# Surface Science Division
# Fachverband Oberflächenphysik (O)

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## Overview of Invited Talks and Sessions

(lecture rooms H1, H2, H31, H32, H33, H34, H36, H37, H38, H40, H42, H46, H48; poster B1, B2)

### Invited Talks

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|---|---|---|---|---|
| O 1.1 | Mon | 10:15–11:00 | H36 | **Manipulation and assembly of single functional molecules: Towards molecular nanotechnology** — •Leonhard Grill |
| O 9.1 | Mon | 14:00–14:45 | H36 | **Sub-Wavelength Patterning of Ultrathin Organic Coatings via Nonlinear Laser Processing** — •Nils Hartmann |
| O 20.1 | Tue | 9:30–10:15 | H36 | **Control of Photon Emitters Coupled to Nano-Antennas** — •Niek F. van Hulst |
| O 31.1 | Tue | 14:00–14:45 | H36 | **Rare earth silicide nanowires on silicon surfaces** — •Mario Dähne |
| O 42.1 | Wed | 9:30–10:15 | H36 | **Electrons in quasi two dimensions: Revelations from photoemission mapping, microscopy, and filming** — •Kai Rossnagel |
| O 51.1 | Wed | 14:00–14:45 | H36 | **Photonic Metamaterials: Novel Optics with Artificial Atoms** — •Stefan Linden |
| O 61.1 | Thu | 9:30–10:15 | H36 | **Shining light on catalysis** — •Jeroen A. van Bokhoven |
| O 70.1 | Thu | 14:00–14:45 | H36 | **Sensing and controlling the spin of an atom by electric current** — •Sebastian Loth |
| O 81.1 | Fri | 10:15–11:00 | H36 | **Towards the computational design of heterogeneous catalysts** — •Thomas Bligaard |
| O 89.1 | Fri | 13:30–14:15 | H36 | **Evidence for exciton condensation in layered TiSe2: A photoemission study** — •Philipp Aebi |
| O 90.1 | Fri | 14:15–15:00 | H36 | **Surface Science and Electrocatalysis - Where do we stand?** — •R. Jürgen Behm |

### Invited Talks Focussed Session Solid/Liquid Interfaces

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| O 64.1 | Thu | 10:30–11:00 | H33 | **Metal/Electrolyte interfaces under atmospheric corrosion conditions** — •Michael Rohwerder |
| O 64.2 | Thu | 11:00–11:30 | H33 | **Copper Damascene Process: From the wafer to the atomic scale** — •Alexander Flügel |
| O 64.3 | Thu | 11:30–12:00 | H33 | **Atomic-scale dynamics and interactions at solid-liquid interfaces** — •Olaf Magnussen |
| O 73.1 | Thu | 15:00–15:30 | H33 | **Theoretical studies on the electrocatalytic Oxygen reduction reaction on Pt** — •Timo Jacob |
| O 73.2 | Thu | 15:30–16:00 | H33 | **Investigations on Pt based catalysts for PEM fuel cells: from model systems to high surface area catalysts** — •Matthias Arenz |
| O 73.3 | Thu | 16:00–16:30 | H33 | **Computer Simulation of Electrolyte / Solid Interfaces** — •Eckhard Spohr |

### Invited talks of the joint symposium SYPN

See SYPN for the full program of the Symposium.

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| SYPN 1.1 | Thu | 9:30–10:00 | H1 | **Growth and applications of N-polar (Al,Ga,In)N** — •Stacia Keller, Umesh K Mishra |

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| SYPN 1.2 | Thu | 10:00–10:30 | H1 | **Green light-emitting diodes and laser heterostructures on semi-polar GaN(11-22)/sapphire substrates** — •Andre Strittmatter |
| SYPN 1.3 | Thu | 10:30–11:00 | H1 | **Pros and cons of green InGaN lasers on polar GaN substrates** — •Uwe Strauss, Adrian Avramescu, Teresa Lermer, Jens Müller, Christoph Eichler, Stephan Lutgen |
| SYPN 1.4 | Thu | 11:15–11:45 | H1 | **Molecular beam epitaxy as a method for the growth of free-standing zinc-blende GaN layers and substrates.** — •Sergei Novikov, Thomas Foxon, Anthony Kent |
| SYPN 1.5 | Thu | 11:45–12:15 | H1 | **Three-dimensional GaN for semipolar light emitters** — •Thomas Wunderer, Frank Lipski, Stephan Schwaiger, Ferdinand Scholz, Martin Feneberg, Klaus Thonke, Andrey Chuvilin, Ute Kaiser, Sebastian Metzner, Frank Bertram, Jürgen Christen, Clemens Vierheilig, Ulrich Schwarz |

## Invited talks of the joint symposium SYDF

See SYDF for the full program of the Symposium.

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| SYDF 1.1 | Thu | 14:45–15:15 | H1 | **Downfolded Self-Energy of Many-Electron Systems and the Hubbard U** — •Ferdi Aryasetiawan |
| SYDF 1.2 | Thu | 15:15–15:45 | H1 | **LDA+Gutzwiller method for correlated electron systems** — •Zhong Fang |
| SYDF 1.3 | Thu | 15:45–16:15 | H1 | **Localized and itinerant states in $d/f$-electron systems unified by $GW$@LDA+$U$** — •Hong Jiang |
| SYDF 1.4 | Thu | 16:30–17:00 | H1 | **Giant polaronic effects in solids and nanstructures** — •Andrea Marini |
| SYDF 1.5 | Thu | 17:00–17:30 | H1 | **Excitation energies with time-dependent density *matrix* functional theory** — •Evert Jan Baerends, Klaas J. H. Giesbertz, Oleg Gritsenko, Katarzyna Pernal |
| SYDF 1.6 | Thu | 17:30–18:00 | H1 | **Calculations of multipoles in magnetic metals and insulators** — •Lars Nordström |

## Invited talks of the joint symposium SYNT

See SYNT for the full program of the Symposium.

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| SYNT 1.1 | Fri | 10:15–10:45 | H1 | **Atomic friction under ultrahigh vacuum conditions** — •Ernst Meyer, Enrico Gnecco, Pascal Steiner, Gregor Fessler, Sascha Koch, Thilo Glatzel, Alexis Baratoff, Mircin Kisiel, Urs Gysin, Akshata Rao, Shigeki Kawai, Sabine Maier |
| SYNT 1.2 | Fri | 10:45–11:15 | H1 | **Layering and Squeeze-out Damping in Confined Liquid Films** — •Frieder Mugele |
| SYNT 1.3 | Fri | 11:15–11:45 | H1 | **Wear on the nanoscale: mechanisms and materials** — •Bernd Gotsmann, Mark A. Lantz, Harish Bhskaran, Abu Sebastian, Ute Drechsler, Michel Despont, Yun Chen, Kumar Sridharan, Papot Jaroenapibal, Robert Carpick |
| SYNT 1.4 | Fri | 11:45–12:15 | H1 | **Friction at the Nanoscale: Insights from Atomistic Simulations** — •Izabela Szlufarska, Yifei Mo, Yun Liu, Maneesh Mishra |
| SYNT 1.5 | Fri | 12:15–12:45 | H1 | **The friction of wrinkles** — •Martin H. Müser, Hamid Mohammadi |
| SYNT 1.6 | Fri | 12:45–13:15 | H1 | **Influence of humidity on nano- and micromechanical contact adhesion** — •Hans-Jürgen Butt |

## Sessions

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| O 1.1–1.1 | Mon | 10:15–11:00 | H36 | **Invited talk (Grill, Leonhard)** |
| O 2.1–2.7 | Mon | 11:15–13:00 | H31 | **Metal substrates: Solid-liquid interfaces** |
| O 3.1–3.7 | Mon | 11:15–13:00 | H32 | **Methods: Scanning probe techniques I** |
| O 4.1–4.7 | Mon | 11:15–13:00 | H33 | **Heterogeneous catalysis I** |
| O 5.1–5.7 | Mon | 11:15–13:00 | H34 | **Electron and spin dynamics I** |
| O 6.1–6.7 | Mon | 11:15–13:00 | H36 | **Metal substrates: Adsorption of organic / bio molecules I** |
| O 7.1–7.6 | Mon | 11:15–12:45 | H38 | **Spin-Orbit Interaction at Surfaces I** |

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| O 8.1–8.9 | Mon | 10:15–12:30 | H8 | **[DS] Organic Electronics and Photovoltaics I (Joint Session DS/CPP/HL/O)** |
| O 9.1–9.1 | Mon | 14:00–14:45 | H36 | **Invited talk (Hartmann, Nils)** |
| O 10.1–10.9 | Mon | 15:00–17:15 | H31 | **Methods: Electronic structure theory & Methods: other (theory)** |
| O 11.1–11.10 | Mon | 15:00–17:30 | H32 | **Methods: Scanning probe techniques II** |
| O 12.1–12.11 | Mon | 15:00–17:45 | H33 | **Oxides and insulators: Adsorption** |
| O 13.1–13.11 | Mon | 15:00–17:45 | H34 | **Semiconductor substrates: Adsorption** |
| O 14.1–14.11 | Mon | 15:00–17:45 | H36 | **Metal substrates: Adsorption of organic / bio molecules II** |
| O 15.1–15.9 | Mon | 15:00–17:15 | H38 | **Spin-Orbit Interaction at Surfaces II** |
| O 16.1–16.10 | Mon | 15:00–17:30 | H46 | **Organic, polymeric, biomolecular films - also with adsorbates** |
| O 17.1–17.6 | Mon | 14:00–15:30 | H8 | **[DS] Organic Electronics and Photovoltaics II (Joint Session DS/CPP/HL/O)** |
| O 18.1–18.7 | Mon | 16:00–17:45 | H15 | **[HL] Organic Semiconductors: Solar Cells (Joint Session DS/CPP/HL/O)** |
| O 19.1–19.6 | Mon | 14:00–17:45 | H1 | **Symposium Spin-Orbit Coupling and Spin Relaxation in Graphene and Carbon Nanotubes** |
| O 20.1–20.1 | Tue | 9:30–10:15 | H36 | **Invited talk (Van Hulst, Niek)** |
| O 21.1–21.10 | Tue | 10:30–13:00 | H2 | **[DS] Plasmonics and Nanophotonics I (Joint Session DS/O/HL)** |
| O 22.1–22.9 | Tue | 10:30–12:45 | H32 | **Methods: Scanning probe techniques III** |
| O 23.1–23.10 | Tue | 10:30–13:00 | H33 | **Nanostructures at surfaces: Dots, particles, clusters** |
| O 24.1–24.8 | Tue | 10:30–12:30 | H34 | **Particles and clusters** |
| O 25.1–25.10 | Tue | 10:30–13:00 | H36 | **Metal substrates: Adsorption of organic / bio molecules III** |
| O 26.1–26.9 | Tue | 10:30–12:45 | H40 | **Oxides and insulators: Clean surfaces** |
| O 27.1–27.8 | Tue | 10:30–12:30 | H42 | **Metal subtrates: Adsorption of O and/or H** |
| O 28.1–28.10 | Tue | 10:30–13:00 | H48 | **Surface or interface magnetism** |
| O 29.1–29.12 | Tue | 9:30–12:45 | H37 | **[CPP] Organic Electronics and Photovoltaics I (Joint Session DS/CPP/HL/O)** |
| O 30.1–30.12 | Tue | 9:30–12:45 | H15 | **[HL] Organic Semiconductors: Transistors and OLEDs (Joint Session DS/CPP/HL/O)** |
| O 31.1–31.1 | Tue | 14:00–14:45 | H36 | **Invited talk (Dähne, Mario)** |
| O 32.1–32.6 | Tue | 15:00–16:30 | H2 | **Plasmonics and Nanophotonics II (Joint Session O/DS/HL)** |
| O 33.1–33.6 | Tue | 15:00–16:30 | H31 | **Nanostructures at surfaces: arrays** |
| O 34.1–34.5 | Tue | 15:00–16:15 | H32 | **Methods: Scanning probe techniques IV** |
| O 35.1–35.6 | Tue | 15:00–16:30 | H33 | **Heterogeneous catalysis II** |
| O 36.1–36.4 | Tue | 15:00–16:00 | H34 | **Methods: Atomic and electronic structure** |
| O 37.1–37.6 | Tue | 15:00–16:30 | H36 | **Metal substrates: Adsorption of organic / bio molecules IV** |
| O 38.1–38.4 | Tue | 15:00–16:00 | H40 | **Semiconductor substrates: clean surfaces** |
| O 39.1–39.5 | Tue | 15:00–16:15 | H42 | **Phase transitions** |
| O 40.1–40.10 | Tue | 13:45–16:15 | H37 | **[CPP] Organic Electronics and Photovoltaics II (Joint Session DS/CPP/HL/O)** |
| O 41.1–41.120 | Tue | 18:30–21:00 | Poster B1 | **Poster Session I (Semiconductor Substrates: Epitaxy and growth; Semiconductor Substrates: Adsorbtion; Semiconductor Substrates: Solid-liquid interfaces; Semiconductor Substrates: Clean surfaces; Oxides and insulators: Epitaxy and growth; Oxides and insulators: Adsorption; Oxides and insulators: Clean surfaces; Organic, polymeric and biomolecular films - also with adsorbates; Organic electronics and photovoltaics, Surface chemical reactions; Heterogeneous catalysis; Phase transitions; Particles and clusters; Surface dynamics; Surface or interface magnetism; Electron and spin dynamics; Spin-Orbit Interaction at Surfaces; Electronic structure; Nanotribology; Solid/liquid interfaces; Graphene; Others)** |
| O 42.1–42.1 | Wed | 9:30–10:15 | H36 | **Invited talk (Rossnagel, Kai)** |
| O 43.1–43.9 | Wed | 10:30–12:45 | H31 | **Graphene I** |
| O 44.1–44.11 | Wed | 10:30–13:15 | H32 | **Plasmonics and Nanooptics III** |
| O 45.1–45.9 | Wed | 10:30–12:45 | H33 | **Electronic structure I** |
| O 46.1–46.11 | Wed | 10:30–13:15 | H34 | **Density functional theory and beyond for real materials I** |
| O 47.1–47.10 | Wed | 10:30–13:00 | H36 | **Metal substrates: Adsorption of organic / bio molecules V** |
| O 48.1–48.9 | Wed | 10:30–12:45 | H40 | **Surface dynamics I** |

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| O 49.1–49.9 | Wed | 10:30–12:45 | H42 | **Surface chemical reactions I** |
| O 50.1–50.12 | Wed | 9:30–12:45 | H37 | **[CPP] Organic Electronics and Photovoltaics III (Joint Session DS/CPP/HL/O)** |
| O 51.1–51.1 | Wed | 14:00–14:45 | H36 | **Gaede-Prize talk (Linden, Stefan)** |
| O 52.1–52.9 | Wed | 15:00–17:15 | H31 | **Graphene II** |
| O 53.1–53.11 | Wed | 15:00–17:45 | H32 | **Plasmonics and Nanooptics IV** |
| O 54.1–54.9 | Wed | 15:00–17:15 | H33 | **Electronic structure II** |
| O 55.1–55.9 | Wed | 15:00–17:15 | H34 | **Density functional theory and beyond for real materials II** |
| O 56.1–56.10 | Wed | 15:00–17:30 | H36 | **Metal substrates: Adsorption of organic / bio molecules VI** |
| O 57.1–57.10 | Wed | 15:00–17:30 | H40 | **Surface dynamics II** |
| O 58.1–58.10 | Wed | 15:00–17:30 | H42 | **Surface chemical reactions II** |
| O 59.1–59.117 | Wed | 17:45–20:30 | Poster B1 | **Poster Session II (Nanostructures at surfaces: Dots, particles, clusters; Nanostructures at surfaces: arrays; Nanostructures at surfaces: Wires, tubes; Nanostructures at surfaces: Other; Plasmonics and nanooptics; Metal substrates: Epitaxy and growth; Metal substrates: Solid-liquid interfaces; Metal substrates: Adsoprtion of organic / bio molecules; Metal substrates: Adsoprtion of inorganic molecules; Metal substrates: Adsoprtion of O and/or H; Metal substrates: Clean surfaces; Density functional theory and beyond for real materials)** |
| O 60.1–60.35 | Wed | 17:45–20:30 | Poster B2 | **Poster Session III (Methods: Atomic and electronic structure; Methods: electronic structure theory; Methods: Molecular simulations and statistical mechanics; Methods: Sanning probe techniques; Methods: other (experimental); Methods: other (theory) )** |
| O 61.1–61.1 | Thu | 9:30–10:15 | H36 | **Invited talk (Van Bokhoven, Jeroen)** |
| O 62.1–62.8 | Thu | 10:30–12:30 | H31 | **Graphene III** |
| O 63.1–63.10 | Thu | 10:30–13:00 | H32 | **Plasmonics and Nanooptics V** |
| O 64.1–64.7 | Thu | 10:30–13:00 | H33 | **Solid/liquid interfaces I (focussed session)** |
| O 65.1–65.11 | Thu | 10:30–13:15 | H34 | **Density functional theory and beyond for real materials III** |
| O 66.1–66.7 | Thu | 10:30–12:15 | H36 | **Nanotribology I** |
| O 67.1–67.5 | Thu | 10:30–13:00 | H37 | **Gerhard Ertl Young Investigator Award (talks of the selected canditates)** |
| O 68.1–68.10 | Thu | 10:30–13:00 | H42 | **Semiconductor substrates: Epitaxy and growth** |
| O 69.1–69.5 | Thu | 9:30–12:15 | H1 | **Symposium Polarization Field Control in Group-III-Nitrides** |
| O 70.1–70.1 | Thu | 14:00–14:45 | H36 | **Invited talk (Loth, Sebastian)** |
| O 71.1–71.12 | Thu | 15:00–18:00 | H31 | **Metal substrates: Epitaxy and growth** |
| O 72.1–72.12 | Thu | 15:00–18:00 | H32 | **Plasmonics and Nanooptics VI** |
| O 73.1–73.8 | Thu | 15:00–17:45 | H33 | **Solid/liquid interfaces II (focussed session)** |
| O 74.1–74.12 | Thu | 15:00–18:00 | H34 | **Nanostructures at surfaces: Other** |
| O 75.1–75.8 | Thu | 15:00–17:00 | H36 | **Nanotribology II** |
| O 76.1–76.9 | Thu | 15:00–17:15 | H38 | **Nanostructures at surfaces: Wires, tubes** |
| O 77.1–77.12 | Thu | 15:00–18:00 | H42 | **Oxides and insulators: Epitaxy and growth** |
| O 78.1–78.6 | Thu | 14:45–18:00 | H1 | **Symposium Density functional theory and beyond for real materials** |
| O 79 | Thu | 19:30–20:00 | H1 | **General Meeting of the Surface Science Division** |
| O 80 | Thu | 20:00–21:00 | H1 | **Post Deadline Session** |
| O 81.1–81.1 | Fri | 10:15–11:00 | H36 | **Invited talk (Bligaard, Thomas)** |
| O 82.1–82.7 | Fri | 11:15–13:00 | H31 | **Graphene IV** |
| O 83.1–83.7 | Fri | 11:15–13:00 | H32 | **Plasmonics and Nanooptics VII** |
| O 84.1–84.8 | Fri | 11:15–13:15 | H34 | **Density functional theory and beyond for real materials IV** |
| O 85.1–85.7 | Fri | 11:15–13:00 | H36 | **Metal substrates: Adsorption of organic / bio molecules VII** |
| O 86.1–86.6 | Fri | 11:15–12:45 | H40 | **Organic, electronics and photovoltaics** |
| O 87.1–87.6 | Fri | 11:15–12:45 | H42 | **Methods: Other (experimental)** |
| O 88.1–88.6 | Fri | 10:15–13:15 | H1 | **Symposium Nanotribology** |
| O 89.1–89.1 | Fri | 13:30–14:15 | H36 | **Invited talk (Aebi, Philipp)** |
| O 90.1–90.1 | Fri | 14:15–15:00 | H36 | **Invited talk (Behm, Jürgen)** |

## Annual General Meeting of the Surface Science Division

Thursday 19:30– 20:00 H1

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

## Post deadline session

Post deadline session O80 on Thursday 20:00-21:00 in H1, followed by the Surface Science "get-together".

## O 1: Invited talk (Grill, Leonhard)

Time: Monday 10:15–11:00 Location: H36

**Invited Talk** O 1.1 Mon 10:15 H36
**Manipulation and assembly of single functional molecules: Towards molecular nanotechnology** — •Leonhard Grill — Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin

Functional molecules are of great interest for future applications in molecular nanotechnology where they should be used as single-molecule devices. The scanning tunneling microscope (STM) is a very important instrument for the investigation of such molecules, because it can image single molecules with submolecular resolution and is also capable to manipulate them by chemical and electrostatic forces or electronic processes [1].

In this talk, various examples of manipulations of single molecules by low temperature STM will be given. The controlled assembly of functional molecules by "on-surface-synthesis" [2] will be presented, whereas covalent bonding is the desired intermolecular interaction, because it provides high stability and the possibility of efficient intermolecular charge transfer. By pulling a polymer from a metallic surface, the conductance can be measured for a single molecular wire as a continuous function of the electrode-electrode distance, revealing electronic and mechanical properties [3]. Finally, the adsorption and growth of such organic nanostructures on inorganic crystallites, thus creating a hybrid system, will be discussed.

[1] L. Grill, J. Phys.: Cond. Matt. 20, 053001 (2008) [2] L. Grill et al., Nature Nanotechn. 2 (2007) 687 [3] L. Lafferentz et al., Science 323, 1193 (2009)

## O 2: Metal substrates: Solid-liquid interfaces

Time: Monday 11:15–13:00 Location: H31

O 2.1 Mon 11:15 H31
**Self-organized Porphyrin monolayers on iodine-modified noble metal surfaces** — •Michael Schneider, Christian Schlaup, and Klaus Wandelt — Inst. f. Phys. u. Theo. Chem., Universität Bonn, Wegelerstr. 12 D-53115, Bonn, Germany

In the field of template chemistry, new and interesting phenomena can be discovered at gold /electrolyte interfaces in the presence of anions and supramolecules as function of electrode potentials. The spontaneous self-assembly of organic molecules is considered a promising bottom-up technique in nanotechnology to create surface patterns and electronic devices. Porphyrins are important organic compounds in the fields of biology and technology. They open a series of potential applications in cancer therapy, or as catalysts and sensors. Halide-modified Au(111)-surfaces are desirable substrates due to their long range order. Iodide-modified Au(111)-surfaces show electrocompression and phase transitions dependent on the electrode potential, as shown in previous works . Our studies with STM and cyclic voltammetry not only reproduce previous works about Tetra (N-methyl-4-pyridyl)-porphyrin molecules (TMPyP) on iodide-modified Au(111)-surfaces, but provide an even more precise understanding. Namely, it is found that the TMPyP layer exhibits a long-range periodic superstructure beyond the molecular arrangement. This research complements one of our previous studies regarding adsorption of the same molecule on halide-modified copper-surfaces , allowing comparisons between systems with the same molecules but different substrates.

O 2.2 Mon 11:30 H31
**Effect of additives on Cu electrodeposition: an in-situ STM study** — •Yuriy Yanson, Geert Wijts, Fred Schenkel, and Marcel J. Rost — Kamerlingh Onnes Laboratory, Leiden University, The Netherlands

Small amounts of specific substances, known as additives, can dramatically influence the growth of electrodeposited thin films. Although additives are often applied in the industry not only to change the film properties but also to enable a specific deposition, the microscopic (atomic) understanding of the additive influence on the growth is usually still lacking. We present an in-situ STM studies of Cu electrodeposition on the Au(111) substrate, in which we clearly show the atomic scale effect of industrially relevant additives on the growth. In particular, we discuss the influence of the accelerator bis-(3-sodiumsulfopropyl) disulfide (SPS) and the inhibitor polyethylene glycol (PEG) on Cu plating. We expect that our newly developed video-rate EC-STM will provide access to even shorter time scales enabling the study of growth dynamics.

O 2.3 Mon 11:45 H31
**Pb adsorption on Cu(100) studied in situ by electrochemical video STM** — •Otavio Alves[1], Hisayoshi Matsushima[2], Harry E. Hoster[1], R. Jürgen Behm[1], and Olaf Magnussen[2] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — [2]Institute of Experimental and Applied Physics, Christian-Albrechts University, D-24118 Kiel, Germany

As a prototype for a lattice-mismatched system, the growth of Pb on Cu(100) was subject of various studies under ultrahigh vacuum conditions (UHV) [1-4]. It has been established that Pb grows on Cu(100) in a Stranski-Krastanov mode, with three well-defined ordered structures appearing in the submonolayer regime up to 0.6 monolayers. In this contribution, we will report on the growth of Pb on Cu(100) at the solid/liquid interface, which we observed in situ by electrochemical video scanning tunnelling microscopy (STM). At low Pb surface concentration, spontaneous formation of a surface alloy takes place on a reconstructed Cu(100). Increasing the Pb surface content leads to dealloying, finally resulting in a saturated Pb overlayer. Our in situ STM atomic-scale pictures are comparable to those obtained in UHV. Atomic Pb diffusion, dynamic structural fluctuation and coexistence of different Pb phases will be discussed.
[1] J. Henrion et al., *Surf. Sci.* 29, **1972**, 20.
[2] C. Nagl et al., *Surf. Sci.* 331, **1995**, 831.
[3] Y. Gauthier et al., *Surf. Sci.* 345, **1996**, 53.
[4] S. Robert et al., *Surf. Sci.* 350, **1996**, 136.

O 2.4 Mon 12:00 H31
**Formation of Ultrathin Copper Sulfide Semiconductor Films under Electrochemical Conditions** — •Christian Schlaup and Klaus Wandelt — Institute for Physical and Theoretical Chemistry, Wegelerstr. 12, D-53115 Bonn, Germany

Ultrathin copper sulfide semiconductor films were prepared in an electrochemical environment using subsequential steps of copper deposition on an inert Au(1 0 0) electrode surface and reaction with bisulfide anions. The thickness of thus prepared copper sulfide films depends only on the initially deposited amount of copper and can be easily tuned within a range of a single monolayer to several layers. Structural characterization using in situ STM reveals commensurate $c(2\times2)$ structure for an only one monolayer thick copper sulfide film, which remains stable over a wide potential range. In addition, these films could also be stabilized in a bisulfide free solution resulting in an even higher stability against anodic potentials. Preparing thicker copper sulfide films yields a mixed phase regime consisting of a bulk-like copper sulfide phase with a granular appearance and a metastable bilayer phase which can be completely converted into the bulky phase by initial oxidation.

O 2.5 Mon 12:15 H31
**About the Orientation of Viologen Monolayers on a Cu [1 0 0] Electrode Surface** — •Melanie Röefzaad[1], Vlad Zamlynny[2], and Klaus Wandelt[1] — [1]Institute for Physical and Theoretical Chemistry, University of Bonn — [2]Chemistry Department, Acadia University, Canada

Detailed investigations of the metal/electrolyte interface in presence of the redox active 4,4‘-Bipyridin with different substituents at 1,1‘-position have been done combining Infrared Reflection Absorption Spectroscopy (IRRAS) and Cyclic Voltammetry (CV). To reveal indications about the orientation of certain parts of the molecule in the adsorbed monolayer and their changes, the Polarization Modulated IR-

RAS was applied.[1,2] Calculations showed that in general all viologen species adsorb with the longer molecular axis parallel to the surface. In contrast the orientation of the ring planes of the bipyridine moiety changes after the reduction process. For Dibenzylviologen (DBV) the angles with respect to the surface normal have been calculated to ~20° for the dication and to ~70° for the radical-cation. In the same way orientations of alkyl substituents were investigated. For example Heptylviologen shows a straightening up of the long alkyl chains, from 50° to 24° with respect to the surface normal, while lowering the potential. This orientation change is mainly caused by decreasing the area per molecule (ApM) with a closer packing of the stacking rows.

[1] H. Seki, K. Kunimatsu, W. G. Golden, Appl. Spectroscopy 1985, 39, 437.

[2] A. N. Parikh, D. L. Allara, J. Chem. Phys. 1992, 96, 927.

O 2.6 Mon 12:30 H31

**X-ray reflectivity studies at the mercury/electrolyte interface** — •Annika Elsen[1], Bridget M. Murphy[1], Ben M. Ocko[2], Lilach Tamam[3], Moshe Deutsch[3], Ivan Kuzmenko[4], and Olaf M. Magnussen[1] — [1]Institut für Experimentelle und Angewandte Physik, CAU, D-24105 Kiel, Germany — [2]Department of Physics, BNL, Upton, New York 11973, USA — [3]Department of Physics, Bar-Ilan University, Ramat Gan 52900, Israel — [4]CMC-CAT, APS, ANL, Argonne, Illinois 60439, USA

The interface between the liquid mercury electrode and an electrolyte solution is one of the most extensively studied electrochemical systems. It was fundamental for verifying traditional and modern theories of the electrochemical double layer. Although the metal contributes significant to the double layer capacity, with its interface structure playing an important role, up to now there is almost no knowledge about this structure. Here we present the first X-ray reflectivity studies at the liquid mercury electrode in electrolyte solution (0.01M NaF), allowing to clarify the interface structure. The experiments exhibited atomic layering of the mercury perpendicular to the surface similar to that found for the mercury vapour interface. We found a significant influence on the width of the interface electron density profile which can be referred to two effects: first of all the potential dependent change in the surface tension causes a change in the capillary wave induced interface roughness. Secondly another potential controlled effect was found due to the intrinsic change in the electron density distribution because of interface polarisation.

O 2.7 Mon 12:45 H31

**Simulating cyclic voltammograms of bimetallic model surfaces** — •Harry E. Hoster, Otavio B. Alves, Albert K. Engstfeld, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

Cyclic voltammograms recorded at bimetallic surfaces reflect the superposition of current contributions from adsorption, desorption, and reaction processes at surface regions with laterally varying chemical properties. As will be demonstrated for some selected well-defined single crystalline model systems including Pt films on Ru(0001) and PtAu/Pt(111) surface alloys, voltammetric features at bimetallic surfaces can be simulated using the corresponding features for the monometallic surfaces in combination with information on the adsorption properties and abundance of the dominating sites at the bimetallic surfaces. Trends in the local adsorption properties can be predicted based on density functional theory calculations, whereas the necessary information about the local vertical and lateral metal distribution is obtained from scanning tunnelling microscopy imaging.

## O 3: Methods: Scanning probe techniques I

Time: Monday 11:15–13:00 Location: H32

O 3.1 Mon 11:15 H32

**Contrast mechanisms for the detection of ferroelectric domains with scanning force microscopy** — •Tobias Jungk, Florian Johann, Akos Hoffmann, and Elisabeth Soergel — Physikalisches Institut, Universität Bonn, Wegelerstrasse 8, 53115 Bonn

We present an analysis of the contrast mechanisms for the detection of ferroelectric domains on all faces of bulk single crystals using scanning force microscopy. The experiments were carried out with hexagonally poled lithium niobate to access well-defined domain structures on every crystal face [1]. Using a rotation stage including subsequent image processing allows for the discrimination of deflection and buckling from the vertical signal, which – together with the lateral signal – yield all accessible information [2]. Thus, the domain contrast can be attributed to three different mechanisms: (i) the thickness change of the sample due to an out-of plane piezoelectric response, (ii) the lateral displacement of the sample surface due to an in-plane piezoresponse and (iii) an expansion/contraction movement in the vicinity of the domain wall on the crystallographic y- and z-faces. A careful analysis of the movement of the cantilever with respect to its orientation relative to the crystallographic axes of the sample allows a clear attribution of the observed domain contrast to the corresponding driving forces.

[1] T. Jungk, A. Hoffmann, and E. Soergel, New J. Phys. 11, 033029 (2009).

[2] F. Johann, T. Jungk, S. Lisinski, A. Hoffmann, L. Ratke, and E. Soergel, Appl. Phys. Lett. 95, 202901 (2009).

O 3.2 Mon 11:30 H32

**SubSurface AFM: towards nondestructive 3D microscopy** — •Gerard J. Verbiest, Johannes Simon, and Marcel J. Rost — Leiden University, Leiden, Netherlands

True nondestructive, subsurface microscopy is desired in many fields ranging from material science over biology to industry. The variety of possible applications include, e.g., microelectronics failure analysis or biological processes within cells. The key to 3D information is the use of nondestructive, ultrasonic acoustic waves, which lead to an interference pattern at the sample surface, that is measured locally with an AFM. This has been demonstrated experimentally [1].

In order to receive insights in the physical contrast mechanism and to design the most suited AFM, we are both developing an analytical model and performing finite element analysis calculations to understand the experimentally determined acoustic wave propagation in artificially created samples. We address questions like: what causes the (surface) contrast; what is the ultimate achievable resolution; and how to extract depth information?

[1] G.S. Shekhawat and V.P. Dravid; Science 310, 89 (2005) 5745

O 3.3 Mon 11:45 H32

**Atomic-resolution force map measurements on single molecules** — •Fabian Mohn, Leo Gross, Nikolaj Moll, Peter Liljeroth, and Gerhard Meyer — IBM Research - Zurich, 8803 Rüschlikon, Switzerland

It was recently shown that atomic resolution can be achieved in AFM imaging of individual molecules by a controlled functionalization of the microscope's tip apex [L. Gross et al., *Science* **325**, 1110 (2009)]. We present measurements that yield further insight into the nature of the contrast mechanism in this atomic-resolution imaging of molecules.

In particular, the distance-dependence of the frequency shift above admolecules was investigated with atomic resolution. The standard technique of 3D force mapping was extended to permit measuring at close tip–sample distances, in the regime of maximal attractive forces. A precise control of the interaction strength during data acquisition is essential to avoid instabilities of the imaged molecules. Our technique enables atomic resolution on both the substrate and the admolecules, simultaneously.

O 3.4 Mon 12:00 H32

**Interaction of the STM/AFM tip with graphite and graphene surfaces - theoretical models** — •Martin Ondráček, Vít Rozsíval, and Pavel Jelínek — Institute of Physics, Academy of Sciences of the Czech Republic, Praha

Although atomic resolution is routinely achieved on the graphite (0001) surface and graphene with scanning probe techniques (STM and AFM), there are still open questions with respect to the identification of the atomic-scale features in the images with the actual atomic and hollow sites on the surface. While it is generally agreed that the low-bias STM sees one of the two non-equivalent surface atoms of the graphite surface (the $\beta$-site atom), the interpretation of contrast in the AFM is not so simple. Depending on the experimental setup, the apparent height maxima may be located at the hollow sites or at the atomic sites. We show that any realistic modeling of the AFM must include the relaxation of the tip and surface atomic structure as well as the chemical composition of the tip. Furthermore, conductance calculations aiming to explain near-to-contact STM measurements cannot neglect multiple electron scattering. In order to meet these requirements, we combine accurate total energy DFT calculations in the PAW method with calculations of electron transport in the Green's function approach. Such an approach allows us to analyze the relation between the chemical short-range force and the electric conductance in the range from the tunneling to the contact regime.

O 3.5 Mon 12:15 H32

**Searching for spin contrast on NiO with Ni tips** — •Florian Pielmeier and Franz J. Giessibl — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Nickel atoms in the NiO(001) surface show antiferromagnetic ordering at room temperature resulting from indirect exchange interactions between neighbouring Ni 3d-electrons [1]. Frequency modulation atomic force microscopy, using extra stiff qPlus sensors, was used to probe the NiO(001) surface at room temperature. At tip-sample distances in the range of a few angstroms, the different spin orientations should provide detectable contributions to the short-range interaction forces between tip and sample. Nickel was used as the tip material as it is rather inert to oxygen and is widely used in spin polarized STM. Atomic resolution images with very good signal-to-noise ratio are presented, but similar to previous measurements with Co and NiO tips [2] evidence for spin contrast has not been found yet.

[1] D. Ködderitzsch, W. Hergert, W. M. Temmerman, Z. Szotek, A. Ernst, H. Winter: Phys. Rev. B 66, 064434 (2002)

[2] M. Schmid, J. Mannhart, F.J. Giessibl: Phys. Rev. B 77, 045402 (2008)

O 3.6 Mon 12:30 H32

**Challenges in constructing spin-polarized scanning probe tips** — •Thorsten Wutscher and Franz J. Giessibl — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg

A central feature of scanning force microscopy (SFM) is the force dependence upon the atomic configuration and chemical identity of the tip [1, 2]. Spin-polarized tips, created with an external magnetic field, have been shown to yield spin contrast at the atomic scale [3]. In order to detect spin contrast, the apex atom has to be a magnetic atom, the spins between tip and sample should be (anti-)parallel to each other and the magnetic moment of the apex atom has to be stable. Given an appropriate tip selection, this should be possible at room temperature without the presence of an external magnetic field. *In situ* cleaved tips can avoid contamination near the tip-sample junction. Nickel oxide was chosen as a candidate tip material because it has a high Néel temperature and a common magnetic bulk and surface alignment. It has a rock salt structure and thus cleaves well. The tips were oriented on a quartz cantilever (qPlus sensor) for SFM experiments.

[1] Y. Sugimoto, P. Pou, M. Abe, P. Jelinek, R. Pérez, S. Morita and Ó. Custance, Nature, 446, 64-67 (2007)

[2] S. Hembacher, F. J. Giessibl, J. Mannhart, Science, 305, 380-383 (2004)

[3] U. Kaiser, A. Schwarz, R. Wiesendanger, Nature, 446, 522-525 (2007)

O 3.7 Mon 12:45 H32

**Characterization of tips for spin-polarized scanning tunneling microscopy** — Guillemin Rodary, •Sebastian Wedekind, Hirofumi Oka, Dirk Sander, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

A common procedure to prepare tips for spin-polarized scanning tunneling microscopy is to deposit magnetic materials onto a W-tip, which was electrochemically etched and subsequently flashed to 2200 K under UHV conditions [1]. However, this macroscopic tip preparation does not necessarily yield a certain magnetic sensitivity. We show that depositing Cr or Co/Cr bilayers on a W-tip can lead to vastly different magnetic tip responses in external fields [2]. We find that the microscopic tip preparation by voltage pulses under imaging conditions is decisive for the resulting magnetic configuration at the tip apex. We propose a conclusive characterization of the magnetic configuration of the tip apex. We show that both careful tip preparation and characterization by tunneling spectroscopy need to be augmented by measurements in magnetic field to ensure a reliable analysis of a magnetic contrast in spin-polarized scanning tunneling microscopy studies. [1] R. Wiesendanger, Rev. Mod. Phys. **81** (2009)1495. [2] G. Rodary, S. Wedekind, H. Oka, D. Sander, J. Kirschner, Appl. Phys. Lett. **95** (2009) 152513.

## O 4: Heterogeneous catalysis I

Time: Monday 11:15–13:00 Location: H33

O 4.1 Mon 11:15 H33

**First-Principles statistical mechanics simulations of catalytic oxidation of ammonia at RuO$_2$(110)** — •Claudia Mangold[1] and Karsten Reuter[1,2] — [1]Fritz-Haber-Institut, Berlin (Germany) — [2]Technische Universität München (Germany)

RuO$_2$(110) has evolved into a frequently studied model oxide surface, with appealing catalytic properties for a range of reactions. Recent experiments by Wang *et al.* [1] determined an almost 100% selectivity for the oxidation of ammonia, adding this first step of the Ostwald process to the list. In order to understand the mechanistic details behind this high selectivity we perform first-principles statistical mechanics simulations, based on density-functional theory for a quantitative account of the surface energetics. The atomistic thermodynamics phase diagram, constructed for a constrained equilibrium with the NH$_3$ and O$_2$ gas phase, points at a prominent role of the coordinatively unsaturated sites offered by the surface. First kinetic Monte Carlo simulations concentrate on the kinetics at these sites and reveal severe diffusion limitations at the nanostructured RuO$_2$(110) surface.
[1] Wang *et al.*, J. Phys. Chem. B **109** (2005) 7883.

O 4.2 Mon 11:30 H33

**Size effects in C$_2$H$_4$ dehydrogenation studied by HR-PES: Pt(111) versus Pt/CeO$_2$/Cu(111) model catalysts.** — •Yaroslava Lykhach[1], Thorsten Staudt[1], Natalia Tsud[2], Tomas Skala[3], Vladimir Matolin[2], Kevin C. Prince[3], and Joerg Libuda[1] — [1]Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany — [2]Charles University, Department of Plasma and Surface Science, 18000 Prague 8, Czech Republic — [3]Sincrotrone Trieste, 34012 Basovizza-Trieste, Italy

Complex catalysts consisting of noble metal particles on reducible CeO$_2$ supports show unique reactivity and reduced carbon precipitation during hydrocarbon reforming. In order to explore these effects at the microscopic level, we have studied the adsorption and dehydrogenation of C$_2$H$_4$ on a Pt/CeO$_2$(111)/Cu(111) and Pt(111)model catalysts. Reaction and decomposition of C$_2$H$_4$ are investigated by means of HR-PES as a function of the CeO$_{2-x}$ stoichiometry and Pt particle size. In contrast to the behavior on Pt(111), where molecular adsorption of C$_2$H$_4$ is observed, dissociation intermediates, namely CCH$_3$ and CHCH$_3$, were found on the Pt nanoparticles even at 100 K. The dehydrogenation of these products to carbonaceous deposits is accompanied by the hydrogen spillover and formation of hydroxyl groups on ceria. The decomposition of the hydroxyl groups and desorption of H$_2$ occurs at 450 K. At higher temperatures, carbonaceous species react with oxygen, which is supplied via reverse spillover from the ceria and, subsequently, desorb in the form of CO and/or CO$_2$.

O 4.3 Mon 11:45 H33

**Nanostructured Cerium Oxide Based Model Catalysts: Structure, Morphology and Reactivity** — •Thorsten Staudt[1], Yaroslava Lykhach[1], Michael Peter Andreas Lorenz[1], Regine Streber[1], Lutz Hammer[2], Hans-Peter Steinrück[1], Alexander Schneider[2], and Jörg Libuda[1] — [1]Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen — [2]Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen

Nanostructured cerium oxide based catalysts offer unique properties in the field of heterogeneous catalysis, e.g. involving the activation of $CO_2$. In our study we prepare model systems starting from $CeO_2(111)$ films on a Cu(111) substrate. Ultra-thin films are grown by PVD in $O_2$ at different sample temperatures. The morphology is analyzed by STM and LEED [1], showing a (1.5x1.5) superstructure. STM reveals a 3d growth mode for films grown at elevated temperatures (520K). Using kinetically limited growth at 100K and subsequent annealing, closed layers of ceria with atomically flat terraces can be prepared, even in the ultra-thin regime (1.5 ML). Via homoepitaxial growth of ceria on this initial film, closed films with larger thickness (3 ML) are available.

In a second step, the ceria substrate is modified by deposition of MgO, which offers basic sites and may further enhance the reactivity. We have investigated the influence of surface structure, oxidation state and composition of these samples on their interaction with $CO_2$.[2] Systematic XPS studies show that two $CO_2$ related species are formed, which are assigned to carbonates and carboxylates. [1] T. Staudt et al., Surface Science 603 (2009) 3382 [2] Y. Lykhach et al., submitted

O 4.4 Mon 12:00 H33

**CO oxidation on Au/$TiO_2$(110) model catalysts - support oxidation state and Au particle size effects** — •Menhild Eyrich, Cihan Topkaya, Joachim Bansmann, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

Since Haruta [1] discovered the unusual catalytic activity of small Au particles on transition metal oxide supports in the late 1980s, numerous studies were carried out on the catalysts to understand the physical origin of the high activity. Especially for the CO oxidation on $TiO_2$ supported Au catalysts, the reaction mechanism is still not completely resolved. Analogously to the respective powder catalysts, also the activity of the planar model catalysts strongly depends on the pretreatment of the catalyst and on the size of the Au nanoparticles. Here, we report the results of a study on fully oxidized and reduced planar Au/$TiO_2$ model catalysts. For each model system, the reaction rates for different Au nanoparticle sizes were determined. The results will be compared to other Au/$TiO_2$ catalysts and possible reasons for the strong influence of the Au nanoparticle size and the oxidation state of the support on the catalytic activity will be discussed.

[1]M. Haruta, N. Yamada, T. Kobayashi, S. Iijima, J. Catal. 115 (1989), 301-309.

O 4.5 Mon 12:15 H33

**Mechanisms of CO oxidation at nanoporous gold: combined TPD and XPS study** — •Sarah Röhe, Tobias Becker, Andreas Schaefer, Arne Wittstock, Volkmar Zielasek, and Marcus Bäumer — Universität Bremen, Institut für Angewandte und Physikalische Chemie, Leobener Str. NW2, 28359 Bremen

Unsupported nanoporous gold (NPG) shows high catalytic activity for CO oxidation with molecular oxygen even below room temperature [1]. So far, the mechanisms of how the surface of NPG catalyzes this reaction have been somehow puzzling. In particular, several experiments on various low-index single crystal gold surfaces had demonstrated that the rate of $O_2$ dissociation at pure gold is negligible - even at higher temperatures and even if the surface had been roughened on the atomic scale by Ar sputtering.

Based on a combined TPD and XPS study in ultrahigh vacuum at NPG we will provide evidence for residual silver in the NPG surface playing a major role for the activation of molecular oxygen for CO oxidation. Since NPG is produced by leaching of silver from Au-Ag alloy, rest silver with total concentrations of 1-5% and up to 20% at the surface remains in the material and was speculated on as an active ingredient in the CO oxidation, before. Our data indicate that at temperatures above 200 K $O_2$ is dissociated at silver sites and atomic oxygen probably binds at silver but also spills over to gold surrounding silver islands.

[1] V. Zielasek, B. Jürgens, C. Schulz, J. Biener, M.M. Biener, A.V. Hamza, M. Bäumer, Angew. Chem. Int. Ed. 45 (2006) 8241.

O 4.6 Mon 12:30 H33

**Oxidation of carbon monoxide on Au/ZnO nanoparticles: an infrared spectroscopy study** — •Heshmat Noei[1], Martin Muhler[1], and Yuemin Wang[1,2] — [1]Lehrstuhl für Technische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, 44801 Bochum, Germany

Recently, supported gold nanoparticles have attracted enormous attention due to their unique catalytic properties for a number of chemical reactions including CO oxidation at low temperatures. In this contribution the catalytic reactivity of different ZnO-supported Au nanoparticles was studied systematically by ultra-high vacuum FTIR spectroscopy (UHV-FTIRS). Exposing negatively charged Au nanoparticles to CO at 110 K leads to the appearance of two C-O stretching bands at 2180 and 2066 $cm^{-1}$, which are assigned to CO species adsorbed on ZnO and Au surfaces, respectively. On oxidized Au/ZnO (with $Au^0$) the IR band for CO adsorption on ZnO is observed at 2183 $cm^{-1}$, while two new C-O bands show up at 2105 and 2112 $cm^{-1}$, which are attributed to the CO species adsorbed on Au/ZnO interface and Au particles, respectively. After further exposing the reduced and oxidized Au/ZnO nanopartcles to oxygen at 110 K, CO oxidation occurs yielding physisorbed $CO_2$ and carbonate species. It was found that the reduced surfaces favour $CO_2$ production, whereas on the oxidized surfaces carbonate species are preferentially formed. The catalytic mechanisms of low temperature CO oxidation will be discussed in details.

O 4.7 Mon 12:45 H33

**First-Principles Approach to Heat and Mass Transfer Effects in Model Catalyst Studies** — •Sebastian Matera[1] and Karsten Reuter[1,2] — [1]Fritz-Haber-Institut Berlin (Germany) — [2]Technische Universität München (Germany)

We assess heat and mass transfer limitations in *in situ* studies of model catalysts with a first-principles based multiscale modeling approach that integrates a detailed description of the surface reaction chemistry and the macro-scale flow structures. Using $RuO_2(110)$ as a representative substrate for the frequently studied CO oxidation reaction we find corresponding limitations to significantly mask the intrinsic catalytic function at the high conversion rates reached at near-ambient gas-phase conditions [1]. Two crucial and hitherto largely unappreciated factors specific to the model catalyst reactor geometry are in this respect the degree of heat dissipation at the back of the thin sample and the propensity to build-up a product boundary layer above the flat-faced surface. A qualified discussion of a possibly different surface chemistry across the "pressure gap" requires accounting for resulting temperature and pressure gradients, both in experimental *in-situ* setups and through predictive-quality integrated models as the one presented here. Otherwise wrong mechanistic conclusions may be derived which hamper our progress towards an atomic-scale understanding of the function of heterogeneous catalysts at technologically relevant gasphase conditions. [1] S. Matera and K. Reuter, Catal. Lett. **133**, 156 (2009).

## O 5: Electron and spin dynamics I

Time: Monday 11:15–13:00 Location: H34

O 5.1 Mon 11:15 H34

**Image-potential states on Au(100) measured by Two-Photon Photoemission** — •Tobias Bierlein, Daniel Niesner, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Most metals do not have reconstructions of their clean surfaces at room temperature. But Au(100) and Ir(100) surfaces always reorder to (5x20) respectively (5x1) reconstructions. There are some methods to break this reconstructions and obtain (1x1) surfaces. The resulting surfaces were examined for work function and image-potential states with Two-Photon Photoelectron Spectroscopy (2PPE). 2PPE uses two short laser pulses for the emission of electrons. The first pulse excites the electrons into the image potential states, the second pulse emits them into free electron states. Measurements were performed using a display analyzer, which allows to detect electrons from a large range of emission angles. With this method binding energies and dispersion of image-potential states were determined.

O 5.2 Mon 11:30 H34

### Image-Potential Resonances on Al(100)

— •Matthias Schult, Manuel Marks, Jens Güdde, and Ulrich Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, 35032 Marburg, Germany

The Hydrogen-like image-potential (IP) states provide a well understood model system to study electron dynamics at metal surfaces. The energy of these states is usually located within the projected bulk band gap, which limits the penetration of the excited electrons into the bulk. In many surface phenomena that are connected to electron transfer, however, electronic resonances, i.e. electronic states at the surface that are resonant with bulk states, play an important role.

At Al(100) the vacuum energy lies 6 eV above the projected bulk band gap and the whole series of IP states form surface resonances with strong coupling to bulk states. Excited electrons in these resonances can not only decay by electron-hole pair excitation, but can also scatter elastically into the bulk. Therefore, much shorter lifetimes and broader linewidths compared to noble metal surfaces can be expected.

In this talk we present experimental results on the energies and lifetimes of IP resonances on the Al(100) surface obtained by time-resolved two-photon photoemission. In the photoelectron spectra the first members of the IP resonance series up to $n = 3$ could be resolved. For $n \geq 3$ lifetimes that are longer than the experimental time-resolution of 60 fs could be observed. We will compare the experimental results to calculations using a one-dimensional model potential, which predict binding energies and the elastic contribution to the lifetimes.

O 5.3 Mon 11:45 H34

### Time and angle-resolved photoelectron spectroscopy of solids using femtosecond high-harmonic-generation pulses

— •Timm Rohwer, Martin Wiesenmayer, Stefan Hellmann, Kai Rossnagel, Lutz Kipp, and Michael Bauer — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel

Angle-resolved photoelectron spectroscopy (ARPES) has emerged as a leading technique in identifying static key properties of complex electron systems. In a pump-probe scheme using femtosecond XUV pulses this technique can be extended to monitor ultrafast changes in the electronic valence and core-level structure in response to an intense optical excitation. In this contribution we present first time-resolved ARPES data from Pt(111) recorded with a 3 kHz high-harmonic-generation source. A multilayer mirror monochromator guarantees a LAPE (laser-assisted photoemission) cross-correlation trace shorter than 35 fs, mainly governed by the width of the 800 nm excitation pulses. We furthermore proof the capability of this technique to monitor ultrafast band structure phenomena over the whole Brillouinzone.

O 5.4 Mon 12:00 H34

### One- and two-photon photoemission from Si(100)

— •Thomas Fauster[1], Shin'ichiro Tanaka[2], and Katsumi Tanimura[2] — [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

One- and two-photon photoelectron spectra with the same total photon energy should give information on the same initial and final states. Differences show the influence of intermediate states in two-photon photoemission (2PPE). Of particular interest are bulk bands where the conservation of perpendicular momentum leads to peak shifts, resonances and peak narrowing [1,2].

We have measured one- and two-photon photoemission from Si(100)(2×1) in normal emission using frequency-quadrupled and -doubled femtosecond laser radiation with a total photon energy around 6 eV for s- and p-polarized light incident at 45°. Differences and common features in the various spectra are analyzed and discussed.

[1] Schattke *et al.*, Phys. Rev. B **78**, 155314 (2008).

[2] Pontius *et al.*, Phys. Rev. B **72**, 115105 (2005).

O 5.5 Mon 12:15 H34

### Ultrafast Electron Transfer Dynamics at Phosphorus-Metal Interfaces

— •Florian Blobner, Stefan Neppl, and Peter Feulner — Physik-Department E20, TU-München, Germany

Ultrafast electron transfer reactions in heterogeneous systems are of paramount interest in both fundamental research and technology.

To obtain a better understanding of the underlying mechanisms of ultrafast charge transfer, we investigated the simplest model system, a reactive atom adsorbed on a surface. Using the core hole clock spectroscopy, we studied the influence of the electronic and structural properties of different adsorbate-substrate systems on the charge transfer dynamics. We investigated the following three systems: P/Ru(0001) with two different adsorbate superstructures and P/Cu(111).

Our analysis shows that the charge transfer of the excited phosphorus P2s electron to the conduction band of the Ru(0001) occurs on a timescale of a few femtoseconds down to several hundred attoseconds and is not affected by the symmetry of the adsorbate superstructure nor by the polarization of the electric field. In contrast to that, no evidence for an electron localization could be found for Phosphorus adsorbed on the Cu(111) surface. Our investigations also proved that both P/Ru(0001) systems are well suited for further analysis with the attosecond streaking technique which allows insight into the real time dynamics of the system.

Supported by the Excellence Cluster Munich-Centre for Advanced Photonics (project C1.5). We also thank the staff of BESSY for help during the experiments.

O 5.6 Mon 12:30 H34

### Attosecond photoelectron spectroscopy of solids

— •Elisabeth Magerl[1], Adrian L. Cavalieri[1], Ralph Ernstorfer[2], Stefan Neppl[2], Nicholas Karpowicz[1], Michael Stanislawski[1], Elisabeth Bothschafter[1], Dietrich Menzel[2], Johannes V. Barth[2], Peter Feulner[2], Ferenc Krausz[1,3], and Reinhard Kienberger[1,2] — [1]Max Planck Institute of Quantum Optics, Garching, Germany — [2]Technical University of Munich - E20, E11, Garching, Germany — [3]Ludwig Maximilians University, Munich, Germany

The dynamics of the photoelectric effect in single-crystals are investigated on the attosecond time scale. An isolated attosecond XUV-pulse is used to excite photoelectrons, while a few-cycle waveform-controlled NIR-pulse modulates the kinetic energy of the emitted photoelectrons. Recently, applying this streaking technique a relative time delay in emission on the order of 100 attoseconds between electrons originating from different electronic levels in tungsten was already revealed [1].

