 Fri 12:30 WIL B321

Phonon-mediated adsorption and desorption of an image bound electron — •Rafael Leslie Heinisch, Franz Xaver Bronold, and Holger Fehske — Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, 17489 Greifswald, Deutschland

We study phonon-mediated physisorption, that is, temporary trapping and desorption, of an electron in polarization-induced external surface states (image states) of a dielectric surface [1,2]. Electron energy relaxation at the surface is enabled by surface vibrations whose energy scale is the Debye energy. Due to the large depth of the surface potential with respect to the Debye energy, multiphonon processes are important. Using a quantum kinetic rate equation for the occupancy of the image states, we calculate desorption times and prompt as well as kinetic sticking coefficients for an electron at a dielectric surface. We show that the classification of the potential depth and bound state level spacing in terms of Debye energies is paramount for a scenario of sticking and desorption and present results for graphite, MgO, CaO, Al_2O_3 and SiO_2.

[1] R. L. Heinisch et al., Phys. Rev. B 81, 155420 (2010)
[2] R. L. Heinisch et al., Phys. Rev. B 82, 125408 (2010)

O 99.7 Fri 12:45 WIL B321

Electron dynamics of atomic gold chains on vicinal Si(111) surfaces — •Kerstin Biedermann and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

Atomic wires of noble metals such as gold serve as a model system for the investigation of one-dimensional electron systems. Recent experiments on Si(557)-Au have provided initial information on the unoccupied part of the electronic band structure [1,2]. We extended our research to Si(111)-(5×2)-Au and Si(553)-Au and investigated the electron dynamics of these systems.

Time-resolved two-photon photoemission experiments were carried out using infrared (IR, $E_{IR} = 1.55$ eV) and ultraviolet (UV, $E_{UV} = 4.65$ eV) femtosecond laser pulses. In normal emission the beams were incident on the sample at a glancing angle of 10° and their electric field vectors could be aligned either perpendicular to (s-pol.) or parallel (p-pol.) to the plane of incidence in order to evaluate the parity of the electronic states.

For all three surfaces we find an even, short-lived ($\tau < 10$ fs) state at about $E = E_{Vac} - 0.6$ eV below the vacuum level, which we assign to the $n = 1$ image-potential resonance, and a long lived feature ($\tau > 600$ fs) within the bulk band gap of silicon. We present here an analysis of our time- and energy-resolved measurements and discuss the similarities and differences between the surfaces investigated.

[1] J. A. Lipton-Duffin et al., Phys. Rev. B **73**, 245418 (2006)
[2] T. K. Rügheimer et al., Phys. Rev. B **75**, 121401(R) (2007)

O 100: Organic electronics and photovoltaics

Time: Friday 11:15–12:30 Location: WIL B122

O 100.1 Fri 11:15 WIL B122

Spin-resolved photoemission study of the interface of transition metal phthalocyanines (CuPc, FePc, CoPc) on Co(100) — •Anna Altenhof, Felix Schmitt, Michael Vogel, Stefan Lach, and Christiane Ziegler — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany

Because of their unpaired electrons the three transition metal phthalocyanines (MePcs) CuPc, FePc and CoPc are promising candidates for the development of molecular spintronics devices based on organic-inorganic hybrid systems. For these future devices the injection of spin-polarized electrons is necessary. Therefore the interface between a ferromagnetic contact material and the organic layer plays a major role for the performance of the device.

In this study the electronic and magnetic properties of the interface between the ferromagnetic cobalt and the metal-organic molecules CuPc, FePc and CoPc were investigated by different means of ultraviolet photoelectron spectroscopy (UPS). Ultrathin MePc films were grown in situ on Co(100) under ultra high vacuum conditions. These were studied by spin-integrated and spin-resolved UPS. Linear dichroism with unpolarized light was used to examine the valence band structure. These studies show that all molecules interact with the cobalt substrate so that new states occur which are located at the interface. They also show that the interaction of FePc and CoPc with the Co substrate is similar to each other but differs from the interaction of CuPc with Co.