In order to further study the delay and its possible dependence on material properties and on laser parameters, several streaking measurements on different systems were carried out: We present results obtained on single-crystalline tungsten and rhenium, measured with XUV photon energies of 90 and 130 eV. We also show measurements on a combined system of a single crystal substrate with an adsorbed monolayer of a rare gas.

[1] A. L. Cavalieri et al., Nature **449**, 1029 (2007)

O 5.7 Mon 12:45 H34

### 1*T*-TiSe$_2$: Ultrafast Dynamics in the CDW Phase

— •Stephan Hilgenfeldt, Martin Wiesenmayer, and Michael Bauer — Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24098 Kiel, Germany

At $T \approx 200$ K the transition metal dichalcogenide 1*T*-TiSe$_2$ undergoes a phase transition into a charge density wave (CDW) phase which is accompanied by the formation of a (2×2×2) superlattice. The origin of this CDW phase has been under discussion for a long time and recent photoemission experiments give evidence for an excitonic insulator phase to play a key role in the understanding of this system. In this talk we present pump-probe photoemission results of 1*T*-TiSe$_2$ in the CDW state in the weak excitation regime. We are able to monitor an optically induced weakening of the CDW phase taking place within 250 fs and we follow the subsequent dynamics of this perturbation further into the picosecond time regime. Our results will be discussed under consideration of the excitonic insulator model for TiSe$_2$.

# O 6: Metal substrates: Adsorption of organic / bio molecules I

Time: Monday 11:15–13:00 Location: H36

O 6.1 Mon 11:15 H36

**Phase boundaries in organic adlayers – a quantitative video-STM study** — •Michael Roos, Harry E. Hoster, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

Bis(terpyridine)derivatives (BTP) form highly ordered hydrogen-bonded networks on different substrates at solid surfaces [1,2]. Using time resolved scanning tunneling microscopy (STM), we have studied dynamic phenomena in such adlayers on Ag/Ru(0001) at room temperature. BTP molecules on Ag/Ru(0001) form coverage dependent networks with different hydrogen bonding configuration. At low coverages, a parallel chain structure (PCS) is formed in coexistence with a two-dimensional admolecule gas. At higher coverages, domains of a locally more densely packed quasi quadratic network (QQN) are formed [2]. Time resolved STM imaging at QQN|PCS phase boundaries reveals a continuous exchange of molecules between both phases as indicative for a dynamic equilibrium. Based on a statistical evaluation of the STM sequences, we show that the anisotropy of the molecule-molecule interactions is not only reflected in the periodic structures of the 2 adlayers, but also in the probability of different types of local rearrangements at the phase boundary.

[1] M. Roos et al., *Phys.Chem.Chem.Phys.* 9, **2007**, 5672.

[2] H. E. Hoster et al., *Langmuir* 23, **2007**, 11570.

O 6.2 Mon 11:30 H36

**Adsorption of Bis(terpyridine) studied with DFT and Force Field Methods** — •Daniela Künzel and Axel Gross — Institute for Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

Bis(terpyridine) (BTP) molecules can form a number of different ordered surface structures on metal and graphite substrates [1]. The structural variability in combination with easily modifiable properties turn the BTP molecules into interesting candidates for theoretical and experimental studies.

Both DFT and force field methods are used to study the formation and modification of 3,3'-BTP and 2,4'-BTP surface structures. Self-assembling into ordered monolayers is directed by the formation of weak intermolecular C-H$\cdots$N hydrogen bonds and by van-der-Waals and $\pi$-$\pi$ interactions with the surface. Depending on the BTP isomer, substrate and adsorption conditions, different phases can be observed and their stability estimated. The modification of the surface structures by the formation of host-guest systems or by the interaction with additional oxygen will also be addressed.

[1] C. Meier, M. Roos, D. Künzel, A. Breitruck, H.E. Hoster, K. Landfester, A. Groß, R. J. Behm and U. Ziener, J. Phys. Chem. C (2009), DOI: 10.1021/jp910029z.

O 6.3 Mon 11:45 H36

**Alkali-Crown Ether Complexes at Metal Surfaces** — •Nicha Thontasen[1], Giacomo Levita[2], Zhitao Deng[1], Nikola Malinowski[1,3], Stephan Rauschenbach[1], and Klaus Kern[1,4] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]University of Trieste, Trieste, Italy — [3]Bulgarian Academy of Sciences, Sofia, Bulgaria — [4]EPFL, Lausanne, Switzerland

Crown ethers are polycyclic ethers which, in solution, selectively bind cations depending on the size of the ring cavity. The study of a single host-guest complex is highly desirable in order to reveal the characteristics of these specific interactions at the atomic scale. Such detailed investigation is possible at the surface where high resolution imaging tools like scanning tunneling microscopy (STM) can be applied.

Here, electrospray ion beam deposition (ES-IBD) is employed for the deposition of Dibenzo-24-crown-8 (DB24C8)-H+, -Na+ and -Cs+ complexes on a solid surface in ultrahigh vacuum (UHV). Where other deposition techniques have not been successful, this deposition technique combines the advantages of solution based preparation of the complex ions with a highly clean and controlled deposition in UHV.

Single molecular structures and the cation-binding of DB24C8 at the surface are studied in situ by STM and MALDI-MS (matrix assisted laser desorption ionization mass spectrometry). The internal structure of the complex, i.e. ring and cavity, is observable only when alkali cations are incorporated. The BD24C8-H+ complex in contrast appears as a compact feature. This result is in good agreement with theoretical models based on density functional theory calculations

O 6.4 Mon 12:00 H36

**STM/STS study of Spiro-DPO molecules on Au(111)** — •Michael H. Waelsch[1], Tatjana Podlich[1], Melanie Klinke[1], Tobat P. I. Saragi[2], Josef Salbeck[2], and René Matzdorf[1] — [1]Universität Kassel, Experimentalphysik II, — [2]Universität Kassel, AG Makromolekulare Chemie und Molekulare Materialien, FB 18 Naturwissenschaften, Heinrich-Plett-Str. 40, 34132 Kassel

In the Spiro-DPO molecule an electron transport material (donor) is linked to a hole transport material (acceptor) via a Spiro-C-atom.

The arrangement of about 1/10 ML Spiro-DPO on a Au(111)-substrate has been investigated with respect to the molecular energy-levels by STM/STS in UHV at 4.8 K. We observed amorphous clusters of molecules, which showed obvious shifts in their HOMO- and LUMO-energies, if the sample was annealed above the glass transition temperature. The shifts may be due to screening by the surrounding molecules. Without annealing the molecules arrange in rings, double rows and chains, depending on the underlying Au(111)-herringbone-reconstruction. In these structures the HOMO/LUMO-levels measured with STS are less shifted than in the amorphous clusters.

O 6.5 Mon 12:15 H36

**Charging and decharging single molecules** — Dagmar Kreikemeyer-Lorenzo, Isabel Fernandez-Torrente, Anna Strozecka, •Katharina J. Franke, and Jose I. Pascual — Fachbereich Physik, Freie Universität Berlin, Germany

The charge state of molecules on surfaces crucially influences their reactivity, electronic transport properties and magnetic state. The mixture of the charge transfer compounds tetramethyl-tetrathiafulvalene (TMTTF) and tetracyanoquinodimethane (TCNQ) on a Au(111) surface leads to a self-assembled monolayer of homomolecular rows. In these structures, the majority of TCNQ becomes charged by accepting a single electron in its lowest unoccupied molecular orbital as evidenced by a Kondo resonance in STM transport experiments. Using the STM tip we can manipulate the charge state and thus its magnetic properties. The charging/decharging depends strongly on the position of the tip above the molecular structures and the applied bias voltage.

O 6.6 Mon 12:30 H36

**An unusual approach to the description of bonding of chemisorbed conjugated molecules on noble metals** — •Gerold M. Rangger[1], Lorenz Romaner[2], Oliver T. Hofmann[1], Michael G. Ramsey[3], and Egbert Zojer[1] — [1]Institut für Festkörperphysik, Technische Universität Graz, Austria — [2]Lehrstuhl für Atomistic Modeling and Design of Materials, Montanuniversität Leoben, Austria — [3]Institut für Physik, Karl-Franzens Universität Graz, Austria

The deposition of organic monolayers on metals has attracted significant interest as a tool to modify surfaces in the field of molecular electronics.

We present a theoretical study of the acceptor F4TCNQ on Ag(111) and the donor viologen on Au(111). There, experiments show pronounced changes in the UPS spectra of the molecules due to strong interactions with the surfaces. To understand the bonding mechanism, we use a projection of the density of states onto atomic and molecular orbitals in combination with a crystal orbital overlap type population analysis. This enables analyzing the molecular orbital occupation and the determination of bonding and anti-bonding contributions of molecular/atomic orbitals on the energy scale. Only a simultaneous examination of adsorption induced changes of the molecular geometry (including a bending of the molecule) and of the interaction between molecule and metal allows to arrive at a consistent picture for the investigated chemisorption processes.

O 6.7 Mon 12:45 H36

**A new charge-transfer complex in UHV-deposited tetramethoxypyrene and TCNQ** — •Katerina Medjanik[1], Sergej Nepijko[1], Gerd Schönhense[1], Milan Rudloff[2], Vita Solovyeva[2], Michael Huth[2], Shahab Naghavi[3], Claudia Felser[3], Martin Baumgarten[4], and Klaus Müllen[4] — [1]Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz, Germany — [2]Physikalisches Institut, Goethe-Universität, 60438 Frankfurt, Germany — [3]Institute für Analytische und Anorganische Chemie, Johannes Gutenberg-Universität, 55099 Mainz, Germany — [4]Max-Planck-Institute for Polymer Research, 55128 Mainz, Germany

A study of the UHV-deposited mixed phase of tetramethoxypyrene (TMP) and TCNQ has been performed using UPS, X-ray-diffraction, and infrared spectroscopy. Formation of a new intermolecular compound is evident from the appearance of new reflexes in XRD ($d_1$=0.911 nm, $d_2$=0.684 nm). In UPS characteristic shifts of the level positions indicate a charge transfer from TMP to TCNQ, being suggested also by the softening of the CN stretching vibration of TCNQ visible in IR spectroscopy (shift by 7 $\mathrm{cm}^{-1}$). The size of the level shift is similar to shifts observed for the acceptor-donor pair hexaketo-/hexamethoxycoronene. In SEM and AFM micro crystals with sizes in the sub-micrometer range are visible, similarly as previously found for BEDT-TTF / TCNQ [1]. A DFT calculation serves as guideline for interpretation of the spectra. Project funded via Transregio SFB TR49 and Graduate School of Excellence MAINZ.

[1] V. Solovyeva *et al.*, Thin Solid Films **517**, 6671 (2009)

## O 7: Spin-Orbit Interaction at Surfaces I

Time: Monday 11:15–12:45 Location: H38

O 7.1 Mon 11:15 H38

**Spin filtering by Self-Assembled Organic Monolayers on gold** — •Benjamin Göhler[1], Volker Hamelbeck[1], Matthias Kettner[1], Georg F. Hanne[1], Helmut Zacharias[1], and Ron Naaman[2] — [1]Physikalisches Institut, Universität Münster — [2]Department of Chemical Physics, The Weizmann Institute, Israel

Electron dichroism has been reported for vapours of chiral molecules [1]. Because of different interactions of spin-polarized electrons with chiral molecules the attenuation of polarized electron beams depends on the helicity of the electrons. Similarly the photoelectron yield of gold covered with organized organic thin films of chiral molecules shows a dependence on the circular polarization of the incident light, because the spin polarized photoelectrons of the gold substrate interact differently with the thin film [2]. In this presentation we show that these photoelectrons are in fact spin-polarized. Photoelectrons are emitted by 210 nm (5.9 eV) laser radiation which is sufficient to emit photoelectrons of the gold substrate but not to ionize the molecules of the organic layer. The self assembled layer of chiral molecules (ds-DNA) filters the electrons with a spin polarization of about 20%. The spin polarization is measured by a calibrated mini Mott analyzer.

[1] J.Phys.B. 30, 5491, 1997. [2] Science 283, 814, 1999.

O 7.2 Mon 11:30 H38

**Spin spirals with unique rotational sense in magnetic thin films: Cr on W(110)** — •Bernd Zimmermann[1], Marcus Heide[1,2], Gustav Bihlmayer[1], and Stefan Blügel[1] — [1]Institut für Festkörperforschung (IFF) und Institute for Advanced Simulation (IAS), Forschungszentrum Jülich — [2]Department of Precision Engineering, Osaka University, Japan

Recently [1] for a Mn monolayer on W(110) a new and unexpected magnetic phase was discovered which exhibits a left rotational sense of the magnetization. The origin was explained by the presence of Dzyaloshinskii-Moriya Interaction (DMI) caused by the spin orbit coupling in a symmetry-broken environment of the surface. In this work we present investigations on the magnetic structure of a single Cr layer on W(110) by means of density functional theory (DFT). We perform spin-spiral calculations including SOC and find that the DMI is strong enough to compete with the symmetric exchange interaction to create a spiraling magnetic structure with unique rotational sense. A layer-resolved analysis shows, that the main contribution to the DMI comes from the W interface atoms. Using a micromagnetic model, we determine how far the spin spiral deviates from a perfectly homogeneous solution. We compare our results to the systems Mn/W(110) and Fe/W(110), where the direction of the spin spiral and the period length are different. Our results are confirmed by SP-STM experiments [2].

[1] Bode *et al.*, Nature **447**, 190 (2007)

[2] Santos *et al.*, New J. of Phys. **10**, 013005 (2008)

O 7.3 Mon 11:45 H38

**Spin-orbit and exchange interaction of the surface state on Au/Ni(111)** — •Andreas Nuber[1], Frank Forster[1], Hendrik Bentmann[1], Jürgen Braun[2], and Friedrich Reinert[1,3] — [1]Experimentelle Physik VII, Universität Würzburg, Germany — [2]Dep. Chemie und Biochemie, LMU München, Germany — [3]Forschungszentrum Karlsruhe, Gemeinschaftslabor für Nanoanalytik, Germany

The surface state of Au(111) is a standard model of spin-orbit Rashba-type splitting, visible in ARUPS as two parabolas shifted in $k_{||}$-direction. On Ni(111), the surface state is split in energy due to exchange interaction. Both interactions are expected to be present on the surface of thin Au films grown on Ni(111). We used high resolution ARUPS to investigate the system Au/Ni(111) for different Au layer thicknesses and compared our experimental data with photoemission calculations based on LSDA and DMFT. Due to the integrating properties of photoemission we could not resolve a combination of spin-orbit and exchange splitting on unmagnetized samples. But magnetizing the Ni(111) substrate in-plane can change this in principle.

O 7.4 Mon 12:00 H38

**Spin-polarized topological surface states of topological insulators $Bi_2Te_3$ and $Bi_2Se_3$** — •Markus R. Scholz[1], Dmitry Marchenko[1], Andrei Varykhalov[1], Oliver Rader[1], Andrey Volykhov[2], and Lada V. Yashina[2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie — [2]Department of Chemistry, Moscow State University

The topological insulator has been proposed as new state of quantum matter in 2005 [1]. A gap in the two-dimensional bulk is crossed by one-dimensional states which occur as pairs in which the spin of each partner is connected to its propagation direction. A generalization towards three-dimensional solids predicted topological insulator properties for Bi10%Sb and $Bi_2Te_3$ [2]. Spin resolution is crucial for distinguishing the topological from ordinary surface states in experiment as was shown for Bi10%Sb [3]. For $Bi_2Te_3$ only spin-averaged data exists [4]. We grew $Bi_2Te_3$ and $Bi_2Se_3$ single crystals by the Bridgeman method and conducted spin- and angle-resolved photoemission. For both systems, the spin-resolved spectra show that the surface state forms a single non-degenerate Dirac cone with the Kramers degeneracy point at $\overline{\Gamma}$. Spin- and angle-resolved spectra above and below the Kramers point and for positive and negative $\mathbf{k}_{||}$ clearly show the spin-momentum relation expected for the surface of a topological insulator.

[1] C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 146802 (2005); 226801 (2005) [2] L. Fu and C. L. Kane, Phys. Rev. 76, 045302 (2007) [3] D. Hsieh et al., Science 323, 920 (2009) [4] Y. Xia et al., Nature Phys. 5, 398 (2009)

O 7.5 Mon 12:15 H38

**Tight-binding treatment of Dzyaloshinskii-Moriya interaction on surfaces** — •Timo Schena[1], Yuriy Mokrousov[1], Phivos Mavropoulos[1], Cyrille Barreteau[2], and Stefan Blügel[1] — [1]Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]CEA Saclay, IRAMIS, SPCSI Bat. 462, F-91191 Gif sur Yvette, France

The Dzyaloshinskii-Moriya interaction (DMI) was recently discovered to be important in determining the magnetic properties of thin films and nanostructures. Little is known about the strength and the sign of DMI as function of the chemical composition. We report the development of a self-consistent, parametrized tight-binding code able to treat bulk-systems, films, one-dimensional structures and clusters of high magnetic complexity. It is optimally designed to study the effects arising due to interplay of non-collinear magnetic order, spin-orbit coupling and broken symmetries at surfaces. The self-consistency is based on a simple Stoner model and consideration of the Mulliken-charges of each atom for charge neutrality. To demonstrate the applicability of the developed method we investigate the occurrence of DMI in 3d transition-metal overlayers on substrates of heavy elements.

O 7.6 Mon 12:30 H38

**In-situ UPS studies into hydrogen terminated surface of amorphous carbon films and its direct effects on electron emission** — •Daniel Chua — National University of Singapore, Singapore

The effects of hydrogen terminated surface of single crystal diamond are well known. This imparts unique properties such as p-type transfer doping and enhanced surface conductivity to the diamond films. In this work, the effects of surface hydrogenation on non-hydrogenated tetrahedral amorphous carbon (ta-C) films are systematically studied and for the first time, we report that the hydrogen termination directly leads to a lowering of the turn-on field for ta-C films, resulting in electron emission from an ultra-smooth thin film without any pre-conditioning process. Prior, HREELS confirmed the presence of C-H bonds on the surface after microwave plasma CVD system was used to hydrogenate the surface of the ta-C films. In-situ UPS shows the hydrogen terminated surface reduces the work function by $> 1$ eV and is highly stable up to 600oC. Surface roughness from an AFM shows minimal changes to the morphology during the various process. Enhancement effects are distinctly observed when the surface hydrogenated ta-C films are directly tip-coated on vertically aligned carbon nanotubes. These hybrid core-shell structures have potential applications as cold cathode source due to the very low turn-on field.

## O 8: [DS] Organic Electronics and Photovoltaics I (Joint Session DS/CPP/HL/O)

Time: Monday 10:15–12:30 Location: H8

O 8.1 Mon 10:15 H8

**Colour tuneable light-emitting transistor** — •Eva J. Feldmeier, Christian Melzer, and Heinz von Seggern — Electronic Materials Department, Institute of Materials Science Technische Universität Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany

In recent years the interest in ambipolar organic light-emitting field-effect transistors has increased steadily as the devices combine switching behaviour of transistors with light emission. Usually, small molecules and polymers with a band gap in the visible spectral range serve as semiconducting materials. Mandatory remain balanced injection and transport properties for both charge carrier types to provide full control of the spatial position of the recombination zone of electrons and holes in the transistor channel via the applied voltages. As will be presented here, the spatial control of the recombination zone opens new possibilities towards light-emitting devices with colour tuneable emission.

In our contribution an organic light-emitting field-effect transistors is presented whose emission colour can be changed by the applied voltages. The organic top-contact field-effect transistor is based on a parallel layer stack of acenes serving as organic transport and emission layers. The transistor displays ambipolar characteristics with a narrow recombination zone within the transistor channel. During operation the recombination zone can be moved by a proper change in the drain and gate bias from one organic semiconductor layer to another one inducing a change in the emission colour. In the presented example the emission maxima can be switched from 530 nm to 580 nm.

O 8.2 Mon 10:30 H8

**Improved transport properties of p-i-i small molecule solar cells deposited on heated substrates** — •Steffen Pfuetzner, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, Technische Universität Dresden

To achieve higher efficiencies in organic solar cells, ideally the open circuit voltage ($V_{OC}$), fill factor (FF) as well as the short current density ($j_{SC}$) have to be improved further. However, in bulk heterojunction (BHJ) solar cells jsc and the FF are typically limited by charge carrier recombination due to transport problems (e.g. low mobility, dead ends) in the BHJ. A suitable way to modify the BHJ layer morphology and to improve solar cell parameters is substrate heating during bulk layer deposition. Furthermore, $j_{SC}$ can be enhanced by replacing $C_{60}$ by $C_{70}$. We show that substrate heating at 90°C leads to improved FF and $j_{SC}$ for a $C_{60}$ and ZnPc containing BHJ solar cell with the following stack structure: ITO/p-Di-NPD/$C_{60}$:ZnPc/$C_{60}$/BPhen/Al. However, in case of similar $C_{70}$:ZnPc solar cells, no significant improvements are observed. Using SEM we show that the preferential aggregation by heating is completely suppressed by the p-doped underlayer Di-NPD. To force aggregation of the heated $C_{70}$:ZnPc bulk, 5 nm intrinsic ZnPc layer is deposited on the p-Di-NPD layer and verified by SEM. J-V characteristics show a drop in FF and Voc with the additional interlayer ZnPc. To overcome this problem probably caused by transport barriers to the neighboring layers, experiments with doped ZnPc are carried out.

O 8.3 Mon 10:45 H8

**Analysis of Chemical Degradation Mechanism of Phosphorescent Organic Light Emitting Devices by Laser-Desorption/Ionization Time-of-Flight Mass Spectrometry** — •Ines Rabelo de Moraes, Sebastian Scholz, Björn Lüssem, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, 01062 Dresden, Germany

Phosphorescent Organic Light Emitting diodes (OLEDs) have attracted much interest for their potential application in full color flat-panel displays and as an alternative lighting source. However, low efficiency, and the short operation lifetime, in particular in the case of blue emitting devices, are the major limitations for the current OLEDs commercialization. In order to overcome these limitations, a deep knowledge about the aging and the degradation mechanism is required [1]. Our work focuses on the chemical degradation mechanism of different iridium based emitter materials like FIrpic (light blue) and Ir(ppy)3 (green), commonly used in OLEDs. For this purpose, the devices were aged by electrical driving until the luminance reached 6% of the initial luminance. The laser-desorption/ionization time-of-flight mass spectrometry was used to determine specific degradation pathways.

[1] Hany Aziz, and Zoran D. Popovic, Chem. Mater. 16, 4522 (2004).

O 8.4 Mon 11:00 H8

**Spatially resolved, polarization dependent absorption and photocurrent measurements of pentacene based OFETs** — •Christian Westermeier, Matthias Fiebig, and Bert Nickel — Department für Physik and CeNS, Ludwig-Maximilians-Universität, Geschwister-Scholl-Platz 1, 80539 München

Pentacene is a promising candidate for organic electronics and optoelectronic applications due to its high charge carrier mobility and strong absorption properties. Forming a triclinic herringbone structure, its optical properties are highly anisotropic [1]. Pentacene films show a thin-film-phase texture. The grains inducing the texture should absorb linear polarised light depending on their orientation with respect to the direction of polarisation.

Here we use local illumination of the transistor channel in a confocal laser scanning setup with a spatial resolution in the submicron regime [2]. The pentacene grains in the channel of our OFETs exhibit a size of a few microns in diameter. The absorption of separate grains is found to be strongly dependent on the polarisation of the incident light, as expected. Thus, the scanning technique allows for imaging of grain orientation with a submicron resolution over large areas.

Absorption being the initialising step to generate excitons is important for optoelectronic devices like solar cells and the photoresponse of transistors. The influence of polarisation on the spatially resolved photocurrent of pentacene OFETs will be discussed.

[1] M. Dressel, et al., Opt. Express 16, 19770-19778 (2008)
[2] M. Fiebig, et al., Appl. Phys. A 95, 1, 113-117 (2009)

O 8.5 Mon 11:15 H8

**In-situ Analysis of Charge Carrier Mobility in Field Effect Transistors During Organic Semiconductor Deposition** — •Christopher Keil, Dominik Klaus, Jan Hartel, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de

Films of $F_{16}PcCu$ prepared by physical vapour deposition under high vacuum conditions were characterized in situ during the growth from the monolayer range up to about 100 nm. The charge carrier mobility in the linear and saturation region as well as the threshold voltage were investigated in real time at deliberate film thickness by help of a real time analysis software routine. The organic films were deposited on thermally grown silicon oxide which also acts as gate dielectric. The underlying Si wafer served as a bottom gate electrode and structured inter-digital metal source- drain contacts were prepared by photolithography. Different channel lengths and widths as well as different metal contacts were used to determine the influence of semiconductor/metal contacts on the characteristics of the field effect transistors.

O 8.6 Mon 11:30 H8

**Investigation of contact properties of organic field effect transistors** — •M. Grobosch[1], I. Hörselmann[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 P3HT were characterized by combined X-ray and ultra violet photoemission spectroscopy (XPS, UPS) and electrical measurements of the OFET whereas the sample preparation for the different measuring principles has been realized in parallel differing in the layer thickness of the polymer. By means of UPS a reduced work function could be demonstrated for different prepared, sputtered, and as-received Au contacts in agreement with previous publications. Furthermore the chemistry and the electronic structure of the interfaces between Au metal deposited onto thin films of solution prepared modified P3HT on sputtered Au contacts have been studied. From the observed well defined molecular orbitals we have found an interface dipole of $+1.5$ eV and a hole injection barrier of about 0.6 eV. However, one cannot expect such a high barrier from the measured characteristics of the OFET because the currents are not contact limited. Clarifying the reason for such a discrepancy we have carried out two-dimensional simulations. These results confirm clearly for a barrier of 0.6 eV strongly reduced drain currents would be measured. The difference in the layer thickness can be the reason for the measured difference but further investigations are necessary to explain more in detail this phenomenon.

O 8.7 Mon 11:45 H8

**Improving the mobility of the CuPc OFETs by variing the substrate preparation** — •Iulia G. Korodi[1], Daniel Lehmann[1], Michael Hietschold[2], and Dietrich R. T. Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Solid Surfaces Analysis Group, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Top-contact organic field-effect transistors (OFETs) using Copper Phthalocyanine (CuPc) as active layer were produced under high vacuum conditions ($p \leq 5 \times 10^{-7}$ mbar). 20 nm thick organic films were deposited by Organic Molecular Beam Deposition on highly p-doped Si(100) substrates with 100 nm $SiO_2$ as the gate dielectric. Source and drain electrodes of gold were deposited through a shadow mask on top of the organic layer with the substrate cooled by liquid nitrogen.
The performance of the OFETs was tested in vacuum as well as in atmosphere. The highest mobility of CuPc OFETs was found to be $\mu_{vacuum} = (1.5 \pm 0.6)\,10^{-3}\,\mathrm{cm}^2/\mathrm{Vs}$. When the substrate was modified by applying an elevated temperature (130 °C) during deposition of the CuPc film the mobility of the OFETs increased by a factor of $\approx 6$. The threshold voltage was also improved from a value of $V_{Th} = -(15.0 \pm 0.3)$ V to $V_{Th} = -(9.6 \pm 1.4)$ V for deposition at room and elevated substrate temperatures, respectively. A similar effect on the electrical characteristics was found after modifying the gate dielectric with a self-assembled monolayer of n-octadecyltrichlorosilane. The improved OFET performance with the variation of the substrate conditions will be discussed.

O 8.8 Mon 12:00 H8

**Electrical characterization of operating OFETs using Kelvin Probe Force Microscopy** — •Franziska Lüttich, Harald Graaf, Iulia G. Korodi, Daniel Lehmann, Dietrich R. T. Zahn, and Christian von Borczyskowski — Center for nanostructured Materials and Analytics, Chemnitz University of Technology, Germany

We present recent results on n-type organic field effect transistors (OFETs) using Atomic Force Microscopy (AFM) and Kelvin Probe Force Microscopy (KPFM). These studies allow the local potential in the channel of OFETs during operation to be determined. The transistor structures investigated differ in gate insulator treatment and substrate temperature during evaporation of the organic material.
All investigated top-contact OFETs were fabricated under high-vacuum conditions ($p < 4 \cdot 10^{-7}$ mbar) by evaporating PDI8-$CN_2$ on top of a p-doped silicon substrate covered by a $SiO_2$ layer. Gold-electrodes were evaporated through a shadow mask on top of the organic layer. The gate insulator modification was implemented prior to the substrate transfer into the vacuum chamber. For this purpose monolayers of N-octadecyltrichlorosilane (OTS) resulting in hydrophobic surfaces were employed. In the case of deposition at elevated temperature the substrate was kept at 130°C.
These variations of preparation influence the structural and electronic properties of the OFET and result in changes of the charge carrier mobility. The effects observed indicate tuning possibilities for organic devices leading to increased charge carrier mobility.

O 8.9 Mon 12:15 H8

**Experimental study and time dependent modeling of OFETs with solid electrolyte gate dielectrics** — •Katharina Schätzler[1], Klaus Schmidt[1], Walter Fix[1], Gottfried Döhler[1], and Heiko Weber[2] — [1]PolyIC GmbH & Co. KG, Fürth — [2]Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität, Erlangen

We successfully investigated and simulated organic field effect transistors (OFETs) with a solid organic insulator containing ionic salt. It is already well known that electrolytes as gate dielectrics in OFETs offer low operating voltages by means of a high capacitance. Hence, the charge carrier density is increased in the channel region of the semiconductor. However, the drain-source current $I_{ds}$ shows a strong time dependency because of the limited mobility of the ions. Consequently we developed a time dependent model for the spatial distribution of the ionic current within the insulator matrix. The ionic current of both cations and anions splits in a diffusion and a drift process. The model very precisely reproduces the time as well as the ion concentration dependency of $I_{ds}$. Parameters like ion and semiconductor mobility are extracted and are in good agreement with parameters extracted from experimental OFET and capacitance characteristics.

## O 9: Invited talk (Hartmann, Nils)

Time: Monday 14:00–14:45 Location: H36

**Invited Talk** O 9.1 Mon 14:00 H36

**Sub-Wavelength Patterning of Ultrathin Organic Coatings via Nonlinear Laser Processing** — •Nils Hartmann — Fakultät für Chemie, CeNIDE, NETZ, Universität Duisburg-Essen, Germany

Laser patterning represents a key step in many technological applications. The lateral resolution, however, usually is limited by optical diffraction. A means to enhance the lateral resolution takes advantage of nonlinear effects. In photothermal laser processing, for example, a focused laser beam is used to locally heat the substrate surface and to thermally initiate chemical reactions. For this reason, photothermal processing is highly nonlinear in laser power density and facilitates sub-wavelength patterning. Femtosecond laser processing, as another example, provides promising perspectives in sub-wavelength patterning via multiphoton absorption processes. A general account on recent achievements in nonlinear laser patterning of ultrathin organic coatings, such as self-assembled monolayers and supported lipid membranes, is given [1-3]. Because of their exceptional stability, nonlinear laser processing of silane-based monolayers is most effective [1-2]. In particular, photothermal laser processing at $\lambda = 514$ nm and a 1/e spot diameter of 1.8 $\mu$m allows one to fabricate functional surface structures with lateral dimensions well below 100 nm [1]. Such structures are used as reactive templates to build up functional surface nanostructures via directed self-assembly of nanoscopic components.

[1] D. Dahlhaus et al., Nano Lett. 6 (2006) 2358.
[2] N. Hartmann et al., APL 92 (2008) 223111.
[3] M. Mathieu et al., Small 5 (2009) 2099.

# O 10: Methods: Electronic structure theory & Methods: other (theory)

Time: Monday 15:00–17:15 Location: H31

O 10.1 Mon 15:00 H31

**The importance of van der Waals dispersion forces in ice** — •Biswajit Santra[1], Angelos Michaelides[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany. — [2]University College London, London, UK.

For decades it is known that the condensed phases of water are held together through a combination of hydrogen bonds (HBs) and van der Waals (vdW) dispersion forces. Whilst HBs have received widespread attention, relatively little is known about the importance of vdW forces. Partly this is down to the now most popular electronic structure theory (density-functional theory (DFT)) providing an inadequate description of vdW forces when standard exchange-correlation functionals are used. However, improved semi-empirical vdW corrections to DFT[1] and the non-local vdW functional[2] mean that it is now possible to shed light on this issue. Here, we report simulations on a range of ambient and high pressure phases of ice to understand the delicate interplay of HBs and vdW. We find that the proportion of the lattice energy coming from vdW forces monotonously increases as the density of the ice phases increases, and as a consequence vdW plays a crucial role in determining the relative stabilities of the high density phases of ice. In addition, our calculations show that the effective volume of the water molecules is reduced when vdW is accounted for and provide general insights into the importance of vdW forces in other condensed phases of water. [1]Tkatchenko *et al.*, PRL **102**, 073005 (2009), [2]Dion *et al.*, PRL **92**, 246401 (2004).

O 10.2 Mon 15:15 H31

**Density functional calculations for thousands of atoms: KKRnano - recent developments and first applications** — •Alexander Thiess[1,2], Rudolf Zeller[2], and Stefan Blügel[2] — [1]German Research School for Simulation Sciences, 52425 Jülich, Germany — [2]Institut für Festkörperforschung and Institute for Advanced Simulation, Research Center Jülich, 52545 Jülich, Germany

KKRnano is a new massively parallel DFT-algorithm in the framework of the KKR Green function method [1] we have developed for large-scaled applications on state-of-the-art supercomputers. The advantageous scaling of our code enables to exceed the limits of most of today's DFT-algorithms of hundreds of atoms per unit cell by one order of magnitude. In order to deal with the enormous computational requirements of such calculations we have parallelized our code in real space, spin space, over energies and with respect to angular momentum. This allows for an efficient use of hundreds of thousands of processors. We present recently developed extensions as a fast parallel Lloyd's formula algorithm, real space calculation of Liechtenstein's formula and preconditioning techniques leading to a significant speed-up. First applications considering complex disordered systems of thousands of inequivalent atoms illustrate the strength of our method.

[1] R. Zeller, J. Phys.: Condens. Matter **20**, 294215 (2008).

O 10.3 Mon 15:30 H31

**Using the kinetic energy density in local density functionals** — •Georg Madsen[1], Lara Ferrighi[2], and Bjork Hammer[2] — [1]ICAMS, Ruhr Universität Bochum, Germany — [2]Department of Physics and Astronomy, Aarhus University, Denmark

Recent developments in local functionals including the kinetic energy density, so-called meta-generalized gradient approximations (MGGAs), are described. It is shown how MGGAs can solve the longstanding problem of the cross over between 2D and 3D structure for cationic and anionic gold clusters. The MGGAs stronger tendency towards 3D structures lies in their smaller gradient enhancement, but contrary to GGAs with smaller gradient enhancements, MGGAs do not overestimate the atomization energy. Furthermore, we find that closed shell interactions are fingerprinted in the kinetic energy density and that MGGAs have enough flexibility to treat correctly both the covalent and the dispersive interactions in layered solids such as Graphite, h-BN and $MoS_2$. It is shown how MGGAs thereby potentially can give a consistent improvement over the GGAs for the adsorption on metal surfaces.

Ferrighi, Hammer, Madsen, J. Am. Chem. Soc. **2009**, *131*, 10605
Madsen, Ferrighi, Hammer, J. Phys. Chem. Lett.

O 10.4 Mon 15:45 H31

**Adsorption behavior of super-heavy elements from 112 to 118 on inert and metal surfaces** — •Josef Anton and Timo Jacob — Institut für Elektrochemie, Universität Ulm, 89069 Ulm

One of the very interesting but also rather challenging topics in modern chemistry are the properties of super-heavy elements at the edge of the periodic table [1]. Due to their very short life times (usually $< 1\,\mathrm{s}$) one is only able to perform extremely short (before the decay of the nucleus) experiments on one atom at a time. Therefore, most standard techniques of "traditional" chemistry are not applicable, leaving only a few possibilities. One of these is the gas-phase thermochromatography [1,2], where the desorption temperature of a species is measured and afterwards analyzed to obtain different element properties such as the volatility.

For the theoretical calculation of the properties of these super-heavy elements as well their adsorption behavior on the detector material (e.g. gold or quartz), a fully-relativistic description of all electrons is required. Therefore, using our four-component DFT code [3], we determined the adoption energies of elements 112 to 118 and their homologues on different metal surfaces. In this presentation we will discuss these results, compare them to available experiments, and provide predictions for future measurements.

O 10.5 Mon 16:00 H31

**Real-Space DFT for large Molecules on Surfaces** — •Paul Baumeister[1], Daniel Wortmann[1], Tomoya Ono[2], and Stefan Blügel[1] — [1]Institut für Festkörperforschung & Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich — [2]Dept. of Precision Science and Technology, Osaka University, Japan

Electronic structure calculations within the framework of density functional theory (DFT) has turned out to be the most powerful tool for a reliable determination of ground state properties of large structures such as big organic molecules on surfaces. Especially complicated systems containing far beyond several hundreds of atoms become move with increasingly into the focus of research. We present a real-space grid density functional simulation code that has been developed in Osaka and Jülich. It combines the flexibility of arbitrary boundary condition with the strength of nearly perfect parallel efficiency on massively parallel computers. The projector augmented wave (PAW) method, proposed by Blöchl[1], provides an accurate description for reproducing the chemical behavior of valence states with a reasonable number of grid points. Grid based methods tend to show Pulay-like forces depending on the atomic position with respect to the nearest grid points, sometimes referred to as egg-box effect. These oscillations of forces and total energies endanger the reliable convergence of structural relaxation. We will discuss how to apply the double grid technique[2] and pre-filtering in Fourier space to avoid this problem.

[1] P.E. Blöchl, PRB 50, 17953 (1994)
[2] T. Ono, K. Hirose, PRB 72, 085115 (2005)

O 10.6 Mon 16:15 H31

**Van der Waals forces in solids: Challenges for density functionals** — •Guo-Xu Zhang, Alexandre Tkatchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany

While the importance of van der Waals (vdW) forces for binding between molecules is well established, their influence on the cohesive properties of solids remains to be quantified from first-principles. In particular, most state-of-the-art density functionals yield systematic deviations for the lattice constants, cohesive energies, bulk moduli and transition pressures for a range of solid-state systems. We evaluate the long-range $C_6$ dispersion coefficients for ions in solids and use them to assess the effect of the long-range vdW forces on the abovementioned cohesive properties of ionic (NaCl, AgCl, MgO) and semiconductor (Si, GaAs) solids. For all of these systems, we obtain consistently accurate results by coupling the long-range $C_6R^{-6}$ dispersion energy with the Perdew-Burke-Ernzerhof functional for the short range. We compare our results for the cohesive properties with recently developed functionals for solids.

O 10.7 Mon 16:30 H31

**Exchange an Correlation effects in the electronic properties**

**of transition metal oxides: the example of NiO** — •Matteo Guzzo[1,3], Matteo Gatti[2,3], and Lucia Reining[1,3] — [1]LSI - ETSF, Ecole Polytechnique, Palaiseau CEDEX 91128, France — [2]Nano-bio group - ETSF, Universidad del Pais Vasco, San Sebastian, Spain — [3]European Theoretical Spectroscopy Facility (ETSF)

This contribution has been rescheduled to O 55.9.

O 10.8 Mon 16:45 H31

**Determination of structural and electronic properties of different titanates by means of XANES** — •Stephan Borek[1], Remya Govind[1], Martin Trautmann[1], Franziska Steudel[1], Michael Huth[1], Liudmilla Makhova[2], Joachim Gräfe[2], Daniel Wett[2], Karl-Michael Schindler[1], Reinhard Denecke[2], and Angelika Chassé[1] — [1]Institute of Physics, Martin-Luther-University Halle-Wittenberg, Germany — [2]Wilhelm-Ostwald Institute for Physical and Theoretical Chemistry, University Leipzig, Germany

Starting from SCF potentials we have calculated near edge XAS spectra on the perovskites $BaTiO_3$ and $SrTiO_3$, both in the cubic and in the tetragonal phase. The resulting spectra could be explained by comparing with the calculated DOS in terms of the dipole-approximation. It has be shown that the observed differences in the XAS spectra for the O K-edge, the Ti $L_{2,3}$-edge and the Ba and Sr $M_{4,5}$-edge, between the cubic and tetragonal phase, may be related to the differences in the calculated DOS. Furthermore we investigate the effect of iron-multilayers on the electronic, e.g. the spectroscopical properties of the different titanates, and compared our calculations with experimental results, measured on the beam-line of BESSY.

O 10.9 Mon 17:00 H31

**Particle redeposition and the non-local damping term in the Kuramoto-Sivashinsky equation** — •Nils Anspach and Stefan Linz — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Deutschland

Ion-beam erosion processes have recently regained the focus of both experimental and theoretical physicists due to the fact that they can induce the formation of regular and well-ordered patterns on surfaces under low-energy ion bombardement. The so far most promising model for the evolution of the surface's height profile under normal ion incidence is the non-local Kuramoto-Sivashinsky equation (KSE) which is able to reproduce the experimentally observed structures. However it is still unclear what the physical origin of the non-local damping term in the KSE might be. Motivated by some speculation in the literature that redeposition of eroded particles back to the surface could possibly be the relevant mechanism here, we have developed a conceptually simple one-dimensional model that catches the essence of a potential redeposition process while simultaneously neglecting all other surface effects included in the KSE. This model and its inherent properties are investigated in considerable detail [1]. After that, the obtained results are then compared to the non-local damping term in order to discuss the potential role of particle redeposition as the driving force behind this term.

[1] N. Anspach, S. J. Linz, submitted for publication.

## O 11: Methods: Scanning probe techniques II

Time: Monday 15:00–17:30 Location: H32

O 11.1 Mon 15:00 H32

**Light emission from single Ag atom contacts** — •Natalia Schneider[1], Guillaume Schull[2], 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 de Chimie de Strasbourg, CNRS UMR 7504, 67034 Strasbourg, France

Using a cryogenic scanning tunneling microscope, we investigated the transition from tunneling to a single atom contact on Ag(111) at voltages between 1.4 and 2.0 V. Contrary to Au/Au(111) junctions, Ag/Ag(111) junctions do not exhibit a jump. This enables a detailed study of the junction luminescence at each step of the contact formation. Optical spectra reflect single and multiple electron processes and their distinct evolution as a single-atom contact is formed.

O 11.2 Mon 15:15 H32

**Investigating the voltage dependence of the apparent barrier height in scanning tunneling microscopy** — •Michael Becker and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Scanning tunneling microscopy measurements of the apparent height of the tunneling barrier on noble metal (111) surfaces and for Pb islands on Ag(111) are analyzed. The apparent barrier height (ABH) is found to vary significantly with the bias voltage. In particular for the coinage metal surfaces, the ABH is asymmetric with respect to the bias polarity, in contrast to simple interpretations in terms of an average work function of tip and sample. For Pb/Ag(111) the bias dependence leads to drastic changes and even inversion of contrast in spatial maps of the ABH. Model calculations of the tunneling current, which take band structure effects into account, describe the experimental observations. Financial support by the Deutsche Forschungsgemeinschaft through SFB 668 is acknowledged.

O 11.3 Mon 15:30 H32

**Deconvolution of the local density of states from constant-current tunneling spectra** — •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 to analyze the local density of states (LDOS) of a sample. An undoubted advantage over I-V measurements at constant tip-sample separation is a wider accessible range of bias especially on delicate samples such as those involving organic molecules. While now-a-days numerical methods are available to include effects of the tunnelling barrier and even to deconvolve the LDOS of tip and sample from I-V measurements [1], for z-V spectroscopy such an analysis is still missing. Recently, Ziegler et al. applied an adopted method to remove effects of the tunnelling barrier from z-V measurements [2]. Here, we introduce an adopted method from [1] to obtain a deconvolution of the LDOS from z-V measurements taken at different set currents on Nb(110) at low temperature.

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

[2] M. Ziegler, N. Néel, A. Sperl, J. Kröger, R. Berndt, Phys. Rev. B 80, 125402 (2009).

O 11.4 Mon 15:45 H32

**Local density of states from constant-current tunneling spectra** — Martin Ziegler, Nicolas Néel, •Alexander Sperl, Jörg Kröger, and Richard Berndt — Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Scanning tunnelling spectroscopy of the differential conductance is often performed at constant tip-surface distance. Sometimes it is advantageous to acquire spectra at constant current. However, the latter method may significantly affect peak positions and line shapes in spectra as well as patterns in spatial maps of the differential conductance. A normalization procedure for constant-current data, which relies on experimental current-distance data, is shown to yield spectral information on the local density of states. Financial support by the Deutsche Forschungsgemeinschaft through SFB 668 and SFB 677 is acknowledged.

O 11.5 Mon 16:00 H32

**Structure and Charge State Characterization of Line Defects in the Alumina Film on NiAl(110) by Dynamic Force Microscopy** — •Leonid Lichtenstein, Lars Heinke, Georg Hermann Simon, Thomas König, Markus Heyde, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14196 Berlin, Germany

Metal oxides play a decisive role in many technological applications such as microelectronics and heterogeneous catalysis. To understand their catalytic performance in detail, it is important to determine the atomic and electronic structure of their surfaces. For this purpose, the thin aluminum oxide film grown on NiAl(110) often serves as model system in catalysis. It has been shown that line defects like step edges and antiphase domain boundaries (APDB) are particularly active sites for, e.g., the decomposition of NO [1]. In this context, frequency modulated dynamic force microscopy (FM-DFM) and scanning tunneling microscopy (STM) are applied to unveil the atomic structure of the thin film and its line defects in ultra high vacuum at 5 K [2]. By means of bias spectroscopy [3] differences in the density of electronic states between domains and line defects were determined. The contact-potential spectroscopy shows different local work functions indicating different charge states for both. This study links catalytic processes to the electronic structure of line defects.

[1] S. Schauermann et al., Chem. Phys. Lett. 381 (2003) 298-305
[2] G. H. Simon et al., New J. Phys. 11 (2009), 093009
[3] N. Nilius et al., Phys. Rev. B 69 (2004), 121401

O 11.6 Mon 16:15 H32

**Lateral Piezoelectric Response at Domain Boundaries in Bulk Single Crystals** — Florian Johann, Tobias Jungk, Martin Lilienblum, Akos Hoffmann, and •Elisabeth Soergel — Physikalisches Institut, Universität Bonn, Wegelerstrasse 8, 53115 Bonn

The lateral signal at domain boundaries using piezoresponse force microscopy has first been described by Wittborn et al. [1] and was later investigated by Scrymgeour et al. [2]. They assumed the signal to originate from the topographical slope of the surface at the domain boundary. A different approach by Jungk et al. [3] ascribed domain specific surface charge distributions to cause the signal. Calculations by Morozovska et al. [4] explained the signal by a sideways motion of the sample surface at the domain boundary. In this contribution, we try to clarify the situation by experimental data obtained on different materials and crystallographic cuts.

[1] J.Wittborn, C.Canalias, K.V.Rao, R.Clemens, H.Karlsson, and F.Laurell, Appl. Phys. Lett. 80, 1622 (2002). [2] D.A.Scrymgeour and V.Gopalan, Phys. Rev. B 72, 024103 (2005). [3] T.Jungk, A.Hoffmann, and E.Soergel, Appl. Phys. Lett. 89, 042901 (2006). [4] A.N.Morozovska, E.A.Eliseev, S.L.Bravina, and S.V.Kalinin, Phys. Rev. B 75, 174109 (2007).

O 11.7 Mon 16:30 H32

**Infrared near-field optical microscopy on sub-surface doped silicon** — •Rainer Jacob[1], Manfred Helm[1], Stephan Winnerl[1], Harald Schneider[1], Marc Tobias Wenzel[2], Hans-Georg von Ribbeck[2], and Lukas M. Eng[2] — [1]Institut für Ionenstrahlphysik und Materialforschung, Forschungszentrum Dresden, 01314 Dresden, Germany — [2]Institut für Angewandte Photophysik, TU Dresden, 01062 Dresden, Germany

Scattering-type scanning near-field optical microscopy (s-SNOM) has proven as a useful tool for surface science. Materials can be distinguished by their interaction with the local probe, hence yielding different intensities of the near-field signal. In semiconductors this can be achieved through doping, allowing a significant variation in the dielectric function. This becomes even more interesting when probing sub-surface interactions of such dopants.

Although s-SNOM is mainly used as a surface sensitive technique, we present here the ability to probe sub-surface doped silicon. To this end we prepared samples by implanting gallium and boron with different energies at a variable depth. Afterwards, the samples were annealed in order to activate the dopants. The carriers were then investigated with IR-s-SNOM using wavelengths between 9 and 15 $\mu$m from the free-electron laser at the FZD. We were able to probe doping layers up to 100 nm below the surface. Furthermore, we could show contrast inversion between doped and undoped areas in the Si-wafer for different wavelengths. From these measurements the carrier density in doped regions can be extracted directly using the Drude model.

O 11.8 Mon 16:45 H32

**Sol-gel derived ferroelectric nanoparticles investigated by piezoresponse force microscopy** — •Florian Johann[1], Tobias Jungk[1], Susanne Lisinski[2], Akos Hoffman[1], Lorenz Ratke[2], and Elisabeth Soergel[1] — [1]Institute of Physics, University of Bonn, Wegelerstr. 8, 53115 Bonn, Germany — [2]Institute for Material Physics in Space, DLR, Linder Höhe, 51147 Cologne, Germany – *Present address of F. Johann: Max Planck Institut for Microstructure Physics, Weinberg 2, 06120 Halle, Germany

Piezoresponse force microscopy (PFM) was used to investigate the ferroelectric properties of sol-gel derived $LiNbO_3$ nanoparticles. To determine the degree of ferroelectricity we took large-area images and performed statistical image-analysis. The ferroelectric behavior of single nanoparticles was verified by poling experiments using the PFM tip. Finally we carried out simultaneous measurements of the in-plane and the out-of-plane piezoresponse of the nanoparticles, followed by measurements of the same area after rotation of the sample by 90° and 180°. Such measurements basically allow to determine the direction of polarization of every single particle.

O 11.9 Mon 17:00 H32

**Mid-Infrared Broadband s-SNOM** — •Sergiu Amarie and Fritz Keilmann — Max Planck Institute for Quantum Optics, 85741 Garching, Germany

We demonstrate continuous infrared spectra from 20 nm sample spots, by combining dispersive Fourier-transform infrared spectroscopy (FTIR) with scattering near-field microscopy (s-SNOM). As a next step we aim for spectroscopic near field images with 20 nm spatial resolution, at 6 cm-1 spectral resolution. The method is to be applied for biomedical imaging.

S. Amarie, T. Ganz, and F. Keilmann, "Mid-infrared near-field spectroscopy," Opt. Express (2009) 17, 21794-21801.

O 11.10 Mon 17:15 H32

**Imaging short-range forces with a scanning tunnelling microscope** — •Temirov Ruslan, Weiss Christian, Wagner Christian, Kleimann Christoph, and Tautz Stefan — Institut für Bio- und Nanosysteme 3, Forschungszentrum Jülich, JARA Fundamentals of Future Information Technology, Germany

One of the unresolved issues in the field of scanning tunnelling microscopy (STM) is the lack of chemical sensitivity. The STM probes the density of states (DOS) close to the Fermi level while the details of the chemical structure are mostly encoded by lower lying orbitals. Thus it is desirable to measure the total electron density (TED) rather than the DOS. Since the TED defines Pauli repulsion, imaging of short-range forces should directly reveal the chemical structure. Indeed, it was demonstrated recently that non-contact atomic force microscopy (AFM) resolves the structure of a complex organic molecule by probing short-range repulsive interactions [1]. In our contribution we show that STM can also be used to map short-range forces and resolve chemical structures. The key to the new functionality is a single hydrogen molecule confined in the STM junction [2]. The molecule acts as a force-sensor/signal transducer, which probes the repulsive branch of the surface adsorption potential and transforms the force signal into variations of the junction conductance [3].

[1] L. Gross et al. Science 325, 1110 (2009). [2] R. Temirov et al. New J. Phys. 10, 053012 (2008) [3] C. Weiss et al. arXiv:cond-mat/0910.5825

## O 12: Oxides and insulators: Adsorption

Time: Monday 15:00–17:45 Location: H33

O 12.1 Mon 15:00 H33

**Water adsorption on $SrTiO_3$(001): A density-functional theory study** — •Hannes Guhl[1,2], Wolfram Miller[1], and Karsten Reuter[2,3] — [1]Leibniz Institut für Kristallzüchtung Berlin (Germany) — [2]Fritz-Haber-Institut Berlin (Germany) — [3]TU München (Germany)

$SrTiO_3$ is a technological oxide, with applications as photo-catalyst, gas-sensor or as substrate for film growth. In many of these applications the surface of $SrTiO_3$ is deliberately or unintended in contact with water molecules. Aiming for the atomic-scale details of this interaction we perform density-functional theory calculations addressing the adsorption of $H_2O$ on both regular terminations of the $SrTiO_3$(001) surface. We find that the binding energetics is crucially controlled

by long-range surface relaxations. Using this energetics to construct a thermodynamic phasediagram we obtain a different propensity for hydroxylation of the two terminations that is consistent with recent experiments by Iwahori *et. al* [1]. Around room temperature the SrO-termination becomes hydroxylated already at lowest background humidity, whereas the $TiO_2$-terminated domains stay practically water-free in the range of low and moderate $H_2O$ vapor pressures.
[1] K. Iwahori *et. al* J. Appl. Phys. **93**, 3227 (2007).

O 12.2 Mon 15:15 H33

**H and $H_2O$ adsorption on $Fe_3O_4$(001): Adsorbate induced charge and orbital order** — •Narasimham Mulakaluri[1,2], Rossitza Pentcheva[1], Wolfgang Moritz[1], and Matthias Scheffler[2] — [1]Section Crystallography, Dept. for Earth and Environmental Sciences, University of Munich — [2]Fritz-Haber-Institut der MPG, Berlin

Besides potential applications in spintronics, magnetite plays an important role in many environmental redox reactions. Using density functional theory together with an on-site Coulomb repulsion term (GGA+$U$), we investigate the adsorption of $H_2O$ and H on $Fe_3O_4$(001) surface and its influence on the electronic structure. The surface phase diagram, compiled within the framework of *ab initio* atomistic thermodynamics reveals dissociative adsorption of water especially at surface defect sites. At higher water vapour pressures a partial dissociation sets in, where a chain of hydrogen bonded $H_2O$ and OH groups forms[1]. The adsorbates ($H_2O$, OH, H) are found to induce a unique charge and orbital ordering in the surface and sub-surface layers. This feature can be used to tailor the catalytic properties as well as half-metallicity of the material.
[1] N. Mulakaluri *et.al*, Phys. Rev. Lett **103**, 176102 (2009).

O 12.3 Mon 15:30 H33

**A Classical Potential to Model Protein Adsorption on the Natively Oxidised Titanium Surface** — •Julian Schneider and Lucio Colombi Ciacchi — Hybrid Materials Interfaces Group, BCCMS, Universität Bremen, 28359 Bremen

In order to investigate the surface properties of metals in a realistic fashion it is crucial to take into account the thin oxide layer that forms spontaneously when the surface is exposed to an oxidising environment. Starting from reference oxide layer structures obtained in extensive first-principles molecular dynamics simulations, we have developed a novel classical potential which is able to reproduce the topological binding features of the amorphous oxide network on Ti as well as the interfacial behaviour of the TiOx/water interface. The analytic form of the potential has been chosen so that it can be easily combined with well-established biomolecular force fields. This allowed us to perform classical simulations of small organic molecules on the oxide surface and compare the results with those of density functional theory calculations. Ongoing work is focusing on the application of our force field to simulate the adsorption of amino acids, small peptides and larger protein fragments on oxidised Ti surfaces.

O 12.4 Mon 15:45 H33

**Anomalous molecular orbital variation upon adsorption on wide band gap insulator: Gluconic acid on $MgSO_4{\cdot}H_2O$(001)** — •Wei Chen[1], Christoph Tegenkamp[1], Herbert Pfnür[1], and Thomas Bredow[2] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany — [2]Institut für Physikalische und Theoretische Chemie, Universität Bonn, Bonn, Germany

The understanding of the interaction between organic molecule and wide band gap insulator is of great importance provided with their elementary roles in organic electronics and optoelectronic devices. It is commonly believed that organic molecules are physisorbed on the ideal non-polar surface of wide band gap insulator with limited variation on the electronic properties of the adsorbate molecule. However, on the basis of first principles calculation on the gluconic acid adsorbed on the (001) surface of a ternary compound $MgSO_4{\cdot}H_2O$, we show that the orbitals of the acid molecule could undergo significant changes upon adsorption. The gluconic acid binds strongly to the $MgSO_4{\cdot}H_2O$(001) via multiple electrostatic interactions from Mg-O, which is further stabilized by the long range dispersion force. The electrostatic interactions result in a pronounced intra-molecular distortion of the adsorbate, yielding a much smaller HOMO-LUMO gap of the acid due to the geometrical change alone. Furthermore, as manifested by the prominent hybridization between the molecule and the surface, the characteristics of the frontier orbital are modified significantly upon adsorption with respect to the isolated molecule.

O 12.5 Mon 16:00 H33

**A comparative study of short-chained alcohols and water adsorbed on TiO2(110) by He atom scattering and DFT** — •David Silber[1], Franziska Traeger[1], Christof Wöll[3], Piotr Kowalski[2], and Dominik Marx[2] — [1]Department for Physical Chemistry I at the university of Bochum — [2]Department for Theoretical Chemistry at the university of Bochum — [3]Institute of Functional Interfaces Karlsruhe at the Karlsruher Institute of Technology

In this combined experimental and theoretical study the adsorption of methanol and ethanol on well defined TiO2(110) was investigated. Theoretical and experimental results will prove that methanol adsorbs molecularly in a c(2x2)-superstructure. Heating the surface to 300 K leads to the deprotonation of methanol. Further heating to 350 K (binding energy - 1 eV) leads to a recombinative desorption process in which solely methanol is detected. In additional experiments predosing of D2O was performed to fill bridge bonded oxygen vacancy sites and to investigate the interaction of water with methanol. TDS reveals that water and methanol compete for adsorption sites, but a pure methanol layer was never formed on water precovered TiO2. These experimental finding is supported by our DFT calculation, which proves that a mixed methanol and water structure is stable. This work is complemented by the analogue investigation of ethanol adsorption on clean and water precoverd TiO2. On clean rutile solely the desorption of ethanol in a recombinative desorption process was detected. Like methanol ethanol competes with water for adsorption sites, but unlike methanol, ethanol is able to completely replace water in the first layer.

O 12.6 Mon 16:15 H33

**Light-induced isomerization of an azobenzene derivate on an insulating surface** — •Jörg Henzl and Karina Morgenstern — Universität Hannover, Institut für Festkörperphysik, Abteilung für Atomare und Molekulare Strukturen (ATMOS), Appelstr. 2, 30167 Hannover

Azobenzene molecules and its derivates are highly attractive for switches in molecular electronics and have a high potential in optoelectronic devices as they exhibit a light-induced *cis-trans* isomerization. Recent studies demonstrated the principle feasibility of isomerization in contact with a metal surface. But circuits on metals are of little technological relevance in contrast to insulators. A model system for an insulating surface is a thin NaCl film grown on metal substrates. Recently, the electron-induced isomerization of aminonitroazobenzene on NaCl/Ag(111) was shown.[1] In this contribution, we present low temperature scanning tunnelling microscopy measurements of p-hydroxy-azobenzene on thin NaCl films on Ag(111). After depositing at 20 K, single molecules are found on the surface. The reversible isomerization can be triggered either with inelastic tunnelling electrons from the STM tip or with photons from a Hg-arc lamp. We characterize the adsorption geometry of both configurations and discuss the wave-length depend light-induced isomerization. [1] A. Safiei, J. Henzl, and K. Morgenstern, O17.8, DPG conference, Dresden 2009

O 12.7 Mon 16:30 H33

**Orbital symmetries in Cu(II)-tetraazaphthtalocyanine isomers** — •Tobias Sonnleitner, Ingmar Swart, Niko Pavliček, Christof Uhlmann, and Jascha Repp — Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Ultrathin insulating films on metal substrates facilitate the use of the scanning tunneling microscope to study the electronic properties of individual molecules, which are electronically decoupled from the metallic substrate. To gain a detailed understanding of the molecular properties, it is desirable to systematically vary the electronic structure of molecules step by step without changing the geometrical structure too strongly. Cu(II)-tetraazaphthalocyanine molecules provide such a model system. For these molecules four classes of isomers with different symmetries exist. These symmetries are directly visualized by imaging of the unperturbed molecular orbitals. This allows us to determine the isomer under study, and locate the nitrogen atoms in the molecular structure. DFT calculations substantiate the experimental findings.

O 12.8 Mon 16:45 H33

**Interaction of $CO_2$ and $H_2O$ with Thin NiO Layers on Cu(111)** — •Karin Gotterbarm, Michael Peter Andreas Lorenz, Regine Streber, Oliver Höfert, Marie-Madeleine Walz, Christian Papp, Andreas Bayer, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-

Nürnberg, Egerlandstr. 3, 91058 Erlangen

NiO is an important material in heterogeneous catalysis. Under ambient conditions, reactions with $CO_2$ and $H_2O$ can lead to the formation of carbonates and hydroxides, which could block active sites and thereby influence the catalytic reactivity. We studied the adsorption of $CO_2$ and $H_2O$ on thin NiO layers (around 2 ML) on Cu(111) as inert substrate by in-situ XPS applying synchrotron radiation at BESSY II.

Upon adsorption of $CO_2$, characteristic peaks in the O 1s and C 1s region indicate the formation of carbonate. When the surface is exposed to water, hydroxide and multilayers of water are formed. In-situ XPS during heating revealed an unusual thermal stability of the carbonate as well as hydroxide layers. Experiments on different NiO layers with varying hydroxide precoverages showed that adsorbed OH species effectively block $CO_2$ adsorption sites, leading to a lower saturation coverage of $CO_3$.

This work was supported by BMBF (05 ES3XBA/5) and the DFG through the Cluster of Excellence ”Engineering of Advanced Materials”.

O 12.9 Mon 17:00 H33

**Adsorption of cobalt phthalocyanine on rutile TiO2 (110) surfaces: interface formation.** — •Pavel Shukrynau, Marius Toader, and Michael Hietschold — Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group. D-09107 Chemnitz, Germany.

We have employed variable temperature scanning tunneling microscopy (STM) to follow the adsorption of cobalt phthalocyanine (CoPc) on rutile TiO2 (110)-1x1 and -1x2 substrates. The coverage of CoPc varied from 0.05 up to 1 monolayer (ML). At room temperature and very low coverage single pthtalocyanine molecules either lay flat on the surface over the bridging oxygen atomic lines or stay tilted in troughs between them. Further deposition of CoPc leads to the agglomeration of the molecules and finally results in the formation of irregularly disordered films on both substrates. At a coverage of about 0.75 ML the surfaces are completely covered with roundly shaped 3D clusters of typical size up to 3 nm. The general structure of the surface, i.e., shape of the step edges, remains unchanged. Subsequent annealing of the samples up to 300°C results in the rearrangement of the adlayer and forms the molecular rows along [001] direction of the substrate. STS spectra taken at different coverages give an information about the electronic properties of the interface, revealing the adsorption mechanism of molecules on this substrate.

O 12.10 Mon 17:15 H33

**NEXAFS/XPS Study of the Organic Molecules on Metal-Oxide Surfaces** — •Michael Naboka[1,2], Alexei Nefedov[1,2], and Christof Wöll[2] — [1]Ruhr University of Bochum, D-44780, Bochum, Germany — [2]Karlsruher Institute of Technology, D-76344, Eggenstein-Leopoldshafen, Germany

Today the investigation of the electronic properties and orientation of the organic molecules adsorbed on metal-oxide single crystal surfaces attracts considerable attention. The reason for that is a search for the new metal organic systems which may become useful in the rapidly developing area of organic electronics and catalysis. The example of such a system can be a terephtalic acid adsorbed on the $TiO_2$ (110) surface. This system offers a possibility to create the monolayer of the carboxyl-terminated up-standing molecules which may in future have an application similar to self-assembling monolayers or may also serve as a linker for Metal Organic Frameworks (MOFs). Near Edge X-Ray Adsorption Fine Structure (NEXAFS) spectroscopy and X-ray Photoelectron Spectroscopy (XPS) are the techniques which were developed particularly for the study and understanding of the organic molecules structure on the surface revealing the molecular electronic structure and its orientation. Since nowadays requirements for such kind of research are increased the new NEXAFS/XPS endstation at synchrotron facility BESSY II has been developed and constructed. The machine functionalizes under ultrahigh vacuum conditions and allows to measure NEXAFS/XPS spectra as well as to use the additional surface science methods such as LEED and TDS.

O 12.11 Mon 17:30 H33

**Coupled cluster calculations for NO and Au adsorption on $CeO_2$ using the method of increments** — Carsten Müller and •Beate Paulus — Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustraße 3, 14195 Berlin

$CeO_2$ is an active constituent in today's car catalysts where it assists in the reduction of $NO_x$ to $N_2$. Here we present results from first principles CCSD(T) calculations for NO physisorption on the $CeO_2$ (111) surface. Many first principles methods fail to describe the physisorption phenomenon. The main binding force is dispersion, which is neglected in the Hartree-Fock theory, not included in common DFT functionals, but recovered by many-body methods such as MP2 or the coupled cluster method. Here we apply this theory in the framework of a local correlation scheme called "The Method of Increments". It was successfully used to determine the adsorption energies for CO and $N_2O$ on the $CeO_2$ (111) surface [1,2]. Now we extend the method to the adsorption of open-shell molecules like NO and to open-shell atoms like Au.

[1] C. Müller, K. Hermansson, and B. Paulus, Chem. Phys. 362, 91 (2009).

[2] C. Müller, B. Paulus, and K. Hermansson, Surf. Sci. 603, 2619 (2009).

## O 13: Semiconductor substrates: Adsorption

Time: Monday 15:00–17:45 Location: H34

O 13.1 Mon 15:00 H34

**metallic transport and Anderson localization on In atomic layers on silicon** — •Shiro Yamazaki[1], Yoshikazu Hosomura[2], Iwao Matsuda[3], Rei Hobara[2], Toyoaki Eguchi[3], Yukio Hasegawa[3], and Shuji Hasegawa[2] — [1]Institute of Applied Physics, University of Hamburg, Hamburg, Germany — [2]Department of Physics, The University of Tokyo, Tokyo, Japan — [3]The Institute for Solid State Physics, The University of Tokyo, Kashiwa, Japan

Metallic electrical transport have not been observed in atomic-scale low-dimensional metal systems at low temperature region due to Anderson localization effect, except to Graphene or extremely conductive polyaniline [1,2]. Si(111)-$\sqrt{7} \times \sqrt{3}$-In surface reconstruction is a In atomic layer supported by Si(111) substrate. According to ARPES study, the surface shows 2D metal state with the very large Fermi wave number ($k_F$=14[$nm^{-1}$]) and the large electron density ($4.6\times10^{14}$ [$eV^{-1}$ $cm^{-2}$]) [3], leading to a low resistance. By using variable-temperature micro-four-point probe method [3], very low resistance and metallic transport was found down to 10 K. It is quantitatively explained by the ARPES result by using 2D Boltzmann equation $R_{2D} = \frac{4\pi^2\lambda m^*}{e^2\hbar k_F^2} k_B T$. By introducing defects, it shows semiconducting temperature dependence of variable range hopping due to Anderson localization. [1]K. S. Novoselov, et al. , Nature **438**, 197 (2005) [2]K. Lee, et al. , Nature **441**, 65 (2006) [3]E. Rotenberg, et al. , Phys. Rev. Lett. **91**, 246404 (2003) [4]T. Tanikawa, et al. , e-J. Surf. Sci. Nanotech. **1**, 50 (2003)

O 13.2 Mon 15:15 H34

**Thermal stability of ultra-thin $ZrO_2$ films and structure determination of $ZrSi_2$ islands on Si(100)** — •Frank Schönbohm[1,2], Christian Rolf Flüchter[1], Daniel Weier[1], Tobias Lühr[1], Ulf Berges[1,2], Sven Döring[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik 1 - Technische Universität Dortmund, Otto-Hahn-Str. 4, D-44221 Dortmund, Germany — [2]DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44221 Dortmund, Germany

The ongoing miniaturisation of semiconductors requires a substitute for the presently used $SiO_2$ gate dielectrics. Below 2 nm film thickness the leakage current increases drastically due to tunneling processes and causes the loss of efficiency. Among the *high-k* materials $HfO_2$ and $ZrO_2$ might be proper candidates to replace the $SiO_2$. We studied the temperature dependence of thin $ZrO_2$ films on clean silicon by means of x-ray photoelectron spectroscopy (XPS) and photoelectron diffraction (XPD). $ZrO_2$ films with a thickness of approximately 11 Å were grown by electron beam evaporation on a (2×1)-reconstructed Si(100) surface. At annealing temperatures of 650°C and above the $ZrO_2$ films were transformed into $ZrSi_2$. The temperature region of structural transformation could be narrowed to the range from 650°C to 725°C. During the formation of $ZrSi_2$ all oxygen was removed from the sample surface. After annealing at 725°C neither zirconia nor silicon oxide could be verified on the sample. From the combined spectroscopy, SEM, and XPD analysis a model for the internal structure of $ZrSi_2$ is proposed.

O 13.3 Mon 15:30 H34

**Characterization of Si(112) and In/Si(112) studied by SPA-LEED** — •Jan Höcker, Moritz Speckmann, Thomas Schmidt, and Jens Falta — Institute of Solid State Physics, University of Bremen, 28359 Bremen

High index surfaces are of strong interest in todays research because of the possibility to grow low dimensional structures. It has for instance already been shown that the adsorption of Ga can induce the formation of 1D metal chains on Si(112) (cf. Snijders et al., PRB **72**, 2005). In this work we investigated the clean Si(112) surface and the adsorption of In on Si(112) to establish an analogy to Ga/Si(112) using spot profile analyzing low energy electron diffraction (SPA-LEED).

By means of reciprocal space mapping we determined the bare Si(112) surface to be decomposed into alternating $(5\,5\,12)$ and (111) facets in $[1\bar{1}0]$ direction with $(2 \times 1)$ and $(7 \times 7)$ reconstruction, respectively (cf. Baski et al., Surf. Sci. **392**, 1997).

With SPA-LEED we were able to observe the decreasing intensity of the facet spots in-situ while depositing In on Si(112) and thus reveal the smoothening of the surface due to the deposition of In. At saturation coverage we found a "$(3.x \times 1)$" reconstruction, where $x$ is dependent on the deposition temperature and changes from $x = 7$ at 400°C to $x = 5$ at 500°C. This leads us to the assumption that the reconstruction is not incommensurate but a mixture of $(3 \times 1)$ and $(4 \times 1)$ building blocks, which is very similar to the super structure of Ga on Si(112).

O 13.4 Mon 15:45 H34

**Adsorption of metalorganic molecules on metal-semiconductor systems** — •Jędrzej Schmeidel, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Abteilung Atomare und Molekulare Strukturen, Appelstrasse 2, 30167 Hannover, Germany

Molecular junctions appropriate for transport trough single molecules can be realized using concepts of surface science. The controlled opening of ultra-thin Ag nanostructures on Si surfaces by electromigration and injection of single ferrocene molecules has been demonstrated recently [1]. In order to model accurately the conductivity of ferrocene-1,1'-dithiol molecules, thiolate bounded molecules are adsorbed on perfect sites of the Ag contacts. However, chemisorption takes place at defect sites, e.g. atomic step [2]. For an detailed understanding of this complex scenario we have investigated the adsorption of metal organic molecules on metal/semiconductor surfaces. As substrate the Ag $\sqrt{3}$ reconstruction, Ag islands and Ag multilayers on Si(111) have been investigated by means of STM and STS. Only without the wetting layer, Ag nanostructures can be electronically decoupled from the substrate as seen by a Coulomb blockade oscillations of the double barrier structure [3]. In order to study the selectivity of defects regarding molecular adsorption, porphyrins and ferrocene-1,1'-dithiol molecules have been adsorbed on these structures. The molecules adsorb predominantly at defects sites, e.g. steps and grain boundaries, as observed in the bias dependence of the STM image contrast.
[1] APL 89, 063120, [2] JCP 128, 064704, [3] PRB 80, 115304

O 13.5 Mon 16:00 H34

**Comparison on the local adsorption of pyridine and cyclopentene on Si(100)** — •Daniel Weier[1,2], Tobias Lühr[1], Frank Schöhnboh[1,2], Axel Beimborn[1], Max Brucker[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

We investigated the chemical and geometrical properties of the systems pyridine on Si(100) and cyclopentene on Si(100) in a combined of photoelectron spectroscopy (XPS) and photoelectron diffraction (XPD) study. The experiment had been performed by applying synchrotron radiation in order to achieve a high resolution with high surface sensitivity. Our XPS and XPD results show that cyclopentene reacts with one silicon-dimer of the (2x1)-reconstructed surface in a [2+2]-cycloaddition, changing the planar molecule to a diverse tilted molecule after adsorption. The pyridine contrariwise reacts with two of the silicon dimers by a combined reaction of cycloaddition and Lewis-acid base reaction. We will provide and compare structure models for both systems including detailed structure parameters obtained within a comprehensive numerical analysis.

O 13.6 Mon 16:15 H34

**Structural study of self-assembled Lead-Phthalocyanine ultra-thin layers on GaAs(001)** — •Linda Riele[1,2], Benjamin Buick[1], Thomas Bruhn[2,3], Eugen Speiser[1,3], Bjørn-Ove Fimland[4], Michael Kneissl[2], Norbert Esser[2,3], Patrick Vogt[2], and Wolfgang Richter[1] — [1]Università di Roma Tor Vergata, Rome, Italy — [2]TU Berlin, Berlin, Germany — [3]ISAS Department Berlin, Berlin, Germany — [4]Dept. of Electronics and Telecommunications, NTNU, Trondheim, Norway

Phthalocyanine molecules attract a growing scientific and technological interest because of their potential use for sensing applications. A systematic design of devices based on heterostructures, however, requires a profound understanding and control of the structural and electronic properties of organic/inorganic interfaces. Here we report on the non-planar lead phthalocyanine (PbPc) layers deposited on GaAs(001) with c(4×4), (2×4) and (4×2) reconstructed surfaces. The samples were investigated with Raman spectroscopy, reflectance anisotropy spectroscopy (RAS) and scanning tunneling microscopy (STM). RAS revealed a strong influence of the initial GaAs(001) surface reconstruction on the molecular arrangement within 20 nm thick PbPc films. Structural differences could also be verified by Raman spectra showing significant differences (frequencies, intensities and angular dependency). Moreover, STM measurements elucidated the influence of the GaAs substrate surface reconstructions on the organic film structure within the first monolayer.

O 13.7 Mon 16:30 H34

**Adsorption of PTCDA on GaN(0001) surfaces** — •Christian Schulz[1], Cherno Jaye[2], Christian Tessarek[1], Stephan Figge[1], Jan Ingo Flege[1], Thomas Schmidt[1], Detlef Hommel[1], Daniel A. Fischer[2], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, 28359 Bremen — [2]Ceramics Division, National Institute of Standards and Technology, Gaithersburg, MD 20899

Ordered growth of thin PTCDA layers is mainly observed on metals but recent reports (S. Yim et al. *J. Phys.: Condens. Matter* **15**, (2003)) have shown that some molecules also show ordered layers on unpassivated III-V semiconductor surfaces. In this work we investigate the adsorption of PTCDA on gallium-polar GaN(0001) with different methods. X-ray photoelectron spectroscopy (XPS) shows that the molecules are not dissociating after deposition, because the peak area ratios (including the shake-up's) for the perylene to carboxylic C1s feature is near the expected ratio for the intact molecule. Scanning tunneling microscopy (STM) and spot profile analyzing low energy electron diffraction (SPA-LEED) measurements reveal an island growth mode. For monolayer equivalent deposits, the near edge X-ray absorption fine structure (NEAFS) data of the C K-edge exhibit no polarization dependence indicating a disordered mixture of molecules in upstanding and down-lying geometry. However, for multilayer equivalent deposits a polarization dependence is observed which suggests a flat-lying geometry of the molecules. These findings are in good agreement with high-resolution STM and SPA-LEED data which reveal lateral ordering, compatible with a bulk-like configuration, within the islands.

O 13.8 Mon 16:45 H34

**SHG Spectroscopy of Potassium-Covered Si(100)(2x1)** — •Dominic Gerlach, Björn Braunschweig, Gerhard Lilienkamp und Winfried Daum — Institute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany

Previous second-harmonic generation (SHG) studies of potassium-modified Si(100)/SiO2 interfaces have revealed dramatic changes in the SHG spectra due to the presence of potassium ions at the interface and electric-field-induced second-harmonic generation in the space charge region of the semiconductor [1]. Here we present results of SHG experiments with a saturation layer of potassium (0.5 monolayer) deposited on clean Si(100)(2x1) surfaces. The main effect of the potassium adlayer on the SHG spectrum is a spectrally flat background contribution similar to a metal surface. The strength of the surface E1 resonance of the undoped Si substrate is almost unaffected by the adlayer, although it appears strongly enhanced in the spectra by interference. An additional resonance at 3.9 eV is tentatively assigned to a surface plasmon excitation in the potassium layer. The SHG results are consistent with a metallic character of the adsorbed potassium.

[1] A. Rumpel et al., Phys. Rev. B 74 081303(R) (2006)

O 13.9 Mon 17:00 H34

**Potential energy diagram for the selective adsorption of $C_{60}$ on Bi terminated Si and Ge surfaces** — •Vasily Cherepanov[1], Stefan Korte[1], Sergey Filimonov[2], and Bert Voigtländer[1] — [1]Institute of Bio and Nanosystems (IBN-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology — [2]Department of Physics, Tomsk State University, Tomsk 634050, Russia

Si/Ge nanostructures can be grown using a surfactant like Bi in order to suppress Si-Ge intermixing. Choosing appropriate growth conditions one can achieve a chemical selectivity for $C_{60}$ adsorption and $C_{60}$ adsorbs only onto the Ge area of the surface. A passivation of dangling bonds on Si and Ge surfaces by Bi atoms results in an adsorption of $C_{60}$ molecules on top of Bi layer in a physisorbed state. At elevated temperatures the deposited $C_{60}$ molecules desorb from the physisorbed state back to the gas phase or transfer to a chemisorbed state by substituting Bi and bonding directly to the substrate. The $C_{60}$ molecules in physisorbed and chemisorbed state can be easily distinguished in Scanning Tunneling Microscopy images. Measurements of the temperature and rate dependences of the density of $C_{60}$ molecules in physisorbed/chemisorbed state allow to plot the potential energy diagram for adsorption of $C_{60}$ on Bi terminated Si and Ge surfaces. The knowledge of the adsorption diagrams for Si and Ge is essential to choose the proper growth condition for selective adsorption and thereby to achieve a desired functionality of the surface.

O 13.10 Mon 17:15 H34

**First-principles study of H diffusion on Si(001)** — •Jürgen Wieferink[1,2], Peter Krüger[1], and Johannes Pollmann[1] — [1]Institut für Festkörpertheorie, Universität Münster — [2]Fritz-Haber-Institut, Berlin

Hydrogen diffusion on the Si(001)-(2×1) surface is crucial for an understanding of molecular $H_2$ desorption. On flat Si(001) terraces, only diffusion along the dimer rows is found for moderate temperatures and low H coverage. On the other hand, the occurrence of vacancy interrow transitions on a monohydride surface has been demonstrated by a recent study combining pulsed laser heating and scanning tunneling microscopy (STM) [1].

After a general introduction of the experimental findings we will present the results of our ab initio study on activation energies and diffusion rates as function of H coverage. The barrier energies depend strongly on the distance between the Si atoms in the transition state. As the monohydride surface is more rigid than the clean surface, isolated vacancies are less mobile than isolated H atoms. Interestingly, two adjacent vacancies may transfer charge from one to another prior to a vacancy transition, which significantly lowers the barrier.

[1] C. H. Schwalb, M. Dürr, U. Höfer, *Phys. Rev. B* **80**, 085317 (2009).

O 13.11 Mon 17:30 H34

**Self-assembly of aromatic heterocyclic molecules on GaAs surfaces** — •Thomas Bruhn[1,2], Bjørn Ove Fimland[3], Michael Kneissl[1], Norbert Esser[1,2], and Patrick Vogt[1] — [1]TU Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany — [2]ISAS Berlin, Albert-Einstein-Str. 9, 12489 Berlin, Germany — [3]NTNU, NO-7491 Trondheim, Norway

Although organic/inorganic interfaces are already used in a variety of technological applications, such as OLEDs or sensors, there is still no sufficient basic understanding of the structural and electronic parameters that influence the interface formation between the organic and the inorganic material. We investigate organic adsorbates on technologically important III-V surfaces. After having gained detailed understanding of the adsorption of unsaturated hydrocarbon ring molecules, we investigate the adsorption of the aromatic heterocyclic molecule Pyrrole ($C_4H_4NH$) on clean GaAs(001) surface reconstructions. The samples were prepared under UHV conditions and the adsorption process was monitored in-situ with reflectance anisotropy spectroscopy (RAS). The interfaces were characterized electronically by scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS) and photoemission spectroscopy (PES). The measurements show a significantly higher surface reactivity for the Ga rich surface reconstructions and indicate a physisorption of the adsorbed molecules at the As-rich $c(4 \times 4)$ reconstruction. Intra-molecular bondings could be identified in the tunneling spectra and molecular adsorption sites could be determined from the STM measurements.

## O 14: Metal substrates: Adsorption of organic / bio molecules II

Time: Monday 15:00–17:45 Location: H36

O 14.1 Mon 15:00 H36

**Random 2D metal-organic string networks based on divergent coordination assembly** — •Matthias Marschall[1,2], Joachim Reichert[1,2], Alexander Weber-Bargioni[2], Knud Seufert[1], Willi Auwärter[1], Svetlana Klyatskaya[3], Giorgio Zoppellaro[3], Mario Ruben[3], and Johannes V. Barth[1,2] — [1]Physik Department E20, TU München, Germany — [2]Department of Physics & Astronomy, University of British Columbia, Vancouver, Canada — [3]Institut für Nanotechnologie, Karlsruhe Institute of Technology, Germany

The molecular-level investigation of random networks becomes possible with two-dimensional supramolecular systems assembled on well-defined surfaces. Such studies allow to identify elementary structural motifs or characteristic defects and thus provide new insights into the intriguing nature of glasses and amorphous solids. Here we report a direct scanning tunneling microscopy investigation of a random metal-organic network, comprising interconnected strings and multiple ramification motifs. We employed a nonlinear prochiral ditopic linker deconvoluted in three stereoisomers upon surface confinement. Metallosupramolecular assembly was induced by codeposited cobalt atoms engaging in lateral metal-ligand interactions with the linker dicarbonitrile endgroups. The resulting complex networks are based on a library of distinct three- and fourfold Co-carbonitrile nodal coordination motifs giving rise to bifurcation or string formation. Thus the linker symmetry deconvolution and coordination multiplicity entails divergent assembly with concomitant random reticulation of the entire surface.

O 14.2 Mon 15:15 H36

**On the Scalability of Supramolecular Networks - High Packing Density vs. Optimized Hydrogen Bonds in Tricarboxylic Acid Monolayers** — •Jürgen F. Dienstmaier[1], Kingsuk Mahata[2], Wolfgang M. Heckl[3], Michael Schmittel[2], and Markus Lackinger[1] — [1]LMU München, Sektion Kristallographie — [2]Universität Siegen, Organische Chemie I — [3]Deutsches Museum

We present a Scanning Tunneling Microscopy (STM) based study of 1,3,5-tris[4*-carboxy(1,1*-biphenyl-4-yl)]benzene (TCBPB) monolayers at the liquid-solid interface. In analogy to smaller aromatic threefold symmetric tricarboxylic acids, this compound was aimed to yield two-dimensional nanoporous networks with large cavities. Depending on the solute concentration, three crystallographically distinct phases with pores of different size and shape were observed on graphite (001) with heptanoic acid as solvent. All three phases have the same dimer motif as basic building block in common. Yet, as opposed to other carboxylic acid assemblies, these dimers are not interconnected by O-H...O hydrogen bonds as anticipated, but by two energetically inferior C-H...O hydrogen bonds. Instead of the common head-to-head arrangement, this bonding pattern results in displaced dimers, which exhibit lower symmetry, allow for higher packing density, and give rise to chirality of all polymorphs. In accordance with studies of comparable systems, a positive correlation between solute concentration and average surface packing density is identified, which is rationalized by thermodynamic arguments.

O 14.3 Mon 15:30 H36

**Simulation of short-range order in a metal-organic network** — •Harry E. Hoster, Achim Breitruck, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

Short-range order (SRO) is a common phenomenon for surfaces and adlayers, where disturbances of a periodically ordered ground state are energetically inexpensive and thus thermally accessible. It has become common to simulate SRO using Monte-Carlo approaches based on additive models for the structure relevant interactions. The necessary parameters are usually obtained from ab-initio calculations or from fitting to experimental data. In this contribution, we will demonstrate that adlayers involving large organic molecules may exhibit a SRO with many similarities to disordered two-dimensional alloys [1]. Specifically, we focus on a structure that consists of a mixture of metal-organic complexes and organic trimers distributed on a hexagonal lattice. This distribution reflects an SRO governed by hydrogen bonds between the different types of lattice occupants. We show that this SRO, which is directly observed by scanning tunneling microscopy, can be simulated using pairwise interaction energy parameters based on a simple counting of hydrogen bonds [2].

[1] A. Bergbreiter et al., *Phys.Chem.Chem.Phys.* 9, **2007**, 5127.
[2] A. Breitruck et al., *J.Phys.Chem.C Letters*, DOI: 10.1021/jp908748w.

O 14.4 Mon 15:45 H36

**Thiolate based 2D Metal-Organic-Frameworks** — •Georg Eder, Hermann Walch, Jürgen Dienstmaier, and Markus Lackinger — LMU Munich, Department of Earth and Environmental Sciences

Self-assembled monolayers of the organic compound 1,3,5-tris(4-mercaptophenyl)benzene on Cu(111) are studied by Scanning Tunneling Microscopy under ultrahigh vacuum conditions. The molecular structure of this threefold symmetric compound aims at the synthesis of open pore networks through symmetric interconnection via their functional groups. Thiol groups can interact via weak hydrogen bonds, whereas deprotonated thiolate groups can form covalent disulphur bridges or metal coordination bonds. After room temperature deposition on Cu(111) we observe a close packed arrangement of deprotonated molecules that do not interact directly via their functional groups. Yet, annealing the sample up to 200°C induces phase transitions which result in two distinctly different phases where molecules bond through their functional groups. Depending on the initial coverage, we observe predominance of one of these phases. In both cases molecules coordinate with metal adatoms, thereby forming S-Cu-S metal coordination bonds. Preliminary results obtained on a Ag(111) surface suggest a similar behavior. Since the thiolate metal coordination bond provides better electronic coupling than for instance carboxylate analogues, this novel type of networks is of particular interest for molecular electronics.

O 14.5 Mon 16:00 H36

**Metal/SAM/Metal junctions studied from first principles** — •Jan Kučera and Axel Gross — Institute for Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

There is currently a strong interest in sandwich structures made of self-assembled monolayers (SAMs) between two metal layers (M/SAM/M) because of their potential in future nanoelectronics [1]. Recently, a M/SAM/M/SAM/M "double decker" junction was realized with two 4-mercaptopyridine SAMs sandwiched between an Au electrode and Pd and Pt monolayers [2]. We have performed periodic electronic structure calculations based on density function theory (DFT) to describe various phenomena playing a role in hybrid systems such as Au/SAM, Au/SAM/Pd, and Au/SAM/Pd/SAM/Pt with the SAMs consisting of the bifunctional thioaromatics 4-aminothiophenol or 4-mercaptopyridine [1-3]. Based on the calculated local density of states (LDOS) of the metal layers, possible explanations for experimental results will be provided which show a reduced DOS at the Fermi energy [2]. In addition, the role of van der Waals forces on the structure and stability of the SAMs has been addressed by performing DFT calculations with semi-empirical corrections for dispersion effects.
[1] M. Manolova et al., Adv. Mater. **21**, 320 (2009)
[2] F. Eberle et. al., Angew. Chem., accepted for publication.
[3] J. Kučera and A. Groß, Langmuir **24**, 13985 (2008)

O 14.6 Mon 16:15 H36

**Adsorption of long-chain alkanethiols on Au(111): a look from the substrate side** — •Frederick Chesneau[1], Jianli Zhao[1], Cai Shen[2], Manfred Buck[2], and Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, Germany — [2]EaStCHEM School of Chemistry, University of St Andrews, UK

The structure of interface between a self-assembled monolayer (SAM) of alkanethiolates and the underlying Au(111) substrate is one of the greatest mysteries of surface science. To cast light on this problem, we took SAMs of hexanethiolate (HT) and dodecanethiolate (DDT) on Au(111) as test systems and studied them by a combination of synchrotron-based high resolution X-ray photoelectron spectroscopy (HRXPS) and scanning tunneling microscopy (STM). The emphasis of the HRXPS characterization was put on the Au 4f emission of the substrate, which could be decomposed into the components related to the bulk and surface. The behavior of the surface component upon the formation of HT and DDT SAMs was monitored in detail. We observed both a shift of this component and its branching into two independent emissions, which were associated with the gold atoms in the topmost layer and gold adatoms, respectively. The branching of the surface component was correlated with the lateral structure of the SAMs as determined by STM. Conclusions on the reliability of different adsorption models for these lateral structures were derived.

O 14.7 Mon 16:30 H36

**Impact of the backbone on the electronic structure of SAMs on gold** — •LinJun Wang[1,2], Gerold M. Rangger[3], Lorenz Romanner[4], Tomas Bučko[5], ZhongYun Ma[1], QiKai Li[1], Zhigang Shuai[1,6], Egbert Zojer[3], and Georg Heimel[7] — [1]Institute of Chemistry, Chinese Academy of Sciences, Beijing, PR China — [2]Chemistry of Novel Materials, University of Mons Hainaut, Mons, Belgium — [3]Institute of Solid State Physics, Graz University of Technology, Graz, Austria — [4]Department of Material Physics, University of Leoben, Leoben, Austria — [5]Fakultät für Physik and Center for Computational Materials Science, Universität Wien, Wien, Austria — [6]Department of Chemistry, Tsinghua University, Beijing, PR China — [7]Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany

Modifying metal electrodes with self-assembled monolayers (SAMs) has promising applications in organic/molecular electronics. Through a comprehensive DFT study on a series of organic thiols on Au(111) surfaces, the impact of the chemical structure of the molecular backbone on the interface electronic structure is discussed. It is found that the backbone significantly impacts the alignment of the SAM conducting states relative to the metal Fermi level; for molecules with small ionization potentials, Fermi-level pinning is observed. For the work-function modification due to SAM adsorption, the main impact of the backbone arises from its influence on the molecular orientation on the surface. The polarizability is of only minor importance as the larger molecular dipole moments achieved with more polarizable backbones are largely compensated by increased depolarization.

O 14.8 Mon 16:45 H36

**Self-assembled monolayers of molecules with dithiol anchor groups: a DFT study** — •Katrin Tonigold and Axel Gross — Institute for Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

Traditionally, either aliphatic or aromatic thiols are used to prepare self-assembled monolayers on gold surfaces. If both types of thiol groups are combined in the anchor group of a molecule, the size of the anchor group as well as its electronic structure are changed. Competing reactions between the two different S-atoms and the Au-surface might take place possibly leading to different surface structures.

A molecule that contains such a dithiol anchor group is 2-Mercaptomethylbenzenethiol (MMBT). In cooperation with experimentalists from the Institute of Functional Interfaces of the Karlsruhe Institute of Technology we have studied the adsorption and structure formation of MMBT on Au(111) using DFT-GGA-calculations with semi-empirical corrections for dispersion effects. IR spectra and STM images have been simulated to allow a comparison with experimental results [1]. Furthermore, the formation of surface defects upon adsorption has been addressed.

[1] X. Stammer, K. Tonigold, M. Kind, A. Groß, Ch. Wöll *et al.*, in preparation.

O 14.9 Mon 17:00 H36

**STM study of fullerene molecules on alcanethiol based monolayers** — •Axel Beimborn[1], Patrick Mehring[1], Daniel Weier[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

Self assembled monolayers (SAMs) of organic molecules on metal surfaces are of great interest for the development of nanoscale mechanic and electric devices. The adsorption of alkanethiolate SAMs on Au(111) has been extensively investigated in a large number of studies. Another system with increasing research activities in the last years are $C_{60}$ fullerenes which have potential applications in several fields of nanotechnology. In this work the assembly of $C_{60}$ buckyballs on a thiolated Au(111) surface was studied with in situ STM investigations. This allows new arrangements of physisorbed buckyballs on metal surfaces. $CH_3S$ on gold was prepared exposuring a clean Au(111) surface to different partial preassures of Dimethyldisulfid (DMDS) yielding SAMs with different surface orientations. On these monolayers $C_{60}$ buckyballs were evaporated. Instead of the standard close packed hexagonal arrays the $C_{60}$ buckyball monolayers form striped phases depending on the underlying $CH_3S$ phases.

O 14.10 Mon 17:15 H36

**Building 2D crystals from fivefold-symmetric molecules** — •Tobias Bauert[1], Leo Merz[1], Manfred Parschau[1], Jay S. Siegel[2], Georg Koller[3], and Karl-Heinz Ernst[1,2] — [1]Empa, Nanoscale Material Science, Dübendorf, Switzerland — [2]Organisch-chemisches Institut, Universität Zürich, Switzerland — [3]Institut für Physik, Karl-Franzens-Universität, Graz, Austria

Curved surface fragments of the fullerene molecule, so-called buckybowls, are promising candidates for surface modifications because of their unique electronic and chemical properties. Corannulene ($C_{20}H_{10}$) is the simplest curved fullerene fragment with a central $C_5$ ring, surrounded by five aromatic $C_6$ rings. Due to this fivefold symmetry, it is also a fascinating molecule for studies of fundamental phenomena in adsorbed monolayers, like molecular and chiral recognition or spontaneous symmetry breaking. Fivefold symmetry is incompatible with the translational order of a classical crystal lattice, which applies to plane group symmetries of 2D crystals grown at surfaces as well. Corannulene forms a quasi-hexagonal lattice by tilting away from the $C_5$ symmetry. Bulky substituents, however, do not allow a tilt and enforce $C_5$ as tiling motif. The observed molecular structures in STM are compatible with mechanical modeling experiments and Monte-Carlo simulations of hard pentagons. Apart from the self-assembly results, adsorbed corannulene shows interesting electronic properties, like induction of a large interface dipole moment (9 D), as determined with workfunction change measurements via UPS.

O 14.11 Mon 17:30 H36

**2D-grids as precursors for 2D-crystals** — •Thomas Waldmann, Christina Nenon, Robert Reichert, Harry E. Hoster, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

The bis(terpyridine) derivative 2,4'-BTP [1,2] forms ordered monolayers (ML) on Ag(111)/Ru(0001) [3-5], Au(111) [3,5], highly ordered pyrolytic graphite (HOPG) [1-3,5], and Ag(100) at coverages between 0.35 and 0.44 molecules/nm$^2$. At T = 300 K and lower coverage, the adsorbates form a two-dimensional (2D) admolecule gas, where they move faster than the STM-tip. At T = 115 K, one can observe (2,4'-BTP)$_n$ oligomer chains stabilized by C-H$\cdots$N-type hydrogen bonds. We show that the local configurations of the molecules and their individual orientations with respect to the substrate are similar to those known from ordered structures formed by the molecules at higher coverages. This confirms our previous suggestion that the corrugation of the molecule-substrate potential and the molecule-molecule interactions play an equally important role for the structures formed by this kind of molecules [3-4].

[1] U. Ziener et al., *Chem.Eur.J.* 8, **2002**, 951.
[2] C. Meier et al., *J.Phys.Chem.B* 109, **2005**, 21015.
[3] H.E. Hoster et al., *Langmuir* 23, **2007**, 11570.
[4] M. Roos et al., *Phys.Chem.Chem.Phys.* 9, **2007**, 5672.
[5] M. Roos et al., *Phys.Chem.Chem.Phys.*, DOI: 10.1039/b920481d

## O 15: Spin-Orbit Interaction at Surfaces II

Time: Monday 15:00–17:15 Location: H38

O 15.1 Mon 15:00 H38

**Graphene with strong extrinsic spin-orbit effects: an ab-initio study** — •Gustav Bihlmayer and Stefan Blügel — Institut für Festkörperforschung & Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

Recent experimental investigations of Au-intercalated graphene on Ni(111) reported strong spin-orbit (SO) induced splittings in the spectrum near the $\overline{K}$-point [1]. Theoretical studies of a model Hamiltonian for graphene with extrinsic SO coupling predict an unusual spectrum and spin-orientation pattern for this case [2].

We present first principles calculations of this system, basically confirming the scenario developed in [2], but including effects from the realistic materials, e.g. modifications due to the substrate. Our calculations show quantitative agreement with the experimental results [1]. Moreover, the complex interplay of the nickel's exchange field and Rashba-type SO-fields (induced by the intercalated Au monolayer) is analysed and compared to other cases, e.g. the Rashba-split surface state of the Gd(0001) surface [3].

[1] A. Varykhalov et al., Phys. Rev. Lett. **101**, 157601 (2008)
[2] E. I. Rashba, Phys. Rev. B **79**, 161409(R) (2009)
[3] O. Krupin et al., Phys. Rev. B **71**, 201403(R) (2005)

O 15.2 Mon 15:15 H38

**Spin-orbit coupling and Rashba effect in graphene: *Ab initio* model studies** — •Samir Abdelouahed[1], Hossein Mirhosseini[1], Igor V. Maznichenko[2], Arthur Ernst[1], and Jürgen Henk[1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Martin Luther University Halle-Wittenberg, Halle, Germany

Significant spin-orbit effects have been found experimentally in graphene, e. g. Rashba-type splittings at the Dirac point. Because the atomic spin-orbit coupling of carbon is very weak, additional mechanisms must come into question to explain these splittings. Theoretical studies already addressed these mechanisms but sometimes relied on empirical methods.

Here, we report on a first-principles investigation of spin-orbit coupling in graphene, in which various ingredients of Rashba-type effects are systematically considered. Besides a potential gradient normal to the carbon sheet which gives rise to the conventional Rashba effect, an in-plane potential gradient and corrugation effects are discussed.

O 15.3 Mon 15:30 H38

**Structural Influence on the Rashba-type Spin-Splitting in Surface Alloys** — •Christian R. Ast[1], Isabella Gierz[1], Benjamin Stadtmüller[1,2], Johannes Vuorinen[3], Matti Lindroos[3], Hugo Dil[4], Fabian Meier[4], and Klaus Kern[1] — [1]MPI für Festkörperforschung, Stuttgart — [2]Exp. Physik II, Universität Würzburg — [3]Tampere University of Technology, Dept. of Physics, Tampere, Finland — [4]PSI, SLS, Villigen, Switzerland

The Rashba-Bychkov (RB) model has been remarkably successful in describing the spin splitting of two-dimensional (2D) electron systems with a structural inversion asymmetry (SIA). It explains how the spin-degeneracy is lifted by an electric field perpendicular to a 2D free electron system. Looking in more detail, different contributions to a strong spin-splitting at surfaces include a strong atomic spin-orbit interaction, orbital character, a SIA as well as other structural modifications. For surface states, the RB effect can only serve as a qualitative model, because it only accounts for an effective electric field. A number of surface alloys (Bi/Ag(111), Pb/Ag(111), etc.) have been identified with an extremely large spin-split surface state. Interestingly, only a fraction of the atoms at the surface feature a sizeable atomic spin-orbit coupling so that the source of the large spin-splitting must be sought in the structure. We present a systematic study of the alloy atom relaxation in different Ag(111) surface alloys using quantitative low-energy electron diffraction (IV-LEED) measurements and calculations. We relate the alloy atom relaxation to the size of the spin-splitting and discuss possible scenarios of the underlying mechanism.

O 15.4 Mon 15:45 H38

**Tuneable Hybridization between Rashba-split Surface States in BiAg$_2$/Ag/Au(111) Trilayer Systems** — •Hendrik Bentmann[1], Frank Forster[1], and Friedrich Reinert[1,2] — [1]Universität Würzburg, Experimentelle Physik VII, Am Hubland, D-97074 Würzburg, Germany — [2]Forschungszentrum Karlsruhe, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe, Germany

We have studied the surface states of a BiAg$_2$ surface alloy grown on thin Ag films on Au(111) by angle-resolved photoelectron spectroscopy. In contrast to the case of the bulk Ag(111) substrate we find the $sp_z$-type and the $p_xp_y$-type surface state to be separated by a hybridization gap that is accompanied by a pronounced kink in the dispersion of the $p_xp_y$-type state. The size of the gap is tunable via the Ag film thickness, whereas the gap closes for higher coverages. Our observations are attributed to slight variations in the protrusion height of the Bi atom. We propose that these variations are induced by thickness-dependent partial charge densities of the Ag quantum well states in the topmost layer. According to previous calculations we anticipate an unconventional sign change of the spin polarization at the hybridization kink of the $p_xp_y$-type state [1,2].

[1] H. Mirhosseini, J. Henk, A. Ernst, S. Ostanin, C.T. Chiang, P. Yu,
A. Winkelmann, and J. Kirschner, Phys. Rev. B **79**, 245428 (2009).
[2] G. Bihlmayer, S. Blügel, and E. V. Chulkov, Phys. Rev. B **75**, 195414 (2007).

O 15.5 Mon 16:00 H38

**Local topography and density of states in the Bi$_x$Pb$_{1-x}$/Ag(111) mixed surface alloy** — •Fabian Zinser, Maximilian Assig, Klaus Kern, and Christian R. Ast — Max Planck Institute for Solid State Research, Stuttgart, Germany

The Bi/Ag(111) and Pb/Ag(111) surface alloys exhibit a 2D electronic structure with an extremely large spin-splitting [1]. Mixing the relative amounts of Bi and Pb atoms at the surface creates a mixed surface alloy where the spin-splitting as well as the band occupation can be tuned continuously [2]. We present a study of the electronic structure and local topography at the surface of the Bi$_x$Pb$_{1-x}$/Ag(111) mixed surface alloy using scanning tunneling microscopy and spectroscopy (STM/STM). We discuss the local disorder of the Pb and Bi alloy atoms as well as the evolution of the local density of states as a function of relative Bi and Pb content.

[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 15.6 Mon 16:15 H38

**Quantum-size induced giant spin-orbit splitting** — •Andreas Ruffing[1], Stefan Mathias[1,2], Martin Wiesenmayer[3], Indranil Sarkar[1], Gustav Biehlmayer[4], Eugene V. Chulkov[5,6], Yury M. Koroteev[7], Pedro M. Echenique[5,6], Michael Bauer[3], and Martin Aeschlimann[1] — [1]Deepartment of Physics, University of Kaiserslautern, Germany — [2]JILA and Department of Physics, University of Colorado, Boulder, USA — [3]Institut für Experimentelle und Angewandte Physik, Universität Kiel, Germany — [4]Institut für Festkörperforschung und Institut for Advanced Simulation, Forschungszentrum Jülich, Germany — [5]Donostia International Physics Center (DIPC), San Sebastián/Donostia, Basque Country, Spain — [6]Departamento de Física de Materiales and Centro Mixto CSIC-UPV/EHU, San Sebastian/Donostia, Basque Country, Spain — [7]Institut of Strength Physics and Materials Science, RAS, Tomsk, Russia

We report on the observation of giant spin-orbit splitting of quantum-well states in the unoccupied electronic structure of a Bismuth monolayer on Cu(111). Up to now, Rashba-type splittings of this size have been reported exclusively for surface states in a partial bandgap. With these quantum-well states we have experimentally identified a second - and broader - class of states that show a huge spin-orbit splitting. First-principle electronic structure calculations show that the origin of the spin-orbit splitting is due to the perpendicular potential at the surface and interface of the ultrathin Bi film. This finding allows for the direct possibility to tailor spin-orbit splitting by means of thin film nanofabrication.

O 15.7 Mon 16:30 H38

**Evolution of Topological Edge-States in Bi$_{1-x}$Sb$_x$ Films on Si(111)** — •Hadj Mohamed Benia, Carola Strasser, Klaus Kern, and Christian R. Ast — Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany

Due to a semimetal-semiconductor transition in the Bi$_{1-x}$Sb$_x$ alloy, Bi is transformed into a topological insulator for Sb concentrations larger than 8% [1]. So far, the evolution of the topological states with Sb concentration has only been studied theoretically [2]. We have experimentally investigated the band structure of high quality Bi$_{1-x}$Sb$_x$ films grown on Si(111) using angular resolved photoemission spectroscopy (ARPES). The evolution of the topological states as function of Sb concentration will be discussed.

[1] D. Hsieh et al. Nature 452, 970 (2008).
[2] L. Fu, C.L. Kane, Phys. Rev. B 76, 45302 (2007).

O 15.8 Mon 16:45 H38

**Towards a ferroelectric control of Rashba spin-orbit coupling: Bi on BaTiO$_3$(001) from first principles** — •Hossein Mirhosseini[1], Igor Maznichenko[2], Samir Abdelouahed[1], Sergey Ostanin[1], Arthur Ernst[1], Ingrid Mertig[1,2], and Jürgen Henk[1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Institute of Physics, Martin Luther University Halle-Wittenberg, Halle, Germany

We propose a new route for controling the Rashba splitting of the electronic states of an adlayer. The Rashba spin splitting in the 6$p$ states of a Bi adlayer on BaTiO$_3$(001) can be manipulated by the electric polarization in the ferroelectric substrate.

The Bi surface states display an anisotropic dispersion with an unmached splitting about 0.2 Å$^{-1}$. Switching of the intrinsic electric polarization $P$ in BaTiO$_3$ affects the strength of the Rashba splitting in the Bi adlayer. The relative change in the splitting is about 5 %. Our findings may pave a route for new spinelectronic devices.

O 15.9 Mon 17:00 H38

**Growth and characterization of Bi$_{1-x}$Sb$_x$ crystalline films on Si(111)** — •Carola Strasser, Hadj Mohamed Benia, Klaus Kern, and Christian R. Ast — Max Planck Institute for Solid State Research, Stuttgart, Germany

Recently, the Bi$_{1-x}$Sb$_x$ alloys have been identified as topological insulators for Sb contents larger than 8%. While studies so far have used single crystals, we have grown Bi$_{1-x}$Sb$_x$ films on Si(111) with a focus on producing a particularly smooth surface.

The quality of the samples was analyzed using different techniques, such as low energy electron diffraction (LEED), secondary ion mass spectrometry (SIMS), X-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS). The preparation and optimization of flat and homogenous films will be presented.

## O 16: Organic, polymeric, biomolecular films - also with adsorbates

Time: Monday 15:00–17:30 Location: H46

O 16.1 Mon 15:00 H46

**Initial growth of crystalline rubrene thin film growth on mica (001)** — •Harald Zaglmayr[1], Lidong Sun[1], Günther Weidlinger[1], Shaima'a Abd Al-Baqi[2], Dmitrii Nabok[3], Peter Zeppenfeld[1], Helmut Sitter[2], and Claudia Ambrosch-Draxl[3] — [1]Institute of Experimental Physics, Johannes Kepler University Linz, Altenbergerstraße 69, A-4040 Linz, Austria — [2]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Altenbergerstraße 69, A-4040 Linz, Austria — [3]Department of Material Physics, Montanuniversity Leoben, Franz-Josef-Straße 18, A-8700 Leoben, Austria

Epi-fluorescence and laser scanning confocal microscopy (LSCM) have been used to investigate the morphology and optical properties of rubrene thin films at the early stage of crystallization and rubrene single crystals with a diameter of several tens of micrometers. The films were prepared on a muscovite mica substrate by hot wall epitaxy. The initial growth proceeds via the formation of a wetting layer and the nucleation of islands with an amorphous structure. Crystallization starts when the amorphous islands coalesce and needle like crystalline fibers are formed in the gap between the islands. The crystalline fibers then grow on top and in between the original amorphous islands leading to an "open network" of islands. The latter acts as a basis for the growth of semi-crystalline spherulites. For the rubrene single crystals, the spatially resolved photoluminescence spectrum shows a strong dependence on the orientation, which can be attibuted to the optical anisotropy of the crystals.