O 100.2 Fri 11:30 WIL B122

Smooth growth of organic semiconductor films on graphene for high efficiency electronics — •Gregor Hlawacek[1,2], Fawad S. Khokhar[1], Raoul van Gastel[1], Bene Poelsema[1], and Christian Teichert[2] — [1]Physics of Interfaces and Nanomaterials, MESA+ Institute for Nanotechnology, University of Twente, P.O. Box 217, NL-7500AE, Enschede, The Netherlands — [2]Institute for Physics, University of Leoben, Franz Josef Str. 18, A-8700 Leoben, Austria

High quality thin films of conjugated molecules with smooth interfaces are important to assist the advent of organic electronics. Here, we report on the layer-by-layer growth of the organic semiconductor molecule para-sexiphenyl on the transparent electrode material graphene. State of the art Low Energy Electron Microscopy, micro Low Energy Electron Diffraction and spot profile analysis techniques revealed the morphological and structural evolution of the thin film. Subtle difference in the molecular arrangement in comparison to graphite are confirmed by molecular dynamics simulations. Initial islands are found to have a meta stable structure that is characterized by flat lying molecules. With increasing coverage this structure changes into a herringbone arrangement similar to the $\{1\bar{1}\bar{1}\}$ bulk layer. The layer-by-layer growth of 6P on graphene proceeds by subsequent adding of $\{1\bar{1}\bar{1}\}$ layers.

O 100.3 Fri 11:45 WIL B122

Elucidation of Partial Charge Transfer from the Methoxy Groups of Substituted Pyrene as Donor in Complexes with Tetracyanoquinodimethane — •Katerina Medjanik[1], Sergej Nepijko[1], Hans-Joachim Elmers[1], Gerd Schönhense[1], Peter Nagel[2], Stefan Schuppler[2], Dennis Chercka[3], Martin Baumgarten[3], and Klaus Müllen[3] — [1]Ins. für Physik, Johannes Gutenberg-Universität,Mainz — [2]Karlsruhe Institute of Technology, ANKA — [3]Max-Planck Ins. for Polymer Research, Mainz

Novel charge transfer (CT) compounds can be synthesized on the basis of large polycyclic aromatic hydrocarbons [1]. Microcrystals of the CT-compounds tetra- and hexamethoxypyrene/tetracyanoquinodimethane (TMP_x/HMP_x-$TCNQ_y$) in different stoichiometries $x : y = 1 : 1$, $1 : 2$ and 2:1 were grown from solution via vapour diffusion. These crystallite fractions were studied by NEXAFS with particular emphasis on direct fingerprints of a charge transfer. Oxygen and nitrogen K-edge NEXAFS gives direct access to the unoccupied orbitals in the donor and acceptor, respectively. With increasing HMP content, a strongly rising O 1s pre-edge signal comes along with a substantial drop of N 1s resonance intensity. Charge is transferred from the π^*-orbital of the methoxy-group to the σ^*-orbitals b_{1g} and b_{2u} and - to a weaker extent

- to the π^*-orbitals b_{3g} and a_u of the cyano-group of TCNQ, particularly strong for the 2:1 compound. Funded by DFG/TR49, Graduate School of Excellence MAINZ, Centre of Complex Materials COMATT.

[1] K. Medjanik *et al.*, Phys. Chem. Chem. Phys. **12**, 7184 (2010)

O 100.4 Fri 12:00 WIL B122

Tuning the hole-injection barrier at the organic-metal interface with a strong organic acceptor — •Jens Niederhausen[1], Patrick Amsalem[1], Johannes Frisch[1], Andreas Wilke[1], Benjamin Bröker[1], Antje Vollmer[2], Ralph Rieger[3], Klaus Müllen[3], Jürgen P. Rabe[1], and Norbert Koch[1] — [1]Humboldt-Universität, Institut für Physik, Berlin, Germany — [2]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [3]Max Planck Institut für Polymerforschung, Mainz, Germany

Ultraviolet photoelectron spectroscopy was used to investigate how pre-adsorption of the strong electron acceptor hexaazatriphenylene-hexanitrile (HATCN) on Ag(111) affects the energy level alignment of two subsequent deposited conjugated organic materials (COM). The tuning of the sample work function (WF) by precovering Ag(111) with HATCN monolayers oriented either in a lying or in a standing fashion is found to induce important variations in the hole injection barrier (HIB) of the COM. An interface dipole of similar magnitude is observed upon adsorption of both COM overlayers on a lying HATCN monolayer with low WF. It is related to the push-back effect, which occurs at specific adsorption sites of the molecules at very low coverage. For COM adsorbed on Ag(111) precovered with a standing HATCN monolayer with high WF, Fermi level pinning is identified in both cases, and appears as a fundamental limit to further HIB lowering. The observed behavior is reminiscent of the adsorption characteristics of COM on high WF conducting polymers substrates. This leads to a situation where the HIB decreases by up to 1.1 eV.