O 16.2 Mon 15:15 H46

**Photoisomerization of azobenzene on layer compound surfaces studied by photoelectron spectroscopy** — •Eric Ludwig[1], Jaroslaw Iwicki[1], Kai Rossnagel[1], Felix Köhler[2], Rainer Herges[2], and Lutz Kipp[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel, Germany — [2]Otto-Diels-Institut für Organische Chemie, Universität Kiel, D-24098 Kiel, Germany

Photoswitchable azobenzene and its derivative Disperse Orange 3 (DO3) molecules were deposited *in situ* under UHV conditions on the surfaces of the metallic and semiconducting layered crystals $TiTe_2$ and $HfS_2$, respectively. Due to weak van der Waals-like coupling between the layers these materials serve as excellent substrates for the analysis of adsorbed molecules and their possible photoswitching behavior. Coverages from sub-monolayer to several monolayers were realized. Photoelectron spectroscopy (PES) experiments were performed using a He discharge lamp and a SPECS Phoibos 150 analyzer. Results imply Stranski-Krastanov-like film growth of azobenzene on $TiTe_2$. Comparison of PES spectra to outer valence green function calculations suggests dimer formation of DO3. To photoisomerize the adsorbed molecules, the samples were irradiated with a LED Power Pen (wavelength 365 nm, 3.5 $W/cm^2$). Experimental data of azobenzene adsorbed on $HfS_2$ shows that the molecules can be partially switched from the *trans* to the *cis* orientation. On $TiTe_2$ no switching has been observed, presumably due to stronger molecule-substrate coupling. This work was supported by the DFG through SFB 677.

O 16.3 Mon 15:30 H46

**Light effective mass of the valence band hole of rubrene single crystal observed by angle-resolved photoelectron spectroscopy** — •Satoshi Kera, Steffen Duhm, Shunsuke Hosoumi, Qian Xin, Nobuo Ueno, Shinichi Machida, Akihiro Funakoshi, Naoki Ogawa, Yasuo Nakayama, and Hisao Ishii — Grad. School of Advanced Integration Science, Chiba University

The mechanism of the carrier transport in organic semiconductor has remained in puzzling at room temperature region, especially. Rubrene ($C_{42}H_{28}$) single crystal has been recognized to exhibit the highest hole mobility among all organic semiconductors [1]. To comprehend the transport nature as well as to improve the device performance, information on the electronic structure is indispensable. In the present study, we successfully observed the valence electronic structures of rubrene single crystal by angle-resolved ultraviolet photoelectron spectroscopy with laser illumination to avoid sample charging. A clear energy dispersion of the highest occupied molecular orbital band was observed, where the dispersion width is 0.4 eV along the well conjugated direction. Effective mass of holes is estimated to be 0.7 $m_0$. The present results suggest that the carrier conduction mechanism in a rubrene single crystal should be described as band transport of a delocalized light quasiparticle [2].

[1] T. Hasegawa and J. Takeya, Sci. Technol. Adv. Mater. 10, 024314 (2009). [2] S. Machida et al, submitted.

O 16.4 Mon 15:45 H46

**Self-assembled monolayers of perfluoroterphenyl-substituted alkanethiolates on coinage metal substrates** — •Frederick Chesneau[1], Björn Schüpbach[2], Katarzyna Szelagowska-Kunstman[3], Nirmalya Ballav[1], Piotr Cyganik[3], Andreas Terfort[2], and Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany — [2]Institut für Anorganische und Analytische Chemie, Goethe-Universität Frankfurt, 60438 Frankfurt, Germany — [3]Faculty of Physics, Astronomy, and Applied Computer Science, Jagiellonian University, 30059 Krakow, Poland

Self-assembled monolayers (SAMs) formed by perfluoroterphenyl-substited alkanethiols (FTPn, with n being the number of the methylene units) with variable length of the aliphatic linker (n = 2 and 3) on (111) Au and Ag were characterized by a combination of several complementary spectroscopic and microscopic techniques. The SAMs were found to be well-defined, highly ordered, and densely packed, which suggest a strong correlation between the orientations of the analogous rings in the adjacent molecules. In addition, the SAMs exhibited pronounced odd-even effects, i.e. dependence of the molecular orientation and packing density on the length of the aliphatic linker, with parity of n being the decisive parameters and the direction of the effects on Au opposite to that on Ag. The presence of the odd-even effects in the FTPn system, characterized by distinctly non-planar conformation of the FTP moieties, brings new aspects into the discussion about the origin of these effects.

O 16.5 Mon 16:00 H46

**Fast and non-invasive optical study of protein films on surfaces** — •Franz-Josef Schmitt[1], Heinrich Südmeyer[2], Kai Reineke[1], Insa Kahlen[1], Joachim Börner[1], Max Schöngen[1], Patrick Hätti[1], Hans Joachim Eichler[1], and Hans-Joachim Cappius[2] — [1]Berlin Institute of Technology, Berlin — [2]Laser- und Medizintechnologie GmbH, Berlin

Thin films of proteins, bacteria and diverse biochemical compounds are always found on surfaces exposed to the environment. Optical methods deliver innovative tools for the study of protein films. Residue of proteins, which exhibit fluorescence when exited in the UV wavelength range, can easily be investigated optically. The results show that protein films are structured inhomogeneously. Ring shaped structures often found after surface drying can be explained by the influence of surface tension during the evaporation process of the protein solvents. We present a specially designed handheld measuring device that can analyse organic contamination levels below $1\mu g/cm^2$ within seconds. By using time-correlated methods the fluorescence detection of contamination level on surfaces is possible even if the fluorescence spectra of contamination and base material overlap.

Financial support by Federal Ministry of Education and Research (BMBF) is greatfully acknowledged.

O 16.6 Mon 16:15 H46

**Protein resistant ethylene glycol terminated self-assembled monolayers by vapour deposition in vacuum** — •Laxman Kankate[1], Helge Grossmann[2], Udo Werner[1], Robert Tampé[2], Andrey Turchanin[1], and Armin Gölzhäuser[1] — [1]Department of Physics, Physics of Supramolecular Systems, University of Bielefeld — [2]Institute of Biochemistry, Johann Wolfgang Goethe-University, Frankfurt am Main

Vacuum vapour deposition (VD) is a method of choice for the preparation of organic interfaces for the in situ characterization and nanofabrication. However, it is usually difficult to prepare the self-assembled monolayers of thiols on gold by vacuum VD with the degree of quality sufficient for applications. Therefore, most of the SAM preparation is usually undertaken in solvents. In this contribution we report the first vacuum VD study of the protein resistant 11-(mercaptoundecyl)-triethylene glycol (C11EG3OH) SAM on gold surfaces. We present a comparison of C11EG3OH SAMs prepared by VD and by solution method using X-ray photoelectron spectroscopy and Fourier transform infrared reflection absorption spectroscopy. Using surface plasmon resonance spectroscopy we demonstrate that SAMs prepared by both methods have comparable protein resistivity to the adsorption of various proteins (bovine serum albumin, trypsin and myoglobin). These results show a new path to the in situ engineering of protein resistant surfaces and patterns by standard nanofabrication techniques.

O 16.7 Mon 16:30 H46

**One- and Two-dimensional Polyamide Films by Vapor Deposition Polymerization** — •Christoph H. Schmitz, Julian Ikonomov, and Moritz Sokolowski — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Germany

Long-range ordered structures on surfaces are mainly based on weak adsorbate-adsorbate interactions, such as van der Waals-forces, dipole interactions and hydrogen bonds. Though, technical applications (*e.g.*, coatings, sensors, catalysis) require more robust and durable layers, which may be realized by covalent networks on the surface.

We herein report on the formation of covalently interlinked structures of a polyamide via condensation polymerization directly on the Ag(111) surface at room-temperature. The vapor deposition polymerization technique was combined with ultra-high vacuum preparation methods to obtain polymer monolayers. Depending on the symmetry (*i.e.* the substitution pattern) of the deposited aromatic amine and acid chloride monomers, one- or two-dimensional polymers can be prepared, which are stable at elevated temperatures up to 620 K. The structures have been characterized by variable temperature scanning tunneling microscopy.

Funded by DFG through SFB 624

O 16.8 Mon 16:45 H46

**Investigation of Cellulose Model-Systems for Paper Fiber-Fiber Bonds with FTIR and AFM** — •Eduard Gilli[1,2],

Mario Djak[1,2], Oliver Miskovic[1,3], Franz Schmied[1,3], Christian Teichert[1,3], Eero Kontturi[4], and Robert Schennach[1,2] — [1]CD-Laborarory for Surf. Chem. and Phys. Fund. of Paper Strength — [2]Institute for Solid State Physics, TU-Graz, Austria — [3]Institute of Physics, University of Leoben, Austria — [4]TKK Helsinki, Finland

Spectroscopic investigation of the properties of fiber-fiber bonds in a sheet of paper often fails due to incorrect interpretation of the spectra, which are influenced heavily by geometrical effects, and scattering. Simulating the geometry as a multi-layer stack can help understanding the properties of paper, but the complex stochastic behavior of fibers cannot be modeled by these means. Investigation of model film systems from cellulose and hemicelluloses on Si can improve the situation, and close the gap between theory and experiment.

The cellulose model films were prepared by spin coating from trimethylsilyl cellulose solution and subsequent hydrolyzation. Further layers of hemicelluloses can be attached by spin coating or by adsorption. From atomic force microscopy measurements comprehensive knowledge of the layer roughness can be obtained, which is used as a prerequisite for spectral simulation. By spectral simulation optical effects can be identified, yielding a better understanding of the chemistry, going on between cellulose and hemicelluloses. Finally bonding strength tests on the model films can correlate the chemistry to the mechanical properties of fiber-fiber bonds.

O 16.9 Mon 17:00 H46

**Growth of alpha-Sexithiophene films on Cu(110)-(2x1)O at elevated substrate temperatures** — •Günther Weidlinger, Harald Zaglmayr, Lidong Sun, Daniel Roman Fritz, Thorsten Wagner, and Peter Zeppenfeld — Johannes Kepler Universität Linz, Institut für Experimentalphysik, Altenberger Straße 69, A-4040 Linz

alpha-Sexithiophene (6T) films were grown on the Cu(110)-(2x1)O surface in UHV with the substrate held at 380 K. Ex-situ atomic force microscopy (AFM), fluorescence microscopy (FM) and laser scanning confocal microscopy (LSCM) reveal elongated 6T islands with a height of up to a few hundred nanometers. These needles consist of crystallites of two distinct orientations with respect to the main axes of the substrate surface. However, polarization dependent FM shows that the 6T molecules in the needles are always aligned along the [001] direction of the substrate. Comparing AFM and FM images, regions of maximum fluorescence emission correspond to defects, e.g. needle ends or grain boundaries, at which light can couple out of the needles whereas defect-free parts appear darker due to a waveguiding effect inside the islands. Photoluminescence spectra obtained by LSCM are in qualitative agreement with reference spectra of single crystalline 6T. No wetting layer of 6T was observed with LSCM. This is in agreement with results from reflectance difference spectroscopy measurements where a quenching of the characteristic wetting layer signal was observed after exposure to air.

O 16.10 Mon 17:15 H46

**Crystalline Inverted Membrane Growth by Electrospray Ion Beam Deposition** — •Stephan Rauschenbach[1], R. Thomas Weitz[1], Ludger Harnau[2], Nikola Malinowski[1,3], Theresa Lutz[1], Nicha Thontasen[1], Zhitao Deng[1], and Klaus Kern[1,4] — [1]MPI Festkoerperforschung, Stuttgart, Germany — [2]MPI Metallforschung, Stuttgart, Germany — [3]Central Laboratory of Photographic Processes, Bulgarian Academy of Sciences, Sofia, Bulgaria — [4]Institut de la Matière Condenseé, EPFL, Lausanne, Switzerland

Amphiphilic molecules assembled in 2D membranes stabilize interfaces by the interplay of intermolecular- and hydrophobic- interactions. The latter interaction is canceled, when the surfactant molecules are transferred to an interface in vacuum.

Ion beam deposition of sodium dodecyl-sulfate (SDS) onto surfaces in vacuum is used as a model system for the assembly of amphiphilic molecules in the absence of solvents. To this end, cluster ion beams of SDS with excess Na+ as charge carrier are deposited on graphite and silicon samples which are analyzed ex-situ by AFM.

Our samples show stable, extended, flat islands of heights corresponding to single and double layers of upright standing SDS molecules. The relative strengths of the ionic- and van-der-Waals-interaction between the molecules without the presence of water suggests an inverted internal structure of the membranes with respect to their liquid grown counterparts. The shape of the islands is found to be characteristic for a crystalline phase of SDS.

## O 17: [DS] Organic Electronics and Photovoltaics II (Joint Session DS/CPP/HL/O)

Time: Monday 14:00–15:30 Location: H8

O 17.1 Mon 14:00 H8

**Influence of the substrate-lattice-geometry on the island shape of organic thin films** — •M. Benedetta Casu[1], Britt-E. Schuster[1], Indro Biswas[1], Christoph Raisch[1], Helder Marchetto[2], Thomas Schmidt[2], T. Onur Menteş[3], Miguel A. Nino[3], Andrea Locatelli[3], and Thomas Chassé[1] — [1]IPTC, University of Tübingen, Tübingen, Germany — [2]Fritz-Haber-Institut, Berlin, Germany — [3]Sincrotrone Trieste S.C.p.A., Trieste, Italy

By using a combination of microscopic imaging and diffraction techniques with structural and chemical sensitivity, we studied the growth of diindenoperylene (DIP) on Au(100), and Au(111). Growth and structure of DIP films of different thickness were monitored in situ including real time PEEM and LEEM performed at the beamlines Nanospectroscopy at Elettra, and UE49-PGM-b-SMART at BESSY. A layer-by-layer mechanism characterizes the initial growth in both cases followed by island nucleation, i.e., the growth follows the Stranski-Krastanov mode. The islands surprisingly show a fractal-like shape when the DIP thin films are deposited on a Au(111) single crystal. DIP thin films deposited on various substrates at RT have been investigated, revealing the tendency to Stranski-Krastanov growth but the observed islands were always compact (i.e. non-fractal). In particular, real time LEEM investigations on Au(100), under the same preparation conditions as on Au(111), show compact islands. We interpret the fractal growth of DIP for these kinetic growth conditions as a consequence of the triangular symmetry of the substrate, as seen in homoepitaxial and heteroepitaxial metal on metal growth.

O 17.2 Mon 14:15 H8

**Can X-ray microspectroscopy probe inhomogeneities in the electron structure of organic devices?** — •Christian Hub, Martin Burkhardt, Marcus Halik, and Rainer Fink — Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen, Egerlandstraße 3, 91058 Erlangen, Germany

The degree of homogeneity in the morphology of organic thin film devices has a major impact on the charge transport properties. Real devices usually strongly deviate from the ideal device structure since epitaxial growth with low defect concentrations cannot be achieved. We have recently started to investigate pentacene-based OFETs, which were prepared using commercial silicon nitride membranes as dielectric showing excellent transport characteristics. The overall device thickness is sufficiently small to perform scanning transmission X-ray microspectroscopy (SXTM) experiments at the PolLux microspectroscope. Grains with varying preferential orientation in the polycrystalline pentacene films are detected using the significant local NEXAFS dichroism. The local NEXAFS contrast is utilized to investigate differences in the electronic structure within these films while the devices are operated. Using the standard photomultiplier tube of the PolLux as detector no pronounced changes were observed when current is driven through the organic films. Therefore electron detection was implemented to further enhance the sensitivity of the microscope to ultrathin films. We will discuss the related problems and opportunities to use local NEXAFS with lateral resolution below 30 nm. The work is funded by the BMBF under contract 05 KS7WE1.

O 17.3 Mon 14:30 H8

**Morphology and electronic properties of an electron acceptor adsorbed on organic insulator pre-covered metal surfaces** — •P. Amsalem[1], J. Frisch[1], A. Wilke[1], A. Vollmer[2], R. Rieger[3], K. Müllen[3], J.-P. Rabe[1], and N. 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

In this work, we explore the possibility of tuning the interface energetics at a pi-conjugated (electron acceptor) molecule-metal interface by modifying the adsorbate-substrate distance through pre-adsorption of insulating organic monolayers. We report a photoemission study of the growth of hexaazatriphenylene-hexacarbonitrale (HATCN) deposited on N,N-bis-(1-naphthyl)-N,N-diphenyl1-1,1-biphenyl1-4,4-diamine($\alpha$-NPD) or tris(8-hydroxyquinoline)aluminum ($Alq_3$) pre-covered Ag(111) surfaces. $\alpha$-NPD and $Alq_3$ are known to be weakly adsorbed on Ag(111) and have both been used as thin organic spacer. The choice of HATCN has been motivated by its high electronic affinity ($\sim$3.5 eV). HATCN molecules deposited on $\alpha$-NPD/Ag(111) are found to diffuse below the $\alpha$-NPD molecules pre-adsorbed on Ag(111). In the case of HATCN on $Alq_3$/Ag(111), an interface state close to the Fermi-level is observed. This interface state differs markedly from the one measured for HATCN in direct contact with Ag(111). The results are discussed in terms of the formation of polaronic states and charge transfer across insulating layers.

O 17.4 Mon 14:45 H8

**Energy levels and work function of ultra-thin polythiophene films on conductive polymer electrodes** — •Johannes Frisch[1], Antje Vollmer[2], Jürgen P. Rabe[1], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Institut f. Physik, Brook-Taylor-Straße 6, D-12489 Berlin — [2]Elektronenspeicherring BESSY II, Albert-Einstein-Str. 15, D-12489 Berlin

In modern organic photovoltaic cells (OPVCs), poly(ethylene-dioxythiophene):poly(styrenesulfonate) (PEDT:PSS) and poly(3-hexylthiophene) (P3HT) are prototypical materials used as transparent anode and as donor polymer, respectively. In this context, it is essential to clarify how the efficiency of OPVCs based on these materials depends on the position of the energy level at the interface. In the present work, the morphology, work function, and energy level alignment of ultra-thin films of P3HT on PEDT:PSS were investigated using photoelectron spectroscopy (XPS, UPS). Ultra-thin films (down to sub-monolayer coverages) were produced by spin coating P3HT films on PEDT:PSS followed by a subsequent washing process. It has been found that the deposition of ultra-thin P3HT films on PEDT:PSS lowers the sample work function ($\Phi$) by 0.4 eV due to doping of P3HT film with positive charges from the PEDT:PSS layer. The valence band edge (VBE) is located only 0.1 eV below the Fermi-level. For thicker P3HT films (ca. 10 nm), $\Phi$ further decreases by 0.2 eV and the VBE is observed 0.2 eV below the Fermi-level. These results are discussed within existing concepts of local work function fluctuations and energy level bending at the P3HT/PEDT:PSS interface.

O 17.5 Mon 15:00 H8

**Electronic properties of Cu-phthalocyanine-fullerene planar and bulk heterojunctions on PEDOT:PSS** — •Andreas Wilke, Toshiko Mizokuro, Ralf Peter Blum, Jürgen P Rabe, and Norbert Koch — Institut für Physik, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 6, D-12489 Berlin

In organic photovoltaic cells (OPVCs) typically two organic materials with electron-acceptor and electron-donor properties are placed between anode and cathode, forming either a layered planar or mixed bulk heterojunction where charge separation should occur. To improve the efficiency of this central process it is important to know and understand the energy levels at such heterojunctions, and how they may depend on heterojunction morphology. We report ultraviolet and X-ray photoelectron spectroscopy studies on layered planar and mixed bulk heterojunctions of Cu-phthalocyanine (CuPc) and $C_{60}$, a prototypical material pair for OPVCs. The respective heterojunctions were formed on poly(ethylene-dioxythiophene):poly(styrenesulfonate) substrates, in order to achieve morphologies comparable to those in actual OPVCs. The energy offset between the highest occupied levels of CuPc and $C_{60}$ was determined to 1.3 eV for both the layered and mixed bulk heterojunction. Our results demonstrate that the energy levels that determined the efficiency of charge separation in OPVCs made of CuPC and $C_{60}$ are independent of particular interface morphology, and that differences in device efficiency are due to other effects.

O 17.6 Mon 15:15 H8

**A high molecular weight donor for electron injection interlayers on metal electrodes** — •Benjamin Bröker[1], Ralf-Peter Blum[1], Luca Beverina[2], Oliver T. Hofmann[3], Georg Heimel[1], Antje Vollmer[4], Johannes Frisch[1], Jürgen P. Rabe[1], Egbert Zojer[3], and Norbert Koch[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstrasse 15, D-12389 Berlin, Germany — [2]Department of Materials Science and INSTM, State University of Milano-Bicocca, Via Cozzi 53,I-20125 Milano, Italy — [3]Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria — [4]Helmholtz-Zentrum Berlin, Bessy II, Albert-Einstein-Str. 15, D-12489 Berlin, Germany

The molecular donor 9,9-ethane-1,2-diylidene-bis(N-methyl-9,10-dihydroacridine) (NMA) has been synthesized, and its electronic properties were characterized at interfaces to metals with photoelectron spectroscopy. Here a decrease of the sample work function is observed that becomes larger with increasing molecular coverage and clearly exceeds values that would be expected for metal surface electron "push back" alone, confirming the electron donating nature of NMA. For tris(8-hydroxyquinoline)aluminum ($Alq_3$) deposited on top of a NMA-modified Au(111) surface, the electron injection barrier (EIB) is reduced by 0.25 eV compared to that on pristine Au(111). Furthermore, the EIB reduction depends linearly on $\Theta$ of the donor-modified Au(111) surface, adjustable by NMA pre-coverage. Comparisons will also be given to the stronger donor MV0.

This work was supported by the EC project ICONTROL.

## O 18: [HL] Organic Semiconductors: Solar Cells (Joint Session DS/CPP/HL/O)

Time: Monday 16:00–17:45 Location: H15

O 18.1 Mon 16:00 H15

**Pulsed Photocurrent Measurements in Bulk Heterojunction Solar Cells** — •Markus Mingebach[1], Moritz Limpinsel[1], Alexander Wagenpfahl[1], Alexander Goldmann[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — [2]Centre of Applied Energy Research (ZAE Bayern e. V.), Am Hubland, D-97074 Würzburg

The performance of organic bulk heterojunction solar cells greatly improved during the last years up to 6% power conversion efficiency. Nevertheless very important properties such as the voltage dependent photocurrent are not fully understood yet. We investigate the photocurrent in poly(3-hexyl thiophene) (P3HT) : [6,6]-phenyl-$C_{61}$ butyric acid methyl ester (PCBM) solar cells by applying a pulsed measurement technique (proposed by Ooi et al.) and also find a point of optimal symmetry (POS) at 0.52-0.64 V. In contrast to Ooi we identify this voltage not as the built-in voltage, but as the case of flat bands in the bulk of the cell (confirmed by macroscopic simulations). [1] To explain the voltage dependent photocurrent, we apply a combination of Onsager–Braun (polaron pair dissociation) and Sokel–Hughes (charge carrier extraction) theory in conjunction with the POS. In addition we observe and investigate a voltage-independent offset of the photocurrent, which is crucial for optimizing the device performance.

[1] M. Limpinsel, A. Wagenpfahl, M. Mingebach, C. Deibel and V. Dyakonov, Investigation of the Photocurrent in Bulk Heterojunction Solar Cells, submitted (2009).

O 18.2 Mon 16:15 H15

**Analytical analysis of the CELIV theory** — •Jens Lorrmann[1], Bekele Homa Badada[2], Carsten Deibel[1], Olle Inganäs[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians University of Würzburg — [2]Biomolecular and Organic Electronics, IFM, Linköping University, Sweden — [3]ZAE Bayern, Div. Functional Materials for Energy Technology, Würzburg

Charge extraction by linearly increasing voltage (CELIV) has attracted much interest in organic semiconductor research, due to its feature of measuring charge carrier mobility and density directly and simultaneously. Up to now the theoretical description of this method has been solved for a low mobility approximation only, because the general solution was impeded by a Ricatti type first order differential equation. In this contribution we present the analytical solution for this Ricatti equation, thus completing the analytical framework of the CE-

LIV method. We compare it with the approximated theory and show that especially for standard organic solar cell materials the low mobility approach is hardly valid. The evaluation of photo-CELIV measurements on poly(3-hexyl thiophene-2,5-diyl):[6,6]-phenyl-$C_{61}$ butyric acid methyl ester solar cells can then be done by fitting the current transients. Surprisingly the fit results are only in a good agreement with the experimental currents, if two extraction currents are taken into account – the origin of which we will discuss. Furthermore we present a new equation for mobility evaluation from numerical analysis within our framework, which can be applied over the entire experimental range.

O 18.3 Mon 16:30 H15

**Oxygen Induced Degradation of P3HT:PCBM Solar Cells** — •Julia Schafferhans, Stefan Neugebauer, Andreas Baumann, Alexander Wagenpfahl, Carsten Deibel, and Vladimir Dyakonov — Experimental Physics VI, Faculty of Physics and Astronomy, Julius-Maximilians-University of Würzburg, Am Hubland, 97074 Würzburg, Germany

Power conversion efficiencies of 6% for organic solar cells have already been achieved, with growing tendency. A critical issue yet to be addressed are the factors influencing the device lifetime. To gain a detailed understanding of the device stability, the underlying degradation mechanisms and their impact on the solar cell performance is an important prerequisite for lifetime enhancement. We investigated the oxygen induced degradation of state of the art (PCE > 3%) P3HT:PCBM (poly(3-hexylthiophene):[6,6]-phenyl C61 butyric acid methyl ester) solar cells in the dark as well as under simultaneous illumination. Current–Voltage measurements are supplemented by Thermally Stimulated Current (TSC) and Charge Extraction by Linearly Increasing Voltage (CELIV) measurements. In the case of dark degradation the influence of oxygen results in a decrease of the short circuit current (Isc), whereas degradation under bias light leads to a decrease of all solar cell parameters. With the aid of a macroscopic simulation we demonstrate that the origin of the loss in Isc is oxygen doping, which we confirmed by CELIV measurements. In addition, TSC and CELIV measurements revealed an increase of deeper traps and a slight decrease of the mobility due to oxygen.

O 18.4 Mon 16:45 H15

**Polaron Recombination Dynamics in Bulk Heterojunction Solar Cells** — •Andreas Baumann[1], Alexander Wagenpfahl[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — [2]Centre of Applied Energy Research (ZAE Bayern e. V.), Am Hubland, D-97074 Würzburg

Organic solar cells with more than 6% power conversion efficiency were recently shown, coming closer to commercialization. For further improvements, a better understanding of the loss mechanisms inside the solar cell are needed, such as the recombination of photo-generated charge carriers. We applied the experimental technique of charge extraction by linearly increasing voltage (Photo-CELIV) to investigate the recombination dynamics in poly(3-hexylthiophene) (P3HT) : [6,6]-phenyl-$C_{61}$ butyric acid methyl ester (PCBM) bulk heterojunction solar cells. It was found experimentally, that the dominating polaron loss mechanism in P3HT:PCBM solar cells is of Langevin type, but reduced by a factor in the range of 0.1 in pristine samples to 0.01 in annealed ones [1]. We propose a model taking the charge carriers profile inside the active layer into account, which describes the origin of the observed reduced Langevin recombination [2].

[1] C. Deibel, A. Baumann, V. Dyakonov, APL 93, 252104 (2008)
[2] C. Deibel, A. Wagenpfahl, V. Dyakonov, PRB 80, 075203 (2009)

O 18.5 Mon 17:00 H15

**Relation of open circuit voltage to charge carrier concentration in organic bulk heterojunction solar cells** — •Daniel Rauh[1], Alexander Wagenpfahl[2], Carsten Deibel[2], and Vladimir Dyakonov[1,2] — [1]Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg — [2]Julius-Maximilians-University of Würzburg, Institute of Physics, Experimental Physics VI, D-97074 Würzburg

A deeper understanding of the open circuit voltage $V_{oc}$ in bulk heterojunction solar cells is crucial for further performance enhancements. In order to investigate $V_{oc}$, we measured temperature dependent current–voltage characteristics of poly(3-hexylthiophene):[6,6]-phenyl C61 butyric acid methyl ester (P3HT:PCBM) solar cells (pristine and annealed) at various light intensities. With charge extraction measurements under the same conditions we could determine the corresponding charge carrier densities $n$ in the operating device. Extrapolating $V_{oc}$ to $T$=0K gives a constant value for all intensities indicating the effective bandgap of the donor–acceptor system. Fitting the data with $V_{oc}$ models [1,2] showed excellent agreement with only one free parameter, the effective density of states. From our analysis, we gain insights into the recombination meachanisms limiting $V_{oc}$.

[1] Koster et al., Appl. Phys. Lett. 86, 123509 (2005)
[2] Cheyns et al., Phys. Rev. B 77, 165332 (2008)

O 18.6 Mon 17:15 H15

**Charge Carrier Concentration and Temperature Dependent Recombination in Polymer-Fullerene Solar Cells** — •Alexander Foertig[1], Andreas Baumann[1], Daniel Rauh[2], Thiemo Gerbich[1], Vladimir Dyakonov[1,2], and Carsten Deibel[1] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — [2]Centre for Applied Energy Research (ZAE Bayern e.V.), Am Hubland, D-97074 Würzburg, Germany

We performed temperature dependent transient photovoltage and photocurrent measurements on poly(3-hexyl thiophene):[6,6]-phenyl-$C_{61}$ butyric acid methyl ester bulk heterojunction solar cells. Thus we determined small perturbation carrier lifetime and charge carrier densities under operating conditions. We found a strongly charge carrier concentration and temperature dependent Langevin recombination prefactor. The observed recombination mechanism is discussed in terms of a bimolecular loss and compared with charge carrier extraction by linearly increasing voltage (photo-CELIV) measurements done on the same blend system. The observed charge carrier dynamics, following an apparent order larger than two, are explained by dynamic trapping of charges in the tail states of the Gaussian density of states.

O 18.7 Mon 17:30 H15

**Charge Carrier Generation Yield in Organic Solar Cells using a C80 Derivative as Acceptor** — •Moritz Liedtke[1,2], Andreas Sperlich[2], Hannes Kraus[2], Andreas Baumann[2], Carsten Deibel[2], Vladimir Dyakonov[1,2], and Claudia Cardona[3] — [1]Centre for Applied Energy Research (ZAE Bayern e. V.), Am Hubland, D-97074 Würzburg, Germany — [2]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — [3]Luna Innovations Incorporated, 521 Bridge Street, Danville, VA 24541 (USA)

Organic solar cells (OSC) with $C_{70}$ and $C_{80}$ fullerenes show a higher open circuit voltage (Voc) than the standard [6,6]-phenyl-C[61]-butyric acid methyl ester (PCBM):poly-3-hexylthiophene (P3HT) bulkheterojunction cells. Devices containing the trimetallic nitride endohedral fullerene $Lu_3$:N@$C_{80}$ showed a Voc of 910mV compared to 600mV with $C_{60}$-PCBM. Still the overall efficiency of these cells remain below the performance of our $C_{60}$-PCBM:P3HT reference cells. We address the origin of the lower efficiency by means of optical, magnetic and current measurement techniques. In samples containing $Lu_3$:N@$C_{80}$ we found photoluminescence quenching 3.2 times weaker, triplet yield higher and short-cut current about 2mA/cm$^2$ lower than in cells with $C_{60}$-PCBM as acceptor. We conclude that less efficient charge carrier generation in the $Lu_3$:N@$C_{80}$:P3HT bulkheterojunction system is the reason for the lower photocurrent.

# O 19: Symposium Spin-Orbit Coupling and Spin Relaxation in Graphene and Carbon Nanotubes

Time: Monday 14:00–17:45 Location: H1

**Invited Talk** O 19.1 Mon 14:00 H1
**Models for spin-orbit coupling in graphene** — •Francisco Guinea — Instituto de Ciencia de Materiales de Madrid. CSIC. Cantoblanco. 28049 Madrid. Spain

The spin-orbit coupling in the carbon atom is relatively weak, due to its low nuclear charge. This makes graphene an interesting material for spintronics applications. Nevertheless, the intrinsic spin-orbit coupling can lead, at least at low temperatures, to the spin Hall effect, with topologically protected edge currents. Extrinsic effects, like electric fields, corrugations, and impurities, can modify significantly the spin-orbit coupling. Similar effects take place in carbon nanotubes. Models for the effect of impurities and corrugations are reviewed[1-3], and compared to available experimental data.

Work done in collaboration with D. Huertas-Herrero, A. Brataas, and A. H. Castro-Neto.

[1] Spin-orbit coupling in curved graphene, fullerenes, nanotubes, and nanotube caps, D. Huertas-Hernando, F. Guinea, A. Brataas, Phys. Rev. B. vol. 74, 155426 (2006). [2] Impurity-Induced Spin-Orbit Coupling in Graphene, A. H. Castro Neto and F. Guinea, Phys. Rev. Lett., vol. 103, 026804 (2009). [3] Spin-Orbit-Mediated Spin Relaxation in Graphene, D. Huertas-Herrero, F. Guinea, A. Brataas, Phys. Rev. Lett. vol. 103, 146801 (2009).

**Invited Talk** O 19.2 Mon 14:35 H1
**Spin-orbit coupling and spin relaxation in carbon nanotube quantum dots** — •Ferdinand Kuemmeth — Harvard University, Cambridge, MA, USA

This talk presents transport measurements through single and double quantum dots that elucidate the role of spin-orbit coupling on the energy spectrum and spin-relaxation in carbon nanotubes.

In a one-electron quantum dot the lowest shell consists of four quantum states associated with spin up/down and clockwise/counterclockwise orbital motion around the circumference of the nanotube. These states are resolved by application of a magnetic field parallel to the nanotube. Sub-Kelvin tunneling spectroscopy reveals that spin-orbit coupling breaks the four-fold degeneracy expected at zero magnetic field, by favoring parallel alignment of the electron's orbital and spin magnetic moment. For the one-hole quantum dot antiparallel alignment is observed, demonstrating that spin-orbit coupling also breaks electron-hole symmetry [Nature 452, 449 (2008)].

In double quantum dots Pauli blockade is observed and utilized to study spin-relaxation. In 12C nanotubes the leakage current displays a minimum at B=0 whereas a maximum is observed in 13C devices. We attribute the first effect to spin-relaxation via spin-orbit coupling - a phenomenon which is suppressed near B=0 due to time reversal symmetry. We explain the second effect by hyperfine coupling to the nuclear spins, resulting in fast electron-nuclear flip-flop processes at B=0 [Nature Phys. 5, 321 (2009)].

**Invited Talk** O 19.3 Mon 15:10 H1
**Spin-orbit interaction in carbon nanotubes probed in pulsed magnetic fields** — •Sungho Jhang[1], Magdalena Marganska[2], Yurii Skourski[3], Dominik Preusche[1], Benoit Witkamp[4], Milena Grifoni[2], Herre van der Zant[4], Joachim Wosnitza[3], and Christoph Strunk[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, Germany — [2]Institute for Theoretical Physics, University of Regensburg, Germany — [3]Dresden High Magnetic Field Laboratory, Forschungszentrum Dresden-Rossendorf, Germany — [4]Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands

A source of spin-polarized electrons is one of the important building blocks of a future spin-based electronics. Very high degrees of polarization can potentially be achieved by exploiting spin-orbit interaction (SOI). Based on the low atomic number Z = 6 of carbon the spin-orbit interaction in carbon nanotubes (CNTs) was mostly believed to be very weak, until a recent experiment [1] has demonstrated the effect of spin-orbit interaction in clean CNT quantum dots. Here we present magneto-conductance (MC) data for an open CNT-quantum wire obtained in pulsed magnetic fields, which exhibit a peculiar split MC peak close to the charge neutrality point. Our analysis of the MC data suggests that this splitting is intimately connected to the SOI and the tube chirality and that the current in the peak regions can be up to 100% spin-polarized, which calls for application in future CNT-based spintronic devices.

[1] F. Kuemmeth et al., Nature (London) 452, 448 (2008).

**15 min. break**

**Invited Talk** O 19.4 Mon 16:00 H1
**Wigner molecules and spin-orbit coupling in carbon-nanotube quantum dots** — •Massimo Rontani — CNR-INFM Research Center S3, Modena, Italy

The paradigm of few-electron complexes in quantum dots (QDs) relies on the 'particle-in-a-box' idea that lowest-energy orbitals are filled according to Pauli's exclusion principle. If Coulomb repulsion is sufficiently strong to overcome the kinetic energy cost of localization, a different scenario is predicted: a 'Wigner' molecule (WM) forms, made of electrons frozen in space according to a geometrical pattern. Despite considerable experimental effort, evidence of the WM in semiconductor QDs has been elusive so far. Here we demonstrate theoretically that WMs occur in gate-defined QDs embedded in typical semiconducting carbon nanotubes (CNTs), even in the presence of strong spin-orbit coupling. The signatures of the WM state must be searched -and indeed have already been observed - in tunneling spectra. Through exact diagonalisation (ED) calculations, we unveil the inherent features of the electron molecular states. We show that, like nuclei in a usual molecule, electrons have localized wave functions and hence negligible exchange interactions. The molecular excitations are vibrations around the equilibrium positions of electrons. ED results are well reproduced by an ansatz vibrational wave function, which provides a simple theoretical model for transport experiments in ultraclean CNTs.

**Invited Talk** O 19.5 Mon 16:35 H1
**Spin relaxation and decoherence in graphene quantum dots** — •Guido Burkard — Dept. of Physics, Univ. of Konstanz, Germany

Graphene is a promising material for electron spin qubits due to its low concentration of nuclear spins and relatively weak spin-orbit coupling [1]. Despite the expected weakness of spin relaxation and decoherence effects, the time scales for these processes are relevant for coherent spin manipulations in graphene. We have calculated the spin relaxation time $T_1$ of a single spin in graphene quantum dots [1,2] as a function of the magnetic field $B$. In quantum dots without coupling between the valleys $K$ and $K'$ in the graphene band structure, there is an effective time-reversal symmetry breaking which prevents the Van Fleck cancellation at $B = 0$ known from semiconductor quantum dots. This leads to a distinct value of the exponent $\alpha$ in the power law $T_1 \propto B^\alpha$ which can be different from the value for semiconductor quantum dots. In the context of spin decoherence, we have also studied the form of the hyperfine interaction with $^{13}C$ atoms in graphene and find that it leads to a spin-valley coupling [3]. In the transport current through a double quantum dot, we find that the valley degeneracy and hyperfine-induced spin-valley coupling in graphene lead to features in the Pauli blockade that are qualitatively different from the known effect for semiconductor quantum dots.

[1] B. Trauzettel, D.V. Bulaev, D. Loss, and G. Burkard, Nature Phys. **3**, 192 (2007). [2] P. Recher, J. Nilsson, G. Burkard, and B. Trauzettel, Phys. Rev. B **79**, 085407 (2009). [3] A. Palyi and G. Burkard, Phys. Rev. B **80**, 201404(R) (2009).

**Invited Talk** O 19.6 Mon 17:10 H1
**Spin transport in graphene field effect transistors** — •Bart van Wees — Zernike Institute of Advanced Materials, University of Groningen, Groningen, The Netherlands

I will give an overview of electron spin injection, spin transport, spin precession and manipulation in graphene. The use of the so-called non-local geometry using graphene FET devices with ferromagnetic contacts allows a detailed experimental investigation. After a basic introduction I will discuss that: a) Spins can be transported through a graphene layer with a spin relaxation length of about 1.5 micrometer. By applying a perpendicular magnetic field Hanle spin precession can be studied and information about spin relaxation and the carrier diffusion can be obtained [1,3]. b) By applying a large DC electric field the transport of spins between injector and detector can be manipulated (sped up or slowed down) using carrier drift [2]. c) Spins can be injected with an injection efficiency up to 20 percent. This injection efficiency can be enhanced by a current bias which takes the carriers away from the injecting contacts [4]. d) We have observed a scaling between the spin relaxation times and lengths and the carrier mobility in graphene [5,6]. I will discuss the possibility that in clean intrinsic graphene spin relaxation lenghts of 100 micrometer in graphene at room temperature might be possible. [1] N. Tombros et al., Nature 448, 571 (2007)[2] N. Tombros et al., Phys. Rev. Lett. 101, 046601 (2008) [3] C. Jozsa et al., Phys. Rev. Lett. 100, 236603 (2008) [4] C. Jozsa et al., Phys. Rev. B 79, 081402 R (2009) [5] M. Popinciuc et al.,accepted for Phys. Rev. B. [6] C. Jozsa et al, Phys. Rev. B 80, 241403 (2009)

## O 20: Invited talk (Van Hulst, Niek)

Time: Tuesday 9:30–10:15 Location: H36

**Invited Talk** O 20.1 Tue 9:30 H36

**Control of Photon Emitters Coupled to Nano-Antennas** — Daan Brinks[1], Tim H. Taminiau[1], Alberto Gonzalez-Curto[1], Richard Hildner[1], Marta Castro-Lopez[1], Fernando D. Stefani[2], and •Niek F. van Hulst[1,3] — [1]ICFO - the Institute of Photonic Sciences, Castelldefels (Barcelona), Spain — [2]Universidad de Buenos Aires, Argentina — [3]ICREA - Barcelona, Spain

We show that the excitation-emission of single photon emitters, such as individual molecules and Q-dots, can be controlled both in time and space, on fs and nm scale. Using broad band excitation (~120nm bandwidth) in combination with a pulse shaper we control the excitation of single molecules and reveal coherent response by 20-40fs vibrational wave-packets. The pulse shape can be tailored to an optimum/minimum for each individual molecule, yielding a coherent control ratio of up to 4 times. Similarly by phase control of individual optical nano-antennas we adapt to the spectral phase development of the antenna, optimize the driving efficiency and generate local spatial hotspots at the antenna. Single molecules are ideal probes of the local antenna field and here we show optical fields spatially localized within 25 nm. Finally the enhancement of the radiative/excitation rates is treated, particularly how the angular emission of the coupled antenna-emitter system is highly directed. A nano-Yagi-Uda antenna is presented acting as a unidirectional single photon emitter for Q-dots in close proximity to the feed element. The controlled directivity makes such antennas a promising candidate for compact easy-to-address single photon sources or planar sensors at the single quantum level.

## O 21: [DS] Plasmonics and Nanophotonics I (Joint Session DS/O/HL)

Time: Tuesday 10:30–13:00 Location: H2

O 21.1 Tue 10:30 H2

**Electrochemically tunable photonic metamaterial** — •Lihua Shao, Stefan Linden, Matthias Ruther, Jörg Weissmüller, and Martin Wegener — Institut für Nanotechnologie and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

We report experiments to combine two approaches for designing functional nanomaterials. Photonic metamaterials provide a strategy for obtaining unconventional optical response - in the extreme, negative refractive indices - by lithographically structured elements like arrays of split-ring resonators (SRR). Nanomaterials with tunable electronic structure exploit large specific surface area of metal nanostructures to tune the surface properties through the controlled space-charge regions for tuning macroscopic properties. The combination is a photonic metamaterial in which the space-charge at the surface of SRR is controlled via an applied potential, leading to a tunable optical resonance. We report first results support this concept. SRR structures with resonance frequencies in the near infrared are immersed into aqueous electrolytes as working electrode in an electrochemical experiment. Varying the electrode potential, E, induces a space-charge layer at the metal surface as part of the electrochemical double-layer. We find the resonance frequencies vary linearly, reversibly, and reproducibly with E, with a blue shift for negative potential. A tentative explanation is based on the effective thickening of the SRR by the excess electrons, which changes the SRR aspect ratio. The observation of larger frequency shift for thinner SRR's is compatible with this scenario.

O 21.2 Tue 10:45 H2

**Mixing colours like nature** — •Mathias Kolle, Maik Scherer, Pedro Cunha, Fumin Huang, Jeremy Baumberg, and Ullrich Steiner — Cavendish Laboratories, University of Cambridge, UK

Biomimetic attempts to produce novel photonic structures have attracted increasing research interest in recent years. Nature offers us an enormous amount of multifunctional micro- and nanostructures, that provide outstanding, distinctive, dynamic and tailored colouration. A “brilliant” example is the indonesian butterfly *papilio blumei*, whose wing scales are covered with 5-10$\mu$m wide concavities, that are cladded with a perforated cuticle multilayer. The regularly shaped multilayer structure gives rise to very impressive colour mixing effects, accompanied by controlled change in light polarisation.

We have successfully replicated the intricate photonic structure of *papilio blumei* on the cm$^2$-scale in four simple steps involving colloidal templating, electrochemical growth and atomic layer deposition. A small conceptual modification of the original photonic structure leads to a completely different optical effect. Any freely chosen colour and its complementary hue can be separated and reflected into different directions while conserving a particular polarisation effect.

Since the procedures are easily up-scaleable, these biomimetic photonic structures have a huge potential for industrial applications in security printing, encoding of information, non-emissive display technology and other fields where distinct colours play an important role.

O 21.3 Tue 11:00 H2

**Optical properties of carpets of randomly grown silicon nanowires on glass** — •Gerald Brönstrup and Silke Christiansen — Institut für Photonische Technologien e.V., Abt. Halbleiter-Nanostrukturen, 07745 Jena

Silicon Nanowires [SiNWs] have attracted much attention in the recent years as possible future building blocks for field effect transistors, sensors, photo detectors and solar cells. For the latter SiNWs grown on a cheap substrate like glass is of special interest. To build solar cells with high efficiencies a high absorption is mandatory. We present a study of the influence of the diameter on the reflection, transmission and absorption spectra of carpet like assembly of SiNWs grown on glass.

We grew SiNWs on glass using gold colloids of different fixed diameters to achieve a control over the diameter of the SiNWs. Then we measured the reflection R and transmission T using an integrating sphere. The absorption A was calculated using the simple formula A=1-T-R.

For a better understanding of the underlying physics of the absorption happening in SiNWs with diameters much smaller than the wavelength of the visible light we present a statistical model based on scattering cross sections calculated for single SiNWs using Mie-theory.

O 21.4 Tue 11:15 H2

**Suppressed transmission through ultrathin metal films by subwavelength hole arrays** — •Julia Braun[1], Bruno Gompf[1], Uwe Huebner[2], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart — [2]IPHT Jena, Albert-Einstein-Straße 9, 07745 Jena

If an opaque metal film is periodically perforated by tiny subwavelength holes, extraordinary high transmission is observed [1]. We investigate the transmission through subwavelength hole arrays (SWHA) in ultrathin semitransparent Au films with various periodicities and hole diameters and observe the opposite behavior: less light is transmitted through the pierced metal compared to the closed film. The samples were fabricated by optical interference and electron beam lithography in 12 nm and 20 nm thick Au films with periodicities between 250 nm and 400 nm, and than characterized in the frequency range 4400 $\mathrm{cm}^{-1}$ to 37000 $\mathrm{cm}^{-1}$ (0.6 eV to 4.6 eV). The optical properties of SWHA cannot be explained by a pure dielectric function, but show a strong $\vec{k}$-dependent behavior. In ultrathin Au films it is marked by the excitation of strongly damped antisymmetric short range surface plasmons. The obtained dispersion curves perfectly agree with this explanation when the altered dielectric function of the ultrathin Au films is taken into account [2].

[1] T.W. Ebessen, H.J. Lezec, H.F. Ghaemi, T. Thio, and P.A. Wolff, *Nature* **391**, 667 (1998).

[2] J. Braun, B. Gompf, G. Kobiela, M. Dressel, *Physical Review Letters* **103**, 203901 (2009)

O 21.5 Tue 11:30 H2

**Manipulation of fluorescence resonance energy transfer in single plasmonic nanoresonators** — •Valerie Faessler, Calin Hrelescu, Sergiy Mayilo, Frank Jäckel, and Jochen Feldmann — Photonics and Optoelectronics Group, Department of Physics and Center for Nano Science (CeNS), Ludwig-Maximilians-Universität München, Amalienstrasse 54, 80799 München, Germany;

We show that fluorescence resonance energy transfer (FRET) between two organic chromophores can be manipulated in plasmonic nanoresonators consisting of two spherical gold nanoparticles.The nanoresonators can be tuned by varying the inter-particle distance or the nanoparticle size. This allows us to selectively modify the decay channels of the chromophores. FRET can be supressed if the molecules are placed in the nanoresonator at a certain distance from the nanoparticle surface. Furthemore we observe spectral shaping and intensity modulation of the fluorophore emision in the nanoresonators [1]. Correlated whitelight Rayleigh scattering and fluorescence microscopy data of the hybrid system are discussed in the framework of generalized Mie theory.

[1] M. Ringler, A. Schwemer, M. Wunderlich, A. Nichtl, K. Kürzinger, T. A. Klar, J. Feldmann Phys. Rev. Lett., 100, 203002 (2008)

O 21.6 Tue 11:45 H2

**Optical antenna thermal emitters** — •Jon Schuller[1], Thomas Taubner[1,2], and Mark Brongersma[1] — [1]Stanford University, Stanford, CA, USA — [2]1. Physikalisches Institut, RWTH Aachen, Germany

Optical antennas are a critical component in nanophotonics research[1] and have been used to enhance nonlinear and Raman cross-sections and to make nanoscale optical probes [2]. In addition to their receiving properties, optical antennas can operate in broadcasting mode, and have been used to modify the emission rate[3] and direction [4] of individual molecules.

In these applications the antenna must operate at frequencies given by existing light emitters. Using thermal excitation of optical antennas, we bypass this limitation and realize emitters at infrared frequencies where sources are less readily available [5].

Specifically, we show that the thermal emission from a single SiC whisker antenna is attributable to well-defined, size- tunable Mie resonances. Furthermore, we derive a fundamental limit on the antenna emittance and argue theoretically that these structures are nearly ideal black-body antennas.

1. Schuck, P. J. et al., PRL 94, 017402 (2005).
2. Farahani, J. N., et al., PRL 95, 017402 (2005).
3. Kuhn, S., et al., PRL 97, 017402 (2006).
4. Taminiau, T. H., et al, Nature Photon. 2, 234-237 (2008).
5. Schuller, J.A. et al., Nature Photon. 3, 658-661 (2009).

O 21.7 Tue 12:00 H2

**Spatial Resolved Near Field Interference on Nanooptical Bowtie Antennas** — •Pascal Melchior, Daniela Bayer, Christian Schneider, Martin Rohmer, Alexander Fischer, and Martin Aeschlimann — Fachbereich Physik and Research Center OPTIMAS, Technische Universität Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany

The response of metallic nanostructures is responsible for interference effects of the electric near field in the vicinity of the structure surface. While the incoming electric field vectors are independent in the far field, spectral interference in the near field can occur since the resulting field vectors are not necessarily perpendicular. On the nanostructure configuration of a Bowtie antenna, we show how the superposition of different plasmonic excitation modes leads to a local enhancement of the effective near field depending on the phase relation between the incoming electric field vectors. Via an interferometric superposition of two laser pulses with cross polarized electric fields the near field interference can be directly observed by means of a photoemission electron microscope (PEEM). Spatial switching of the photoemission yield depending on the relative phase between the two superposed laser pulses will be demonstrated.

O 21.8 Tue 12:15 H2

**Interaction effects of gold nanoantenna arrays in the infrared** — •Daniel Weber[1], Frank Neubrech[1], Dominik Enders[2], Tadaaki Nagao[2], and Annemarie Pucci[1] — [1]Kirchhoff Institute for Physics, University of Heidelberg, Germany — [2]National Institute for Materials Science, Tsukuba, Japan

Gold nanoantennas are of great interest for applied spectroscopy due to their tuneable plasmonic properties including local electromagnetic (EM) field enhancement (FE). Excited resonantly by EM radiation, they are able to strongly enhance the local EM field. In the past, we exploited this strong effect for surface-enhanced infrared spectroscopy (SEIRS) with gold nanoantennas. We want to further improve the sensitivity of SEIRS by making use of nanoantenna coupling. Coupling may increase local FE but also strongly modify the spectral distribution of the FE, which provides further options for optimum resonance tuning as necessary for specific sensor applications.

We report on the IR optical properties of gold-nanoantenna arrays with different gap sizes and show the relation between plasmonic resonances and geometrical arrangement on the substrate. Stripe-like, polycrystalline gold nanoantennas (nanorods) with rectangular cross-sections were produced by electron beam lithography on silicon wafers. IR measurements were performed by micro-spectroscopy in our laboratories and at the synchrotron light source ANKA (Karlsruhe Institute of Technology). Special focus is on the preparation of very small gaps between the tip ends of nanorods, where the highest local FE is expected.

O 21.9 Tue 12:30 H2

**Structural and Optical Properties of Gold and Iron Nanowires** — •Piotr Patoka[1,2], Georgios Ctistis[3], Michael Hilgendorff[1], and Michael Giersig[1] — [1]Freie Universität Berlin — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH — [3]University of Twente, MESA+ Institute & Dept. of Science and Technology, Complex Photonic Systems (COPS), Enschede, The Netherlands

Plasmonic nanostructures gained a tremendous interest during the last decade due to their structural and optical properties, which make them promising materials for opto-electronic as well as bio-sensing-applications.

Here we will present results on gold and iron nanowires prepared by means of nanosphere lithography as a cheap method of preparation of large areas of such nanostructures. The 30nm thick lines with 440nm in periodicity have been characterized with atomic force microscopy and scanning electron microscopy. The investigation showed strong influences of the preparation steps to the final structure. For optical investigation UV-VIS-NIR spectrometry and scanning near field optical microscopy have been used showing extraordinary light transmission.

O 21.10 Tue 12:45 H2

**Surface Plasmon Resonance Coupling on Magnetically Capped Gold Nanorods** — •Gillian Doyle and Dominic Zerulla — Plasmonic and Ultrafast Optics Group, School of Physics, University College Dublin, Belfield, Dublin 4, Ireland

Nanorods compared to their spherical counterparts exhibit enhanced sensitivity and are used for a wide variety of applications from biosensing to solar cells. The presence of two resonance peaks in their scattering spectra allows their two geometrical axes, the longitudinal and transverse axes to be separately distinguished. In this research we use iron capped gold nanorods with geometrical dimensions in the range of 60 x 700 nm. Coupling of the surface plasmons between the two axes is investigated both in multiple particle and single particle experiments and the effect of the proximity of particles to each other and their associated coupling is considered. In the single particle experiments a 532 nm laser beam is used to optically trap and manipulate a nanorod, while coupling white light to the setup allows Mie Scattering Spectroscopy (MSS) to be performed on a single particle. Large sample MSS experiments provide more intense signals for detection and give an insight into phenomena occurring at the surface of the nanoparticle [1]. In addition, the intensity of the scattering cross section by these nanorods is examined by magnetically manipulating the particles themselves and opening a novel method of optimum signal detection of SP resonances on nanorods.