O 100.5 Fri 12:15 WIL B122

Experimental and theoretical spin-resolved investigations of the electronic structure of open shell metal-phthalocyanines. — •Michael Vogel, Anna Altenhof, Felix Schmitt, Jens Sauther, Benedikt Baumann, Stefan Lach und Christiane Ziegler — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin- Schroedinger-Strasse 56, D-67663 Kaiserslautern Tel.: +49-631-205- 2855 Fax: +49-631-205-2854 E-mail: cz@physik.uni-kl.de

The valence band structure of different metal-phthalocyanines (MePcs) was investigated by comparison of gas-phase ultraviolet photoelectron spectra (UPS) and spin-resolved thin film UPS spectra with simulated spectra calculated using density functional theory (DFT). High resolution gas phase UPS spectra of cobalt phthalocyanine (CoPc) and iron phthalocyanine (FePc) show states which were unresolved in earlier studies. They were compared to Kohn-Sham eigenvalue spectra, derived from unrestricted DFT calculations. The composition of the molecular orbitals (MOs) just below the highest occupied molecular orbital (HOMO) was studied using UPS thin film spectra recorded at different excitation energies and thus different cross sections for s-, p-, and d-orbitals. Further the spin polarization of these MOs was derived from the DFT calculations and compared to thin film spin-resolved UPS spectra. The combination of these methods leads to a detailed image of the ground state electron system configuration with new insights into the behavior of the spin system.

O 101: Particles and clusters II

Time: Friday 11:15–13:00 Location: WIL C107

O 101.1 Fri 11:15 WIL C107

Orbital and spin magnetic moments of small, size-selected CoRh alloy clusters, deposited on Ni/Cu(100) — •Torben Beeck, Ivan Baev, Kai Chen, Michael Martins, and Wilfried Wurth — Institute of Experimental Physics, University of Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

Besides their high potential for applications in magnetic materials and chemical catalysis, transition metal clusters of few atoms are excellent candidates for comparison with complex theoretical calculations, including correlation effects which become very important on the nanoscale.

X-ray magnetic circular dichroism (XMCD) studies on small, size-selected Co_xRh_y transition metal clusters have been carried out at the Co $L_{2,3}$ absorption edges. Under UHV conditions the clusters were deposited in situ on a remanently magnetized Ni thin film evaporated upon a Cu(100) crystal. All the measurements were performed at the BESSY II, UE52 SGM beamline.

We will show the orbital and spin magnetic moments of the Co_xRh_y clusters which exhibit changes with cluster size and composition. A comparison to other transition metal alloy clusters will be given.

This work is supported by the DFG in the framework of the SFB 668 subproject A7

O 101.2 Fri 11:30 WIL C107

Surface enhanced Raman spectroscopy using tailored noble metal nanoparticles — •Robert Ossig, Frank Hubenthal, and Frank Träger — Institut für Physik and Center for Interdisciplinary Nanostructure Science and Technology – CINSaT, Universität Kassel, Kassel, Germany

Surface enhanced Raman spectroscopy (SERS) is a powerful technique in the field of molecular spectroscopy, which exploits the superior optical properties of metal nanoparticles. In principle SERS allows to detect and to measure spectra of single molecules. However, stable and reproducible SERS substrates, which are necessary for routine applications, are only rarely available. Furthermore, to achieve the optimum enhancement for certain excitation wavelength and molecule combinations, a tailoring of the optical properties is desired. To meet these requirements, our samples were produced by Volmer-Weber growth, in combination with laser tailoring. The combination of both methods allows a tuning of the surface plasmon resonance of the metal nanoparticles in the vicinity of the excitation wavelength for the SERS measurements, independently from the nanoparticle size. Hence, the influence of the wavelength on the SERS spectra can be studied. In this contribution we present SERS measurements of pyrene as a function of the excitation wavelengths. We will show that for all excitation wavelengths the SERS spectra are highly reproducible and strongly enhanced, if tailored nanoparticles serve as substrates. However, only for an excitation wavelength near the infrared, a background free Raman signal with an excellent signal-to-noise ratio is achieved.