[1] G Doyle, D. Zerulla, Applied Physics A, Vol 89, No. 2, 2007

# O 22: Methods: Scanning probe techniques III

Time: Tuesday 10:30–12:45 Location: H32

O 22.1 Tue 10:30 H32

**Scanning Probe Microscopy with a Hydrogen atom** — •Jay Weymouth, Thorsten Wutscher, and Franz Giessibl — Institute for Experimental and Applied Physics, Universität Regensburg, D-93040 Regensburg, Germany

Scanning probe microscopy requires atomically sharp tips in order to image surfaces with atomic resolution. One way to increase the spatial resolution of a single-atom tip is to use a lighter atom as the front atom. While tungsten, with a covalent radius of 130 pm, is common as a tip material for SPM, it has been shown that carbon, with a covalent radius of 77 pm, can be used to probe the orbitals of a tungsten atom [Hembacher et al., Science (2004)]. Carrying on, hydrogen has the smallest covalent radius and is thus an ideal candidate for the front atom. Hydrogen has the additional benefit of passivating the tip and thus strongly decreasing reactivity, which may be beneficial for SPM tips operating in the repulsive force regime. We report on our work creating and characterizing hydrogen-terminated silicon tips.

O 22.2 Tue 10:45 H32

**Imaging surfaces with scanning tunneling hydrogen microscopy** — •Christian Weiss[1,2], Stefan Tautz[1,2], and Ruslan Temirov[1,2] — [1]Institut für Bio- und Nanosysteme (IBN-3) and — [2]JARA Fundamentals of Future Information Technology

Recently it has been demonstrated that a single hydrogen molecule confined in the junction of a scanning tunneling microscope (STM) acts as a combined force-sensor/signal transducer that probes the local surface adsorption potential and converts the force signal into variations of the junction conductance [1]. Images taken with the new method, called scanning tunnelling hydrogen microscopy (STHM), show an ultra-high geometric resolution, which resembles chemical structure formulae of the imaged compounds [2]. In our contribution we discuss applications of the STHM to imaging of various surfaces and show the operation in two different regimes. In one regime the hydrogen sensor maps the repulsive short-range interactions [1], while in the other possibly the attractive ones.
References:
[1] C. Weiss et al. arXiv:condmat/0910.5825
[2] R. Temirov et al. 2008 New. J. Phys 10 053012

O 22.3 Tue 11:00 H32

**An atomic force microscope scanner for high speed, large range and high resolution imaging** — •Christoph Braunsmann and Tilman Schäffer — Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Staudtstr. 7, Bau A3, 91058 Erlangen

We constructed a high-speed AFM for imaging large areas at high resolution. This involved significantly increasing the bandwidth of every single AFM component. Besides the electronics, the data acquisition system and the cantilever, one important such component is the scanner. By using finite element modeling we developed a fast three-dimensional scanner based on piezo stacks and flexures. The scanner design is modular and allows for an easy exchange of the $x$- and $y$-piezos. Large $x$- and $y$-piezos achieve scan sizes of up to 23 $\mu$m × 23 $\mu$m, which is the largest scan size for a feedback-controlled $xyz$ high-speed scanner reported to-date. Smaller $x$- and $y$-piezos can be employed giving high lateral resolution. We demonstrated the high speed performance of the new scanner by imaging collagen fibrils in air (14 images/s) and calcite dissolution in hydrochloric acid (10 images/s) with small cantilevers (18 $\mu$m in length). Tip-sample velocities of up to 8.8 mm/s and z-piezo velocities of up to 11 mm/s were reached while scanning. By resolving the hexagonal lattice of the (001) cleavage plane of muscovite mica with a small cantilever in water we showed that the scanner is not only suited for high-speed imaging at large range, but can also give resolution on the atomic scale.

O 22.4 Tue 11:15 H32

**AFM with Light-Atom Tip** — •Thomas Hofmann, Joachim Welker, and Franz J. Giessibl — University of Regensburg, Faculty of Experimental and Applied Physics II - Physics, Universitätsstrasse 31, D-93053 Regensburg

STM and AFM images are a convolution of the tip and the sample wave functions. Hence, for maximal resolution, the size of the protruding tip orbital has to be minimized. Beryllium is a promising candidate as tip material because a Beryllium atom has just four electrons, leading to a covalent radius of only 89 pm. In addition to being conductive, it has a high binding energy, which is a necessity for a stable tip cluster. For imaging with Beryllium tips a new tip preparation method was developed: High voltage is applied to the tip and the tip is crashed into a metal plate, resulting in a clean, oxide-free surface. After the preparation, dynamic STM images of the Si-(111)-(7×7) surface can be obtained and compared with images recorded with a Silicon tip. To specify the resolution of the images, the apparent radii of curvature of the imaged atoms are determined. With a Beryllium tip atom a radius of curvature of minimal 4.0 Å can be achieved. In comparison, a tip terminated by a Silicon atom only provides a radius of 8 Å. Furthermore, FM-AFM images with atomic resolution can be obtained with Beryllium tips. These images indicate even smaller radii of curvature (2.6 Å) than the STM images.

O 22.5 Tue 11:30 H32

**Simulations of metastable states near the apex of a KBr tip** — •Regina Hoffmann[1] and Alexis Baratoff[2] — [1]Physikalisches Institut, Karlsruhe Institute of Technology — [2]Institut für Physik, Universität Basel

Telegraph-like noise in the low-temperature resistance of small conductors has been explained by a single defect hopping between two energy minima separated by a barrier. A similar phenomenon correlated with additional energy dissipation has been observed in dynamic AFM near contact to a KBr(001) sample [1]. The authors attributed this behaviour to a KBr molecule hopping near the apex of the tip, rather than between tip and sample. We report results of atomistic simulations for such a system using a code validated in studies of AFM on ionic crystals [2]. The simulated system consists of a 4*4*4 cube supplemented by one additional K ion bound to a nearby Br ion. Relaxation led to the first stable configuration A. Another stable configuration was found by flipping one of the Br coordinates (x) by about one lattice constant; subsequent relaxation led to the more stable position E. In order to map the potential energy landscape between positions A to E, we incremented the Br x-coordinate forward and backward while relaxing its other coordinates and those of the other ions. Simulations in the presence of a KBr(001) sample indicate that the molecule stays near the tip apex and that additional states with lower energy barriers occur. This may account for the observed jumps. [1] R. Hoffmann et al., Nanotechnology 18, 395503 (2007). [2] T. Trevethan and L. Kantorovich, Nanotechnology 15, S34 (2004)

O 22.6 Tue 11:45 H32

**Advances in Quantitative Nanomechanical Mapping, and robust, user-friendly AFM tapping** — •Johannes Kindt[1], Chanmin Su[2], Shuiqing Hu[2], and Bede Pittenger[2] — [1]Veeco GmbH, Dynamostr. 19, 68165 Mannheim — [2]Veeco Metrology, 112 Robin Hill Road, Santa Barbara, CA 93117

The AFM has long been recognized for its ability to resolve surfaces at nm-resolution, and to probe mechanical properties and interactions on the sample surface by local mechanical measurement. However, until recently, the combination of these two capabilities was often a compromise between achievable imaging rate, and amount of property data collected - Examples are force volume maps collected over hours, or AFM images with a few select measurement points for mechanical properties. Here, we present recent advances in AFM technology that allow the collection of mechanical data (modulus, adhesion, deformation, dissipation) at normal AFM imaging rates. We also present an implementation of this technology that greatly simplifies AFM tapping operation while at the same time making it more robust, and the interaction more controlled.

O 22.7 Tue 12:00 H32

**Magnetic Force Microscopy with a qPlus Sensor** — •Maximilian Schneiderbauer and Franz J. Giessibl — Institute for Experimental and Applied Physics, Universität Regensburg, Universitätsstrasse 31, 93053 Regensburg, Germany

Magnetic Force Microscopy (MFM) plays an important role in investigating magnetic storage materials. Until now experiments were mainly performed with standard silicon cantilevers whose tips have been coated with ferromagnetic materials. Such cantilevers have a resonance frequency on the order of 200 kHz and spring static constant k of about 20 N/m. This enables spatial resolution of approximately 15 nm. To prevent snap to contact from strong magneto static forces at closest separation one needs a much stiffer cantilever. The qPlus sensor with k approximately 2000 N/m is therefore a promising candidate for MFM measurements. In this talk preliminary results achieved with a qPlus based force sensor are presented.

O 22.8 Tue 12:15 H32

**Observing a qPlus sensor oscillate** — Joachim Welker, •Alfred J. Weymouth, and Franz J. Giessibl — Institute for Expermental and Applied Physics, University of Regensburg, Germany

The qPlus sensor [1] has been widely used in FM AFM for investigations of various surfaces. The qPlus sensor consists of a quartz tuning fork with one prong fixed to a massive substrate, so that the motion is can be described as harmonic oscillator. Real time observation of the oscillations of a qPlus sensor would require a high-speed video recorder with a framerate on the order of 50 kHz. However, by using a stroboscopic light with frequency $f_{\text{light}} = f_{\text{qPlus}} \pm \Delta f$, the oscillation of the sensor can be recorded at the beat frequency $\Delta f$ with a much lower frame rate. This allows us to explore the single harmonic oscillation motion that is used to model the movement of the tip. In the new three-contact design of the qPlus sensor, a gold wire is used to bias the tip for STM operations. This measurement also provides information about the role of the gold wire on tip oscillations.

[1] F. J. Giessibl, et al., Nanotechnology 15, S79-S86 (2004)

O 22.9 Tue 12:30 H32

**Dynamic Force Microscopy with Small Amplitudes at Ambient Conditions** — •Elisabeth Köstner and Franz J. Giessibl — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg

Yamada et al. [1,2] have shown that it is possible to obtain atomic resolution on cleaved mica and calcite in water with frequency-modulation force microscopy. These impressive results were acquired with a setup that enabled them to get very low deflection noise density, which is decisive for atomic resolution.

We have approached the problem of ambient condition imaging with quartz tuning fork based (qPlus) cantilevers. We tried to simplify our setup by using very stiff cantilevers (spring constant of 4300 N/m) with small amplitudes (around one nanometer). However, independent of the cantilever, small amplitudes appear to be necessary for high resolution imaging. Results made in frequency-modulation force microscopy mode with this setup are presented showing monoatomic steps on silicon in air and on calcite in PEG (polyethylenglycol).

[1] T. Fukuma, K. Kobayashi, K. Matsushige, and H. Yamada, Appl. Phys. Lett. 87, 034101 (2005)

[2] S. Rode, N. Oyabu, K. Kobayashi, H. Yamada and A. Kühnle, Langmuir 25, 2850-2853 (2009)

## O 23: Nanostructures at surfaces: Dots, particles, clusters

Time: Tuesday 10:30–13:00 Location: H33

O 23.1 Tue 10:30 H33

**Surface Photovoltage of Ag Nanoparticles and Au Chains on Si(111)** — •Kristian Sell, Ingo Barke, Stefan Polei, Viola von Oeynhausen, and Karl-Heinz Meiwes-Broer — Universität Rostock, Institut für Physik, 18051 Rostock

We present surface photo voltage (SPV) measurements of deposited Ag nanoparticles on Si(111)7x7 and of the quasi one-dimensional Si(111)5x2-Au structure. Quantitative results are obtained from spatially resolved I(V) spectra under laser illumination. On Si(111)5x2-Au we determine the SPV as a function of laser power at different locations. An accurate value for the Fermi-level pinning position is obtained. Based on these results we establish and discuss a simple model for the band topology. It is confirmed by spatially-resolved local work function measurements utilizing the image-state derived field emission resonances. These results have interesting implications on the electronic properties of metal nanostructures on semiconductors with metallic surface states.

O 23.2 Tue 10:45 H33

**Identifying low-coordinated atoms on oxide-supported Au clusters** — Xiao Lin[1], •Niklas Nilius[1], Pekka Koskinen[2], Hannu Häkkinen[2], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institut der MPG, Faradayweg 4-6, D-14195 Berlin, Germany — [2]Department of Physics, University of Jyväskylä, P.O. Box 35, FI-40014 Finland

The outstanding chemical properties of small metal particles are partly governed by the perimeter atoms that are located at the boundary to the oxide support. Those edge and corner sites are unique due to their low coordination, a peculiar electronic structure and charge state. We have employed STM and DFT to characterize the perimeter atoms around planar Au clusters grown on a MgO/Ag(001) thin film. The atoms exhibit an enhanced state density with respect to the island center in conductance spectra taken around the Fermi level. Furthermore, they carry extra electrons resulting from a charge transfer from the MgO-Ag interface into the Au islands. Both effects render the perimeter atoms highly attractive for binding molecules, as demonstrated via CO adsorption experiments on the system.

O 23.3 Tue 11:00 H33

**Gundlach oscillations and Coulomb blockade of Co nano-islands on MgO/Mo(100)** — •Marco Pratzer, Christian Pauly, Martin Grob, and Markus Morgenstern — II. Physikalisches Institut B and JARA-FIT, Otto-Blumenthal-Straße, RWTH Aachen, 52074 Aachen

We studied the electronic properties of ultra thin MgO films (thickness 2 ML to 11 ML) on Mo(100) by scanning tunneling microscopy and spectroscopy at room temperature. Preparation of MgO has been done by molecular beam epitaxy of magnesium in $O_2$ partial pressure of $p = 10^{-7}$ mbar. The work function differences of the MgO film are mapped by field emission resonance states (Gundlach oscillations) by $dz/dU$-spectroscopy. We found parts of islands with significantly reduced workfunction ($\Delta\Phi = 0.6\,\text{eV}$), which are tentatively assigned to charged defects within the MgO film. On top of the MgO films we prepared Co nano-islands with an area of about $A = 4\,\text{nm}^2$ by molecular beam epitaxy. Due to the small capacity of the Co islands we observed Coulomb staircases at room temperature, respectively peaks in $dI/dU$-spectroscopy. Good agreement with orthodox theory is achieved showing variations of $Q_0$ for islands at different positions.

O 23.4 Tue 11:15 H33

**Spatial and temporal resolved microscopic processes in dielectrics irradiated with swift heavy ions** — •Orkhan Osmani[1,2], Nikita Medvedev[2], Marika Schleberger[1], and Baerbel Rethfeld[2] — [1]Universität Duisburg-Essen, Fakultät für Physik, Duisburg — [2]Technische Universität Kaiserslautern, Fachbereich Physik, Kasierslautern

When an ion with kinetic energies of some 100 MeV irradiated a target insulator structural modifications can be observed on the surface. These modifications originate from strong localized electronic excitations induced by the penetrating ion. These excited electrons propagate through the crystal and excite secondary electrons on their path thus creating an electronic cascade. Such excited electrons will thermalize with the target lattice by exciting phonons. The heating of the target lattice will result finally in a molten zone that can be detected by AFM for instance. The aim of this presentation is to give an understanding of the processes involved during irradiation of dielectrics. To this end we study the excitation and relaxation of the electronic system and the creation of phonons theoretically applying classical kinetic Monte Carlo method and the two temperature model.

O 23.5 Tue 11:30 H33

**Oxygen-induced shape changes of Pt nanoparticles on MgO(100)** — •Uta Hejral, Andreas Stierle, Alina Vlad, Mélissa Delheusy, and Helmut Dosch — Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart, Germany

Platinum nanoparticles on oxide carrier materials are used in heterogenous catalysis and are applied successfully in reactions like the oxidation of hydrocarbons or carbon monoxide [1]. In order to achieve better catalyst efficiency, lifetime and selectivity it is important to comprehend catalytic processes on an atomic basis. Thus, the interplay between particle shape, adsorbed oxygen, bulk oxides and catalytic activity needs to be understood. Therefore Pt nanoparticles have been grown epitaxially on MgO(100) substrates under controlled conditions. It has previously been reported that Rh nanoparticles undergo reversible shape changes induced by surface oxides [2]. We have studied oxygen-induced shape changes of Pt nanoparticles on MgO(100) by means of in situ x-ray diffraction. The experiment was performed at 300°C and oxygen pressures ranging from UHV to 500 mbar. The experimental results are compared to the theoretically predicted ones reported in [3].

[1] G. Rupprechter, in: Advances in Catalysis, eds. B. Gates and H. Knözinger, Vol. 51 (Elsevier, Amsterdam, (2007) p.134).

[2] P. Nolte et al., Science 321, 1654 (2008).

[3] N. Seriani et al., Journal of Physics: Condensed Matter 20, 184023 (2008).

O 23.6 Tue 11:45 H33

**Towards nanocatalytic and -magnetic applications of cluster superlattices on the Ir(111)/graphene moiré** — •Timm Gerber, Alpha T. N'Diaye, Carsten Busse, and Thomas Michely — II. Physikalisches Institut, Universität zu Köln

The graphene moiré on Ir(111) is a versatile template for the growth of well ordered cluster superlattices. Employing a newly developed method to ensure full graphene coverage without any rotational variants, we demonstrate entire sample coverage with a cluster superlattice. As a second step towards applications we introduce methods to enhance the thermal stabilty of cluster superlattices and to keep them intact under ambient conditions. In view of nanocatalytic applications we investigated formation and thermal decay of Au and Pt cluster superlattices. The interaction of Pt clusters upon adsorption of CO and O is reported. For the ferromagnetic metals Co, Fe, Ni and for Rh (being magnetic as small clusters) we investigated the ability to form cluster superlattices. For those elements that do not form cluster superlattices upon room temperature deposition cluster seeding with Ir or Pt was employed. The latter offers the possibility to create bimetallic clusters such as FePt and CoPt.

O 23.7 Tue 12:00 H33

**Spectroscopy of Mass Selected Clusters** — •Niklas Grönhagen[1], Ben Wortmann[1], Kolja Mende[1], Natalie Miroslawski[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

We deposited mass selected Ag clusters on $C_{60}$ films at low temperatures. Their size ranged from $Ag_{55}^{+}$ to $Ag_{923\pm9}^{+}$ which correspond to closed shell icosahedra and in STM images they were found to stay size selected after the soft landing process. We investigated the electronic properties with ultraviolet photoemission spectroscopy (UPS). Because the dominant signal of $C_{60}$ masks the signal of the clusters, for UPS experiments HOPG was used as a substrate instead. Coalescence was avoided by depositing and measuring at 40 K, which reduces the mobility of the clusters. For these samples we could detect the Ag UPS signal. In further analysis we measured the size of the deposition spot using the spatial distribution of the energy integrated UPS cluster signal.

In addition we investigated clusters on 1 ML $C_{60}$/Au(111), which ranged from $Ag_{55}$ to $Ag_{138\pm1}$ by using STS and compared them to previous STS measurements of Ag clusters on $C_{60}$/HOPG.

O 23.8 Tue 12:15 H33

**Size-dependent alignment of Fe nanoparticles upon deposition onto W(110)** — •Armin Kleibert[1], Andris Voitkans[2], and Karl-Heinz Meiwes-Broer[3] — [1]Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen, Switzerland — [2]Institute of Solid State Physics, University of Latvia, LV-1063 Riga, Latvia — [3]Institute of Physics, University of Rostock, D-18051 Rostock, Germany

Size, shape, structure and orientation of supported nanostructures have crucial impact on their catalytic, electronic, optical and magnetic properties. Thus, gaining control over these parameters is subject of intense research. Deposition of preformed clusters has attracted much attention in the past since it enables stabilization of nanostructures far from equilibrium and virtually any material and particle size combination. While fragmentation, diffusion and sintering of deposited nanoparticles have been intensively studied in the past, still little is known about the orientation of the nanoparticles upon deposition. In this contribution we present an in situ reflection high energy electron diffraction (RHEED) study on mass-filtered Fe nanoparticles upon deposition onto W(110). We find that clusters below a critical diameter align spontaneously in an epitaxial manner on W(110). Larger particles land preferentially on their surface facets but with random azimuthal orientation with respect to the substrate lattice [1]. These results show that even a random deposition process can lead to uniformly oriented nanostructures.

[1] A. Kleibert, A. Voitkans, and K.-H. Meiwes-Broer, submitted.

O 23.9 Tue 12:30 H33

**Mechanism of metal nanostructure self-ordering during oblique deposition on pre-patterned surfaces** — •Satoshi Numazawa and Karl-Heinz Heinig — Forschungszentrum Dresden-Rossendorf, Dresden, Germany

During oblique metal vapor deposition perpendicular to ripples of prepatterned surfaces, a chain-like formation of metal nanoclusters along the ripples has been observed. The metal nanoclusters are located on the slopes which point towards the evaporation source. The self-ordering of metal nanoclusters has not been observed for normal deposition and for low-angle deposition parallel to the ripple direction. The features of the metal nanostructure depend strongly on the evaporation angle. Here, by means of 3D lattice kinetic Monte Carlo simulations, we studied the process of silver deposition on pre-patterned, oxidized Si surfaces. The experimentally observed Ag nanostructures could be reproduced. It was shown that the extremely low sticking probability of deposited Ag together with a slope-dependent deposition rate leads to a strongly selective Ag nanocluster nucleation on the surface because the nucleation rate depends on the square of the adatom concentration.

O 23.10 Tue 12:45 H33

**Electrospray Ion Beam Deposition: A New Approach to Investigate the Mn12-Acetate Molecular Magnets on Metal Surfaces by Scanning Tunneling Microscopy** — •Zhitao Deng[1], Christian Michaelis[1], Alicia Forment-Aliaga[1,2], Nicha Thontasen[1], Steffen Kahle[1], Nicola Malinowski[1], Markus Ternes[1], Stephan Rauschenbach[1], and Klaus Kern[1,3] — [1]MPI-FKF, Stuttgart, Germany — [2]Instituto de Ciencia Molecular, Universitat de València, Paterna, Spain — [3]Institut de la Matière Condenseé, EPFL, Lausanne, Switzerland

A well defined sample preparation is crucial in order to achieve the ultimate goal of probing the single spin properties of a single molecular magnet. Films of monolayer and submonolayer coverage of the single molecule magnet $Mn_{12}$-acetate ($[Mn_{12}O_{12}(CH_3COO)_{16}(H_2O)_4] \cdot 2CH_3COOH \cdot 4H_2O$) were prepared in-situ on Au(111) surface in ultra high vacuum using electrospray ion beam deposition (ES-IBD). The samples were characterized by several surface sensitive techniques including matrix assisted laser desorption ionization mass spectrometry (MALDI-MS) and scanning tunneling microscopy (STM). The $Mn_{12}$-acetate molecules were deposited by a electrospray ionization source[1] in negative mode. STM measurements at a temperature of 40K show that the molecules are trapped at the elbow sites of the reconstructed Au(111) surface at the initial stage. With increasing molecular coverage, molecules aggregate in the fcc region of the Au(111) surface at first and in the hcp region for even higher coverage. [1] Small **2** (2006), 540-547

# O 24: Particles and clusters

Time: Tuesday 10:30–12:30 Location: H34

O 24.1 Tue 10:30 H34

**Not so loosely bound: temperature dependent vibrational fingerprints of $Au_NKr_M$ clusters** — •Luca M. Ghiringhelli, Philipp Gruene, Gerard Meijer, Andrè Fielicke, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

In order to interpret the vibrational spectra of *neutral* $Au_NKr_M$ clusters, as measured in a Multiple Photon Dissociation Far-IR experiment (P. Gruene *et al.*, Science **321**, 674 (2008)), we calculated their finite temperature vibrational spectra, by means of all electron density functional theory, including the Tkatchenko-Scheffler van der Waals correction. We surprisingly find that Kr forms weak chemical bonds (binding energy around 0.2 eV per Kr atom) with 1- to 3-fold coordinated Au atoms belonging to small $Au_N$ clusters ($N \leq 4$). Such $Au_NKr_M$ clusters have a vibrational spectrum which is different from the related $Au_N$ clusters. For bigger $Au_N$ clusters, Kr physisorbs to the clusters, forming a complex whose vibrational spectrum is practically identical to the spectrum of the bare cluster. Anharmonicities affect the spectrum by changing (with respect to the harmonic spectrum) the relative intensity of the peaks and by showing new peaks, due to interactions among eigenmodes.

O 24.2 Tue 10:45 H34

**RHEED Study of Au-induced Surface Reconstructions and 3D AuSi Nanoparticles** — •Stephan Bartling, 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 Au/Si(111). Three different surface reconstructions can be observed in recorded RHEED patterns during Au evaporation in the sub-monolayer regime. Recently, the ideal Au coverage for the Si(111)$5\times2$-Au reconstruction has been revised [1]. The result of $\Theta = 0.6$ML is confirmed by the coverage-dependent intensity of spots.

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. We do not observe flat top facets reported for similar preparation conditions [2]. This is in agreement with the crystal orientation determined by RHEED.

[1] I. Barke et al., Phys. Rev. B 79, 155301 (2009)
[2] E. Moyen et al., Appl. Phys. Lett. 94, 233101 (2009)

O 24.3 Tue 11:00 H34

**Orbital and spin magnetic moments of small, deposited CoPd alloy clusters on Ni/Cu(100)** — •Steffen Fiedler[1], Ivan Baev[1], Kai Chen[1], Leif Glaser[1], Paolo Imperia[2], Stephan Klumpp[1], Michael Martins[1], and Wilfried Wurth[1] — [1]Institut für Experimentalphysik, Universität Hamburg — [2]Institute of Materials and Engineering Science, Australian Nuclear Science and Technology Organisation New Illawarra Road, Lucas Heights, NSW Australia

It has been shown that the orbital magnetic moments of Co clusters can be exceptionally large on a platinum substrate [1]. Together with a strong induced spin-orbit-coupling this leads to a high magnetic anisotropy.

We examine the magnetic moments of transition metal elements in small, mass selected alloy clusters on ferromagnetic substrates with the method of X-ray circular magnetic dichroism (XMCD). The measurements are performed at the storage ring of the synchrotron radiation source Bessy II in Berlin. Starting with $Co_xPt_y$ clusters we proceeded with the investigation of $Co_xPd_y$ clusters. We will classify the results in the light of the previous measurements also including pure $Co_x$ clusters as a reference.

This work was funded by the DFG through the SPP 1153.

[1] P. Gambardella et al., Science 300, 1130 (2003)

O 24.4 Tue 11:15 H34

**Structural properties of individual mass-filtered *3d*-metal nanoparticles deposited on W(110)** — •Wolfgang Rosellen[1], Christian Kleinhans[1], Volker Hückelkamp[1], Furkan Bulut[1], Joachim Bansmann[2], Armin Kleibert[3], and Mathias Getzlaff[1] — [1]Institute of Applied Physics, University of Düsseldorf — [2]Dep. of Surface Chemistry, Ulm University — [3]Swiss Light Source, Paul Scherrer Institute

Nano-sized clusters and particles are regarded as a new class of material because their physical and chemical properties can significantly change with size. Thus, new features are accessible and additionally tunable by size-selection. Due to the high surface-to-volume ratio and the reduction of the coordination numbers the properties also differ from the respective bulk material such as melting point, conductance or electronic and, for magnetic particles, magnetic behavior. Fe, Co and FeCo alloy nanoparticles were produced by a continuously working arc cluster ion source (ACIS), mass-filtered by means of an electrostatic quadrupole and subsequently deposited on a W(110) surface. We discuss the structural properties of *individual* nanoparticles with diameters between 3 nm and 15 nm. High-resolution transmission electron microscopy (HR-TEM) is used to estimate the size and the crystallographic structure of the nanoparticles before deposition. The height and shape after deposition is investigated by scanning tunneling microscopy (STM). Additionally, the melting behaviour of the nanoparticles at elevated temperatures will be discussed.

O 24.5 Tue 11:30 H34

**Molecular Dynamics Studies on the Morphology of PtNi-alloy Particles** — •Donato Fantauzzi and Timo Jacob — Ulm University, Albert-Einstein-Allee 47, D-89069 Ulm, Germany

Platinum-based catalysts supported on carbon still serve as the preferred electrocatalyst for the oxygen reduction reaction (ORR), which is one of the most important reactions in basic electrochemistry but also in various applications such as low-temperature polymer electrolyte fuel cells. In order to find a more active catalyst than pure Pt, in the past years various platinum alloys such as PtNi, PtCo, etc. with different atom ratios were synthesized and investigated [1]. Since Pt is limited and rather expensive, these multi-metallic catalysts are not only saving precious metal but also show enhanced reactivity and selectivity.

Motivated by recent experimental work on the morphology of $Pt_xNi_1$ *(x=1,2,3)* nanoparticles, we investigated the bulk and surface structure as well as the segregation behavior of differently sized (1.0-3.0 nm) alloy nanoparticles using ReaxFF [2], a reactive molecular dynamics (MD), with a self-optimized forcefield. By applying subsequent simulated annealing cycles to particles of variable size and bulk composition direct comparison to the experimental results was possible [3].

[1] U. A. Paulus *et al.*, *J. Phys. Chem. B*, **106**, 4181 (2002).
[2] A. C. T. van Duin, S. Dasgupta, F. Lorant, W. A. Goddard III., *J. Phys. Chem. A*, **105**, 9396 (2001).
[3] E. Favry, D. Wang, D. S. Su, N. Alonso-Vante, D. Fantauzzi, T. Jacob, *to be published.*

O 24.6 Tue 11:45 H34

**X-ray absorption fine-structure spectroscopy of bimetallic Pt nanoparticles** — •Torsten Laurus[1], Ardalan Zargham[1], Edyta Piskorska-Hommel[1,2], Jan Ingo Flege[1], Sarah Röhe[3], Patrick Sonström[3], Xiaodong Wang[3], Marcus Bäumer[3], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee, 28359 Bremen, Germany — [2]Institute of Physics, Polish Academy of Science, Al. Lotnikow 32/46, 02-668 Warsaw, Poland — [3]Institute for Applied and Physical Chemistry, University of Bremen, Leobener Straße, 28359 Bremen, Germany

Bimetallic nanoparticles have generated great interest in recent years because of their huge number of possible applications, e. g., in future electronic and magnetic devices as well as in heterogeneous catalysis. Since the physical and chemical properties of the nanoparticles significantly depend on both their atomic structure and chemical composition, their material characteristics may individually be tailored provided that these parameters can be controlled.

Several Pt-containing bimetallic nanoparticles, produced by wet chemical synthesis, have been studied by means of fluorescence x-ray absorption fine-structure spectroscopy (XAFS), which was performed at beamlines C and E2 at the Hamburg Synchrotron Radiation Laboratory (HASYLAB/DESY). Our data allow the identification of the crystalline structure of the nanoparticles and the quantification of the local atomic coordination of the constituents. Furthermore, the analysis reveals details on their compositional inhomogeneity and the concomitant oxidation states of the individual components.

O 24.7 Tue 12:00 H34

**Structural metastability of endohedral $M$@Si$_{20}$ cages: A first-principles sampling study** — Alexander Willand[1], •Matthias Gramzow[2], Stefan Goedecker[1], and Karsten Reuter[2,3] — [1]Univ. Basel (Switzerland) — [2]Fritz-Haber-Institut Berlin (Germany) — [3]Technische Universität München (Germany)

Cage-like clusters are considered as appealing building units for nanoscale materials. Their hollow structure facilitates the incorporation of guest atoms, which can either be viewed as an atomic-scale tailoring of the materials properties of the cage through doping or as a perfect shielding of the encapsulated moiety. With Si in general favoring tetrahedral $sp^3$-coordination, corresponding endohedral metal doping appears as a primary avenue to accomplish the stabilization of Si cage geometries at all. C$_{20}$ is the smallest known fullerene cage and Si$_{20}$ cages are building blocks of clathrate materials. We therefore investigate the structural stability of endohedral Si$_{20}$ structures for a large variety of metal dopants. For this purpose we combine global optimization within minima hopping [1] with a DFT potential energy surface using different levels of xc approximation (LDA, GGA, hybrid functionals). In contrast to previous work proposing endohedral $M$@Si$_{20}$ cages as ground state (e.g. [2]) we find for all investigated systems largely more stable isomers, in which the cage structure is broken into smaller cages with additional surface atoms or into completely exohedral isomers. [1] S. Goedecker, JCP **120**, 9911 (2004) [2] Q. Sun *et al.*, PRB **65**, 235417 (2002).

O 24.8 Tue 12:15 H34

**Magnetic coupling and anisotropy of Fe nanoclusters deposited onto Cu(111)** — •Christian Praetorius[1], Greg A. Ballentine[2,4], Armin Kleibert[3,5], Norman Wilken[3], Andris Voitkans[3], Karl-Heinz Meiwes-Broer[3], and Kai Fauth[1,2] — [1]Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]MPI für Metallforschung, Heisenbergstr. 3, 70689 Stuttgart, Germany — [3]Physikalisches Institut, Universität Rostock, 18051 Rostock, Germany — [4]Dpt. of Physics, Brandon University, 270 18th street, Brandon, Canada R7A 6A9 — [5]Swiss Light Source, Paul Scherrer Institute, 5232 Villigen, Switzerland

Magnetization and magnetic response of Fe nanoclusters is studied by temperature and density dependent in situ X-ray magnetic circular dichroism after deposition onto Cu(111). At particle diameters of 6 nm, ferromagnetic response is obtained at ambient temperature for nanocluster densities well below percolation threshold. Both, enhanced intrinsic magnetic anisotropy energy (MAE) density as well as collective effects contribute to this effect. This enhancement of MAE is not accompanied by enhanced orbital magnetic moments. At elevated cluster densities we observe sizeable macroscopic magnetic in plane anisotropy. This anisotropy can quantitatively be understood as the effect of a demagnetizing field, and thus the average effect of diplar interactions of the nanoclusters.

## O 25: Metal substrates: Adsorption of organic / bio molecules III

Time: Tuesday 10:30–13:00 Location: H36

O 25.1 Tue 10:30 H36

**Tuning molecule-mediated spin coupling in bottom-up fabricated vanadium-TCNE nanostructures** — •Daniel Wegner[1,2], Ryan Yamachika[2], Xiaowei Zhang[2], Yayu Wang[2], Tunna Baruah[3], Mark R. Pederson[4], Bart M. Bartlett[2], and Jeffrey R. Long[2] — [1]Physikalisches Intsitut & CeNTech, WWU Münster, Germany — [2]University of California, Berkeley, and Lawrence Berkeley National Laboratory, Berkeley, CA, USA — [3]University of Texas, El Paso, TX, USA — [4]Naval Research Laboratory, Washington, DC, USA

We have fabricated hybrid organic/inorganic magnetic molecules based on vanadium atoms and tetracyanoethylene (TCNE) ligands in an atom-by-atom fashion using a cryogenic scanning tunneling microscope. By means of local tunneling spectroscopy we observe spin-polarized molecular orbitals as well as a structure-dependent Kondo resonance. For complexes having two V atoms, the Kondo behavior can be switched on and off by a minute structural change that leaves the spin-containing orbital essentially unchanged. This can be explained by a tunable, structure-dependent change in the vanadium spin-spin coupling strength through the TCNE molecule, as confirmed by density functional calculations. The present findings offer a new route for designing molecular spin nanostructures with atomic-scale precision.

O 25.2 Tue 10:45 H36

**Positioning Co atoms with organic molecular templates** — •Wolfgang Krenner[1], Dirk Kühne[1], Florian Klappenberger[1], Svetlana Klyatskaya[2], Mario Ruben[2], and Johannes V Barth[1] — [1]Physikdepartment E20, TU München, München, Germany — [2]Institute of Nanotechnology, Forschungszentrum Karlsruhe, Karlsruhe, Germany

In this work the adsorption of atomic Cobalt onto organic molecular templates is investigated by means of low-temperature scanning tunneling microscopy under UHV conditions. When evaporated onto a Ag(111) surface held at room temperature, diphenyl oxalic amides can be grown into strings across the surface at submonolayer coverages or as densely packed monolayers. Co is evaporated at low temperatures around 140 K onto submonolayers and monolayers, displaying different behavior depending on the coverage, which will be discussed.

The presence of the molecular layer prevents the formation of Co-clusters and instead leads to an adsorption of atomic Co onto the phenyl rings of the oxalic amides. Annealing the sample leads to a redistribution of the Co atoms on the monolayer. At coverages well below a single monolayer a bending of the molecular strings in the presence of Co is observed, which is no longer the case for coverages just below a monolayer. Through annealing it is found, that diffusion of Co atoms away from the molecular strings takes place. In both cases it is possible to assemble ordered arrays of single Co atoms sitting on top the phenyl rings of the oxalic amides, therefore forming chains of ferromagnetic atoms.

O 25.3 Tue 11:00 H36

**Scanning Tunneling Microscopy investigation of different porphynoids on a Ni-prestructured Cu(111) surface** — •Michael Röckert, Florian Buchner, Elisabeth Zillner, Stefanie Glässel, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstraße 3, D-91058 Erlangen

The assembly of organic molecules on single-crystal surfaces is an approach towards the creation of novel materials with outstanding properties. Porphyrins appear to be ideal candidates to generate functional molecular devices, due to their self-assembly properties and their versatile functionality. In the present work we study the possibility to locally anchor or functionalize porphyrins on a prestructured surface, namely a composite Ni/Cu(111) surface, by scanning tunneling microscopy (STM) in ultra-high vacuum at room temperature. Based on scanning tunneling micrographs and movies the dynamics, assembly and intramolecular conformation of the corresponding porphyrins (2HTPP, CoTPP, OEP) as well as the role of molecule-molecule and molecule-substrate interactions are discussed. The obtained findings indeed indicate the possibility to locally anchor and/or functionalize (e.g. metalate [1-2]) the porphyrins on a Cu(111) surface prestructured either with atomically flat Ni- or oxygen-islands. This work has been funded by the DFG through Sonderforschungsbereich 583.

[1] F. Buchner et al., ChemPhysChem, 2007. 8(2): p. 241-243 [2] T.E. Shubina et al., JACS, 2007. 129(30): p. 9476-9483.

O 25.4 Tue 11:15 H36

**Dynamics of Tetraphenylporphyrins on a Copper (111) surface: A Scanning Tunneling Microscopy Study** — •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 properties of large organic molecules at surfaces is a requirement to utilize their functional properties either in single-molecule devices or in organized supramolecular architectures. Here we concentrate on the investigation of the dynamics and self-assembly of tetraphenylporphyrins (TPP) on Cu(111) using scanning tunneling microscopy (STM) in ultra-high vacuum (UHV). STM images of ordered molecular arrays and individual molecules with submolecular resolution enable to determine the supramolecular and intramolecular conformation of the porphyrins. Interestingly, 2HTPP molecules exhibit a mainly one dimensional diffusion along the main crystallographic axes of Cu(111) at room temperature, whereas CoTPP molecules form ordered arrays. Based on STM movies acquired at varying sample temperatures fundamental parameters of the molecular motion of 2HTPP on Cu(111), like the activation energy for diffusion and rotation could be estimated. These results allow a deeper understanding of the corresponding molecule-molecule and molecule-substrate interactions and thus the assembly of the observed porphyrins.

Funded by the DFG through Sonderforschungsbereich 583.

O 25.5 Tue 11:30 H36

**Vibrational spectroscopy of 4-mercaptopyridine on Au(111): A comparison of scanning tunneling spectroscopy and calculations** — •Norbert Maurer[1], Anna Tschetschetkin[1], Berndt Koslowski[1], Paul Ziemann[1], Inga Respondek[2], and David M. Benoit[2] — [1]Institut für Festkörperphysik — [2]Nachwuchsgruppe Theorie SFB 569, Universität Ulm, Albert-Einstein-Allee 11, D-89081 Ulm

Notion of the adsorption structure and vibrational properties is essential to understand electronic transport across molecules and, therefore, is an essential issue in the field of molecular electronics. Scanning tunnelling microscopy (STM), scanning tunnelling spectroscopy (STS), and especially inelastic electron tunnelling spectroscopy (IETS) is ideal to investigate these properties on a single-molecular basis. We employ these techniques to reveal the properties of 4-mercaptopyridine (4MPy) on Au(111) and compare those to, e.g., DFT calculations. We put emphasis on IETS where we find about 20 excitations in the energy range 0-200 meV. Results are compared to calculations based on the vibrational self-consistent field method [1] and earlier experimental results [2,3]. We conclude that 4MPy adsorbs at elbow sites, in the fcc region, and at step edges preferentially in a bridge configuration thereby ruling out a model proposed earlier which suggests that adsorption of a single 4MPy is accompanied by a Au ad-atom.

[1] I. Respondek and D.M. Benoit, J. Chem. Phys 131, 054109 (2009). [2] Yu, et al., Nano Lett. 8 (7), 1923 (2008). [3] Zhang, et al., J. Raman. Spec. 38, 1106 (2007).

O 25.6 Tue 11:45 H36

**The local structure of the methoxy reaction intermediate on Cu(110): a scanned-energy mode photoelectron diffraction study** — •Dagmar Kreikemeyer Lorenzo[1], Werner Unterberger[1], David Duncan[2], Tsenolo Lerotholi[2], Matt Bradley[2], Jim Robinson[2], and David Philipp Woodruff[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]University of Warwick, Great Britain

Scanned-energy mode photoelectron diffraction (PhD) is a well-established method to determine quantitatively the local structure of adsorbates at surfaces. We apply this method to study the adsorption on a copper surface, Cu{110}, of the methoxy species, an intermediate in the catalytic decomposition of methanol. Previous STM [1] and XPD [2] studies have concluded that methoxy bonds to Cu {110} through the oxygen atom on a three-fold coordinated site. However, our O1s PhD spectra show the strongest modulation at 30° and 40° polar emission angles in the azimuth, consistent only with a short bridge adsorption site. More quantitative analysis, as well as a parallel DFT study, identifies the structure as involving two distinct short-bridge adsorption sites, one on Cu adatoms, with slightly different bond-lengths to the copper atoms below. The results indicate a tilt of the O-C axes of 37° in the azimuth, with the carbon atoms pointing in opposite directions at alternate adsorption site. This tilt is consistent with the XPD results, and creates a zig-zag structure that accounts for the STM images [1].[1] F.M. Leibsle et al., Surf. Sci. 318 (1994)46[2] E. Holub-Krappe et al., Surf. Sci. 173 (1986)176

O 25.7 Tue 12:00 H36

**Planar chain structure of formic acid on Au(111) surfaces studied by Micro-Channel Plate (MCP)-LEED** — •Mirko Müller, Michel Kazempoor, and Gerhard Pirug — Institut für Bio- und Nanosysteme (IBN 3) and JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Vibrational spectroscopy (HREELS) indicates that formic acid adsorbs in a molecular reversible manner on Au(111) surfaces.(1) The vibrational signature points to the formation of flat lying chains of H-bonded formic acid molecules. This hypothesis could not be proven by structure investigations using conventional LEED systems. The electron beam sensitivity of the adsorbed layer prevents from the observation of clear LEED patterns. On the contrary bright LEED spots could be observed using a micro-channel plate (MCP) LEED system which allows a more gentle examination with reduced electron beam current in the pA regime. Consistent with the weak chemical interaction of physisorbed formic acid molecules the reconstruction of the Au(111) surface is not lifted. In addition an incommensurate rectangular superlattice could be identified. Missing (0,2n+1) spots indicates the presence of mirror glide plane symmetry p2mg consistent with the formation of zig-zag chains containing links of cis formic acid molecules oriented accordingly.

(1) M. Kazempoor, and G. Pirug, Appl. Phys. A 87, 435-441 (2007)

O 25.8 Tue 12:15 H36

**Oxidation of Formic Acid on Pt(111)** — •Wang Gao and Timo Jacob — Universität Ulm, Albert-Einstein-Allee 47, D-89069 Ulm, Germany

Oxidation of formic acid (HCOOH) on Pt(111) surfaces, which can be considered a benchmark reaction to probe the corresponding electrocatalytic HCOOH conversion in fuel cells, has been studied using density functional theory. The effects of water and adsorption coverage on the process from HCOOH to $CO_2$ were investigated in detail. For each reaction pathway we evaluated relative energies under different environmental conditions, including activation barriers, reaction energies, and intermediate and transition state structures. Our results indicate that while the direct conversion is energetically unfavorable both HCOO and COOH could be reactive intermediates. Moreover, surrounding or co-adsorbed water turned out to play a key role in the whole process, which drastically influences the stability of reactants and products on Pt(111), as well as the correlated reaction barriers. Meanwhile, the entire catalytic process additionally varies with surface coverage, making the formic acid oxidation a rather complex reaction. Based on our energetics, future analysis of the reaction kinetics will elucidate preferred reaction mechanisms.

O 25.9 Tue 12:30 H36

**Joint experimental and theoretical studies of complex adsorption structures: Adsorption versus Interaction Strength** — •J. Haubrich[1], D. Loffreda[2], F. Delbecq[2], P. Sautet[2], Y. Jugnet[3], C. Becker[1], and K. Wandelt[1] — [1]Inst. f. Phys. und Theo. Chemie, Universitaet Bonn — [2]Lab. de Chimie, Ecole Normale Superieure de Lyon, France — [3]Inst. de Rech. sur la Catalyse et Env., Villeurbanne, France

Model catalysis studies in UHV represent a crucial strategy to identify surface species, reaction mechanisms, and separate the roles of the catalysts, promoters and supports in heterogeneous catalysis. Combining powerful experimental tools with theoretical methods, surface processes can be studied nowadays in atomic level detail. Here we present a combined HREELS and DFT study of the adsorption and interaction of multifunctional molecules, crotonaldehyde and prenal, on Pt(111) and two Pt-Sn surface alloys. The identification of adsorption structures is a fundamental step towards understanding of the molecule-surface bonding and the reaction mechanisms in the selective hydrogenation of $\alpha,\beta$-unsaturated aldehydes. We identified the stable adsorption structures on the three model surfaces and surprisingly find that the tin-induced changes in the vibrational properties disagree with the electronic modifications of the surfaces and the adsorption energies. Our detailed energetic analysis of the molecule-surface bonding reveals that the interaction energies of complex molecules with the substrate are very different than the adsorption energies and allow us to rationalize the vibrational frequencies.

O 25.10 Tue 12:45 H36

**Nitrogen Adsorption on Graphite: Defying Physisorption** — •Alexandre Tkatchenko and Matthias Scheffler — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany

The adsorption of a nitrogen molecule at the graphite surface can be considered a paradigm of molecular physisorption [1]. The binding of $N_2$ can be phenomenologically described in terms of a competition between quadrupole–quadrupole and van der Waals dispersion energies. Of particular interest is the relative stability of the so-called "in-plane", "out-of-plane" and "pin-wheel" monolayer structures, in which the nitrogen molecules alternate between parallel and perpendicular configurations on the surface. By combining state-of-the-art electronic structure methods, such as dispersion-corrected density-functional theory and Møller-Plesset second-order perturbation theory along with high-level coupled cluster [CCSD(T)] calculations, we are able to gain quantitative insight into the adsorption mechanism of $N_2$@graphite and achieve very good agreement with experimental desorption enthalpy. We challenge the commonly held view of a closed-shell adsorbed $N_2$ molecule, finding a noticeable charge-density polarization for nitrogen in a perpendicular configuration on the surface. We map out the $N_2$@graphite potential energy surface as a function of sliding and orientation and discuss the influence of quantum zero-point energy for different adsorption sites. [1] D. Marx and H. Wiechert, Adv. Chem. Phys. **95**, 213 (1996).

# O 26: Oxides and insulators: Clean surfaces

Time: Tuesday 10:30–12:45 Location: H40

O 26.1 Tue 10:30 H40

**Improved atomic scale contrast via bimodal dynamic force microscopy** — Shigeki Kawai, Thilo Glatzel, •Sascha Koch, Bartosz Such, Alexis Baratoff, and Ernst Meyer — Department of Physics, University of Basel, Klingelbergstr. 82, CH-4056 Basel, Switzerland

We implemented a multi-frequency technique into atomically resolved frequency-modulation dynamic force microscopy for a further improvement of force sensitivity in ultra-high vacuum [1]. The first and second flexural resonance modes of a commercially available Si cantilever are simultaneously excited by controlled amplitudes, while the resonance frequency shifts (Δf_1st and Δf_2nd) are demodulated by two phase-locked loop circuits (Nanonis: Dual-OC4). The combination of sub-angstrom amplitude oscillation A_2nd at the second resonance with the commonly used large amplitude oscillation A_1st at the first resonance enables a high force sensitivity at Δf_2nd while avoiding atomic jump-to-contact instabilities caused by controlling the tip sample distance with Δf_1st [2-4].

Simultaneously in quasi-constant height mode recorded Δf_1st and Δf_2nd maps of KBr(001) show that the Δf_2nd signal has a higher tip-sample distance dependence. With A_1st=16 nm and A_2nd=50 pm at different tip-sample distances in the attractive region the signal-to-noise of Df2nd was higher than that of Δf_1st especially at close tip-sample distances. This high-sensitive detection of the short-range interaction clearly revealed tip/sample deformations.

O 26.2 Tue 10:45 H40

**The valence band structure of $\beta-Ga_2O_3$ single crystals** — •Mansour Mohamed[1], Christoph Janowitz[1], Zbigniew Galazka[2], Reinhard Uecker[2], Roberto Fornari[2], and Recardo Manzke[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany

The valence band structure of the (100) surface of high-quality $\beta-Ga_2O_3$ single crystals grown by the Czochralski method has been investigated by angle-resolved photoelectron spectroscopy utilizing He I and synchrotron radiation along the symmetry directions of the surface Brillouin zone. The surface of $\beta-Ga_2O_3$ single crystal was characterized by different techniques (LEED, Laue, and STM). From the ultraviolet photoemission spectra measured along the parallel directions of the Brillouin zone, it is found that the valence bands along ($k_b$) and ($k_c$) do not show so much dispersion. On the other hand, the measurements performed with synchrotron radiation to probe the direction normal to the surface ($k_a$) indicate much stronger dispersion of the valence bands. The experimental valence band structure of $\beta-Ga_2O_3$ single crystals will be discussed and compared with theoretical results.

O 26.3 Tue 11:00 H40

**Interaction potential for fast atoms in front of KCl(001) surface** — •Uwe Specht[1], Marco Busch[1], Konrad Gärtner[2], and Helmut Winter[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstraße 15, D-12489 Berlin, Germany — [2]Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Max-Wien-Platz 1, D-07743 Jena, Germany

Fast He, Ne, Ar and N atoms with energies from 1 kev up to 60 keV are scattered under grazing angles of incidence ($\leq 2°$) from a clean and flat KCl(001) surface. For scattering along low-index directions (axial surface channeling), we observe pronounced peaks in the angular distribution of the scattered projectiles. This can be attributed to rainbow-scattering caused by the corrugated interaction potential. On the basis of classical trajectory calculations, we derive from comparison with the experimental data the effective interaction potential of He, Ne, Ar and N atoms in front of a KCl(001) surface. Fair agreement is found for individual pair potentials calculated from Hartree-Fock wave functions, where the charge state of K and Cl ions located at lattice sites of the ionic crystal is taken into account. For the generalized ZBL (Ziegler, Biersack and Littmark) and OCB (O'Connor and Biersack) potentials, the agreement for interaction energies below 20 eV is found to be poor.

O 26.4 Tue 11:15 H40

**3D force spectroscopy on KBr(001) by tuning fork based nc-AFM at low temperatures** — Bartosz Such[1], •Sweetlana Fremy[2], Shigeki Kawai[2], Sascha Koch[2], Thilo Glatzel[2], and Ernst Meyer[2] — [1]Research Center for Nanometer-Scale Science and Advanced Materials (NANOSAM), Faculty of Physics, Astronomy, and Applied Computer Science, Jagiellonian University, Reymonta 4, 30-059 Krakow, Poland — [2]University of Basel, Klingelbergstrasse 82, 4056 Basel

We will present 3D dynamic force spectroscopy measurements on KBr(001) by tuning fork based nc-AFM [1] at low temperatures. The high stiffness of a tuning fork enables high-sensitive measurements of the short-range interaction with small oscillation amplitudes [2]. We performed the topographic method to collect 3D frequency shift and energy dissipation maps while keeping an amplitude of 200 pm [3]. The results suggest that significant tip relaxation is present at the smallest tip-sample separations. Analyzing the shape of force vs. distance curves and the cross sections of the 3D frequency shift dataset allows the identification of chemical identity of the tip apex as K+ ion.

[1] F.J. Giessibl, Appl. Phys. Lett. 76, 1470 (2000). [2] S. Hembacher and F. J. Giessibl and J. Mannhart, Science 305, 380 (2004). [3] B. J. Albers, T. C. Schwendemann, M. Z. Baykara, N. Pilet, M. Liebmann, E. I. Altman, U. D. Schwarz, Nature Nano. 4, 307 (2009).

O 26.5 Tue 11:30 H40

**Polarity healing at the local scale: MgO on Au(111)** — •Philipp Myrach[1], Niklas Nilius[1], Stefania Benedetti[2], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institut der MPG, Faradayweg 4-6, D-14195 Berlin, Germany — [2]CNR-INFM S3, Via G. Campi 213/a, I-41125 Modena, Italy

Polar MgO films prepared on Au(111) have been investigated with scanning tunnelling microscopy and spectroscopy. The amount of oxide polarity is derived from the MgO band positions and the local surface potential. Both quantities have been measured as a function of the oxide thickness and are good indicators for the strength of the surface dipole. Whereas bi-layer MgO islands exhibit uncompensated polarity, the dipole gradually decreases in thicker films due to surface roughening. The formation of nano-pyramids and pits is hereby identified as the initial step for polarity healing. Above such structural inhomogeneities, the measured surface potential is drastically reduced with respect to flat MgO(111) patches. This effect is reproduced with simple model structures that enable an estimation of the vertical dipole strength.

O 26.6 Tue 11:45 H40

**Diffraction of fast light atoms and molecules during grazing scattering from a KCl(001) surface** — •Marco Busch, Uwe Specht, and Helmut Winter — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstraße 15, D-12489 Berlin, Germany

Fast light atoms and molecules with energies from 200 eV up to several keV are grazingly scattered from a clean and flat KCl(001) surface. For scattering along low-indexed axial channels, we observe defined diffraction patterns in the angular distributions for scattered projectiles. The experimental results for the scattering of H, D, $^3$He, and $^4$He atoms as well as $H_2$, $D_2$, and HD molecules can be ascribed to atom diffraction with de Broglie wavelengths as low as about $10^{-3}$ Å. From the evaluation of diffraction patterns we derive the widths of axial channels and the corrugation of the interaction potential across these channels. Our analysis is based on a semiclassical model using the hard-wall approximation and individual potentials for the interaction of the atomic projectiles with the atoms of the topmost surface layer of the surface.

O 26.7 Tue 12:00 H40

**Temperature stabilised surface reconstructions at polar ZnO(0001)** — •Mira Todorova[1], Markus Valtiner[2], Guido Grundmeier[2,3], and Jörg Neugebauer[1] — [1]Department for Computational Materials Design, Max-Planck-Insitut für Eisenforschung GmbH, Düsseldorf — [2]Christian Doppler Laboratory for Polymer/Metal Interfaces, Max-Planck-Insitut für Eisenforschung GmbH, Düsseldorf — [3]Technical and Macromolecular Chemistry, University of Paderborn, Paderborn

Combining diffraction experiments with density-functional theory calculations and thermodynamic considerations we study the atomic structure of the polar ZnO(0001) surfaces. We show that a large number of very different reconstructions with similar stoichiometry are energetically almost degenerate, thus surface vibrational entropy contributions significantly affect their stabilisation. The large impact of the vibrational entropy on the surface structure gives rise to a strong dependence of surface phase diagrams on temperature and enables us to consistently describe and explain the experimentally observed surface structures on polar ZnO(0001) surfaces.