O 101.3 Fri 11:45 WIL C107

Stabilization mechanism for cage-like $Si_{16}M^+$ clusters: From global structure optimization to understanding — •Dennis Palagin[1], Matthias Gramzow[2], and Karsten Reuter[1,2] — [1]Technische Universität München — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Doping with endohedral metal atoms appears as a remarkable avenue to tailor the intrinsic properties of silicon clusters, as well as to stabilize cage-like geometries as suitable building blocks for novel engineered materials. A prevalent concept to rationalize this stabilization is that injection of metal electrons into the Si electron gas leads to electronic shell closure. A prominent example is $Si_{16}V^+$, which with 68 valence electrons corresponds to a closed-shell configuration. Intriguingly, $Si_{16}Ti^+$ and $Si_{16}Cr^+$ with 67 and 69 electrons, respectively, are equally believed to stabilize in cage-like geometries [1]. Aiming to further clarify the stabilization mechanism we first use density-functional theory based basin-hopping to ascertain that the cage-like geometry indeed represents the ground-state structure for all three dopant atoms. From this basis we proceed to a detailed analysis of the obtained charge distributions to identify the nature of the bond and the stabilization mechanism in this dopant sequence. [1] J.T. Lau *et al.*, Phys. Rev. A **79**, 053201 (2009).

O 101.4 Fri 12:00 WIL C107

Using STM-Lithography to study interface properties: Footprints of Cu-clusters on single crystalline $ZnO(10\bar{1}0)$ — •Martin Kroll and Ulrich Köhler — Institut für Experimentalphysik IV / AG Oberflächen, Ruhr-Universität Bochum

As model systems in heterogeneous catalysis Cu clusters on single ZnO crystals grown under UHV conditions are used as a first step to understand complex reactions under real catalytical conditions. STM and STS were used to study the annealing behaviour of Cu clusters deposited by MBE on the nonpolar ZnO($10\bar{1}0$) surface. As already found for the polar ZnO(0001)-Zn surface [1], separated Cu clusters are formed at room temperature and a partial entrenching of Cu into the ZnO substrate at elevated temperatures of T > 670K was found. To investigate what happens at the Cu-ZnO interface in more detail Cu clusters were removed from the ZnO surface after different annealing steps using STM-tip induced diffusion. The remaining footprints of the Cu clusters on the undisturbed ZnO substrate were analysed with STM and STS. The results point to a pure thermally driven interaction of the Cu-clusters with ZnO at the borderline between the cluster and the free ZnO substrate surface.

[1] Kroll, M.; Köhler, U.; Surf. Sci. 601 (2007) 2182

O 101.5 Fri 12:15 WIL C107

Deformation of Ag Clusters Deposited on Au(111) - Experiment and Molecular Dynamics — •Natalie Miroslawski[1], Niklas Grönhagen[1], Bernd von Issendorff[2], Tommi Järvi[3], Michael Moseler[2,3,4], and Heinz Hövel[1] — [1]TU Dortmund, Experimentelle Physik I — [2]Universität Freiburg, Fakultät Physik — [3]Fraunhofer Institut für Werkstoffmechanik, Freiburg — [4]Freiburger Materialforschungszentrum

Mass selected clusters from Ag_{55}^{+} to $Ag_{147\pm2}^{+}$ were deposited with different deposition energies at 77 K on Au(111) and imaged with STM at 77 K. We observed a deformation of the cluster shape due to the strong metallic interaction between the cluster and the substrate. The clusters became epitaxial and developed a structure composed of several Ag monolayers. The number of these monolayers depends on the number of atoms in the cluster and the deposition energy. The larger the cluster mass the more monolayers the cluster develops on Au(111) and the larger the deposition energy the fewer monolayers occur. These results were verified by molecular dynamic simulations. Additionally the behaviour of Ag_N clusters on Au(111) after different annealing steps was investigated.