M. Valtiner, M. Todorova, G. Grundmeier, and J. Neugebauer, Phys. Rev. Lett. 103, 065502 (2009).

O 26.8 Tue 12:15 H40

**Relaxation and thermal vibrations at the NaF(100) surface** — •Stephan Härtel, Jochen Vogt, and Helmut Weiss — Chemisches Institut der Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Various theoretical models predict that the (100) surfaces of ionic solids with the rocksalt structure should exhibit a surface rumpling, i. e. cations and anions in the surface layer have different vertical positions. While this type of relaxation has been measured for various alkali halides the rumpling of the NaF(100) surface is expected to be very small. We present results of an experimental determination of the relaxation of the NaF(100) surface based on low-current LEED experiments and a subsequent tensor-LEED analysis of diffraction peak intensities as a function of electron energy at various crystal temperatures. Moreover, we present experimental values of the mean amplitudes of the thermal motions of the surface ions. The experimental data are compared to the results of density functional theory (DFT) calculations using a slab model and ultrasoft pseudopotentials. According to both experiment and theory, the average vertical positions of the $Na^+$ and $F^-$ ions in the topmost surface layer differ at most by 0.02Å. While the measured rumpling is smaller than the error-bars, the model calculations predict a weak inward-displacement of the $Na^+$ ions of 0.01Å, and an outward-shift of $F^-$ of 0.01Å with respect to the truncated bulk geometry. The thermal motions of the ions in the topmost surface layer appear to be enhanced compared to the respective bulk mean amplitudes by a factor of 1.3 to 1.4.

O 26.9 Tue 12:30 H40

**Surface termination of $NdGaO_3$(110) and $DyScO_3$(110)** — •Jens Lienemann[1], Marco Busch[1], Rasuole Dirsyte[2], Jutta Scharzkopf[2], Günter Wagner[2], Helmut Winter[1], and Roberto Fornari[2] — [1]Department of Physics, Humboldt University, Newtonstraße 15, D-12489 Berlin, Germany — [2]Leibniz Institute for Crystal Growth, Max Born Straße 2, D-12489 Berlin, Germany

Auger electron spectroscopy using excitation via grazing impact of protons was applied to determine the elemental composition of the topmost layer of $NdGaO_3$(110) and $DyScO_3$(110) substrates. The preparation conditions of vicinal $NdGaO_3$ and $DyScO_3$ substrates were optimized with respect to annealing temperature, time, and gas atmosphere. Well prepared surfaces show regularly arranged, smooth terraces with single-layer steps as observed by atomic force microscopy. The surfaces of $NdGaO_3$(110) were always NdO terminated with a small amount of Ga (2-4%) atoms at the surface [1]. A Ga and O depletion layer with a thickness of about 4 nm was detected at optimized preparation conditions. $DyScO_3$(110) substrates show a dependence of the termination on the annealing gas. A $ScO_2$ terminated surface was prepared with annealing in argon while an DyO-Termination was found after annealing in oxygen. A depletion layer of Dy and O was also detected.

[1] R. Dirsyte, J. Schwarzkopf, G. Wagner, J. Lienemann, M. Busch, H. Winter and R. Fornari, Appl. Surf. Sci. 255, 8685 (2009)

## O 27: Metal subtrates: Adsorption of O and/or H

Time: Tuesday 10:30–12:30 Location: H42

O 27.1 Tue 10:30 H42

**New Surfaces Stabilized by Adsorbate-Induced Faceting of Ir(210)** — •Payam Kaghazchi[1], Ivan Ermanoski[2], Wenhua Chen[3], and Timo Jacob[1] — [1]Universität Ulm, Albert-Einstein-Allee 47, D-89069 Ulm, Germany — [2]Sandia National Laboratories, USA — [3]Rutgers University, Piscataway, NJ 08854, USA

When atomically-rough Ir(210) is exposed to more than 0.5 ML of oxygen and annealed to 600 K, nanoscale three-sided pyramidal facets grow and cover the surface. Experimental measurements revealed that these facets expose faces of Ir(311), Ir($31\bar{1}$), and Ir(110) orientation. Furthermore, while the (311) and ($31\bar{1}$) faces are always smooth, some (110) faces were found to be partially rough [1]. As a combined effort of experiment (STM) and theory (DFT) we investigated the nature of these rough areas on the (110) faces. It was found that these regions consist of a complicated Ir(110) reconstruction, leading to a stepped double-missing-row (110) superstructure. Interestingly, while this structure is not observable on a Ir(110) single crystal surface, it only becomes thermodynamically favorable on the (110) faces of the nanopyramids formed after the oxygen-induced faceting of Ir(210). This indicates that with the aid of facet formation one can stabilize new surfaces, which cannot be stabilized neither by cleavage of a crystal nor through by reconstruction. [1] T. E. Madey, W. Chen, H. Wang, P. Kaghazchi, T. Jacob, *Chem. Soc. Rev.*, **37**, 2310 (2008).

O 27.2 Tue 10:45 H42

**The interaction of oxygen with AgPd/Pd(111) surface alloys - A case study for ensemble effects on bimetallic surfaces** — •Thomas Diemant, Joachim Bansmann, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

AgPd/Pd(111) surface alloys, which consist of a reactive and an inert metal, represent an ideal test case for the study of ensemble effects on bimetallic surfaces. The structural properties of these planar model systems (surface contents and atom distribution) are accessible by high-resolution scanning tunnelling microscopy (STM), while the chemical/adsorption properties can be studied by a combination of temperature-programmed desorption (TPD) and vibrational spectroscopy, such as high-resolution electron energy loss spectroscopy (HREELS). We have used this approach to correlate the structural properties of structurally well-defined AgPd/Pd(111) surface alloys to their oxygen adsorption behaviour. The modification of the oxygen adsorption properties can be attributed predominantly to ensemble effects. Ligand effects only play a minor role. The results will be compared to findings on the interaction of CO with these surface alloys.

[1] Yunsheng Ma et al., Surf. Sci. 603 (2009) 1046.

O 27.3 Tue 11:00 H42

**Oxidation kinetics of Ru(0001)** — •Marius Ernst[1] and Wim Sloof[2] — [1]Universität Würzburg, Experimentelle Physik 7 — [2]Delft University of Technology, Department of Materials Sciences

Ru is a candidate material to be used as protective capping layers on mirrors for extreme ultraviolet (EUV) lithography. These mirrors are subject to contamination due to reaction of the mirror surface with hydrocarbons and oxygen under influence of the EUV radiation. In order to find a method of mitigating the effects of this contamination, it is necessary to understand the interaction process of the contaminating species and the Ru mirror surface. In this study the oxidation kinetics of a monocrystalline Ru(0001) surface was studied with ellipsometry and XPS. During the oxide growth, first a monolayer of chemisorbed oxygen was formed on the surface. After this monolayer was formed in its entirety, ruthenium dioxide could start to grow. The change from the chemisorbed oxygen layer to $RuO_2$ is related to a phase transition from a (1x1) overlayer structure to the (110) plane of $RuO_2$ and only occurs after a constant exposure of the Ru(0001) surface to oxygen. In the second stage the growth of $RuO_2$ is linear with time, indicating an adsorption limited growth mode. Finally, in the third stage, the growth levels off due to a transport limited behavior. The EUV light can accelerate the transition from the chemisorbed monolayer to $RuO_2$ but has no significant effect on the thickness and structure of the oxide after longer oxidation times.

O 27.4 Tue 11:15 H42

**Surface stress driven population of an "unusual" adsorption site** — •Zhen Tian[1], Dirk Sander[1], Holger Meyerheim[1], Larissa Niebergall[1], Nikolay Negulyaev[2], Katayoon Mohseni[1], Valeriy Stepanyuk[1], and Jürgen Kirschner[1] — [1]Max-Planck-Institute of Microstructure Physics,Halle, Germany — [2]Fachbereich Physik,Martin-Luther-Universität, Halle

Adsorption on (001) surfaces of fcc metals often leads to the population of the fourfold hollow site. This is not the case for small coverage of O on Ir(001), where adsorption on bridge sites is observed[1]. We perform combined surface X-ray diffraction (SXRD) [2], and adsorbate-induced surface stress measurement to elucidate the correlation between structure, stress and adsorption site. We find from SXRD that at 550 K up to a coverage of 0.5 O adsorbs in the unusual bridge site, whereas for $\theta_O > 0.5$, the hollow sites are populated in addition. Our calculations offer an explanation for hollow site adsorption, as O-adsorption for $\theta_O > 0.5$ in bridge sites would induce a prohibitively large lattice corrugation. Our stress measurements reveal a compressive surface stress change of $-2.2$ N/m for the population of both p(1×2) and hollow sites at a total coverage of 0.75. Our experimental results on the atomic structure and the O-induced surface stress change are supported by ab initio calculations. [1] K. Johnson, Q. Ge, S. Titmus, and D. A. King, J. Chem. Phys. 112 (2000) 10460. [2] We thank the staff at ID-03, E.S.R.F., Grenoble for expert support.

O 27.5 Tue 11:30 H42

**Dispersion effects in the dissociative adsorption of $O_2$ on Al(111)** — •Christian Carbogno[1], Jörg Behler[2], Karsten Reuter[3,4], and Axel Gross[1] — [1]Universität Ulm, Germany — [2]Ruhr-Universität Bochum, Germany — [3]Fritz-Haber-Institut, Berlin, Germany — [4]Technische Universität München, Germany

We have recently shown that the low sticking probability of thermal $O_2$ molecules at Al(111) can be reproduced from first principles if spin selection rules are explicitly accounted for [1,2]. These hinder transitions from the initial $O_2$ gas-phase triplet state to the singlet state of the adsorbed O atoms. In spite of the good agreement with the experimental sticking coefficient at normal incidence, its non-monotonic dependence on the incidence angle [3] is only partially reproduced by our calculations. A possible explanation for this discrepancy is the lack of dispersion forces in such a pure DFT approach. As a consequence, the calculated potential energy surfaces do not feature a physisorbed precursor state whose existence is assumed to lead to the observed non-monotonic dependence [3]. We inspect if and how various semi-empirical dispersion corrections (DFT-D) can compensate for this flaw in the description of this system. In addition, we discuss the implications of such corrections on the molecule-metal surface interaction.

[1] J. Behler *et al.*, Phys. Rev. Lett. **94**, 036104 (2005).

[2] C. Carbogno *et al.*, Phys. Rev. Lett. **101**, 096104 (2008).

[3] O. Weiße *et al.*, J. Chem. Phys. **118** 8010 (2003).

O 27.6 Tue 11:45 H42

**Growth and morphology of ultrathin TiOx films on Pt3Ti(111)** — •Marco Moors[1], Séverine Le Moal[2,3], Jan Markus Essen[1], Conrad Becker[2], and Klaus Wandelt[1] — [1]Institut für phys. und theoret. Chemie, Universität Bonn — [2]Centre Interdisciplinaire de Nanoscience de Marseille — [3]Technische Universität München

The morphology as well as the surface composition of ultrathin titanium oxide films grown on a Pt3Ti(111) single crystal surface have been investigated as a function of oxidation temperature (700 K to 1000 K) and oxygen exposure (up to 4500 L) using LEED, HREELS and AES. The oxidation of the alloy surface starts at sample temperatures over 500 K but ordered phases are not formed below 800 K. Depending on the used preparation conditions four different ordered oxide phases with both rectangular and hexagonal symmetry have been observed caused by the competitive influence of the hexagonal symmetry of the substrate and the favoured rectangular oxide symmetry. The found structures show a high degree of surface order. Our studies indicate the preference for a two dimensional oxide growth despite very high oxygen exposures (> 900 L). The thicker films are only metastable in a rather small temperature range between 800 and 900 K. Annealing to higher temperatures results in an immediate surface reduction. A complete oxidation to TiO2 is not possible under UHV conditions (p(O2) up to 10-5 mbar). By comparison with the parameters of known stable bulk oxide surfaces a structure proposal of the found oxide phases can be made.

O 27.7 Tue 12:00 H42

**The molecular structure of ice on Pt(111)** — •Sebastian Standop[1], Alex Redinger[1], Markus Morgenstern[2], Thomas Michely[1], and Carsten Busse[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, D-50937 Köln — [2]II. Physikalisches Institut (IIB), RWTH Aachen, D-52056 Aachen

Using Scanning Tunneling Microscopy the molecular arrangement of the wetting layer of $H_2O$ on Pt(111) is resolved. The water molecules arrange in a hexagonal pattern resembling the (0001) surface of ice $I_h$. The dense packed molecular rows are slightly rotated with respect to the dense packed rows of the underlying metal. This leads to a complex superstructure in accordance with scattering experiments [1]. Due to the tendency of single water molecules to adsorb flat on Pt(111) the structure is geometrically frustrated as each monomer donates two hydrogen bonds but can in turn accept only one. The system escapes this frustration by the introduction of a disordered arrangement of vacancy clusters.

Our results show that the degree of order in the globally disordered phase may be increased artificially. On an appropriate substrate both the $\sqrt{39} \times \sqrt{39}$ R16.1° structure for a full monolayer as well as the $\sqrt{37} \times \sqrt{37}$ R25.3° structure for submonolayer water islands could be identified. Based on the well known binding mechanism of single molecules we propose criteria for the structure formation, domain size enhancement and thermodynamic stability of these high order commensurate phases.

[1] A. Glebov *et al.*, Journal of Chemical Physics 106 (1997) 9382

O 27.8 Tue 12:15 H42

**Effects of substituted palladium on hydrogen adsorption to stepped Au(111) surfaces** — •Jonathan E. Mueller[1,2], Sudha Venkatachalam[1], and Timo Jacob[1] — [1]Ulm University, Albert-Einstein-Allee 47, D-89069 Ulm, Germany — [2]Materials and Process Simulation Center, California Institute of Technology, Pasadena, California 91125, United States of America

Configurations of different Pd-containing Au(111) bimetallic surfaces with Pd substituents varying from one to three atoms have been studied using density functional theory. The stability of the so-formed Pd monomers, dimers or trimers in the surface and subsurface layers of a Au(111) terrace and their influence on the adsorption of hydrogen have been investigated [1]. We find that before hydrogen adsorption the surface prefers to form Pd monomers over dimers or trimers located in subsurface positions, which is in agreement with experimental observations. However, adsorption of atomic hydrogen reverses this trend, leading to a stabilization of Pd trimers over dimers or monomers all located in the surface layer. Since realistic surfaces usually contain step edges, we extended our studies to the (100) and (111) steps of Au(111), finding that Pd does prefer substituting Au at bulk sites over edge sites, a behavior again modified by the presence of surface hydrogen [2].

[1] S. Venkatachalam, T. Jacob, Phys. Chem. Chem. Phys., 11, 3263-3270 (2009) [2] J. E. Mueller, S. Venkatachalam, T. Jacob, in preparation.

# O 28: Surface or interface magnetism

Time: Tuesday 10:30–13:00 Location: H48

O 28.1 Tue 10:30 H48

**Electron pair emission from ferromagnetic surfaces** — •Frank O. Schumann[1], Carsten Winkler[1], Jürgen Kirschner[1], Franz Giebels[2], Herbert Gollisch[2], and Roland Feder[2] — [1]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany — [2]Theoretische Festkörperphysik,Universität Duisburg-Essen, 47048 Duisburg, Germany

We present a combined experimental and theoretical study of the electron pair emission from a Fe(001) surface which is excited by a spin-polarized primary electron beam. The aim is to study the spin dependence of the exchange-correlation hole. The in-plane magnetization direction of the Fe sample can be controlled by an external magnetic field. A spin-polarized primary beam hits the Fe(001) surface along the surface normal and the spin polarization of the beam is either parallel or antiparallel to the magnetization direction. The emitted electron pairs are detected via a time-of-flight coincidence set-up. The data are grouped into two subsets for which the spin polarization of the majority electrons is either parallel or antiparallel to the primary beam. We find that the angular distributions of the coincidence intensity are spin dependent. Furthermore, we are able to identify favorable conditions, which ensure that the scattering partner of the primary electron has a high spin polarization. This allows us to separate the contribution of the exchange from the Coulomb correlation to the size of the exchange-correlation hole. We find that the exchange part has a larger extension than the Coulomb part confirming a suggestion by Slater more than 75 years ago.

O 28.2 Tue 10:45 H48

**Spin Polarized PES on interface states of MgO/Fe/GaAs(100)** — •Daniel Gottlob[1,2], Lukasz Plucinski[2], Carsten Westphal[1], and Claus M. Schneider[2] — [1]Experimentelle Physik 1 - Technische Universität Dortmund, Otto-Hahn-Str. 4, D-44221 Dortmund, Germany — [2]Institurte of Solid State Research - IFF-9 Electronic Properties - Research Center Jülich, D-52425 Jülich, Germany

Spintronics is an important field of current Solid State Research and Magnetic Tunnel Junctions (MTJ's) now are within our grasp. In MTJ's the nature of the electronic structure at the interface determins the tunneling process, and thereby the magnetoresistive potential of the MTJ.

Electronic interface states can have influence on the tunneling process in epitaxial MTJs especially for thinner tunnel barriers. At our ongoing research we will take a closer look at an off-normal surface state of Fe/GaAs(100) and see whether it still exists as an interface state if we cap the Fe by 1-3 monolayers of MgO. We will collect spin-polarized spectra to confirm the spin polarization in this band after the evaporation of MgO.

The measurements take place at Beamline 5 at DELTA, Dortmund, with a unique detector setup. We can acquire 2-dimensional angle resolved data for band mapping and spin-polarized one-dimensional data quasi-simultaneously. Our samples are prepared in-situ by e-beam evaporation and characterized by LEED and Auger spectroscopy.

O 28.3 Tue 11:00 H48

**Range of spin-polarization on the (111) surface of platinum induced by the proximity of cobalt stripes** — •Focko Meier, Lihui Zhou, Jens Wiebe, and Roland Wiesendanger — Institute of Applied Physics, Hamburg University, Germany

The properties of magnetic nanostructures supported by metallic substrates are strongly governed by the electronic interaction between nanostructure atoms and substrate atoms. For the model system of Co impurities dissolved in Pt it is well known that these interactions lead to induced magnetic moments in the neighbouring Pt atoms forming a so called giant moment systems [1]. Furthermore it has been revealed that Pt conduction electrons mediate an RKKY exchange interaction between localized magnetic moments which relies on a spatially oscillating spin-polarization [2]. However it is yet unclear how these two effects interfere. By applying spin-resolved scanning tunnelling spectroscopy at 0.3 K we investigated how the polarization of Pt is influenced in the vicinity of Co stripes on a Pt(111) surface. Our results show that the Pt density of states near the Fermi energy shows a response to the magnetic orientation of the Co stripe. Interestingly this response can be observed for distances larger than 1 nm from the stripe where the RKKY interaction is already antiferromagnetic.

[1] Graham and Schreiber, PRL 17, 650 (1966) [2] Meier et al., Science 320, 82 (2008)

O 28.4 Tue 11:15 H48

**The effect of postgrowth oxygen exposure on the magnetic properties of Ni on the Cu-CuO stripe phase** — •Mariella Denk, Richard Denk, Michael Hohage, Lidong Sun, and Peter Zeppenfeld — Institut für Experimentalphysik, Johannes Kepler Universität Linz, A-4040 Linz, Austria

The magnetism and morphology of thin Ni films deposited on clean and oxygen covered Cu(110) has been studied. Scanning Tunneling Microscopy (STM), as well as Reflectance Difference Spectroscopy (RDS) are used to characterise the sample properties. The sensitivity of the RDS to the polar Magneto-Optic Kerr Effect has been exploited (RD-MOKE). Contrary to growth on pristine Cu(110), thin Ni films on oxygen covered Cu(110)-(2x1)O show a spin reorientation transition from in-plane to out-of-plane magnetisation at 9 ML Ni coverage [1], [2]. For Ni films evaporated on the Cu-CuO stripe phase, which consists of a periodic array of (2x1) reconstructed CuO stripes separated by bare Cu, the magnetic easy axis lies completely in-plane up to a coverage of 22.5 ML. Exceeding this coverage, a small remanent magnetisation component pointing out-of-plane evolves. Upon postgrowth oxygen exposure the Ni film becomes completely out-of-plane magnetised. STM images show a fully (2x1)O reconstructed surface after the oxygen exposure, but no morphological changes of the Ni film. We thus conclude that the oxygen strongly modifies the surface magnetic anisotropy.

[1] Th. Herrmann et al., Phys. Rev. B 73, 134408 (2006)

[2] R. Denk et al., Phys. Rev. B 79, 073407 (2009)

O 28.5 Tue 11:30 H48

**Nanoscale Iron with Extraordinary Magnetic Anisotropy** — •Thomas Lödding[1], Christian Praetorius[1], Greg A. Ballentine[1,4], Kai Fauth[1,3], Armin Kleibert[2,5], Norman Wilken[2], Andris Voitkans[2], and Karl-Heinz Meiwes-Broer[2] — [1]Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute of Physics, Rostock University, 18051 Rostock, Germany — [3]MPI for Metals Research, Heisenbergstr. 3, 70569 Stuttgart, Germany — [4]Physics Dpt., Brandon University, 270 18th street, Brandon, Canada R7A 6A9 — [5]Swiss Light Source, Paul Scherrer Institute, 5232 Villigen, Switzerland

We shall show that iron nanocluster ensembles, prepared by deposition of preformed particles onto Cu(111), possess unusual and unexpected features in their magnetic response. We have studied the magnetic moments and response to applied fields using X-ray magnetic circular dichroism as a sensitive element specific probe of the nanocluster magetism. We show that clusters with average diameters of 4 nm and 6 nm not only possess an enhanced magnetization at low temperature but also display an enhanced magnetic anisotropy energy density.

Overmore, a small but non-negligible fraction ($\approx$ 10 %) of the deposited clusters possess extraordinarily large switching fields, i. e. $\mu_0 H_{SW} > 0.5$ T at $T = 12$ K for particles with 6 nm diameter. It is evident from our experiments that these large switching fields correspond to intrinsic properties of individual deposited nanoclusters. We shall discuss possible origins of this behavior.

O 28.6 Tue 11:45 H48

**Correlation between stress, intermixing and magnetic anisotropy of Pt/Co/Pt (111) monolayers** — •Anita Dhaka, Safia Ouazi, Zhen Tian, Dirk Sander, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 061120 Halle (Germany)

We present the results of a combined stress, low energy electron diffraction (LEED) and magneto-optical kerr-effect (MOKE) study on the spin reorientation transition (SRT) of Co monolayers (ML) on Pt(111). We observe a SRT from out-of-plane to in-plane with increasing Co thickness at 3 ML at 300 K. The deposition of one layer Pt on top of 5 ML Co induces a SRT from in-plane to out-of plane. Our stress and LEED measurements identify intermixing at the Co/Pt(111) interface [1].Stress measurements reveal a stronger intermixing at 370

K, as compared to growth at 300 K. Co growth at 370 K leads to a shift of the SRT from out-of-plane to in-plane to a larger thickness of 5 ML. Our results suggest that an intermixed Pt-Co interface favors an out-of-plane easy magnetisation direction, whereas a Co-vacuum interface favors an in-plane easy magnetization direction.

[1] O. Robach, C. Quiros, P. Steadman, K. F. Peters, E. Lundgren, J.Alvarez, H.Isern, and S. Ferrer: Phys. Rev. B **65**, 054423 (2002)

O 28.7 Tue 12:00 H48

**Switching a single spin on metal surfaces: ab initio studies** — •Kun Tao[1], Valeri.S Stepanyuk[1], Wolfram Hergert[2], Ivan Rungger[3], Stefano Sanvito[3], and Patrick Bruno[4] — [1]Max-Planck-Institute of Microstructure Physics, Halle, Germany — [2]Fachbereich Physik, Martin-Luther-University, Halle-Wittenberg, Friedemann-Bach-Platz 6, D-06099 Halle, Germany — [3]School of Physics and CRANN, Trinity College, Dublin 2, Ireland — [4]European Synchrotron Radiation Facility, F-38043 Grenoble Cedex, France

We perform ab initio calculations of the the exchange coupling between single magnetic adatoms adsorbed on metal surfaces and a spin polarized STM tip. We apply density functional theory (DFT) based methods and perform calculations in the fully relaxed geometries for the tip and the substrate. We demonstrate that the spin direction of single adatoms can be controlled by varying the tip-substrate distance. The sign of the exchange energy is determined by the competition of the direct and the indirect interactions between the tip and the adatom[1]. Based the nonequilibrium Green function method, we perform the spin-dependent transport calculations and find a large magnetoresistance of the junction at short tip-substrate distances.

[1] Kun Tao, V.S. Stepanyuk, W. Herget, I. Rungger, S. Sanvito, P. Bruno, Phys. Rev. Lett 103, 057202 (2009)

O 28.8 Tue 12:15 H48

**Size-dependent spin structures in individual Fe nanoparticles observed by XPEEM** — Arantxa Fraile Rodriguez[1], Armin Kleibert[1], •Joachim Bansmann[2], Laura Heyderman[1], and Frithjof Nolting[1] — [1]Paul Scherrer Institut, Villigen PSI, CH-5232 Switzerland — [2]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

By combining x-ray magnetic circular dichroism (XMCD) with photoemission electron microscopy (PEEM), we present in situ observations of the magnetization orientation of individual Fe nanoparticles in a size range from 5 to 25 nm being in contact with a ferromagnetic Co support. Our results reveal that the magnetic moments of smaller particles (below 8 nm) are aligned parallel to the magnetic domains of the substrate while a non-collinear alignment between particles and substrate is observed for larger sizes. Numerical model calculations reproduce the experimental trend and reveal a transition from an exchange- to an anisotropy-dominated regime: the smaller particles are in a single-domain state collinearly aligned to the substrate while the larger particles exhibit a spiral-like magnetic structure determined by the magnetic anisotropy energy. These results demonstrate that the balance between the local particle-substrate interaction and the individual properties of the particles can lead to unexpected spin arrangements.

O 28.9 Tue 12:30 H48

**Intercalation of iron underneath graphene on Ni(111): PES and XMCD study** — •Martin Weser, Karsten Horn, and Yuriy Dedkov — Fritz-Haber Institut der Max-Planck Gesellschaft, Berlin, Germany

Magnetic thin films with out-of-plane or perpendicular magnetic anisotropy play an important role in nanotechnology. Such systems can be used as perpendicular recording media, which is predicted to allow information storage densities of up to 1 Tbit/in.$^2$ a quadrupling of today's highest areal densities. Along with the widely used materials with out-of-plane magnetic anisotropy such as CoPt or FePt alloys, $fcc$ Fe thin films also showing perpendicular magnetic anisotropy have recently attracted considerable interest as possible candidates for applications in novel magnetic data storage devices. Here Fe which originally has *bcc* structure can be stabilized in $fcc$ $\gamma$-phase at room temperature in thin epitaxial films grown on suitable $fcc$ substrates. The aim of the present work is the preparation of a $fcc$ Fe-based system with potential out-of-plane magnetic anisotropy which behaves inert against an aggressive environment. Here we demonstrate the possibility to prepare such a system via intercalation of a thin Fe film underneath a graphene layer formed on a Ni(111) substrate. Here, we demonstrate that graphene behaves like a passivation layer conserving the underlying epitaxial Fe film. Electronic and magnetic properties of this system were studied by means of angle-resolved PES and XMCD, respectively.

O 28.10 Tue 12:45 H48

**Hard x-ray standing-wave excited photoemission experiments on the MgO/Fe interface** — •Sven Döring[1], Frank Schönbohm[1], Ulf Berges[1], Charles S. Fadley[2,3], Daniel E. Bürgler[4], Mihaela Gorgoi[5], Walter Braun[5], Claus M. Schneider[4], and Carsten Westphal[1] — [1]DELTA/Experimentelle Physik I, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany — [2]Materials and Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA — [3]University of California, Davis, CA 95616, USA — [4]Institut für Festkörperforschung, IFF-9, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [5]Helmholtz-Zentrum Berlin - BESSY, Albert-Einstein-Str. 15, 12489 Berlin, Germany

For layer systems, photoemission experiments with high and reliable depth resolution are essential in order to distinguish between interface effects and bulk photoemission signals. Here we extend the soft x-ray standing-wave photoemission method into the hard x-ray regime to achieve the required high depth resolution and high probing depth. An Fe wedge was grown on top of a $MoSi_2$/Si multilayer with a period of about 40 Å and subsequently covered by a thin MgO film. By moving the wedge structure with respect to the x-ray beam we were able to observe several cycles of the x-ray standing wave field moving through the sample layers. The analysis of the photoemission intensity modulations results in a well-resolved depth-profile of the sample. At the interface the intermixing of Fe and MgO can be studied due to the enhanced interface sensitivity provided by the x-ray standing field.

## O 29: [CPP] Organic Electronics and Photovoltaics I (Joint Session DS/CPP/HL/O)

Time: Tuesday 9:30–12:45 Location: H37

O 29.1 Tue 9:30 H37

**Side chain variations on dicyanovinyl-oligothiophenes studied by photoinduced absorption spectroscopy: consequences for small molecule organic solar cells** — •Hannah Ziehlke[1], Roland Fitzner[2], Christian Koerner[1], Egon Reinold[2], Peter Baeuerle[2], Karl Leo[1], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden — [2]Institut für Organische Chemie II und Neue Materialien, Universität Ulm

Oligothiophenes capped with electron-withdrawing dicyanovinyl groups (DCVnT) are promising candidates for applications in small molecule organic solar cells. These oligothiophene derivatives can act as electron donor in blend layers with $C_{60}$. Single heterojunction devices reach efficiencies above 4 %. The introduction of side chains as intermolecular spacer has little effect on the energetics and mainly influences the morphology of the evaporated thin film. In addition, the distance between donor and acceptor molecules and thus the energy transfer and charge separation at the interface can be controlled. The energetic and dynamic properties of the long lived photoexcitations in pristine and blend layers can be obtained by photoinduced absorption spectroscopy (PIA). We here characterize of DCV3T with zero, two, and four alkyl chains (Methyl and Butyl) via PIA spectroscopy complemented with morphological studies. Our results indicate that the energy transfer process at the heterojunction is more efficient for smaller spatial distances between donor and acceptor molecules.

O 29.2 Tue 9:45 H37

**New multiwall molecular organic nanotubes** — •Maren Rastedt[1], Frauke Kutscher[1], Okko Frey[2], Rüdiger Beckhaus[2], Christian Maibohm[3], and Katharina Al-Shamery[1] — [1]University of Oldenburg, Physical Chemistry 1, Germany — [2]University of Oldenburg, Inorganic Chemistry, Germany —

[3]NanoSYD, Sonderborg, Denmark

Nanotubes can be described as the newest star in the evening sky of nanotechnology. Since the discovery of carbon nanotubes , this nanostructure has grasped the mind of many. This structure has many application possibilities ranging from liquid and gas storage to microelectronics and sub wavelength optical components and fibers. In our presentation we will give an introduction to multiwall nanotubes made from Tetrabenzofluorene(Tbf)-derivates. These Tbf-nanotubes have attracted interest because of their many properties, e.g. crystallization and waveguiding. Our nanotubes are prepared by the elegant and simple process of template assisted assembly. The assembly process will be presented together with specific properties of different Tbf-nanotubes. By changing growth parameters in the assembly process we have a method for probing fundamental questions and properties of our nanotubes. One future application of our nanotubes could be as an active element in a photovoltaic device.

O 29.3 Tue 10:00 H37

**Radical Molecular Wires** — •Georg Heimel[1], Egbert Zojer[2], Lorenz Romaner[3], Jean-Luc Brédas[4], and Francesco Stellacci[5] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Germany — [2]Institut of Solid State Physics, Graz University of Technology, Austria — [3]Chair of Atomistic Modeling and Design of Materials, University of Leoben, Austria — [4]School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, USA — [5]Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, USA

The technological relevance and the functionality of semiconducting materials originate in the fact that their conductivity and the band alignment at the interfaces with other materials can be controlled through doping. Here, we consider the ultimate miniaturization of functional devices by computationally investigating the doping of molecular wires suspended between two metal electrodes.[1] For representative systems we find that, upon doping, the molecular conductivity is enhanced by more than two orders of magnitude. We elucidate the microscopic origin of this dramatic effect and present an intuitive picture, which rationalizes our observations in terms of *Fermi-level pinning.* Our results shed new light on recent experimental findings and, most importantly, in-depth understanding of the doping mechanism enables the targeted development of new functional components for sensing and switching at the single-molecule scale.

[1] G. Heimel et al., *Nano Lett.* **9**, 2559 (2009).

O 29.4 Tue 10:15 H37

**Structure property relationship in aza-bodipy absorber materials for organic photovoltaics** — •Roland Gresser, Toni Mueller, Moritz Philipp Hein, Karl Leo, and Moritz Riede — Institute of Applied Photophysics, Dresden University of Technology, Germany

In this joint experimental and theoretical study, we focus on the structure property relationship of aza-bodipy dyes as active donor materials in vacuum deposited small molecule solar cells.

The position of the materials HOMO can be intentionally varied by the choice of the functional group attached to the molecule. The absorption spectra show a red shift of the maximum with increasing donor strength of the substituents due to the increasing HOMO energy and decreasing band gap.

Based on crystal structure data, the charge carrier mobility determining parameters like reorganization energies and transfer integrals are calculated. The results show an increasing molecular orbital overlap and significant higher transfer integrals upon planarization and rigidification of the molecule. With this information, the observed charge carrier mobility differences from experiment can be explained.

In addition to the electronic properties a high thermal and photo stability is essential. From combined thermogravimetric analysis and mass spectroscopy we could determine the degradation process of the material and were able to increase the thermal stability by substitution of the involved species.

O 29.5 Tue 10:30 H37

**Dicyanovinyl sexithiophenes: self-organization and photovoltaic properties** — •Marieta Levichkova[1], David Wynands[1], Alexandr Levin[1], Karl Leo[1], Karsten Walzer[2], Dirk Hildebrandt[2], Peter Bäuerle[3], Rosina Rentenberger[4], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, TU Dresden, Germany — [2]Heliatek GmbH, Dresden, Germany — [3]Institut für Organische Chemie II und Neue Materialien, Universität Ulm, Germany — [4]Institut für Physik, TU Ilmenau, Germany

Recently, vacuum deposited films consisting of conjugated dicyanovinyl-capped (DCV) oligothiophenes have shown significant potential as photoactive layers in small molecule solar cells [1]. Here, we study the structural and optical properties of films of two DCV-derivatives both comprising six thiophene rings (DCV6Ts) but having different side groups. For both derivatives, neat DCV6T and mixed DCV6T:C60 films are compared using UV-VIS absorption and photoluminescence spectroscopy, X-ray diffraction (XRD), and Atomic Force Microscopy. It is shown that the modification of the molecular structure results in a structured and red shifted absorption band, which indicates better molecular arrangement in the solid state. The improved self-organization at room temperature deposition is confirmed by XRD. Furthermore, the nanomorphology of the mixed DCV6T:C60 films is optimized using substrate heating. Bulk heterojunction solar cells with power conversion efficiencies exceeding 4% are presented.

[1] K. Schulze et al., Adv. Mater. 2006, 18, 2872-2875

**15 min. break**

O 29.6 Tue 11:00 H37

**Hexaazatriphenylene and hexaazatrinaphthylene derivatives as electron transport materials in organic solar cells** — •Christiane Falkenberg[1], Martin Baumgarten[2], Ralph Rieger[2], Selina Olthof[1], Karl Leo[1], Moritz Riede[1], and Klaus Müllen[2] — [1]Institut für Angewandte Photophysik, TU Dresden, 01069 Dresden — [2]MPI für Polymerforschung, 55128 Mainz

There is increasing interest in molecularly doped organic materials for the fabrication of efficient organic electronic devices. In small molecule organic solar cells, the so-called p-i-n concept is advantageous for the independent optimization of electrical and optical properties. Here, the absorbing donor-acceptor heterojunction is sandwiched between a p-doped hole transport layer and an n-doped electron transport layer. The design of suitable functional molecules for the transport layers is currently an important issue, however, the choice of available wide-gap materials for the n-side of organic solar cells is very limited. Here, we investigate hexaazatriphenylene and hexaazatrinaphthylene derivatives as substitutes for the common electron transport materials $C_{60}$ or BPhen and BCP. Having bandgaps of $> 2.7$eV the new materials are transparent which, in combination with a suitable position of the energy levels, enables exciton blocking. Furthermore molecular doping with either acridine orange base (AOB) or NDN1 (Novaled AG) leads to an increase of the conductivity by several orders of magnitude, reaching values beyond $1{\cdot}10^{-6}$ S/cm. Altogether the beneficial optical and electrical properties allow the fabrication of organic solar cells with increased efficiency compared to the standard devices.

O 29.7 Tue 11:15 H37

**Structure - property relationship of thiophene based materials bearing different accepting groups** — •Marion Wrackmeyer, Markus Hummert, Horst Hartmann, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, Technische Universität Dresden, Germany

Organic solar cells require new materials for improved efficiencies. The relationship of molecular structure and properties is very important to optimise the devices. An interesting class of materials are thiophene block co-oligomers. The materials obtain electron donating (D) and accepting (A) groups and have the general structure A-D-A or D-A-D. In particular, the investigation of electron accepting groups is very important, because they have a high influence on the electronic structure of an organic molecule and are therefore an influential impact in the performance of a small molecule p-i-n solar cell. We present investigations on thiophene based materials bearing different accepting groups. The accepting groups are eg dicyanovinyl, dioxaborine, and benzthiadiazole. The materials were synthesised by Stille-coupling. Basic precondition for all materials is the thermal stability for deposition by vacuum-techniques. Subsequent investigations focus on absorption (solution and thin films), electrochemical behaviour (cyclic voltammetry to investigate the frontier molecular orbital energy levels), DFT-calculations (to show the location of HOMO and LUMO), mobility, morphology, dopability, and the properties of a solar cell.

O 29.8 Tue 11:30 H37

**Charge transport in self-assembled semiconducting organic layers: role of dynamic and static disorder** — •Thorsten

Vehoff[1], Yeon Sook Chung[2], Karen Johnston[1], Alessandro Troisi[3], Do Yeung Yoon[2], and Denis Andrienko[1] — [1]Max Planck Institut fuer Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany — [2]Department of Chemistry, Seoul National University, Seoul 151-747, Republic of Korea — [3]Department of Chemistry and Centre of Scientific Computing, University of Warwick, Coventry, CV4 7AL, United Kingdom

Partial disorder is an inherent property of self-assembled organic semiconductors that complicates their rational design, since electronic structure, self-assembling properties and stability all have to be accounted for simultaneously. Therefore, the understanding of charge transport mechanisms in these systems is still in its infancy. A theoretical study of charge transport in organic semiconductors was performed on self-assembled layers of [1]Benzothieno[3,2-b]benzothiophene functionalized with alkyl side chains. Analysis showed that semiclassical dynamics misses static (on timescales of charge transport) disorder while the solution of the master equation combined with the high-temperature limit Marcus theory for charge transfer rates does not take into account molecular dynamic modes relaxing on a timescale of charge hopping. A comparison between predictions based on a perfectly ordered and a realistic crystal structure reveals the strong influence of static and dynamic disorder. The advantage of two-dimensional charge transporting materials over one-dimensional ones is clearly shown.

O 29.9 Tue 11:45 H37

**Charge Transport in rr-P3HT:PCBM Blends - The Impact of Ultrahigh Regioregularity on Hole Transport and Device Performance** — •Ralf Mauer and Frédéric Laquai — Max-Planck-Institut für Polymerforschung, Mainz, Deutschland

Blends of poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl $C_{61}$ butyric acid methyl ester (PCBM) have emerged as a prototypical material system for bulk heterojunction solar cells with reasonable efficiencies during the past five years. Despite tremendous engineering efforts to push devices to 5% power conversion efficiency (PCE), the correlation between charge carrier mobility and device performance is still up for debate. Theoretical models range from "the higher - the better" over optimum finite mobilities to no effect of mobility on PCE at all.

We investigate charge transport in pristine P3HT films and in blends with PCBM by the time of flight (TOF) technique and analyse the results in the framework of the Gaussian disorder model. In order to understand the effect of charge transport on solar cell efficiency, we examine P3HT with three different regioregularities, i.e. regiorandom P3HT, rr-P3HT with high (rr=94%) and with ultrahigh (rr>98%) regioregularity. While the regioregularity is known to have a strong influence on the charge carrier mobility, its effect on other transport parameters, especially on the energetic disorder of hole transport in P3HT, is reported by us for the first time.

Finally, we correlate the TOF results and spectroscopic measurements with device performance to determine the influence of charge transport on the power conversion efficiency.

O 29.10 Tue 12:00 H37

**Charge transport in conjugated polymers with energetic disorder** — •James C Blakesley[1,2], Helen S Clubb[1], Christopher Groves[1], Louise M Hopkins[1], and Neil C Greenham[1] — [1]University of Cambridge, Cambridge, UK — [2]Universität Potsdam, Potsdam, Germany

We investigate charge transport in sandwich-type devices with two polyfluorene-based copolymers: poly(9,9-dioctylfluorene-co-bis(N,N'-(4,butylphenyl))bis(N,N'-phenyl-1,4-phenylene)diamine) (PFB) and poly(9,9-dioctylfluorene-co-benzothiadiazole) (F8BT). A standard analysis of the data produces a poor fit to the data, with an apparent dependence of mobility on device thickness. Previously, such behaviour in electron transport has been attributed to trapping[1]. However, we find that a good fit is obtained by using a numerical simulation based on energetic disorder that takes into account the effects of electric field and carrier density on mobility (Extended Gaussian Disorder model). The amount of energetic disorder is quantified by 110+/-10meV and 100+/-10meV respectively. When the two materials are blended together, hole mobility remains constant when the fraction of PFB is 50% or greater, but drops dramatically for low concentrations of PFB. The amount of energetic disorder remains unaffected by any degree of blending, suggesting that there is no change in microscopic ordering of the polymers upon blending.

[1] R. Steyrleuthner, S. Bange and D. Neher, J. Appl. Phys. 105, 064509 (2009)

O 29.11 Tue 12:15 H37

**Towards high charge carrier mobilities by rational design of organic semiconductors** — •Denis Andrienko[1], Valentina Marcon[2], James Kirkpatrick[3], Victor Ruehle[1], Bjoern Baumeier[1], Thorsten Vehoff[1], Alexander Lukyanov[1], Kurt Kremer[1], Jenny Nelson[3], and Christian Lennartz[4] — [1]Max Planck Institute for Polymer Research, Mainz — [2]Technische Universität Darmstadt, Germany — [3]Imperial College London, UK — [4]BASF AG, Ludwigshafen

The role of material morphology on charge carrier mobility in partially disordered organic semiconductors is discussed for several classes of materials: derivatives of hexabenzocoronenens [1], perylenediimides [2], triangularly-shaped polyaromatic hydrocarbons [3], and Alq3. Simulations are performed using a package developed by Imperial College, London and Max Planck Institute for Polymer Research, Mainz (votca.org). This package combines several techniques into one scheme: quantum chemical methods for the calculation of molecular electronic structures and reorganization energies; molecular dynamics and systematic coarse-graining approaches for simulation of self-assembly and relative positions and orientations of molecules on large scales; kinetic Monte Carlo and master equation for studies of charge transport.

[1] J. Kirkpatrick, et al, Phys. Rev. Lett., 98, 227402, 2007; [2] V. Marcon, et al, J. Am. Chem. Soc., 131, 11426, 2009; [3] X. Feng et al, Nature Materials 8, 421, 2009

O 29.12 Tue 12:30 H37

**Fully functionalized block copolymers for organic electronic applications** — •Sven Hüttner[1,2], Michael Sommer[2], Justin Hodgkiss[1], Peter Kohn[3], Thomas Thurn-Albrecht[3], Richard Friend[1], Ullrich Steiner[1], and Mukundan Thelakkat[2] — [1]Cavendish Laboratory, University of Cambridge — [2]Angewandte Funktionspolymere, Makromolekulare Chemie I, Universität Bayreuth — [3]Experimentelle Polymerphysik, Universität Halle-Wittenberg

Block copolymers are well known to phase separate in highly ordered nanostructures on length scales commensurate with the exciton diffusion length. We use fully functionalized block copolymers for photovoltaic devices, where a donor and an acceptor polymer are covalently linked. The acceptor block consists of a polyacrylate backbone with pendant perylene bisimide moieties and the donor block consists of poly(3-hexylthiophene) (P3HT). We combine temperature dependent small angle and wide-angle X-ray scattering measurements to investigate the block copolymer phase separation as well as the influence of the crystallisation kinetics of the two blocks. Intermolecular and intramolecular interactions drive the self-assembly of structures from molecular lengthscales to larger mesostructures of some nanometers to microphase separation of some tens of nanometers. The investigation of the morphology is accompanied by steady state spectroscopy and transient absorption spectroscopy. Furthermore organic thin film transistors are used to characterize the transport properties in these novel materials which are found to exhibit unique properties such as the tunability between n-type, p-type or ambipolar transport.

## O 30: [HL] Organic Semiconductors: Transistors and OLEDs (Joint Session DS/CPP/HL/O)

Time: Tuesday 9:30–12:45 Location: H15

O 30.1 Tue 9:30 H15

**Ionic liquid gated polymer transistor** — •Johannes Schöck, Daniel Secker, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Staudtstr. 7/A3, D-91058 Erlangen, Germany

We fabricate field-effect transistors with a polymer semiconductor using an ionic liquid top-gate, replacing the gate insulator. The geometry is bottom contact, liquid top gate. Electrical characterization yields a low conductance threshold of the device ($\sim -2.5\,\mathrm{V}$), and a steep increase of the source-drain current. An analysis points towards unusually high charge carrier mobility of the semi-conducting channel, with very favorable leakage currents through the gate. Strong hysteretic effects are observed.

O 30.2 Tue 9:45 H15

**Electrolyte-gated organic thin film transistors** — •Felix Buth[1], Marin Steenackers[2], Deepu Kumar[1], Martin Stutzmann[1], and Jose Antonio Garrido[1] — [1]Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching, Germany — [2]Institute for Advanced Study, Technische Universität München, Arcisstr. 21, 80333 München, Germany

Organic semiconductors are today widely used as the active material in several applications based on thin film transistors. For most of these devices large operational voltages are required. One approach to reduce the gate voltage is increasing the capacitance of the gate dielectric. Several materials, including high-k dielectrics, ultra-thin cross-linked polymers or polyelectrolytes have been tested for this purpose. Among those, polyelectrolytes offer extraordinarily high capacitances with a relatively low technology cost. The high capacitance results from the electrical double layer formed at the polyelectrolyte/semiconductor interface, opening the possibility of using organic thin film transistors for biological and chemical sensors, in which in-electrolyte operation is required. Since, however, water stable organic semiconductors are generally deposited by evaporation in UHV, the surface of the polyelectrolyte needs to be smooth to enable the growth of high quality films. In this contribution the properties of different polyelectrolyte dielectrics are investigated. We show how polyelectrolytes can be directly prepared on conductive substrates, resulting in homogeneous films with high interfacial capacitances. Furthermore, we show the preparation of high quality pentacene thin films onto the polyelectrolyte films.

O 30.3 Tue 10:00 H15

**Molecular weight dependent short channel effect in MDMO-PPV** — •Ali Veysel Tunc, Elizabeth von Hauff, and Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, Carl-von-Ossietzky Str. 9-11, 26129 Oldenburg, Germany

In this study, organic field effect transistors (OFETs) based on poly [2-methoxy,5-(3',7'-dimethyl-octyloxy)]-p-phenylene vinylene (MDMO-PPV) with two different weight-average molecular weights (Mw) were fabricated and the effect of the molecular weight on the device properties was investigated. It was observed that the operation performance of the OFET depends on the molecular weight and channel length. The short channel effect was observed, i.e. a lack of saturation in the output characteristic with a fixed gate voltage. We found that the saturation behavior and hole mobility of a given material strongly depend on molecular weight. Short channel effects were observed in higher molecular weight for MDMO-PPV. The hole mobility around 10 times better for higher molecular weight that has been shown in literature.

O 30.4 Tue 10:15 H15

**Electron Mobility in Methanofullerens** — •Maria S Hammer[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 W\"urzburg — [2]ZAE Bayern, Div. Functional Materials for Energy Technology, Am Hubland, D-97074 Würzburg

Methanofullerenes are the state of the art acceptor-type semiconductors applied in flexible and printed electronic devices, e.g. they are used together with a donor-type polymer in (i) solar cells or (ii) complementary circuits. While the hole transport in polymers has been intensely investigated within the last years, less attention has been drawn to the fundamentals of the transport within methanofullerenes. In the present study, the electron mobility, which strongly depends on the electron density, is investigated.

We utilize the organic field effect transistor (OFET) as it provides a way of probing the mobility within a wide range of electron densities via gate voltage. Nevertheless, the performance of an OFET sensitively depends on electron injection from the contacts and trapping at the dielectric interface. Therefore, in order to assess the transport parameters of methanofullerenes, it is indispensable to vary the work function of the electrodes as well as the insulator. We will investigate and discuss the ambipolar charge transport in dependence of the charge carrier density in [6,6]-phenyl-C61-butyric acid methyl ester and other derivatives, employing a variation of dielectric surfaces and injecting metals.

O 30.5 Tue 10:30 H15

**Correlation between the effective contact resistance and the charge carrier transport in organic semiconductors of different mobility** — R. Winter[1], F. Wörner[1], M.S. Hammer[1], C. Deibel[1], and •J. Pflaum[1,2] — [1]Experimental Physics VI, Julius-Maximilians-University, 97074 Würzburg — [2]Bavarian Center For Applied Energy Research, 97074 Würzburg

In this presentation we address questions on the impact of the charge carrier mobility on the injection behavior in organic thin film transistors (OTFTs). Though many theoretical models treat the contact resistance, R, and the mobility, $\mu$, independently, we demonstrate a significant correlation between these two quantities for P3HT and pentacene. Corresponding TFT measurements have been performed between 40 - 300K. To modify the effective contact resistance, monolayers of different oligoacenes were deposited between the Au bottom contacts and the active organic transport layer. Despite significant differences in the room temperature mobilities, $10^{-4}$cm$^2$/Vs for P3HT and $10^{-2}$cm$^2$/Vs for pentacene, the temperature dependent variations of the mobility as well as of the effective contact resistance prove to be similar. For both materials a change in the slope of the R(T) and $\mu$(T)-slope can be detected. However, the cross-over temperature for pentacene amounts to 80K whereas that for P3HT is shifted to 185K. We will discuss this observation in the context of a balanced transport, i.e. that the injection at the metal contact interfaces is strongly related to the charge carrier transport in the semiconducting layer.
Financial support by BMBF (project GREKOS) is acknowledged.

O 30.6 Tue 10:45 H15

**Thickness dependence of contact and sheet resistance of thiophene and pentacene based organic field effect transistors** — •Torsten Balster, Steve Pittner, Dagmawi Belaineh, Arne Hoppe, and Veit Wagner — School of Engineering and Science, Campus Ring 1, Jacobs University Bremen, 28759 Bremen, Germany

The electrical properties of evaporated organic semiconductors in dependence on the film thickness are affected by the growth mode of the thin film. While dihexyl-substituted oligothiophenes (DHnT) show a typical layer-by-layer growth mode on hexamethyldisilazane(HMDS)-treated silicon oxide, pentacene exhibits 3-dimensional growth. The growth mode as determined by AFM investigations is also reflected in the integral in-situ IV-measurements during growth. DHnT shows oscillatory behaviour in the mobility and the contact resistance within the first two monolayers, whereas the pentacene saturates without oscillations for 10nm. The total contact resistance with gold electrodes has been evaluated by the transfer line method. Furthermore the potential barriers at source and drain contact are determined separately by a four probe setup. For this purpose, additional sense fingers are prepared within the channel allowing the direct access to the channel potential. Major contact effects are identified for channel length smaller than 10 microns.

O 30.7 Tue 11:00 H15

**Semiconducting Thin Films of Fluorinated and Unsubstituted Phthalocyanines for Applications in Organic Field Effect Transistors** — •Harry Brinkmann[1], Christopher Keil[1], Olga Tsaryova[2], Dieter Wöhrle[2], and Derck Schlettwein[1] — [1]Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de — [2]Institute of Organic and Macromolecular Chemistry, University of Bremen, Germany.

Perfluorinated phthalocyanines ($F_{16}Pc$) show n-type characteristics as active layers in organic field transistors while organic field transistors with unsubstituted phthalocyanines ($Pc$) exhibit p-type characteristics. The growth of $F_{16}Pc$ and $Pc$ films has been studied in OFETs on organic (polyimide, $PMMA$) and inorganic insulating layers ($SiO_2$) with different surface modifications ($HMDS$ treatments). We report here about the dependence of the growth mode of the films and the field effect mobility on the used substrate for the copper complexes. The development of the electrical conduction was studied in-situ during film growth and the field effect mobility was determined for various film thicknesses in different regimes of the Stranski-Krastanov growth mechanism that led to the formation of ultrathin conductive layers in the monolayer range followed by reorganization towards island growth. Optical absorbance was measured in reflection or transmission in dependence of the used substrate to investigate details of the intermolecular coupling.

**15 Min. Coffee Break**

O 30.8 Tue 11:30 H15

**Carrier density in a Gaussian density of states: Approximation for the Gauss- Fermi integral** — •Gernot Paasch[1] and Susanne Scheinert[2] — [1]IFW Dresden — [2]TU Ilmenau

The density of hopping transport states in organics can be approximated by a Gaussian DOS. As a consequence, the mobility becomes a function of carrier density, field and of course temperature. Such dependencies can now be implemented easily in advanced device simulation programs as Sentaurus Device. However, the carrier density as function of the Fermi energy is not taken into account until now. For inorganic semiconductors with a square root DOS the situation was similar with the carrier density expressed by the Fermi- Dirac integral F1/2. Further Fermi-Dirac integrals are needed for the electronic energy density and for Einstein's relation. For these cases analytical approximations have been developed early allowing for fast simulation. For the Gaussian DOS the carrier density is given by the integral over the product of Gaussian DOS and Fermi-Dirac distribution, the Gauss-Fermi integral. Related integrals describe the electronic energy density and occur in Einstein's relation. Here we present an extremely simple and accurate approximation for the Gauss-Fermi integral and discuss its potential applicability in simulation of organic devices.

O 30.9 Tue 11:45 H15

**Comparative transport studies in Bridgman and sublimation grown 9,10-Diphenylanthracene single crystals.** — •Andreas Steindamm[1], Ashutosh K. Tripathi[2], Rainer Stöhr[3], Jörg Wrachtrup[3], and Jens Pflaum[1] — [1]Institute of Experimental Physics VI, Julius-Maximilians-University, 97074 Würzburg, Germany — [2]Holst Centre/TNO, 5656 AE Eindhoven, NL — [3]Physikalisches Institut, University of Stuttgart, 70550 Stuttgart, Germany

To improve organic electronic applications, knowledge about microscopic mechanisms determining the charge carrier mobilities is pivotal. 9,10-Diphenylanthracene (DPA) has been identified as model system to study those correlations due to its high electron and hole mobilities at room temperature [1] and its complex structural phase behaviour. We will demonstrate our temperature dependent Time-Of-Flight data on single crystals grown by vapor phase transport (VPT) and by Bridgman growth technique. Both preparation techniques revealed crystals of different morphologies resulting in significant variations of the related bipolar mobilities. As a key result, the charge carrier mobility of $\sim 1cm^2/Vs$ at room temperature along the (111)-direction of Bridgman crystals exceeds that along the (001)-direction of VPT grown crystals by about one order of magnitude. The observed differences in the mobility data will be discussed in the context of the microscopic molecular arrangement within the respective crystal structure. Financial support by BMBF (project GREKOS) is acknowledged.

[1] Tripathi A. K. et al., Adv. Mater. 19 (2007) 2097

O 30.10 Tue 12:00 H15

**Probing charge carrier dynamics in conducting polymers using single molecules as sensors** — •Maximilian Nothaft[1], Steffen Höhla[2], Aurélien Nicolet[3], Jens Pflaum[4], Fedor Jelezko[1], and Jörg Wrachtrup[1] — [1]3. Phys. Ins., Univ. Stuttgart — [2]Chair of Display Technology, Univ. Stuttgart — [3]MoNOS, Huygens Laboratory Leiden — [4]Exp. Phys. VI, Univ. Wuerzburg and ZAE Bayern

Doping of conducting polymers by guest molecules is widely applied in organic light emitting devices to improve their efficiency. By reducing the concentration of suited guest molecules it becomes possible to study the dynamics of single molecule emitters using confocal microscopy.

In our contribution we discuss the optical properties of single Dibenzoterrylene dye molecules dispersed in an OLED consisting of PPV as host material. It will be shown how to prepare devices of photostable single molecules in PPV emitting a constant flux of single photons at room temperature by excitation from a Ti:sapphire laser.

By simultaneous laser excitation and electrical operation it is possible to detect the effect of injected charge carriers on the dynamics of single quantum emitters. Since the ratio of singlet to triplet exciton formation in the device is 1:3, this leads to an effective pumping to the triplet state of the single molecule thereby reducing its fluorescence intensity. Modeling this process it becomes possible to associate the reduced fluorescence intensity with the local current density at the position of the molecule. This correlation enables us to optically probe the current density in an OLED with nm spatial resolution.

O 30.11 Tue 12:15 H15

**Energy band alignment at the oxide-organic interface ITO/ZnPC determined by photoelectron spectroscopy** — •Jürgen Gassmann and Andreas Klein — Surface Science Department, Istitute of Materials Science, TU Darmstadt, Germany

The possibility to generate light on the front- and backside of an organic light-emitting diode (OLED) is given for inverted top-emitting OLEDs. For them the transparency of the back contact is crucial. Here transparent conductive oxides (TCO) like indium tin oxide (ITO) or zinc oxide are of special interest, because these films can be deposited with magnetron sputtering at room temperature. In this work the energy band alignment between the organic material zinc phthanalocyanine (ZnPC) and the transparent oxide ITO is evaluated. For this the X-ray photoelectron spectroscopy technique (XPS) is used and combined with an in-situ preparation of the films. The energy band alignments of the deposition sequences ITO on ZnPC and vice versa are compared. Here valence band offsets up to 1.3eV can be detected. The energy band alignment shows a strong dependence on the deposition sequence. Additionally the electrical and optical properties of ITO films sputtered at room temperature are investigated.

O 30.12 Tue 12:30 H15

**Highly efficient white top-emitting organic light-emitting diodes with forward directed light emission** — •Patricia Freitag, Sebastian Reineke, Mauro Furno, Björn Lüssem, and Karl Leo — Institut für Angewandte Photophysik, TU Dresden, George-Bähr-Straße 1, 01069 Dresden, Germany

The demand for highly efficient and energy saving illumination has increased considerably during the last decades. Organic light emitting diodes (OLEDs) are promising candidates for future lighting technologies. They offer high efficiency along with excellent color quality, allowing substantially lower power consumption than traditional illuminants. Recently, especially top-emitting devices have attracted high interest due to their compatibility with opaque substrates like metal sheets. In this contribution, we demonstrate top-emitting OLEDs with white emission spectra employing a multilayer hybrid cavity structure with two highly efficient phosphorescent emitter materials for orange-red (Ir(MDQ)2(acac)) and green (Ir(ppy)3) emission as well as the stable fluorescent blue emitter TBPe. To improve the OLED performance and modify the color quality, two different electron blocking layers and anode material combinations are tested. Compared to Lambertian emission, our devices show considerably enhanced forward emission, which is preferred for most lighting applications. Besides broadband emission and angle independent emission maxima, power efficiencies of 13.3 lm/W at 3 V and external quantum efficiencies of 5.3% are achieved. The emission shows excellent CIE coordinates of (0.420, 0.407) at approx. 1000 cd/m2 and color rendering indices up to 77.

## O 31: Invited talk (Dähne, Mario)

Time: Tuesday 14:00–14:45 Location: H36

**Invited Talk** O 31.1 Tue 14:00 H36

**Rare earth silicide nanowires on silicon surfaces** — •Mario Dähne — Institut für Festkörperphysik, Technische Universität Berlin, Germany

Rare earth silicide nanowires on silicon are a fascinating research subject because of their self-organized formation and their low-dimensional physical properties. In this talk I will give an overview on recent work on such nanowires on Si(001) and Si(557) surfaces, where two different mechanisms are responsible for nanowire formation. While on Si(001) the anisotropies of the substrate surface as well as of the silicide strain result in nanowire formation, on Si(557) the stepped structure leads to nanowire growth along the step edges. I will present scanning tunnelling microscopy results on the atomic structure as well as angle-resolved photoelectron spectroscopy data on the electronic properties. Depending on the specific structure, both one-dimensional and two-dimensional electronic dispersions are found, which will be discussed in the context of the band structure of the corresponding bulk silicides.

# O 32: Plasmonics and Nanophotonics II (Joint Session O/DS/HL)

Time: Tuesday 15:00–16:30 Location: H2

O 32.1 Tue 15:00 H2

**Nanolocalization of time-reversed optical fields propagating in random scattering media** — •Dominik Differt[1], F. Javier García de Abajo[2], and Walter Pfeiffer[1] — [1]Fakultät für Physik, Universität Bielefeld, Universitätstr. 25, 33516 Bielefeld, Germany — [2]Instituto de Optica, CSIC, Serrano 121, 28006 Madrid, Spain

The far field emission pattern of a nanoscale light emitter positioned in a nanoscale random scattering environment contains information about the localized emission. Because of the reciprocity of electromagnetic wave propagation time-reversing the outgoing wave creates an excitation that propagates back to the emitter and localizes on a sub-diffraction length scale. The electromagnetic response of a random scattering environment is calculated based on a multiple scattering approach. The here investigated scattering environment is characterized by a geometrical hierarchy. On a subwavelength scale the emitter is surrounded by metal nanoparticles acting as a random antenna coupling radiation to the far field. On the scale of tens of microns, several wavelengths distance to the emitter, this structure is embedded in randomly distributed dielectric scatterers acting a permeable reverberation shell. The degree of nanolocalization of a time-reversed planar wave component of the outgoing scattered wave depends on this geometrical hierarchy and the density of scatterers, i.e. the wave mixing occurring in the reverberation shell.

O 32.2 Tue 15:15 H2

**Towards Nanostructure-Enhanced High-Harmonic Generation** — Murat Sivis[1], Katrin Siefermann[2], Yaxing Liu[2], Bernd Abel[2,3], and •Claus Ropers[1] — [1]University of Göttingen, Courant Research Center Nano-Spectroscopy and X-Ray Imaging, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [2]University of Göttingen, Department of Physical Chemistry, Tammannstr. 6, D-37077 Göttingen, Germany — [3]University of Leipzig, Wilhelm-Ostwald-Institute for Physical and Theoretical Chemistry, Linnestr. 2, D-04103 Leipzig, Germany

Recent efforts to utilize optical field enhancements in metallic nanostructures for high-harmonic generation (HHG) have generated significant interest [S. Kim *et al.*, Nature **453**, 575 (2008)]. Using local plasmon resonances, the threshold for HHG can be substantially reduced, allowing for HHG by using unamplified few femtosecond laser oscillators. To date, rather limited information on the characteristics and scaling behavior of the relevant processes is available.

Here, we present the first results of our study on harmonic generation with metallic nanostructures in the presence of a noble gas jet. We demonstrate the significant enhancement of harmonic generation of low orders. Experimental limitations and prospects of the approach are discussed.

O 32.3 Tue 15:30 H2

**Third-Harmonic Generation Spectroscopy in Hybrid Plasmonic Systems** — •Tobias Utikal[1,2], Thomas Zentgraf[3], Markus Lippitz[1,2], and Harald Giessen[1] — [1]4. Physikalisches Institut, Universität Stuttgart — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart — [3]NFS Nano-Scale Science and Engineering Center, University of California, Berkeley, USA

In this work we perform third-harmonic generation (THG) spectroscopy in metallic photonic crystals consisting of gold nanowires buried in a dielectric slab waveguide. In these structures particle plasmon polaritons, which are optically excited in the wires, can be hybridized with photonic waveguide modes, which are excited due to the periodic arrangement of the wires. By tailoring the structure geometry the spectrally broad particle plasmon resonance can exhibit an ultra-narrow and pronounced extinction dip. We excite this hybrid plasmonic system with 150 fs laser pulses which can be spectrally tuned over the modulated plasmonic resonance and measure the generated third-harmonic light. The experiments show that it is insufficient to deduce the shape of the THG spectrum from the linear extinction. It is rather essential to consider the full information of the linear response, i.e. amplitude and phase. We find indications that the increased group index and the associated slow light around the extinction dip leads to an increase in the THG signal.

O 32.4 Tue 15:45 H2

**Ultrafast optical nonlinearities in hybrid metal-semiconductor nanostructures** — •Parinda Vasa[1], Robert Pomraenke[1], Wei Wang[1], Stephan Schwieger[2], Erich Runge[2], and Christoph Lienau[1] — [1]Carl von Ossietzky Universitaet, Institut fuer Physik, 26111 Oldenburg, Germany — [2]Technische Universitaet Ilmenau, Institut fuer Physik, 98684 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 such as nanolasers or ultrafast optical switches. We report the first measurement of an ultrafast optical nonlinearity resulting from the strong interaction between SPPs excited on a gold grating and excitons in either a semiconductor QW or a J-aggregated cyanine dye. The hybrid nanostructures are characterized using far-field linear reflectivity as well as photoluminescence measurements and exhibit enhanced SPP-exciton coupling in the linear optical regime. The experimental results are explained within a phenomenological, coupled oscillator model. The nonlinearity is investigated by low-temperature, angle-resolved, ultrafast pump-probe spectroscopy with 20-fs-time resolution. Due to the strong coupling a significant shift in the resonance wavelength and changes in the response time of the third order nonlinearity of the exciton are observed. Such a strong ultrafast nonlinear interaction between metal and excitons will be of key importance to amplify SPP excitations in such hybrid structures.

O 32.5 Tue 16:00 H2

**Plasmon Hybridization Enhances the Nonlinear Response of Single Metal Nanoparticles** — •Thorsten Schumacher[1,2], Kai Kratzer[1,2], David Molnar[1,2], and Markus Lippitz[1,2] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart — [2]4. Physikalisches Institut, Universität Stuttgart

The optical investigation of single metal nanoparticles is limited to rather large sizes due to their weak influence on focused laser radiation. Therefore it is very difficult to detect small dielectric variations, which is crucial for modern plasmonic nanosensors. We induce small, periodic variations of a nanoparticle's plasmonic properties by a heating pump puls that triggers acoustical breathing oscillations. The particle's response is monitored by a probe pulse. An optical nanoantenna increases the influence of these single dielectric objects on the laser focus. Such an antenna can be implemented by placing a bigger nanoparticle close to the smaller one that is probed.

We will show measurements of single metal nanoparticles' acoustic breathing modes as well as their first antenna enhanced detection. A model of the antenna-effect of plasmon hybridisation is presented. At the end, it allows us to analyze the individual nanomechanical properties of tiny single metal nanoparticles and study plasmonic coupling effects, without averaging over big ensembles.

O 32.6 Tue 16:15 H2

**Enhanced Raman scattering at nanoparticles and gratings with nanoparticles** — •Manuel Gonçalves and Othmar Marti — Universität Ulm - Inst. für Experimentelle Physik, Albert-Einstein-Allee 11, 89081 Ulm, Deutschland

Silver and gold nanoparticles of triangular shape in periodic arrays are appropriate templates for molecular detection by means of surface enhanced Raman scattering (SERS). The near-field enhancements may reach 100 and the corresponding Raman electromagnetic enhancements are of the order of $10^8$. On the other hand, surface plasmon modes supported in gratings contribute as well to near-field enhancements, and allow an easy excitation of the long-range surface plasmons in the grating.

We show how plasmonic systems built of gratings and nanoparticles can be of interest for SERS, and how strong near-fields may be achieved. SERS measurements done with a confocal Raman microscope permit to study the dependence of near-field intensity on the shape of the particle and on the excitation conditions.

## O 33: Nanostructures at surfaces: arrays

Time: Tuesday 15:00–16:30 Location: H31

O 33.1 Tue 15:00 H31

**Fabrication of protein patterns by electron-beam writing in a protein-repelling matrix** — Nirmalya Ballav[1], Heidi Thomas[2], Tobias Winkler[2], Andreas Terfort[2], and •Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany — [2]Institut für Anorganische und Analytische Chemie, Goethe-Universität Frankfurt, 60438 Frankfurt, Germany

One of the challenges of nanotechnology is the development of reliable, efficient, and flexible methods for the fabrication of protein patterns. An essential element of almost all available approaches is a protein-repelling "background" matrix, surrounding the active protein-adsorbing areas - the matrix prevents adsorption of proteins beyond these areas. Such a matrix is usually comprised of oligo- or poly(ethylene glycol)-based materials and is generally prepared by a backfilling procedure after the fabrication of the protein-attracting patterns. We present an alternative approach, showing that the protein-repelling matrix, both SAM- and polymer-like, can be used as a primary template for direct electron-beam writing of both non-specific and specific protein patterns of any desirable shape, including gradient ones, on a flexible length scale. The above factors make the approach quite versatile, which is additionally strengthened by intrinsic flexibility of electron-beam lithography, a wide range of suitable electron energies, broad availability of commercial oligoethylene glycol compounds, variable substrate material, and flexible choice of the target proteins. Complex gradient patterns fabricated by the approach can become an important tool for mimicking natural biological interfaces.

O 33.2 Tue 15:15 H31

**UTAM Surface Nano-Patterning in Fabricating Quantum-Sized Nanodots** — •Yong Lei, Stefan Ostendorp, Stefan Bartels, and Gerhard Wilde — Institute of Materials Physics and Center for Nanotechnology, University of Muenster, Wilhelm-Klemm-Str. 10, D-48149 Muenster, Germany

Two challenging technical points prevent the UTAM (ultra-thin alumina mask) surface patterning technique to synthesize surface structures within the quantum-sized range: (1) the arrangement regularity and monodispersity of UTAM pores are poor when the pore diameter is smaller than 20-25 nm; (2) it is difficult to obtain small-pore UTAMs that are suitable for the surface patterning. This prevents the fabrication of quantum-sized surface structures using the UTAM technique, thus an attractive feature of nanomaterials - the quantum confinement effect - is missing in the UTAM technique. Recently, we found a new route to prepare UTAMs with pores in the quantum-sized range and consequently to synthesize ordered arrays of quantum-dots. First, a modulated anodization process largely decreased the growth rate of UTAMs, and thus results in UTAMs with a thickness of about 80 nm. Regular arrays of nanodots with diameters of about 20 nm were fabricated using the UTAMs. Moreover, we proposed a pore-opening process of UTAMs that can well-control the pore-size of UTAMs in the range of 5 to 27 nm. Ordered arrays of surface nanodots within the similar size range can be fabricated. This is the first time in realizing regularly arrayed surface nanostructures in the quantum-sized range using the UTAM surface nano-patterning technique.

O 33.3 Tue 15:30 H31

**ArF excimer laser irradiation of metallic nanoparticles on Silicon** — Martin Kunz, •Alfred Plettl, and Paul Ziemann — Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm

Distinct methods like a micellar technique [1], miniemulsion / emulsion techniques [2,3] or extended Polysterene (PS) colloid lithography [4] were developed for the preparation of self-assembled arrays of metal (Au, Pt) or polymer (PS, PMMA) nanoparticles (NPs). A short introduction into the various preparation routes, with emphasis on the progress of the micellar technique, will be given.

Studies on the effect of ArF-laser irradiation of extended metal NP arrays with diameters of about 10 or 30 nm respectively, deposited on Si- and $SiO_2$-substrates, are reviewed. The optical and thermal properties of different sample arrangements are analysed, the experimental set-up is presented and some observations at different laser energy densities are reported and discussed. Various phenomena can clearly be identified: small NPs show particle melting and shape rounding at low fluences or complete removal. Under special conditions also sinking of Pt-NPs into Si-oxide was observed. Large Au-particles behave different, e.g. are resulting in fragmentation. If fluences locally higher than the ablation threshold of the Si are reached on the substrate, additional phenomena become visible.

[1] G.Kästle, et al., Adv. Funct. Mat. 13, 853 (2003).
[2] A. Manzke, et al., Adv. Mater. 19, 1337 (2007).
[3] E.Schreiber, et al., Chem. Mater. 21, 1750 (2009).
[4] A. Plettl, et al., Adv. Funct. Mat. 19, 3279 (2009).

O 33.4 Tue 15:45 H31

**Photochemical deposition of gold on ordered FePt nanoparticle arrays** — •Thomas Härtling[1], Tino Uhlig[1], Axel Seidenstücker[2], Ulf Wiedwald[2], Alfred Plettl[2], Paul Ziemann[2], Lukas M. Eng[1], and Phillip Olk[1] — [1]TU Dresden, Institut für Angewandte Photophysik, 01062 Dresden (Germany) — [2]Universität Ulm, Institut für Festkörperphysik, 89069 Ulm (Germany)

Gold-coated magnetic nanoparticles are interesting candidates for biomedical, magneto-optical, or data storage applications. The gold coating of the particles improves their stability as well as biocompatability, and broadens the possibilities for surface functionalization. Here we use a photochemical approach to deposit an ultrathin gold shell around FePt nanoparticles arranged in a two-dimensional, hexagonally ordered array. We investigate the deposition process, the qualitiy of the gold coating, and the magnetic properties of the core-shell particles obtained with our technique. First results indicate an improved long-term stability of the magnetization.

O 33.5 Tue 16:00 H31

**Optical properties of nanopore arrays based on porous alumina** — •Hongdan Yan[1,2], Dirk Wulferding[1,2], Peter Lemmens[1,2], Jianmin Shi[3], Klaus-Dieter Becker[3], Frank Ludwig[4,2], and Meinhard Schilling[4,2] — [1]IPKM, TU-BS, Braunschweig — [2]IGSM, TU-BS, Braunschweig — [3]IPTC, TU-BS, Braunschweig — [4]EMG, TU-BS, Braunschweig

Anodic alumina templates with nanopores show photoluminescence peaks and optical absorption that can be divided into three Gaussian bands. Two kinds of oxygen vacancy centers are responsible for these processes. The defects can be tuned using thermal annealing. Work supported by DFG and B-IGSM.

O 33.6 Tue 16:15 H31

**Terrace-Width Distributions (TWDs) of Touching Steps: Modification of the Fermion Analogy, with Implications for Measuring Step-Step Interactions on Vicinal Surfaces*** — •Theodore L. Einstein[1], Rajesh Sathiyanarayanan[1,2], Ajmi BH. Hamouda[1,3], and Kwangmoo Kim[1] — [1]U. Maryland, College Park, USA — [2]Pennsylvania State U., USA — [3]Monastir U., Tunisia

Using Monte Carlo simulations, we compute[1] the TWDs of surfaces in which steps can touch each other, forming multiple-atomic height steps, but cannot cross (no overhangs), and so inconsistent with the standard mapping to spinless fermions. Our numerical results show that the generalized Wigner distribution, with minor modifications at small step separations, gives a very good fit for TWDs of touching steps. (We also generate analytic results by generalizing results for extended fermions.[2]) The interaction strength derived from the fit parameter $\varrho$ indicates an effective attraction between steps, weakening the overall repulsion. The strength of this effective attraction decreases for larger mean-step separations and decreasing step-touching energies; describable via finite-size scaling. Hence, accurate extraction of the true repulsion strength requires multiple vicinalities.

*Supported by UMD NSF MRSEC Grant DMR 05-20471
[1] RS, ABH, and TLE, Phys. Rev. B 80 (2009) 153415.
[2] Siew-Ann Cheong and C.L. Henley, arXiv:0907.4228v1.

# O 34: Methods: Scanning probe techniques IV

Time: Tuesday 15:00–16:15 Location: H32

O 34.1 Tue 15:00 H32

**Temperature Performance and Concept of an Ultra High Vacuum Compatible Dilution Refrigerator System for Scanning Tunneling Microscopy Applications** — •Maximilian Assig[1], Fabian Zinser[1], Vladimir Shvarts[2], Zuyu Zhao[2], Christian R. Ast[1], and Klaus Kern[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]JANIS research company, USA

The investigation of novel physical phenomena implies the design and the construction of new setups and measurement techniques, which can break through instrumental limitations and open new areas in measurement accuracy. Scanning Tunneling Microscopy (STM) is a technique for probing the electronic structure of single adsorbed atoms and nanostructures at surfaces with atomic resolution. This contribution deals with the concept and performance of an ultra high vacuum (UHV) compatible dilution refrigerator (DR) system which is specially adapted for STM measurements in high magnetic field of 14 T perpendicular and 0.5 T parallel to the sample surface. We will give an overview of the temperature calibration in combination with base temperature and cooling power characterisation of our DR system. First tests of the STM head attached to the DR show heating at the tip and the sample due to the motion of the piezo in the scanning process. In idle conditions it was possible to reach a base temperature of 14mK at tip and sample. In addition, we will present further milestones in the project realisation.

O 34.2 Tue 15:15 H32

**Design of a combined Scanning Tunneling / Atomic Force Microscope working at low temperatures** — •Matthias Emmrich, Anja Merkel, and Franz J. Giessibl — University of Regensburg, Faculty of Experimental and Applied Physics, Universitätsstrasse 31, D-93053 Regensburg, Germany

It is well-known that Scanning Probe Microscopes (SPMs) can yield atomic resolution of surfaces in real space. Custom-built low-noise SPMs can push this envelope and yield chemical information [Sugimoto et al, Nature (2007)], sub atomic resolution [Hembacher et al, Science (2004)], spin contrast [Kaiser et al, Nature (2007)] and submolecular resolution [Gross et al, Science (2009)]. While many commercial microscopes are available, home-built microscopes do not need to sacrifice signal to noise ratio (SNR) in order to accommodate a wide variety of users.

Our goal is a microscope with a vibrational noise level well below 1 pm when operating at liquid He temperatures. Low temperatures reduce thermal motion and increase SNR. More importantly, however, is a stable tip-sample junction.

The current status and preliminary results of this new instrument will be presented.

O 34.3 Tue 15:30 H32

**A sub-Kelvin scanning tunneling microscope with high energy resolution and high stability** — •Lei Zhang and Wulf Wulfhekel — Physikalisches Institut, Karlsruhe Institut of Technology, Germany

We designed a new scanning tunneling microscope (STM) working at sub-Kelvin temperatures in ultra-high vacuum (UHV) in oder to study the magnetic properties on the nanoscale. Detecting excitations of single atoms and molecules, a high energy resolution instrument is needed. To achieve this, the set-up is operated at low temperatures and with high stability. A base temperature of 930 mK at the STM head is achieved using Joule-Thomson expansion of Helium-4, which can be reduced to approx. 400 mK when using Helium-3. Test experiments with a superconducting tip show a high energy resolution of 300 $\mu$eV when performing scanning tunneling spectroscopy (STS). The vertical stability of the tunnel junction is below 1pm (peak to peak) and the electric noise floor of tunneling current is about 6 fm/$\sqrt{Hz}$. The spatial drift is below 10 pm/h. Atomic resolution with a setpoint of 0.5 pA and 1 mV was achieved on Au (111). The set-up allow in-situ preparation of tip and samples under UHV condition. The fast cooling down of the samples (4h) guarantees high sample throughput.

O 34.4 Tue 15:45 H32

**Quantum Point Contact Microscopy of a Noble Metal Surface** — •Yong-hui Zhang[1], Peter Wahl[1], Jakob Bork[1,2], and Klaus Kern[1,3] — [1]Max-Planck-Institut für Festkörperforschung; Heisenbergstr. 1; 70569 Stuttgart — [2]Institut for Fysik og Nanoteknologi, and Interdisciplinary Nanoscience Center (iNANO), Aalborg Universitet, Denmark — [3]Institut de Physique des Nanostructures, Ecole Polytechnique Federale de Lausanne (EPFL), Switzerland

Scanning tunneling microscopy is usually performed in the tunneling regime, with a tunneling junction conductance far below one conductance quantum ($G_0 = \frac{2e^2}{h} = 77.5\mu S$). Here, we present imaging of the noble metal (111) surfaces in point contact ($G \sim 1G_0$) by low-temperature STM. The point contact images routinely provide atomic resolution of the substrate. Details of point contact imaging are discussed exemplarily for Cu(111). Specifically, the threefold symmetric hollow sites of the hexagonal surface lattice are resolved. From an analysis of point contact images, the dynamics of the atomic contact is studied. A clear transition is found at a critical conductance $G_c$ (e.g. $G_c \sim 0.5G_0$ , $G_c$ varies with STM tips) between two regimes. We propose a geometrical model to interpret point contact images below the critical conductance $G_c$ which accounts for vertical relaxations. While the model works very well for conductances smaller than $G_c$, it clearly fails in the point contact regime at conductances above $G_c$. We discuss this finding in terms of relaxations of the tip-sample geometry.

O 34.5 Tue 16:00 H32

**A calibration device for Scanning Thermal Microscopy based on the 3-$\omega$-method** — •Uli F. Wischnath, Adrian Czicholewski, and Achim Kittel — Energy and semiconductor research, Dept. of Physics, Univ. Oldenburg, 26111 Oldenburg

Near-field Scanning Thermal Microscopy (NSThM) measures the heating or cooling of a probe tip by a sample for distances of up to some nm [1]. The tip temperature has to be linked to theoretically calculated values of the heat flow for comparison with the theory of thermal near-field radiation.

We have constructed a calibration device for this purpose, consisting of a 4 $\mu$m thick glass fiber of about 5 mm length bridging two banks. The banks and the fiber are evaporated with a 80 nm thin metal film forming the heat source for the 3$\omega$-method. The glass fiber has to be considered for the thermal properties while it merely serves as a passive support concerning the electrical properties. The thermal resistances for such composites are determined with the 3$\omega$ method to be of the order of $10^6$ K/W. This value would not be accessible with a metal wire of sufficient mechanical stability.

A NSThM brought into tunneling distance forms an additional heat sink. The alteration of the 3$\omega$ signal is then used to quantify the heat flow corresponding to the thermovoltages.

[1] U. F. Wischnath, J. Welker, M. Munzel, and A. Kittel, Rev. Sci. Instrum.79, 073708, 2008.

# O 35: Heterogeneous catalysis II

Time: Tuesday 15:00–16:30 Location: H33

O 35.1 Tue 15:00 H33

**ReactorAFM; imaging supported catalysts at work** — •M.E. Cañas-Ventura[1], A. Ofitserov[2], W. Onderwaater[1], P.C. van der Tuijn[1], G.J.C. van Baarle[2], R.C.T. Koehler[1], and J.W.M. Frenken[1] — [1]Kamerlingh Onnes Laboratory, Leiden Uni, Netherlands — [2]Leiden Probe Microscopy BV, Netherlands

The atomic-scale investigation of supported catalysts is on the move towards experiments with state-of-the-art techniques close to industrial conditions: high pressures (P) and high temperatures (T). After successful experiments with a ReactorSTM[1], a miniature flow reactor integrated with a STM, we feel urged to widen range of model catalysts that can be studied under reaction conditions with atomic/near-atomic resolution, to the oxide-supported metal nanoparticle geometry. In this way we bridge not only the so-called "P gap" but also the "materials gap". For this purpose we have now developed the ReactorAFM. With special attention paid to vibration isolation, low-expansion materials and fast electronics, the instrument operates at T up to 570 K, P up to 5 bar and relatively high speeds. A new gas-flow system provides full control over the gas mixture and excellent time resolution and precise distribution of reaction products. The AFM is housed in a UHV system with several additional preparation and surface analysis techniques. The ReactorAFM also measures a tunneling current, which allows operation in a variety of modes with a wide range of simultaneously acquired signals. First scans and $\Delta f$ vs. Z curves demonstrate the good behavior of the new setup.[1]B.L.M.Hendriksen et al.PRL 89,046101(2002)

O 35.2 Tue 15:15 H33

**Steps to detect catalytic ethylene oxide formation on single crystals** — •Sebastian Böcklein, Sebastian Günther, Robert Reichelt, Markus Seibald, Andreas Preimesser, Martin Ehrensberger, Gergely Rozsa, and Joost Wintterlin — Ludwig-Maximilians-Universität, 81377 München, Germany

As part of a project to bridge the "pressure gap" for the catalytic synthesis of ethylene oxide (EtO) on Ag surfaces we have undertaken extensive studies in a model reactor. The investigations aimed at finding conditions under which the production of EtO can be unambiguously and quantitatively detected on single crystal Ag surfaces, a challenging task because of the extremely low ethylene-to-EtO reaction probability. The experiments were performed in a specially designed reactor, and they involved the variation of partial pressures, temperature, and type of Ag samples (powders and polycrystalline sheets), and great effort was expended for proper background subtraction. We find that for the sheets an essential ingredient is an activation treatment by annealing in oxygen, which raises the activity by more than one order of magnitude. There are indications that subsurface O atoms are created by this pretreatment. The maximum values obtained for activity, selectivity, yield, and reaction probability allow us to predict that EtO produced on a single Ag crystal can indeed be detected under flow conditions in a UHV chamber. Experiments on the deactivation show that sintering plays an important role for the dispersed samples, but that there is an additional deactivation process for the sheets that is not caused by sintering or poisoning.

O 35.3 Tue 15:30 H33

**The role of surface oxides in NOx storage reduction (NSR) catalysts** — •Jelena Jelic[1,2], Randall Meyer[1], and Karsten Reuter[2,3] — [1]Univ. of Illinois at Chicago (USA) — [2]Fritz-Haber-Institut Berlin (Germany) — [3]TU München (Germany)

In the NSR approach to lean burn automotive emissions a longer O-rich mode in the cyclic operation first oxidizes and stores the excess NO before a short O-poor mode reduces the stored NOx. Bulk oxide formation in the oxidizing environment is commonly perceived as detrimental to the catalytic activity of the employed platinum metals. To qualify this notion we perform first-principles atomistic thermodynamics and kinetic Monte Carlo simulations determining the surface structure and composition, as well as catalytic performance of Pd(100) under gas-phase conditions typical for the NO oxidation. With bulk oxide formation prevented on the time scale of the O-rich mode, we identify an ultrathin PdO(101)/Pd(100) surface oxide film as the stable surface termination. Moreover, its turnover frequencies are similar to those measured for platinum metal, demonstrating that a surface oxide may be a viable catalyst for NO oxidation.

O 35.4 Tue 15:45 H33

**The Selective Catalytic Reduction (SCR) of NO with $NH_3$ at Vanadium Oxide Catalysts: Adsorption, Diffusion, Reaction.** — •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. Even though it is widely used in commercial applications details of the reaction mechanism are still under debate. Experiments show that adsorption, diffusion, and reactions with NO and (de)hydrogenation processes at the VOx surface 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 ideal $V_2O_5(010)$ surface where peripheral oxygen bonds are saturated by hydrogen. Apart from the perfect oxide surface also differently reduced surfaces are considered by introducing oxygen vacancies. $NH_3$ is found to interact only weakly with the perfect $V_2O_5(010)$ surface. In the presence of OH groups (Brønsted acid sites) $NH_3$ can form a surface $NH_4^+$ species. $NH_3$ can also interact with the surface near oxygen vacancies, adsorbing at vanadium centers of lower coordination (Lewis acid sites). In contrast, NO interacts much more weakly with the surface. Further, simultaneous NO, $NH_3$ adsorption and SCR reaction scenarios at Brønsted and Lewis acid sites are examined. They result in different reaction paths and intermediates as will be discussed in detail.

O 35.5 Tue 16:00 H33

**Electrochemical promotion of catalytic ethylene oxidation on Pt/YSZ catalyst under low pressure conditions** — •Arafat Toghan, Liz Michaela Rösken, and Ronald Imbihl — Institut für Physikalische Chemie und Elektrochemie, Universität Hannover, Callinstrasse 3-3a, D-30167 Hannover, Germany

The catalytic oxidation of C2H4 on Pt catalyst film interfaced with the oxygen-ion conducting yttria-stabilized zirconia solid electrolyte (YSZ) has been studied in the 10-5 and 10-4 mbar range. Photoemission electron microscopy (PEEM) was used as spatially resolving method. Under open circuit conditions (VWR= 0 V) the CO2 production increases by rising p(C2H4) and then at a critical point decreases sharply, showing a pronounced hysteresis. The hysteresis and the abrupt rate decrease are attributed to the build-up of a carbonaceous CHx layer inhibiting O2 adsorption and hence poisoning the catalyst. Applying an anodic potential of +1V leads to trigger a transition from the unreactive branch of the reaction to an active branch. The huge non-Faradayicity reported in the literature for this reaction system is explained as an ignition effect caused by the partial removal of the inhibiting carbonaceous layer. The electrode has been characterized by SEM, XRD and a profilometer.

[1] S. Bebelis and C. G. Vayenas, J. Catal. 1989, 118, 125-146.

O 35.6 Tue 16:15 H33

**Formation of islands of substitutional Li defects on the MgO (001) surface** — •Sergey V. Levchenko and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, Germany

We use density functional theory (DFT) calculations to evaluate electronic structure and formation energies of the substitutional Li defects in the (001) surface, subsurface, and bulk MgO. We analyze the sensitivity of the results to the approximations in the exchange-correlation functional by comparing semi-local (GGA PBE) and non-local (PBE0 and B3LYP) approximations. Calculated defect formation energy as a function of coverage and layer depth indicates that the Li defects prefer to form islands with molar concentration 50% at the top layer, but not in the deeper layers. The formation energy of an isolated substitutional Li defect increases with the depth of the layer in which the defect is formed [1]. We perform an *ab initio* atomistic thermodynamics [2] analysis to determine the average island size under realistic conditions. This shows that, despite the loss in the configurational entropy due to the island formation, the islands containing 10-20 Li defects are present on the surface at relevant temperatures (900-1000 K). Within the islands, the oxygen vacancy formation energy is greatly decreased due to an electron transfer from the O vacancy state to the lower energy states near the top of the valence band, associated with the Li defects.—[1] Z. Yang, G. Liu, and R. Wu, Phys. Rev. B **65**, 235432 (2002)—[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); M. Scheffler and J. Dabrowski, Phil. Mag. A **58**, 107 (1988)

# O 36: Methods: Atomic and electronic structure

Time: Tuesday 15:00–16:00 Location: H34

O 36.1 Tue 15:00 H34

**Constructing fully numerical optimum atomic basis-sets** — •Björn Lange, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck Institut für Eisenforschung GmbH, 40237 Düsseldorf, Deutschland

Minimum atomic basis-sets as used e.g. for tight-binding calculations are commonly constructed by fitting them or even only their matrix elements to experimental or theoretical data. The resulting models are often optimized only for a specific environment, making a systematic analysis of their transferability impossible. In order to achieve systematically analyzable atom-centered basis-sets, we start from a plane-wave density-functional theory (DFT) calculation where the basis-set convergence is well controlled. The optimum radial shape for each angular momentum channel is determined by maximizing the overlap of the orbitals with the Bloch-states of the underlying plane-wave calculation. While previous approaches employ auxiliary radial basis functions, our orbitals are fully numerical. An analysis of the Bloch state residues shows that part which is not covered by the atomic orbitals and reveals transferability issues and improvement opportunities. To demonstrate the performance of this approach we provide results of an extensive analysis of the transferability characteristics for a wide array of materials such as molecules, semiconductors and metals. Furthermore, we demonstrate the advantages of our basis-sets compared to atomic orbitals obtained from the free atom. For example, detailed convergence checks show that they provide a much better starting point for iterative diagonalization approaches in DFT.

O 36.2 Tue 15:15 H34

**Atomic structure of monolayer silica studied by new ion scattering techniques** — •Jan Seifert, David Blauth, Andreas Schüller, Stephan Wethekam, and Helmut Winter — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin, Germany

The structure of ultrathin silica ($SiO_2$) films grown on a Mo(112) substrate is investigated by three recent experimental techniques using grazing scattering of fast atoms (keV energies) from the film surface: (1) Ion beam triangulation (IBT) where electron emission is recorded for scattering of hydrogen atoms as function of azimuthal orientation of the target. From directions of axial surface channels the position of surface atoms is deduced [1]. (2) Rainbow scattering under axial surface channeling conditions [2]. (3) Fast atom diffraction (FAD). For sufficiently small angles of incidence and projectile energies (2 keV), diffraction patterns can be observed in the angular distribution of scattered atoms and molecules. From the Bragg relation, the periodicity of the interaction potential and from the intensity modulation of the diffraction spots the corrugation of the potential and vertical positions of surface atoms can be determined [3]. Our examples demonstrate the attractive features of grazing fast atom scattering as a powerful tool for structure analysis in surface science.

[1] J. Seifert, D. Blauth, and H. Winter, PRL 103, 017601 (2009)
[2] J. Seifert and H. Winter, Surf. Sci. 603, L109 (2009)
[3] J. Seifert, A. Schüller, H. Winter, R. Włodarczyk, M. Sierka, and J. Sauer, to be published

O 36.3 Tue 15:30 H34

**Modeling of interfaces and nanostructures: Effects of structure mismatch, bond polarity and interface charges** — •Roman Leitsmann — GWT-TUD mbH, Material Calculations, Chemnitz, Germany

The characterization of interface and nanostructure properties versus dimension is of increasing importance [1]. Combinations of strongly ionic semiconductors such as PbTe and CdTe crystallizing in different structures may serve as prototypical systems. However, the theoretical ab initio description of interfaces between polar materials is controversially discussed in the literature [1].

We use ab initio methods to investigate structural and electronic properties of PbTe/CdTe interfaces and nanostructures. For this purpose 4 supercell schemes have been developed to treat internal electric fields, stoichiometry, orientation and thereby to model different experimental situations. The advantages and disadvantages of these models will be discussed at the prototypical example of PbTe/CdTe systems. The obtained interface energies are applied to PbTe nanodots embedded in a CdTe semiconductor matrix. For this system we predict an equilibrium rhombo-cubo-octahedron shape. It is used to show that the special arrangement of polar dot-matrix interfaces induces an electrostatic field, which strongly influences the geometrical and electronic properties and reduces the symmetry of the system [3].

[1] APL 88, 192109 (2006), NJP 8, 317 (2006); [2] PRB 79, 235331 (2009); [3] PRB 78, 205324 (2008), PRB accepted (2009)

O 36.4 Tue 15:45 H34

**Characterization of the angular resolution of an inverse-photoemission experiment** — •Anna Zumbülte, Kathrin Wulff, Anke B. Schmidt, and Markus Donath — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Inverse photoemission (IPE) is an experimental method to investigate the unoccupied part of the electronic structure above the Fermi level with **k** resolution within a wide range of the Brillouin zone. The setup consists of a detection system for photons and an electron gun, whose beam divergence determines the angular resolution of the IPE experiment. While the improvement of the energy resolution has been addressed before [1], the improvement of the angular resolution was often neglected so far.

We present a quantitative approach to investigate the electron-beam divergence based on angle-resolved IPE spectra for dispersing sp-derived surface states on Cu(111). The simulation of spectra with different beam divergences shows a strong sensitivity of the peak intensities on the angular resolution. We discuss different criteria, which can be used to evaluate the beam divergence by comparing the simulated with the measured spectra. We apply these criteria to spectra measured with a high-resolution electron gun and compare the results with beam-profile measurements.

[1] M. Budke et al., Rev. Sci. Instrum. **78**, 113909 (2007)

# O 37: Metal substrates: Adsorption of organic / bio molecules IV

Time: Tuesday 15:00–16:30 Location: H36

O 37.1 Tue 15:00 H36

**Structural dependence of metal organic interface state dynamics studied with 2PPE** — •Manuel Marks[1], Christian H. Schwalb[1], Andreas Namgalies[1], Sönke Sachs[2], 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

Time- and angle-resolved 2-photon photoemission (2PPE) has proven to be a powerful experimental approach to study the electron dynamics at metal organic interfaces. With adsorption of the first monolayer (ML) PTCDA on Ag(111) an unoccupied strongly dispersing interface state (IS) emerges at 0.6 eV above the Fermi Level $E_\mathrm{F}$ [1]. Also for 1 ML NTCDA/Ag(111) a similar unoccupied state arises at 0.37 eV above $E_\mathrm{F}$. The respective inelastic electron lifetimes of 54 fs and 110 fs indicate that the states have a significant overlap with the metal substrate and mainly originate from an upshifted Shockley surface state. We systematically studied the disordered precursor phase of the PTCDA monolayer [2]. For this interface a non-dispersing unoccupied state at 0.45 eV above $E_\mathrm{F}$ can be observed that has an electron lifetime of 63 fs. The influence of the adsorbate morphology and the origin of this non-dispersing feature will be discussed. Either the disorder leads to a localization of the surface state or the signal stems from a molecular state shifted in energy due to the chemical interaction.

[1] C. H. Schwalb *et al.*, Phys. Rev. Lett. **101**, 146801 (2008)
[2] L. Kilian *et al.*, Phys. Rev. Lett. **100**, 136103 (2008)

O 37.2 Tue 15:15 H36

**A FT-IRAS study on the adsorption and growth of ultrathin films of PTCDA on Au(111) and Ag(111) surfaces** — •Gregor Öhl, Carolin R. Braatz, and Peter Jakob — Surface Spectroscopy Group, Philipps-University, Marburg, Germany

The vibrational properties of ultrathin films of 3,4,9,10 perylene tetracarboxylic dianhydride (PTCDA) adsorbed on Au(111) and Ag(111) as investigated by means of Fourier-transform infrared absorption spectroscopy (FT-IRAS) will be presented. The films were grown by organic molecular beam deposition (OMBD) in an UHV environment and analyzed *in situ*. Our excellent spectral resolution accompanied by a formidable sensitivity allows us to clearly distinguish the various phases encountered during the growth and follow the thermal evolution of the layers from cryogenic up to elevated temperatures. Results will be presented for coverages from the sub-monolayer to the lower multilayer regime. Furthermore, the effects of preadsorbed spacer layers of rare gases will be discussed.

O 37.3 Tue 15:30 H36

**DFT study of PTCDA on Ag(111) including a STM tip** — •Andreas Greuling, Marcin Kaczmarski, and Michael Rohlfing — Universität Osnabrück, Fachbereich Physik, Barbarastraße 7, 49069 Osnabrück

Any progress in the field of molecular electronics requires a detailed knowledge of conduction through molecules. As a prerequisite, detailed knowledge of the geometrical structure of a model system like the system 'PTCDA on Ag(111) probed with a STM tip' is of big importance. In experiment it is possible to peel the PTCDA from the surface by using a STM tip above a corner oxygen atom. Furthermore, the molecule flips from the surface to the tip and back under certain tip-surface distance and voltage conditions. Here, we investigate these mechanisms by employing ab initio calculations applying the widely used SIESTA code. Using Density Functional Theory (DFT) in the Local Density Approximation (LDA) we present calculated geometries for the process of peeling of the molecule. Additionally we show tip-surface interaction potentials also considering the influence of a homogen electrical field.

O 37.4 Tue 15:45 H36

**Island decay studies of PTCDA on Ag(100)** — •Julian Ikonomov, Christoph H. Schmitz, and Moritz Sokolowski — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Germany

We have studied two-dimensional islands of perylene-3,4,9,10-tetracarboxylic acid dianhydride (PTCDA) deposited on the Ag(100) surface. For submonolayers, the attractive interactions between the molecules lead to two-dimensional islands with a quadratic equilibrium shape. The ordered PTCDA islands are surrounded by a disordered two-dimensional gas-like phase, consisting of highly mobile molecules [1]. The island ripening and decay were investigated with scanning tunneling microscopy (STM) at room temperature. The decay curves follow the classical continuum model for time evolution of clusters (Ostwald theory). The island area changes with a power low $t^{\alpha}$ with an exponent $\alpha$ of about 2/3 which clearly reveals that the decay of the PTCDA islands is diffusion limited. For an ensemble of more closely to each other located PTCDA islands, a mass transport from the smaller to the larger islands has been observed. We have performed numerical simulations of the decay curves of the islands in this ensemble and obtained values for relevant parameters, e.g., the step line tension of the PTCDA islands, the attachment-detachment rate, and the equilibrium density of the two-dimensional gas-phase.

Funded by DFG through SFB 624

[1] J. Ikonomov, O. Bauer, and M. Sokolowski, Surface Science **602**, 2061 (2008).

O 37.5 Tue 16:00 H36

**The orbital structure of $\pi$-conjugated organic molecules on metal surfaces probed by angle-resolved photoemission** — Johannes Ziroff[1], •Michael Wiessner[1], Frank Forster[1], Peter Puschnig[2], Achim Schöll[1], and Friedrich Reinert[1,3] — [1]Universität Würzburg, Experimentelle Physik VII, D-97074 Würzburg — [2]University of Leoben, Chair of Atomistic Modelling and Design of Materials, A-8700 Leoben — [3]FZ Karlsruhe, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe

We present angle resolved photoemission spectra of monolayers of $\pi$-conjugated molecules adsorbed on single-crystalline metal surfaces. Comparing the experimental $k$-dependant intensity distribution of the molecular states to DFT calculations for the free molecule allows to detect sophisticated modifications of the molecular orbitals at the interface.

In case of the single-domain system PTCDA on Ag(110) the 2D emission pattern confirms that the now occupied interface state is mainly derived from the former LUMO-orbital. Moreover, a clear contribution of metal states is evident from additional intensity in normal emission. In the contrary, the structure of the molecular HOMO changes only slightly upon chemisorption on Ag surfaces. Additional data on other planar $\pi$-conjugated organic molecules such as coronene or NTCDA demonstrates the potential of this approach in analysing the interaction at metal-organic interfaces in great detail.

O 37.6 Tue 16:15 H36

**Observing free-electron-like states in a Ferrocene layer** — •Mircea V. Rastei, Benjamin W. Heinrich, Cristian Iacovita, Mauro Boero, Laurent Limot, and Jean-Pierre Bucher — Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, Université de Strasbourg, France

We use low-temperature scanning tunneling microscopy and spectroscopy to study Ferrocene on Cu(111). Unlike the decomposition observed on Au(111), here the molecules are preserved upon adsorption and form ordered layers. Differential conductance spectra and maps reveal the existence of interface states of free-electron-like character in the HOMO-LUMO gap. Similar states were reported for other adlayers (NaCl, Xe, PTCDA), but this is the first interface state observed by STM at an organometallic layer. Additionally, we show that these states can be localized by depositing Cu atoms onto the Ferrocene layer, while for other metal atoms (Co, Au) a complex behavior is observed.

## O 38: Semiconductor substrates: clean surfaces

Time: Tuesday 15:00–16:00 Location: H40

O 38.1 Tue 15:00 H40

**Angle-resolved low-energy photoemission at clean Si(111)(7x7) surface** — •Wolfgang Heckel, Kerstin Biedermann, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Former experiments on Si(111)(7x7) have shown the existence of three filled surface states below the Fermi level [1].

For a detailed investigation of these states we carried out angle-resolved photoemission experiments (ARUPS) with high energy and momentum resolution at a photon energy of 6.20 eV using the fourth harmonic from a Ti-sapphire laser. The light was incident at an angle of 80° relative to the surface normal so states of $\Lambda_1$ and $\Lambda_3$ symmetry could be distinguished unambiguously by switching the light polarisation between p and s. All measurements were undertaken under flat band condition at 90 K.

Several new bands are identified and their dispersion along the $\overline{\Gamma M}$ and $\overline{\Gamma K}$ symmetry lines is presented.

[1] R. I. G. Uhrberg et al., Phys. Rev. B **58**, R1730 (1998)

O 38.2 Tue 15:15 H40

**SHG Spectroscopy of Si(100)(2x1) Interband Transitions** — Dominic Gerlach, Björn Braunschweig, Gerhard Lilienkamp, and •Winfried Daum — Institute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany

It is well established that optical second-harmonic generation (SHG) at Si surfaces and interfaces with fundamental photon energies above 1.5 eV results from resonant excitation of Si interband transitions. Nevertheless, apart from the contribution due to electric-field-induced SHG in the space charge region the origin of SHG interband resonances is not well understood. We present results of the first SHG experiments on the bare Si(100)(2x1) surface with excitation of transitions for a wide range of energies. Much different to Si(100)/SiO2 systems, the SHG spectrum of the bare Si(100)(2x1) surface does not show interband excitations with energies different from the bulk-type E1 and E2 transitions. Moreover, the surface contribution to the E1 band observed for undoped Si(100)(2x1) is much stronger than that of oxidized surfaces and comparable to the bulk contribution from the space charge region of doped samples. Implications of our spectra for Si bonding at the bare and oxidized Si(100) surface are discussed.

O 38.3 Tue 15:30 H40

**Cleaning of GaN($\bar{2}$110) surfaces by Ga deposition and desorption** — •Simon Kuhr, Christian Schulz, Timo Aschenbrenner, Jan Ingo Flege, Thomas Schmidt, Detlef Hommel, and Jens Falta — Institute of Solid State Physics, University of Bremen, Germany

Cleanliness of substrates is a key issue in fabrication of optoelectronic devices since impurities sensitively affect atomic structure, electronic properties and reactivity of the surfaces being the basis of semiconductor devices. One promising cleaning technique concerning especially the removal of oxygen and carbon on polar GaN(0001) surfaces is the deposition of several monolayers of metallic gallium followed by thermal desorption (Schulz et al., pss (c), **6** (2009)). We present first results of the application of this technique to non-polar GaN($\bar{2}$110) surfaces heteroepitaxially grown on r-plane sapphire substrates by metalorganic vapor phase epitaxy. The cleaning process has been monitored by x-ray photoelectron spectroscopy measurements in order to perform a quantitative analysis of the reduction of contaminations and of the surface stoichiometry. In the course of investigation we have developed a cleaning cycle combining thermal degassing and Ga deposition/desorption steps leading to an effective reduction of the contaminants oxygen and carbon. In addition, the impact of the cleaning method on atomic structure and surface roughness has been investigated by low-energy electron diffraction as well as scanning tunnelling microscopy.

O 38.4 Tue 15:45 H40

**The role of Hydrogen for the formation of the GaP(001) surface** — •Marcel Ewald[1,2], Michael Kneissl[1], Norbert Esser[1,2], and Patrick Vogt[1,2] — [1]ISAS Berlin, Albert-Einstein-Str.9, 12489 Berlin, Germany — [2]TU Berlin, Institut für Festkörperphysik, Hardenbergstr.36, 10623 Berlin, Germany

Previous investigation have shown that the preparation of InP(001)(2×1) refers to a hydrogen terminated surface structure which gives rise to a very specific zig-zag pattern in STM. Hence, it is formed under MOVPE growth conditions but not in standard MBE where no reactive hydrogen is present. Also for the GaP(001)(2×1) such structures have been observed by STM for MOVPE grown samples, suggesting a similar H-termination as found for the InP(001). However, it has not been shown that this surface structure is indeed stabilized by hydrogen. We have prepared GaP(001)(2×1) under MBE-like conditions under supply of activated hydrogen. We find that only under these conditions a (2×1) surface is observed giving rise to a RAS signature similar to the one under MOVPE conditions. This surface is explained by a H-terminated structure model similar to the InP(001)(2×1).

# O 39: Phase transitions

Time: Tuesday 15:00–16:15 Location: H42

O 39.1 Tue 15:00 H42

**On the phase transition behaviour of confined molecular assemblies: The influence of the crystal structure on the freezing-melting transition** — •Sebastian Mörz[1], Christof Schäfer[1], Andriy Kityk[2], Klaus Knorr[1], and Patrick Huber[1] — [1]Technische Physik, Universität des Saarlandes, Saarbrücken, Germany — [2]Institute for Computer Science, Czestochowa University of Technology, Czestochowa, Poland

The phase transition behaviour of simple fluids is strongly altered when confined to a mesoporous sorbent. The formation of supercooled states during cooling gives rise to a pronounced hysteresis between freezing and melting of pore confined liquids. The nucleation mechanisms which initiate the solidification of the supercooled liquid are to date not entirely understood.

We present a comparative calorimetric study on different confined liquids ($N_2$, Ar, CO) which elucidates the decisive influence of grain boundaries and crystal structure of the solidified material on the freezing transition.

O 39.2 Tue 15:15 H42

**Modelling laser-induced dielectric breakdown: Application of the multiple rate equation** — •Oliver Brenk, Nikita Medvedev, and Baerbel Rethfeld — TU Kaiserslautern, 67663 Kaiserslautern, Deutschland

Material processing with ultrashort laser pulses is in the focus of experimental and theoretical research. In order to provide a tool for numerical simulation of the effects of ultrashort laserpulse irradiation on dielectrics the multiple rate equation (MRE) has been introduced [1]. The MRE allows to investigate the temporal evolution of the electronic density in the conduction band with very good agreement to a full kinetic approach [2], using Boltzman's equation, but with considerably less computational effort. We have extended the MRE model to include additional effects, namely the reflectivity and the recombination into Self-Trapped Excitons (STE-States). The reflectivity, depending on the electronic density, influences the laser intensity inside the material. STEs are localized electron-hole pairs formed by free electrons having recombined with localized holes, energetically lying between valence band and conduction band. Re-excitation out of these states is considered as well. We study the influence of these processes on the optical parameters and on the threshold behavior of dielectric breakdown. To further expand the model we plan to add a spatial dimension, to study the spatially resolved evolution of the electronic densities to the already implemented time evolution.