O 101.6 Fri 12:30 WIL C107

Adsorbate-induced smoothing of Re particles on the atomic scale — •Payam Kaghazchi and Timo Jacob — Universität Ulm, Albert-Einstein-Allee 47, D-89069 Ulm, Germany

Using density functional theory in combination with the *ab initio* atomistic thermodynamics approach we studied the equilibrium shape of Re particles in the presence of strongly interacting O and N adsorbates. At low and intermediate coverages, oxygen adsorption has minor influence on the equilibrium shape of the corresponding clean particles, i.e., truncated polyhedra, while nitrogen adsorption leads to stabilization of spherical-like polyhedra with a large contribution from atomically-rough ($13\bar{4}2$) faces[1]. At very high coverages of O and N, particles are perfect prisms consisting of the (0001) and ($10\bar{1}0$) faces. Since the close-packed surfaces are often less active in O and N-involved reactions than atomically-rough ones, these results offer a possible explanation for the experimentally-observed reduction in the activity of Re particles for ammonia synthesis and also predict a decrease in the activity of this system in oxidation reactions at high coverages. This study suggests that, besides the site-blocking effect, adsorbate-induced smoothing of particles on the atomic scale can reduce catalytic activity of transition metals[2]. [1] P. Kaghazchi and T. Jacob, Phys. Rev. B, **82**, 165448 (2010). [2] P. Kaghazchi and T. Jacob, in preparation.

O 101.7 Fri 12:45 WIL C107

Linear and nonlinear optical properties of supported metal clusters and adsorbed molecules — •Philipp Heister, Martin Thämer, Aras Kartouzian, and Ueli Heiz — Lehrstuhl für Physikalische Chemie, Technische Universität München

Metal clusters in the non-scalable size regime supported on oxide surfaces have unknown optical properties, which are essential for the understanding of photochemical properties of cluster-assembled materials and their use in optical applications. Cavity ring-down spectroscopy (CRDS) and surface second harmonic generation spectroscopy (S-SHGS) have been applied to samples of various metal clusters, in order to investigate their optical properties in the wavelength range from 215 to 700 nm. The performance of the employed experimental apparatus is characterized by measuring organic laser dye molecules adsorbed on surfaces as a model system.

We show that both these highly sensitive spectroscopic methods are applicable and are of complementary nature. CRDS for supported samples is limited to wavelengths above 400 nm. S-SHGS is readily extended into the far UV up to 215 nm but for the interpretation of the results the linear spectra obtained by CRDS are needed.

O 102: Epitaxy and growth: Metals and semiconductors II

Time: Friday 11:15–13:00 Location: WIL C307

O 102.1 Fri 11:15 WIL C307

Growth of Pb on Mo(110) studied by scanning tunneling microscopy. Comparison with the growth of Au, Ag and Sn on Mo(110) — •Aleksander Krupski — Institute of Experimental Physics, University of Wrocław, pl. Maxa Borna 9, 50-204 Wrocław, Poland

Scanning tunneling microscopy (STM) has been used for the first time to investigate the growth behaviour of ultra-thin Pb, Ag, Au and Sn films on the Mo(110) surface. The analysis of STM measurements indicates that for a coverage < 1 ML two-dimensional growth of the first Pb monolayer (wetting layer) took place. Above > 1 ML, the three-dimensional growth of the Pb islands with strongly preferred atomic scale *magic height* and flat top is observed. At coverages between 1 ML and 2 ML, only islands containing two atomic layers of Pb are observed. At coverages between 2 ML and 3 ML, islands containing two and four atomic layers of Pb are observed. At higher coverages above 3 ML, the island height distribution shows peaks at relative heights corresponding to N = (2, 4, 6, 7 and 9) of Pb atomic layers. In addition, closer view show coexistence of two well-ordered surface superstructures in the first lead layer. Results presented for growth of Pb will be compared with growth of Ag, Au, and Sn on Mo(110).

O 102.2 Fri 11:30 WIL C307

Stress induced by NiO monolayers on Ag (100) — •Anita Dhaka, Dirk Sander, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 061120 Halle (Germany)

We performed in-situ stress and medium energy electron diffraction (MEED) measurements simultaneously during the formation of NiO monolayers (ML) on Ag (100).We deposit Ni at 300 K in an O_2 partial pressure of 2×10^{-7} mbar [1]. Our stress measurement reveals a compressive stress change of -6.5 N/m after growth of 5 ML NiO.This stress measurement is ascribed to misfit stress, which is calculated as -6.3 N/m for 5 ML. From 5 to 10 ML almost constant stress is observed, and low energy electron diffractin (LEED) shows broadened spots, developing into a streaky diffraction pattern. We conclude that misfit distortions are formed, and pseudomorphic growth ends at 5 ML. MEED oscillations indicate layer-by-layer growth from 2 to 10 ML. The first ML NiO gives a (1×2) LEED pattern [2], and the stress change is +0.48 N/m. We ascribe this to an inhomogeneous surface coverage, which is composed of Ni, NiO and Ag areas, as suggested in STM work [2]. We conclude that combined stress and diffraction measurements identify different growth regimes and film stress in epitaxial oxide monolayers, quantitatively. Financial support by SFB 762 is gratefully acknowledged. [1] K.Marre and H.Neddermeyer, Suf. Sci. **287/288**, 995 (1993)

[2] Stephan Groβer, Christian Hagendorf, Henning Neddermeyer and Wolf Widdra, Surf. Interface Anal. **40**, 1741-1746 (2008)

O 102.3 Fri 11:45 WIL C307

DFT studies of small metal ad-atom clusters on fcc(111) surfaces — •Andreas Garhofer[1,2], Claudia Lenauer[2], Florian Wimmer[2], Philipp Scheiber[2], Michael Schmid[2], Peter Varga[2], and Josef Redinger[1,2] — [1]Computational Materials Science TU Wien, Vienna, Austria — [2]Institute for Applied Physics TU Wien, Vienna, Austria

Bonding of face-centered-cubic metals is usually characterized by a preference of a high coordination number for each atom. However by creating a large amount of Pt clusters with pulsed laser deposition on a Pt(111) surface, up to 1/3 of all clusters were found to be linear chains with lengths of up to 9 atoms. We studied different Pt ad-atom arrangements on Pt(111) with first principles DFT methods and found that for 3 and 4 ad-atom structures a linear chain is most stable. A three atom Pt chain is also more stable than a triangular configuration on other substrates such as fcc Rh(111), Pd(111), Ir(111), Au(111) and hcp Ru(0001), which all have similar lattice constants to Pt(111). For the homoepitaxial systems of these transition metals, only the 5d elements form stable linear ad-atom arrangements i.e. only Ir on Ir(111), Pt on Pt(111) and Au on Au(111). The main reason for the stabilization of the ad-atom chain is a strong d_{z^2} orbital interaction, which pushes the corresponding antibonding state above E_F. The formation of longer Pt chains as seen by experiment on Pt(111) is due to steering by lower diffusion barriers towards the end of the chain.

O 102.4 Fri 12:00 WIL C307

SPA-LEED investigation of a thin hexagonal iron-oxide-layer on Ag(001) — •Irena Kiesel[1], Daniel Bruns[2], and Joachim Wollschläger[2] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Fachbereich Physik, Universität Osnabrück, 49069 Osnabrück, Germany

We present a SPA-LEED (spot-profile-analysis low-energy-electron-diffraction) investigation of a thin iron-oxide-layer on Ag(001). The layer was produced by reactive vapour-deposition of iron in a thin oxygen atmosphere at different substrate temperatures.

The SPA-LEED anaysis of the films produced at 300°C and 400°C has shown a hexagonal structure of the iron-oxide-layer in addition to the cubic structure of the silver-substrate. Accessorily the reflexes of the hexagonal structure split in one direction. The splitting could be explained by an height-modulation of a FeO(111)-film on Ag(001). This height-modulation acts as a phase-grating for the diffracted electrons.

O 102.5 Fri 12:15 WIL C307

Phase diagrams of two dimensional $\mathrm{Pd}_x\mathrm{Ag}_{1-x}$/Pd(111) and $\mathrm{Pt}_x\mathrm{Ag}_{1-x}$/Pt(111) surface alloys — •Albert K. Engstfeld[1], Ralf T. Rötter[1], Andreas Bergbreiter[1], Harry E. Hoster[1,2], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — [2]Current address: Technische Universität München, Centre for Electromobility, 50 Nanyang Drive, Singapore 637553

The distribution of Ag and Pd or Pt in $\mathrm{Ag}_x\mathrm{Pd}_{1-x}$/Pd(111) and $\mathrm{Ag}_x\mathrm{Pt}_{1-x}$/Pt(111) surface alloys was studied by high resolution UHV-STM. The alloys were prepared by evaporating Ag on the respective substrate and subsequent annealing to 800 K. From quantitative 2D atom distributions we can show that AgPt tends towards two dimensional clustering and AgPd towards a 'quasi' random distribution, with small deviations for low and high coverages. From effective pair interactions, we are able to calculate the surface mixing energy and determine 2D phase diagrams. Furthermore we will elucidate whether the size mismatch or the differences in the intermetallic bonding are the dominant factor for the respective distribution in the surface alloy.

O 102.6 Fri 12:30 WIL C307

Properties of Cu on Ru(10-10) revealed by AES, LEED and DEPES — •Michal Jurczyszyn, Jacek Brona, Ireneusz Morawski, and Marek Nowicki — Institute of Experimental Physics, University of Wroclaw, Pl. Maxa Borna 9, 50-204 Wroclaw, Poland

The growth of Cu and the crystalline structure of the Cu/Ru(10-10) system was investigated by means of Auger electron spectroscopy (AES), low energy electron diffraction (LEED) and directional elastic peak electron spectroscopy (DEPES). All experiments were performed by using an RFA analyzer. The Auger signal from the substrate and adsorbate recorded during continuous Cu deposition shows the formation of two monolayers of Cu at early stages of growth. Further evaporation leads to 3D growth of Cu. In DEPES the intensity of elastically backscattered electrons was measured as a function of the incidence angle of the primary electron beam at energies: 0.6keV, 0.9keV, 1.2keV, 1.5keV, and 1.8keV. Due to the forward scattering of primaries the enhancement of the recorded signal was obtained at incidence angles parallel to the close packed rows of atoms in clean and covered substrate. The distribution of intensity maxima reflects very well the twofold symmetry of the Ru(10-10) sample. The stereographic distributions obtained for 6ML of Cu reflect threefold symmetry pattern, characteristic for a (111) surface of the fcc structure. The latter was confirmed by LEED pattern observations. The experimental DEPES results were compared to theoretical distributions obtained by using the multiple scattering (MS) theory.

O 102.7 Fri 12:45 WIL C307

Comparing Zn on Pd(110) with Zn on Pd(111) with LEED, LEIS and TDS — •Werner Stadlmayr, Christoph Rameshan, Simon Penner, Bernhard Klötzer, and Norbert Memmel — Physikalische Chemie, Universität Innsbruck, Austria

Methanol-steam-reforming (MSR) is an important catalytic reaction with regards to hydrogen usage and storage. PdZn-systems were found to show promising properties regarding MSR-capability. In several recent works, Zn on the densely-packed Pd(111)-surface was studied as possible model system and compared with catalytic studies on a polycrystalline Pd-foil. In the present work we present thermodesorption (TDS), low-energy electron diffraction (LEED) and angle-resolved low-energy ion scattering (LEIS) data for the growth and alloying of Zn on the more open Pd(110)-surface. We compare these results with Zn on Pd(111) and discuss differences and similarities.

O 103: Invited Talk (Karsten Reuter)

Time: Friday 13:15–14:00 Location: TRE Phy

Invited Talk O 103.1 Fri 13:15 TRE Phy

Beat the heat! First-principles based modeling of micro- and macroscopic heat dissipation in heterogeneous catalysis — •Karsten Reuter — Technische Universität München — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

First-principles electronic structure theory calculations are the indispensable basis for a predictive-quality modeling of catalytic activity. For a more comprehensive understanding of the catalytic function this basis needs to be linked to more coarse-grained approaches. First-principles kinetic Monte Carlo (kMC) simulations represent such an approach, which allows following the full system dynamics from picoseconds up to seconds, while fully accounting for the correlations, fluctuations and spatial distributions of the chemicals at the catalyst surface. A major challenge to the approach comes from the energy released in the exothermic surface reactions. I will sketch our recent efforts to augment the kMC simulations with an appropriate account of energy dissipation both at the atomistic and continuum level [1].

[1] S. Matera and K. Reuter, Catalysis Letters, 2009, 133, 156.