[1] B. Rethfeld, Phys. Rev. Lett., 92:187401, 2004.
[2] A. Kaiser et al., Phys. Rev. B, 61:11437, 2000.

O 39.3 Tue 15:30 H42

**Influence of $H_2O$ adsorption on the charge-density wave phase of 1T-TiSe$_2$** — •Matthias May, Stephan Thürmer, Cristoph Janowitz, and Recardo Manzke — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin, Germany

The transition-metal dichalcogenide $TiSe_2$ reveals a charge-density wave (CDW) phase transition at low temperatures and the driving force of this CDW is still under discussion (see e.g. [1]). One crucial question for the microscopic origin was that on the electric character, i.e. whether $TiSe_2$ is a semiconductor or a semimetal [1,2]. This has been answered by Rasch et al. [2] by means of angle-resolved photoemission (ARPES) and applying the effect of $H_2O$ adsorption onto the van der Waals-like surface, bending the bands and resulting in a filled lowest conduction band. These ARPES experiments were continued at BESSY investigating now the influence of $H_2O$ adsorption on the CDW transition at different temperatures. Results are discussed in context of the related theories.

[1] H. Cercellier, C. Monney, F. Clerc, C. Battaglia, L. Despont, M. G. Garnier, H. Beck, and P. Aebi, Phys. Rev. Letters 99, 146403 (2007)
[2] J. Rasch, T. Stemmler, B. Mueller, L. Dudy, and R. Manzke, Phys. Rev. Letters 101, 237602 (2008)

O 39.4 Tue 15:45 H42

**New self-consistent model of ultrashort laser irradiation of materials** — •Nikita Medvedev and Baerbel Rethfeld — Technical University of Kaiserslautern, Department of Physics, Erwin Schroedinger Str. 46, 67663 Kaiserslautern, Germany

We present a new model describing femtosecond laser interaction with a semiconductor or dielectric target. Based on the earlier developed Multiple Rate Equations [1], the model includes interaction of electrons with the phononic subsystem, allowing direct determination of conditions for crystal damage. Taking into account dynamical changes of the optical properties of the target (reflectivity, absorption coefficients), the developed model gives access to a criterion of the damage self-consistently, tracing a change of optical properties as well as a lattice heating and melting.

In contrast with commonly used approaches based on the thermodynamical description of the material (like two temperature model), our model is widely applicable for nonequilibrium electronic conditions, where one cannot use such thermodynamical property as temperature. On the other hand, the model is still simple to use. Applying experimental parameters, we found perfect agreement with the measured reflectivity of the material during irradiation with a femto-second laser pulse and also obtained the damage fluence threshold in very good agreement. The developed model is a powerful tool to describe the dynamics of the electronic subsystem as well as lattice heating.

[1] B. Rethfeld, Phys. Rev. Lett. 92, 187401 (2004)

O 39.5 Tue 16:00 H42

**Lattice Gas Monte Carlo Simulations of Pentacene on Cu (110) - $(2 \times 1)$O** — •Johannes Gall, Michael Hohage, Chunyang Liu, Daniel Queteschiner, Günther Weidlinger, Lidong Sun, and Peter Zeppenfeld — Institute of Experimental Physics, Johannes Kepler University, Linz, Austria.

A reversible two-dimensional phase transition of pentacene (5A) submonolayer films on the Cu(110) - $(2 \times 1)$O reconstructed surface has been observed. Several Monte Carlo (MC) and Kinetic Monte Carlo (KMC) simulations of a lattice gas Ising model have been performed to understand the behavior of the system. The combination of MC and KMC simulations allows investigating the role of kinetic processes during the phase transition. In the simulations different interaction models have been investigated. In particular, we find that the characteristics of the phase transitions strongly depend on the anisotropy of the lateral interactions. The simulation results are compared to recent RDS (reflectance difference spectroscopy) and STM (scanning tunneling microscopy) experiments.

## O 40: [CPP] Organic Electronics and Photovoltaics II (Joint Session DS/CPP/HL/O)

Time: Tuesday 13:45–16:15 Location: H37

O 40.1 Tue 13:45 H37

**Spectroscopic signatures of C$_{70}$-Anions in Polymer-Fullerene composites** — •Andreas Sperlich[1], Moritz Liedtke[2], Hannes Kraus[1], Oleg Poluektov[4], Carsten Deibel[1], Nazario Martin[3], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, Div. Functional Materials for Energy Technology, D-97074 Würzburg — [3]Departamento de Quimica Organica, Facultad de Quimica, Universidad Complutense, E-28040 Madrid — [4]Chemical Sciences and Engineering Division, Argonne National Laboratory, 9700, USA

C$_{70}$-derivates are used in the most efficient organic bulk heterojunction solar cells. However, the detailed photophysical processes in composites containing C$_{70}$ are still unresolved. In this contribution, our focus is on the light-induced charge transfer from the polymer to the fullerene, generating negatively charged C$_{70}$ radicals. Photoinduced absorption (PIA), electron spin resonance (ESR 9.5GHz) and optically detected magnetic resonance (ODMR) were used to draw a picture of the photoinduced charge transfer from polymers to C$_{70}$. We provide the first experimental identification of the light induced C$_{70}$ radical anion in blends with P3HT using high frequency ESR (130GHz). Comparing spectra from C$_{70}$-derivates with different sidechains, we could confirm that the electron is indeed localized on the C$_{70}$-cage. Further, we identify an additional absorption band at 0.9eV due to $C_{70}^{-}$ by PIA.

O 40.2 Tue 14:00 H37

**The Localized Nature of Charge Transfer in F$_4$TCNQ-Doped Thiophene-Based Donor Polymers** — •Patrick Pingel[1], Lingyun Zhu[2], Kue Surk Park[1], Jörn-Oliver Vogel[1], Silvia Janietz[3], Eung-Gun Kim[2], Jürgen P. Rabe[1], Jean-Luc Brédas[2], and Norbert Koch[1] — [1]Department of Physics, Humboldt University Berlin, Germany — [2]School of Chemistry and Biochemistry, and Center for Organic Photonics and Electronics, Georgia Institute of Technology, USA — [3]Fraunhofer IAP, Potsdam, Germany

Recently, polymer layers exhibited exceptionally high conductivities upon p-type doping with the molecular acceptor tetrafluorotetracyanoquinodimethane (F$_4$TCNQ). Here, we present experimental and theoretical results on blend layers of F$_4$TCNQ and a series of poly(3-hexylthiophene-*co*-dithienyltetrafluorobenzene) (P3HT-TFT) copolymers with systematically varied TFT content. Regardless of the amount of TFT in the donor polymer, we find that only a single charge transfer (CT) species is formed, which we assign to the interaction of F$_4$TCNQ with an oligothiophene segment of the main chain. The degree of CT remains constant, even if the dopant concentration is increased up to a point, where closely neighbouring CT complexes exist at the same uninterrupted thiophene segment. Our findings show that the CT between F$_4$TCNQ and an oligothiophene segment has a localized, isolated nature, possibly comprising less than five connected thiophene units. Thus, CT is dictated by the local electronic structure on the nm scale, rather than depending, e.g., on the macroscopic ionization potential determined from photoemission methods.

O 40.3 Tue 14:15 H37

**Charge Transfer Exciton Dynamics in Polymer/Fullerene Blend** — •Josef M. Berger, Markus Hallermann, Enrico Da Como, and Jochen Feldmann — Lehrstuhl für Photonik und Optoelektronik, CeNS, LMU München

Polymer fullerene blends are one of the most promising material systems for organic photovoltaics. A major loss channel in these cells is the formation and recombination of charge transfer excitons. These excitons emit light as a consequence of radiative recombination of the hole on the polymer and the electron on the fullerene [1]. Here, we report on time resolved emission experiments with the aim of understanding the parameters controlling the recombination lifetime. For the blend of MDMO-PPV/PCBM we correlate the decay profile with the morphology obtained by transmission electron microscopy [2]. [1] Markus Hallermann, Stephan Haneder, and Enrico Da Como, Appl. Phys. Lett 93, 053307 (2008) [2] Markus Hallermann, Ilka Kriegel, Enrico Da Como, Josef M. Berger, Elizabeth von Hauff, Jochen Feldmann, Advanced Functional Materials 19, 3662 (2009)

O 40.4 Tue 14:30 H37

**The Relationship between the Electric Field Induced Dissociation of Charge Transfer (CT) Excitons and the Photocurrent in Novel Hybrid Small Molecular/Polymeric Solar Cells** — •Sahika Inal[1], Alan Sellinger[2], and Dieter Neher[1] — [1]Universität Potsdam, Institut für Physik und Astronomie, 14476 Potsdam-Golm — [2]Institute of Materials Research & Engineering, Singapore 117602

Complete dissociation of coulombically bound interfacial states is an ultimate step accounting for photovoltaic performance. Recent work has proposed that the emission of CT-exciton, i.e. an exciplex, is a competing process to the generation of free charges [Appl. Phys. Lett. 2007, 90, 092117]. Here, we investigated the photophysical processes in a bulk heterojunction system using a soluble poly(p-phenylenevinylene) donor and a novel small molecular electron acceptor based on Vinazene (2-vinyl-4,5-dicyanoimidazole). Recent work has shown that this blend exhibits a featureless emission, prominent at long wavelengths of the spectrum, which was attributed to a CT-exciton [J. Chem. Phys. 2009, 130, 094703]. We monitored the field induced dissociation of these CT-excitons by means of steady state and time resolved PL spectroscopy. Shortened decay times and reduced PL emission in blend film evidence the dissociation of the emissive intermolecular pair by the external electric field. Analyzing the dependence of the photocurrent and external quantum efficiency on the external field, the fate of the separated exciplex pairs is tackled. It is suggested that the formation of free carriers involves channels other than CT-excitons in such blends.

O 40.5 Tue 14:45 H37

**Study of Sub-Bandgap States in Polymer-Fullerene Solar Cells** — •Martin Presselt[1], Felix Herrmann[1], Marco Seeland[1], Maik Bärenklau[1], Sebastian Engmann[1], Roland Rösch[1], Wichard J. D. Beenken[2], Sviatoslav Shokhovets[1], Harald Hoppe[1], and Gerhard Gobsch[1] — [1]Experimental Physics I, Institute of Physics & Institute of Micro- und Nanotechnologies, Ilmenau University of Technology, Weimarer Str. 32, 98693 Ilmenau, Germany — [2]Theoretical Physics I, Institute of Physics, Ilmenau University of Technology, Weimarer Str. 25, 98693 Ilmenau, Germany

At present polymer-fullerene blends are widely used to build organic solar cells. The main contribution to their photocurrent originates from optical transitions between occupied states below the HOMO level and unoccupied states above the LUMO level of the polymer.

In this work, we investigated the origin of states contributing to the optical absorption in the sub-bandgap spectral range and the resulting photocurrent in P3HT-PCBM bulk heterojunction solar cells. Photothermal deflection spectroscopy, temperature dependent external quantum efficiency, photoluminescence and electroluminescence as well as spectroscopic ellipsometry measurements have been carried out. Effects due to different P3HT-PCBM blending ratios and annealing temperatures have been studied.

Two models are discussed to explain the experimental observations: optical transitions involving (a) disorder and/or defect related states, and (b) charge transfer complexes.

O 40.6 Tue 15:00 H37

**Influence of system size on simulated charge mobility in amorphous films of tris(8-hydroxyquinolinato)aluminium (Alq3)** — •Alexander Lukyanov and Denis Andrienko — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

We present the results of a modeling study of the charge transport in amorphous films of tris(8-hydroxyquinolinato)aluminium (Alq3). In our multiscale approach we combine molecular dynamics to generate material morphologies, Marcus theory to evaluate charge hopping rates and kinetic Monte Carlo to simulate charge dynamics. Energetic disorder is taken into account by assigning partial charges to the hopping sites, obtained from DFT B3LYP, 6-311g(d) calculations. In contrast to the previous studies Poole-Frenkel behavior of the mobility is reproduced. Our results indicate strong finite-size effects, meaning that the absolute value of the calculated mobility decreases with the increase of the simulation box size. Simple analogy with a classical percolation problem suggests that very large systems are required to obtain a reliable estimate of the charge carrier mobility.

O 40.7 Tue 15:15 H37

**Influence of injection and extraction barriers realized by choice of donor and HTL on organic solar cell performance** — •Wolfgang Tress, Ellen Siebert, Karl Leo, and Moritz Riede — TU Dresden, Institut für Angewandte Photophysik

In the p-i-n solar cell architecture, the active materials of a donor/acceptor flat heterojunction are sandwiched between two doped transport layers, which provide a highly conductive contact to the cathode metal and the ITO, respectively. This concept allows for a systematic study of the influence of the HOMO of the donor and the adjacent hole transport layer (HTL) on the open circuit voltage ($V_{oc}$) and the shape of the IV curve. This approach avoids the main problems emerging by metal-organic interfaces like varying work functions, unpredictable interface dipoles, etc.. Additionally, extraction barriers, which cannot be realized by the choice of metal, can be adjusted in a controlled way by a HOMO of the HTL lying deeper than the HOMO of the donor. Using donor and HTL materials with a HOMO between 5.0 and 5.6 eV in combination with $C_{60}$ as acceptor, we demonstrate a systematic dependence of $V_{oc}$ on the HOMO of the donor, whereas the built in field is goverened by the HOMO of the strongly doped HTL. The fill factor (FF) is mainly influenced by the HOMO offset between donor and HTL. Both types of barriers (extraction and injection) decrease FF resulting in s-shaped curves with different characteristics. The experimental results are interpreted by comparison to simulation data of a drift-diffusion model, treating the HOMO barrier with a field dependent lowering effect.

O 40.8 Tue 15:30 H37

**Hole transport characteristics of pentacene studied with Green functions and real-time propagation** — •Sebastian Radke[1], Caroline Gollub[1,2], Stanislav Avdoshenko[1], Rafael Gutiérrez[1], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology — [2]Max Planck Institute for the Physics of complex Systems, Dresden

For temperatures higher than 150 Kelvin the charge carrier mobility in organic semiconductors depends sensitively upon an interplay of band-like and hopping transport [1]. In this contribution, the hole transport characteristics of an organic semiconducting material are studied with two different theoretical methods and both approaches are compared. As a model system a pentacene structure is selected, which is well-characterized in the context of organic electronics. The first approach is based on a Green function formulation of the Holstein-Peierls model, accounting for local and non-local electron-phonon coupling and it addresses the transport problem in the energy space, so that fluctuations are taken into account only within a static picture. In the second approach, a real-time propagation of the charge carrier wave function is performed and this provides a deeper insight into the different time scales appearing in the problem. The Hamiltonian is formulated in the tight-binding representation, where the parametrization is evaluated for different levels of theory of the MD trajectories and of the electronic structure calculations.

[1] Y. C. Cheng, *et al.*, J. Chem. Phys. **118**, 3764 (2002).

O 40.9 Tue 15:45 H37

**Ab initio based modeling of charge transport in organic semiconductors** — •Caroline Gollub[1,2], Stanislav Avdoshenko[1], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology — [2]Max Planck Institute for the Physics of complex Systems, Dresden

In organic electronics, theory is expected to play an important role for the search of organic semiconducting materials with improved charge carrier mobilities. Current theoretical efforts are devoted to the understanding of the charge transport mechanism and the accurate prediction of the structure-mobility relationship. In this contribution, an approach for the charge migration in organic semicondutors is presented based on a self-consistent propagation of the charge carrier wave function effected by the molecular dynamics of the system, i.e. the electronic and nuclear dynamics are treated on an equal footing. The simulation comprises the evaluation of charge transfer parameters from ab initio calculations, the quantum dynamical calculation of the evolution of the charge carrier wave function and the molecular dynamics of the studied system. The method allows to follow the real-time and real-space transport and can be used to extract charge carrier mobilities in dependence of the chemical functionality, the temperature or the structure assembly. The technique will be demonstrated for hole transport in a 1D stack of coronene molecules.

O 40.10 Tue 16:00 H37

**Energetics of Excited States in the Conjugated Polymer Poly(3-hexylthiophene)** — Julien Gorenflot[1], •Daniel Mack[1], Daniel Rauh[4], Stefan Krause[2], Carsten Deibel[1], Achim Schöll[2], Friedrich Reinert[2,3], and Vladimir Dyakonov[1,4] — [1]Experimental Physics VI, University of Würzburg, D-97074 Würzburg — [2]Experimental Physics II, University of Würzburg, D-97074 Würzburg — [3]FZK Karlsruhe, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe — [4]Bavarian Centre for Applied Energy Research (ZAE Bayern), D-97074 Würzburg

Although prototypes and first commercial polymer-based solar panels already exist, a comprehensive understanding of the fundamental processes and energetics involved in photocurrent generation is still missing and limits further device optimisations. We present a complementary set of experiments on poly(3-hexylthiophene(P3HT), which enables us to draw general conclusions on the energy levels and barriers involved in the processes from light absorption to polaron pair dissociation. From photoemission spectroscopy of occupied and unoccupied states we determine the transport gap to 2.6 eV, which we show to be in agreement with the onset of photoconductivity by spectrally resolved photocurrent measurements. We also find that photogenerated singlet excitons, generated with light at the absorption edge, require 0.7 eV of excess energy to overcome the binding energy. The intermediate charge transfer state, also called polaron pair, is situated only 0.3 eV above the singlet exciton. We discuss our results in view of their impact on charge generation.

# O 41: Poster Session I (Semiconductor Substrates: Epitaxy and growth; Semiconductor Substrates: Adsorbtion; Semiconductor Substrates: Solid-liquid interfaces; Semiconductor Substrates: Clean surfaces; Oxides and insulators: Epitaxy and growth; Oxides and insulators: Adsorption; Oxides and insulators: Clean surfaces; Organic, polymeric and biomolecular films - also with adsorbates; Organic electronics and photovoltaics, Surface chemical reactions; Heterogeneous catalysis; Phase transitions; Particles and clusters; Surface dynamics; Surface or interface magnetism; Electron and spin dynamics; Spin-Orbit Interaction at Surfaces; Electronic structure; Nanotribology; Solid/liquid interfaces; Graphene; Others)

Time: Tuesday 18:30–21:00 Location: Poster B1

O 41.1 Tue 18:30 Poster B1

**SPM characterization of GaN formed by ion-beam assisted epitaxy** — •Lena Neumann, Jürgen W. Gerlach, Moharram Abd El Khair, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstrasse 15, 04318 Leipzig

Gallium nitride (GaN) films were formed using the ion-beam assisted epitaxy technique. The influence of the nitrogen ion-to-gallium atom flux ratio (I/A ratio) on the early stages of GaN thin films nucleation and growth on super-polished 6H-SiC(0001) substrates is studied, here. The deposition process was performed by evaporation of gallium using a conventional effusion cell and irradiation with hyperthermal nitrogen ions from a constricted glow-discharge ion source at a constant substrate temperature of 630°C. The nitrogen ions flow was kept constant and their kinetic energy did not exceed 25 eV. The selection of different I/A flux ratios was done by varying the gallium effusion cell temperature in the range between 950°C and 1020°C. For comparison, a constant amount of deposited GaN was achieved by adapting the deposition time. The surface structure during the GaN growth was monitored in situ by reflection high-energy electron diffraction (RHEED). The nucleation and subsequent film formation were observed using a scanning probe microscope (SPM) attached to the deposition system. The results show that the initial stages of the ion-beam assisted GaN formation are strongly influenced by the I/A ratio.

O 41.2 Tue 18:30 Poster B1

**Growth of epitaxial micrometer-sized Cu- and Cu-Ni pyramides on Silicon** — •Sarah Hoffmann, Benedikt Ernst, Regina Nowak, Susanne Seyffarth, and Hans-Ulrich Krebs — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen

Thin Cu and Cu-Ni films were prepared on Si(111) substrates using pulsed laser deposition (PLD) in ultra high vacuum. At elevated substrate temperatures above 200°C, either during deposition or afterwards, epitaxial growth of three dimensional pyramides with edge lengths of about five micrometers and heights up to 500 nm is observed using scanning electron microscopy (SEM) and atomic force microscopy (AFM). In the case of pure Cu, the base area of these islands is a triangle. With increasing Ni-content, shape changes occur, which can be explained by a reduction of surface diffusion. The influence of the $SiO_2$ layer thickness and the formation of a Cu-Si interlayer was studied by ellipsometry. The transformation of the Cu and Cu-Ni films into the pyramids during heating were studied by resistance and x-ray measurements.

O 41.3 Tue 18:30 Poster B1

**Surface analysis for the characterization of thin heteroepitaxial GaP films on Si(100)** — •Henning Döscher[1], Peter Kleinschmidt[1], Anja Dobrich[1], Sebastian Brückner[1], Oliver Supplie[1], Christian Höhn[1], Ulrike Bloeck[1], Benjamin Borkenhagen[2], Gerhard Lilienkamp[2], Winfried Daum[2], and Thomas Hannappel[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin — [2]IEPT, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld

The combination of superior III-V semiconductors with Si(100) substrates via metal-organic vapour phase epitaxy (MOVPE) is a technological and scientific challenge. The growth of nearly lattice-matched GaP on Si(100) represents an important model system for the specific defect mechanisms induced by polar on non-polar epitaxy such as anti-phase disorder. Applying a contamination free transfer system between the MOVPE and ultra high vacuum (UHV), we are able to correlate UHV based surface characterization with in situ optical measurements and post-growth ex situ analysis.

The applied instruments include X-ray photoelectron spectroscopy (XPS) for chemical analysis, X-ray diffraction (XRD) and transmission electron microscopy (TEM) for film characterization, scanning tunnelling (STM) and atomic force (AFM) microscopy for surface investigations, low energy electron diffraction (LEED) and reflectance anisotropy spectroscopy (RAS) for averaged information about the anti-phase domain distribution as well as low energy electron microscopy (LEEM) and dark field TEM for its lateral resolution.

O 41.4 Tue 18:30 Poster B1

**MOVPE growth processes monitored simultaneously by in-situ scanning tunneling microscope and spectroscopic ellipsometry** — •Matthias Schmies, Raimund Kremzow, Markus Pristovsek, and Michael Kneissl — TU Berlin, Institut für Feskörperphysik, EW 6-1, Hardenbergstr. 36, D-10623 Berlin, Germany

Optoelectronic devices, such as single-photon emitters and semiconductor lasers, demand an excellent understanding of the growth processes during metal organic vapor phase epitaxy (MOVPE). Typical MOVPE growth conditions, e.g. 100 mbar reactor pressure and 700°C temperatures, require optical techniques for in-situ control. However, these techniques do not provide sufficient information about surface topology. Especially monitoring the changes in the InGaAs quantum dot (QD) morphology during MOVPE is very challenging. In order to obtain information about the structural changes during MOVPE, we have built a special in-situ scanning tunneling microscope (STM). In order to also measure layer thickness and composition we combined this STM with an in-situ ellipsometer and present measurements on QD formation during MOVPE containing simultaneous information of topography and layer properties. This allows us to investigate the QD shape depending on layer thickness and composition.

O 41.5 Tue 18:30 Poster B1

**Adsorption Characteristics of Gallium on Si(112)** — •Inga Heidmann, Moritz Speckmann, Thomas Schmidt, and Jens Falta — Institute for Solid State Physics, University of Bremen, 28359 Bremen

We studied the morphology of the clean and gallium-terminated Si(112) surface by means of scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED). The Si(112) surface is of great interest for technological applications due to the fact that the clean surface is faceted [1], and the deposition of Ga atoms at the step edges of vicinal surfaces is favoured energetically. This leads to a self-organized formation of quasi one-dimensional atomic wires along the direction of the wires [2].

Our investigations on the bare surface showed two different typs of regions, one exhibiting stepped Si(112) surface areas and the other consisting of (111)-(7 × 7)- and (337)-(2 × 1)-facets orientated along the $[\bar{1}10]$ direction. Due to the adsorption of gallium the surface is smoothened and large-area (112)-orientated domains are established with a $(N \times 1)$-reconstruction, where $N = 4 - 7$ with an averaged value of roughly 5.5. The Ga atoms are arranged in rows parallel to the $[\bar{1}10]$ direction, but are interrupted by perpendicular quasiperiodic vacancy lines.

[1]: Baski et al., Phys. Rev. Lett. **74(6)**, 1995.
[2]: Snijders et al., Phys. Rev. B **72**, 2005.

O 41.6 Tue 18:30 Poster B1

**Aluminium induced facetting of Si(113) studied by SPA-LEED and AFM** — Inga Heidmann[1], •Moritz Speckmann[1], Tobias Nabbefeld[2], Claudius Klein[2], Michael Horn-von Hoegen[2], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, 28359 Bremen — [2]Experimental Physics, University of Duisburg-Essen, 47057 Duisburg

Due to its anisotropy and lack of rotational symmetry the Si(113) surface is a candidate for the growth of low dimensional structures like nanowires. Though it is one of a very few stable high-index silicon surfaces, Si(113) appears to be unstable against facetting after adsorption of metals, e.g., Ga [1,2] or Ag [3].

By means of spot profile analysing low-energy electron diffraction (SPA-LEED) and atomic force microscopy (AFM) we analysed the Al adsorption on Si(113) in a temperature range of 600 to 800°C in dependence on both, the deposition temperature and deposition time. We find that Al, very similar to the adsorption of Ga, decomposes the Si(113) surface into a regular facet pattern along the $[1\bar{1}0]$ direction. This pattern consists of alternating (112) and (115) facets, which are $(6 \times 1)$ and $(4 \times 1)$ reconstructed, respectively. The width of the facets increases strongly with increasing deposition temperature. For temperatures above 750°C, however, only the (112) facets are found to be stable.

[1]: H. Suzuki et al., Surf. Sci. **492**, 166 (2001).
[2]: T. Clausen et al., e-J. Surf. Sci. Nanotech. **3**, 379 (2005).
[3]: M. Speckmann et al., Phys. Status Solidi RRL **3**, 305 (2009).

O 41.7 Tue 18:30 Poster B1

**Influence of the pre-adsorption of group III metals on the growth of Ge nanostructures on vicinal Si surfaces** — •Moritz Speckmann, Thomas Schmidt, Jan Ingo Flege, Inga Heidmann, Jan Höcker, Torsten Wilkens, and Jens Falta — Institute of Solid State Physics, University of Bremen

The employment of metals as surfactants (surface active agents) is a promising approach to influence the growth of Ge nanostructures on Si surfaces. Especially for group III and group V elements an enhanced or suppressed Stranski-Krastanov growth behaviour is found, respectively.

For all group III metal on silicon systems presented in this study we observe a drastic change of the surface morphology after adsorption of a few monolayers. For the investigations we used a variety of surface sensitive techniques, e.g., scanning tunneling microscopy (STM), spot profile analysing low-energy electron diffraction (SPA-LEED), low-energy electron microscopy (LEEM), and x-ray standing waves (XSW). On the one hand, the adsorption of Ga and In leads to a smoothening of the intrinsically unstable Si(112) surface and the development of 1D metal chains. But on the other hand, the stable Si(113) is decomposed into a regular array of nanofacets after adsorption of Ga. For all cases shown here the possibility of growing highly anisotropic Ge islands is demonstrated (Ga/Si(113) [1], Ga/Si(112) [2], In/Si(112)).

[1]: Th. Schmidt et al., New J. Phys. **9**, 392 (2007).
[2]: M. Speckmann et al., J. Phys.: Condens. Matter **21**, 314020 (2009).

O 41.8 Tue 18:30 Poster B1

**STM study of Cu interaction with Pb/Si(111) surface at room and low temperatures.** — •Pavel Shukrynau[1,2], Marius Toader[1], Michael Hietschold[1], and Vladimir Chab[2] — [1]Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group. D-09107 Chemnitz, Germany. — [2]Institute of Physics, Academy of Sciences of the Czech Republic. CZ 162 53, Prague, Czech Republic.

Upon evaporation of a small amount of Cu on the (rt3xrt3)R30-Pb/Si(111) and (1x1)-Pb/Si(111) surfaces at room temperature followed by annealing, new clusters of hexagonal shape are formed. These clusters have a protruded border and are found randomly distributed in the (rt3xrt3)R30-Pb phase or attached to (1x1)-Pb/Si(111) islands with one side. Some of them are agglomerated in bigger clusters of a complex shape. Annealing at higher temperatures induces Pb and Cu segregation in characteristic structures observed at Si surface with a single metal adsorption. Cu atoms agglomerate in quasi-5x5 phase and Pb atoms are found in the "mosaic" structure corresponding to 1/6 ML. The formation of the clusters may be the result of Pb-Cu interaction mediated with Si substrate. Cooling the surface down to 200 K leads to significant changes in the 1x1-Pb islands. The original structure dissipates into small domains of 3x3 nm in size partially keeping the Si(111)-c(5xrt3)-Pb reconstruction. The detailed inspection of this surface reveals a local ordering in a mosaic-like pattern.

O 41.9 Tue 18:30 Poster B1

**HR-EELS-study of the adsorption of propionic acid on clean and $H_2O$ saturated Si(001) surfaces** — •Bochra Boughaled Ellakhmissi[1], Miriam Lange[1], Stefan Kubsky[2], Francois Rochet[3], and Ulrich Köhler[1] — [1]Experimentalphysik IV, Ruhr-Universität Bochum, Germany — [2]Synchrotron Soleil, St. Aubin (Paris), France — [3]Laboratoire de Chimie Physique Matière et Rayonnement, Univ. P. et M. Curie, Paris, France

High resolution electron energy loss (HR-EELS) spectroscopy is used to study the reaction of propanoic acid ($CH_3$-$CH_2$-COOH) with the clean and the hydroxylated Si(001) surface. The results are compared to photoemission data. For the adsorption on the clean Si(001)-2x1 surface the results point to the simultaneous presence of different adsorption geometries, monodentate and bidentate. To circumvent the inhomogeneity caused by multiple adsorption geometries, in a second set of experiments the silicon surface was first modified by the adsorption of water leading to a grafting layer of Si-H and Si-O-H. During the reaction of the hydroxylated surface with propionic acid the strongly diminished O-H stretching mode together with the appearance of the C-H mode clearly shows a reaction of the acid with the water layer. Further information is gained by replacing the $H_2O$ grafting layer by a $D_2O$ layer to distinguish hydrogen (deuterium) related vibrational excitations of the grafting layers from the ones coming from the carboxylic acid. The vibrational data are consistent with the selective adsorption of the propionic acid with the Si-O-H groups via an esterification reaction in a monodentate geometry.

O 41.10 Tue 18:30 Poster B1

**Investigations of PTCDA-growth on passivated silicon surfaces with SPA-LEED** — •André Kubelka, Christian Schulz, and Jens Falta — Institute for Solid State Physics, University of Bremen, 28359 Bremen

Research and utilization of organic semiconductor materials have raised increasing interest in the last years. The organic molecule 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) is often used as an model system for the investigation of physical and chemical properties of organic thin films. PTCDA is a promising candidate for epitaxial layer growth due to its flat molecular structure. We investigated the growth of PTCDA on passivated silicon surfaces with spot profile analysis low energy electron diffraction (SPA-LEED).

After deposition by molecular beam epitaxy on the H-passivated Si(111) the SPA-LEED images showed ring-like patterns with one visible diffuse ring, which indicates the growth of small or weakly-ordered islands with no preferential orientation with respect to the substrate. Further investigations using other experimental methods are in progress.

O 41.11 Tue 18:30 Poster B1

**XPS studies of organosilanes attached to 6H-SiC(0001)** — •Nabi Aghdassi[1], Deb Kumar Bhowmick[1], Steffen Linden[1], Michael Hirtz[1], André Devaux[1,2], Lifeng Chi[1,2], Luisa De Cola[1,2], and Helmut Zacharias[1,2] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster — [2]CeNTech, Center for Nanotechnology, Heisenbergstraße 11, 48149 Münster

Octadecyltrichlorosilane (OTS) represents an organic molecule which has gained much interest in respect of the formation of self-assembled monolayers on silicon dioxide substrates. Silicon carbide (SiC) is a semiconducting substrate well-suited to attach organic complexes due to its outstanding properties like a large bandgap, a high electron drift velocity and its non-toxicity. We have attached OTS molecules to the hydroxyl-terminated 6H-SiC(0001) surface via a wet chemical treatment. This system is studied by XPS. Before the functionalization of the surface the C1s region shows two peaks separated by about 2 eV. The peak with lower binding energy can be attributed to the carbidic component while the second one can be related to a silicon oxycarbide layer. After surface functionalization the peak with higher binding energy shows a large increase in intensity which can be explained by the attached alkyl chains. A covalent bonding of organosilanes with functional end groups may provide a linker for a further functionalization of the surface.

O 41.12 Tue 18:30 Poster B1

**Photocatalytic $CO_2$ reduction investigatet with in situ ATR IR spectroscopy** — •Leo Pöttinger — PCI Universität Heidelberg, Deutschland, Heidelberg

The recycling of $CO_2$ e.g. from exhaust gases to hydrocarbons or even fuels like methanol or methane is of high interest. The chemical storage of energy in fuels with renewable energies is considered. Cheap and good availabe semiconductors like $TiO_2$ are known to reduce $CO_2$ when illuminated with UV light to hydrocarbons. ATR IR spectroscopy is used to investigate the interface of porous $TiO_2$ layer and in water dissolved $CO_2$ . With an in situ flow through cell and light irradiation the reduction process can be tracked. With FTIR ATR spectroscopy vibrational bands are used to identify arising intermediates on the surface. The high bandgap of $TiO_2$ does not allow the process to run with visible light. To drive the process with visible light dye sensitsed $TiO_2$ porous layers are needed. Also the use of cocatalysts is under investigation.

O 41.13 Tue 18:30 Poster B1

**Characterisation of a Titania($TiO_2$)-Water-Interface under UV illumination in the Visible Region** — •Thomas Kriesche — PCI Universität Heidelberg

Photoassisted reactions on $TiO_2$ have attracted much interest for e.g. decomposition of organic pollutants in wastewater. As a result of this it is necessary to understand the dynamic surface charge of titania and its interaction with water to better comprehend reactions involved. In situ ATR IR Spectroscopy is a powerful tool used to investigate the interface between $TiO_2$ and water. Because of the porosity of the titania powder, measurements yield information about dissolved and adsorbed species and their dynamics. LEDs with a wavelength of 350nm for photocatalytic excitation and a ZnSe-ATR-crystal were integrated in a flow cell and used in a Bruker IFS66vS spectrometer. We observed a change in absorption between 9000 and 9500cm$^{-1}$ during UV-illumination. Additionally, we compare the results with the dynamics of the infrared region using a germanium ATR-crystal. Thin titania layer were deposited on the crystal by dropping a titania-ethanol-mixture on the ATR-surface and annealing it overnight. These layers were observed via SEM. The increase of fundamental knowledge about titania will allow a better understanding of photocatalytic reactions.

O 41.14 Tue 18:30 Poster B1

**Coexistence of forward and backward buckled $\pi$-bonded chains on the Si(111)-2×1 surface** — •Thomas K. A. Spaeth, Martin Wenderoth, Karolin Löser, and Rainer G. Ulbrich — IV. Physikalisches Institut, Georg-August Univ. Göttingen, Germany

The (2×1) reconstructed Si(111) surface, prepared by cleaving in ultra-high vacuum, has been studied for more then forty years. Different models for the description of this basic reconstruction have been proposed. The model of $\pi$-bonded chains is widely accepted, but it is still an open question whether forward or backward buckled chains are formed. This ambiguity is due to the small energetic difference between the two variants. Even though the STM cannot directly distinguish between forward and backward buckled $\pi$-bonded chains, we find indications of the coexistence of both chain types by analyzing anti-phase-boundaries between domains of given buckling type on the Si(111)-2×1 surface. The anti-phase-boundaries show a lateral shift of the $\pi$-bonded chains which is not compatible with a model of only one type of buckling. But it can be readily explained by "colliding" domains of differently buckled chains. This finding is supported by STS data taken across the anti-phase-boundaries. They show different electronic structures on both sides. We acknowledge financial support by the DFG via project WE 1889/3.

O 41.15 Tue 18:30 Poster B1

**Formation of the Si(111)-2×1 reconstruction** — Thomas K. A. Spaeth, Martin Wenderoth, •Karolin Löser, and Rainer G. Ulbrich — IV. Physikalisches Institut, Georg-August Universität Göttingen, Germany

The Si(111)-2×1 reconstructed surface is obtained by cleavage at RT in the UHV. It consists of $\pi$-bonded chains which can run in the three equivalent lattice directions $[0\bar{1}1]$, $[\bar{1}10]$ and $[10\bar{1}]$. Different kinds of anti-phase-boundaries (APB) are theoretically possible between domains of reconstructed $\pi$-bonded chains: (i) APB separating domains of different chain orientations or (ii) APB resulting from a 'stacking fault' of the 2×1 reconstruction along or across the chains, i.e. the displacement can be either between two chains or within each chain. We have studied cleaved Si(111)-2×1 samples with high-resolution STM in UHV and observed APBs separating domains with different chain orientations as well as APBs with the displacement within each chain of the same direction. A displacement between two parallel chains was not found. In sample areas containing surface steps, APBs typically run parallel to the steps, within a few nm distance. We also find a clear preference for the $[\bar{1}10]$ and the $[10\bar{1}]$ direction while chains running parallel to the nominal propagation of the cleavage in $[0\bar{1}1]$ direction occur only in very few and small domains, and often linked with steps nearby. Our results provide strong indication that cleavage related surface steps control the formation of the 2×1 reconstruction domains on the Si(111) surface. We acknowledge financial support by the DFG via project WE 1889/3.

O 41.16 Tue 18:30 Poster B1

**Si(100) surface preparation under VPE conditions** — •Anja Dobrich, Henning Döscher, Sebastian Brückner, Christian Höhn, Peter Kleinschmidt, and Thomas Hannappel — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin

The preparation of Si(100) surfaces in vapor phase environments (VPE) suitable for subsequent III-V epitaxy was characterized by surface sensitive instruments available through a dedicated sample transfer to ultra high vacuum (UHV). Using X-ray photoelectron spectroscopy (XPS) for inspection of the chemical surface composition, we verified the ability to obtain clean Si(100) free of oxygen or other contaminations. We checked the process extensively regarding reliability, influences of the process parameters (time, surface temperature, pressure and type of process gas, presence of precursors) and dependencies on type of substrate. Because the results obtained in alternative atmospheres ($N_2$ and Ar) differed from those in $H_2$, we considered an active role of the process gas in the removal of $SiO_2$-layers. Fourier-transform infrared spectroscopy (FTIR) proved the presence of Si-monohydrides while low energy electron diffraction confirmed a two-domain (2x1)/(1x2) reconstruction for all Si(100) surfaces. Since these results implied a predominance of single-layer steps undesirable for subsequent III-V layers, we investigated the atomic surface structure of the samples with scanning tunnelling microscopy (STM). Depending on the off-orientation, the images revealed complex step structures and opposing trends of partial double-layer step formation.

O 41.17 Tue 18:30 Poster B1

**Charge Switching of Donor Ensembles in a Semiconductor** — •Karen Teichmann[1], Martin Wenderoth[1], Sebastian Loth[1], Rainer G. Ulbrich[1], Jens K. Garleff[2], A. P. Wijnheijmer[2], and Paul M. Koenraad[2] — [1]IV. Physikalisches Institut, Georg-August Universität Göttingen, Germany — [2]PSN, Eindhoven University of Technology, the Netherlands

We investigated the charge state switching behaviour of interacting donors near the GaAs (110) surface, by Scanning Tunnelling Microscopy (STM). Silicon doped ($n \approx 6 \cdot 10^{18}$ cm$^{-3}$) GaAs is cleaved in UHV to obtain a clean and atomically flat surface, directly afterwards the sample is transferred into a home build STM, working at 5 Kelvin. Using the STM tip as a movable gate the charge state of each donor can be switched from the neutral to the ionized state [1]. The charge configuration of a single isolated donor is unambiguously determined by the position of the tip and the applied voltage. In contrast, even a two donor system with inter donor distances smaller than 5 nm shows a more complex behavior. The electrostatic interaction of two donors close together can result in ionization gaps. In certain geometrical configurations the modified electronic properties of donors close to the surface [2] can result in bistable and time dependent charge switching behavior. We acknowledge financial support by the DFG SPP 1285.

[1] PRL 101, 076103 (2008)
[2] PRL 102, 166101 (2009)

O 41.18 Tue 18:30 Poster B1

**Characterization of Oxide-based Modelcatalysts- Growth, Morphology and Structure of ultrathin Titaniumoxide- and Ceriumoxide-Films prepared by Oxidation of the Pt-based binary alloys.** — •Jan Markus Essen[1], Severine Le Moal[2], Marco Moors[1], Christian Breinlich[1], Conrad Becker[2], and Klaus Wandelt[1] — [1]Institute of Physical and Theoretical Chemistry, Wegelerstr. 12, D-53115 Bonn — [2]CINaM-CNRS-UPR 3118, Case 913, Marseille Cedex 9, F-13288

Oxidation of bimetallic alloys is a versatile tool for the preparation of ultrathin oxide films. In this study we compare the growth of cerium- and titanium oxide-films obtained by oxidation of $Pt_xCe/Pt(111)$- or $Pt_3Ti(111)$-alloys. For both oxides depending on the oxidation temperature, oxygen pressure, or for the $Pt_xCe$-alloyphases, the amount of cerium, different structures occur. For cerium oxides only 3 different hexagonal phases are observed, while for the titanium oxides 5, hexagonal and rectangular, phases can be distinguished. This can be interpreted as a result of the interplay between the hexagonal substrate symmetry and the oxide favored symmetry, namely hexagonal for the cerium oxides and rectangular for the titanium oxides. For the cerium oxide a stoichiometric oxidation is possible, while for the titanium oxides, caused by strong realloying, this is not the case. For titanium oxides contrarily to the cerium oxides predominantly a 2D-Growth is observed. This is caused by the good matching of the lattice parameters with the underlying substrate. For cerium oxides a lattice the mismatch leads to cluster-formation and thus to a 3D growth mode.

O 41.19 Tue 18:30 Poster B1

**In-situ preparation and characterisation of thick films of Calcium hydroxide** — •Sebastian Dahle[1] und 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 interaction of Calcium hydroxide with different gases is of technological interest for various applications. For example Calcium hydroxide is used as absorbent and reacting agent for neutralisation and desulphurisation, as well as a plaster. Understanding the behaviour of Calcium hydroxide in different environments is expected to lead to increased environmental protection und energy efficiency. The investigation of the interaction processes starts in a clean environment under controlled conditions. Therefore clean films of Calcium hydroxide have to be prepared.

The preparation of thick films of Calcium hydroxide in an Ultra High Vacuum environment using a metal evaporator in combination with a gas inlet system is presented on this poster. In contrast to Calcium oxide that can easily be prepared, Calcium hydroxide shows effects of reduction via impinging Calcium atoms during the preparation. These effects have been studied with Metastable Induced Electron Spectroscopy (MIES), Photoelectron Spectroscopy (UPS(HeI) and XPS), as well as Atomic Force Microscopy (AFM).

O 41.20 Tue 18:30 Poster B1

**STM and STS measurements on thin cerium oxide films grown on Pt(111)** — •Christian Breinlich, Enrico Barletta, Jan Markus Essen, and Klaus Wandelt — Institute for Physical and Theoretical Chemistry, Wegelerstr. 12, 53115 Bonn, Germany

Thin oxide films, grown on a metal support, are showing interesting electronic properties. Therefore they are of great interest for the use as insulating layers in electronic devices and as a support for model catalysts. Cerium oxide has a high dielectric constant, which makes it useful in the fabrication of small capacitor devices. In this study we employed STM and STS to investigate the structural and electronic properties of thin cerium oxide films grown on Pt(111). The preparation process was studied by AES, LEED and HREELS. In a first step a Pt-Ce/Pt(111) surface alloy was prepared by evaporating a thin cerium film at 300 K with subsequent annealing to 1000 K. Then this alloy was oxidised under different conditions. Large amounts of oxygen at 900 K are leading to completely oxidised $CeO_2$ films, whereas smaller amounts of oxygen at 700 K are yielding mixed oxide phases. The former shows a $(1.34 \times 1.34)$ superstructure in LEED and rough, two to three layers high islands in STM. The mixed oxide phase shows a $(4 \times 4)$ superstructure and consists of flat islands with sharp edges. By employing STS it was possible to measure the band gap of the oxide films, which strongly depends on film thickness and stoichiometry.

O 41.21 Tue 18:30 Poster B1

**Structural and electronic characterization of ultra thin MgO films on Mo(100) by scanning tunneling spectroscopy** — •Christian Pauly, Martin Grob, Mike Pezzotta, Marco Pratzer, and Markus Morgenstern — II. Physikalisches Institut B and JARA-FIT, Otto-Blumenthal-Straße, RWTH Aachen, 52074 Aachen

We investigated MgO films on Mo(100) with a thickness of up to 11 monolayers (ML) by scanning tunneling microscopy (STM) and spectroscopy at room temperature. The MgO films were prepared by evaporation of magnesium in oxygen atmosphere.

The appearance of the MgO islands (e.g. island heights) imaged by STM strongly depends on the applied bias voltage at the onset of the conduction band. In particular, the edges appear brighter than the interior of the islands, which we attribute to a spectroscopic effect probably related to defects. The characteristic moiré pattern caused by the lattice mismatch of Mo and MgO has been found on up to 11 ML thick MgO islands. The width of the band gap was measured with respect to the film thickness by $dI/dU$-spectroscopy. The MgO films partly show a characteristic peak in the band gap, which could be assigned to charged defect states.

O 41.22 Tue 18:30 Poster B1

**Mosaic and facet structures of epitaxial MnO films on Au(110)** — •Klaus Meinel, Michael Huth, Hannes Beyer, Henning Neddermeyer, and Wolf Widdra — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Germany

Theoretical studies of rocksalt-like MnO predict for MnO(110) surfaces a (2x1) missing row reconstruction where (100) microfacets run along the [100] direction [1]. For proving this prediction, epitaxial MnO films (thickness 5 - 10 monolayers) have been prepared on an Au(110) substrate and analyzed by means of STM and SPA-LEED. Immediately after film deposition at room temperature, a diffuse background was visible in SPALEED indicating that there is initially poor structural order. Annealing at about 750 K induces long range ordering and relaxation of film structure. Simultaneously, a partly dewetting of the Au(110) substrate occurs. The MnO(110) film displays no (110) terraces. Instead, a furrowed surface is observed with the trenches running parallel to [100]. Along this direction, the film is locally tilted by about +/- 2° due to the misfit which induces a mosaic structure. The surface of the furrows is formed by alternating stripes of (010) and (100) facets having a mean width of about 3 nm. Annealing the films at temperatures around 850 K induces a vanishing of the mosaic structure and an increasing of the width of the (001) facets. Hence, the predicted tendency of (100) faceting is confirmed by experiment. However, the facets are much broader than expected and no (2x1) missing row reconstruction is found within the investigated film thicknesses.

[1] V. Bayer et al., Phys. Rev. B 75, 035404 (2007).

O 41.23 Tue 18:30 Poster B1

**Change of adsorption kinetics of $CH_4$ in the presence of $O^-$ centers on MgO: a TPD study** — •Philipp Giese[1], Harald Kirsch[1], Christian Frischkorn[1,2], and Martin Wolf[1,2] — [1]Institut für Experimentalphysik, FU Berlin, Arnimallee 14, 14195 Berlin — [2]Fritz-Haber-Institut, Abt. Physikalische Chemie, Faradayweg 4-6, 14195 Berlin

In order to obtain a deeper understanding of the interaction between localized holes and adsorbed $CH_4$, its adsorption kinetics are studied on in-situ prepared MgO/Ag(001). Different methods to increase the amount of localized holes or more specifically $O^-$ sites on MgO-surfaces were examined. The detection method is temperature programmed desorption (TPD). After running several cycles of photoinduced $N_2O$ reduction on MgO, the monolayer of $CH_4$ is slightly more strongly bound (increase of desorption temperature by $\sim 5$ K) compared to $CH_4$ adsorbed on untreated MgO. Furthermore, the whole TPD spectrum is broadened and its intensity is smaller. We conclude that the $CH_4$ adsorbate rearranges itself after subsequent reduction of $N_2O$ on MgO. This behaviour cannot be induced by direct UV irradiation, so the interaction between a localized hole and $CH_4$ is much less favourable than the recombination of excited electron-hole pairs, in contrast to the activation of the $N_2O$ bond in photoinduced $N_2O$ reduction. As these localized holes reduce the activation barrier of the C-H abstraction to 0.7 eV, the aforementioned adsorbed state can be interpreted as a precursor in the process of the oxidative coupling of $CH_4$ on oxide surfaces.

O 41.24 Tue 18:30 Poster B1

**Bond formation between single molecules on ultrathin insulating films** — •Niko Pavliček, Tobias Sonnleitner, Ingmar Swart, and Jascha Repp — Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Scanning tunneling microscopy (STM) and spectroscopy (STS) studies on very thin insulating films have shown to be powerful tools in atomic-scale science [1]. These techniques have opened up exciting possibilities by enabling the investigation of the unperturbed electronic properties of single molecules [2] and artificial engineered structures.

Aromatic hydrocarbons with large delocalized $\pi$-systems are promising as functional building blocks for future molecular electronics. Consequently, bond formation between individual organic molecules is essential. First achievements in this field were the imaging of bond formation between pentacene molecules and gold atoms [3], and the formation of coordination-bonded complexes [4].

Here, we present STM and STS studies of molecules comprising nitrile groups, which facilitate the formation of direct molecule-molecule bonds, adsorbed on ultrathin insulating films. We demonstrate such synthesis, characterization, and subsequent manipulation of anthracenedicarbonitrile dimers using the STM tip.

[1] J. Repp and G. Meyer, Applied Physics A **85**, 399 (2006).
[2] J. Repp et al., Physical Review Letters **95**, 225503 (2005).
[3] J. Repp et al., Science **312**, 1196 (2006).
[4] P. Liljeroth et al., submitted (2009).

O 41.25 Tue 18:30 Poster B1

**A Scanning tunneling microscope study of single Phthalocyanine molecules on ultra thin insulating layers on different metal substrates** — Jens Brede, •Jörg Schwöbel, Stefan Kuck, Germar Hoffmann, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, D-20355 Hamburg, Germany

Recent scanning tunnelling microscopy (STM) investigations of pristine molecular features probed with sub-molecular resolution have opened a gateway for future single-molecule-devices. Among these experiments are the study of electron transport via electronic and vibronic excitations [1], the current induced switching of Hydrogen atoms[2] or the spin state of a central magnetic ion[3]. It shows that a sufficient electronic decoupling of the molecule from a metallic substrate is mandatory to grant access to the immaculate molecular properties.

Here, we study single Metal-Phthalocyanine (M-Pc) molecules on insulating layers on different noble metal surfaces with a low temperature STM operated at 6K.

We use atomic resolution to determine the adsorption site of the M-Pc with respect to the underlying layer and probe locally the electronic properties, in particular the highest occupied and the lowest unoccupied molecular orbital (HOMO & LUMO), by scanning tunnelling spectroscopy (STS).

[1] Proc. Natl. Acad. Sci. U. S. A., 2005, 102, 8832-8837 [2] Science, 2007, 317, 1203-1206 [3] Phys. Rev. Lett., 2009, 102, 167203

O 41.26 Tue 18:30 Poster B1

**Reduction and Reoxidation of Thin NiO Films by CO and $O_2$** — •Oliver Höfert, Michael Peter Andreas Lorenz, Regine Streber, Wei Zhao, Karin Gotterbarm, Andreas Bayer, Christian Papp, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

NiO is one important material in heterogeneous catalysis. Surface defects and dislocations are considered to be the active sites; furthermore the size of particles influences the catalysts activity. We studied the reactivity of different thin NiO films on Pd(100) by in situ XPS applying synchrotron radiation at BESSY II. Due to the large lattice mismatch of 7.8% between NiO and Pd, NiO films on Pd(100) are expected to exhibit many defects such as dislocations leading to a large number of potentially active sites. To determine the reactivity of different NiO films we studied their sensitivity towards CO oxidation. Our XPS data revealed that NiO films in the submonolayer regime are indeed reduced to metallic Ni by exposure to CO at 400 K. In contrast, closed layers of NiO show a significantly lower tendency towards CO oxidation. We attribute the observed reactivity to specific sites in close vicinity of the border of uncovered Pd regions and the NiO islands. The reduction of NiO by CO is fully reversible as could be shown by subsequent reoxidation of the metallic Ni by $O_2$.

This work was supported by BMBF (05 ES3XBA/5) and the DFG through the Cluster of Excellence "Engineering of Advanced Materials".

O 41.27 Tue 18:30 Poster B1

**Tunneling Spectroscopy of Cl Divacancies in Ultrathin NaCl Films** — •Jascha Repp[1], Gerhard Meyer[2], Sami Paavilainen[3], Fredrik Olsson[4], and Mats Persson[5] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]IBM Research - Zurich, 8803 Rüschlikon, Switzerland — [3]Institute of Physics, Tampere University of Technology, 33720 Tampere, Finland — [4]Department of Applied Physics, Chalmers University, 41296 Göteborg, Sweden — [5]Surface Science Research Centre and Department of Chemistry, The University of Liverpool, Liverpool, L69 3BX, United Kingdom

In recent years, ultrathin insulating films on metal substrates have gained appreciable attention as templates for the study of individual adsorbates. Cl-vacancies in NaCl films on copper substrates exhibit an unoccupied state localized directly at the vacancy. In this work we study pairs of Cl vacancies in NaCl layers on copper substrates with mutual distances ranging from ~4 Å to ~12 Å by means of scanning tunneling spectroscopy and density functional theory. The close vicinity of these vacancies results in an coupling of the electronic states associated with the individual vacancies. The unoccupied states located directly at the vacancies couple and form a symmetric and an antisymmetric state in analogy to the bonding and antibonding states in a hydrogen molecule. Theoretical analysis shows that the energy splitting of these states is appreciably increased by the zero-point fluctuations of the phonons in the polar insulator.

O 41.28 Tue 18:30 Poster B1

**First-principles study of the interaction of CO, $CO_2$ and water with NiO surfaces** — •Tobias Schaub, Volker Strauss, and Bernd Meyer — Interdisziplinäres Zentrum für Molekulare Materialien ICMM, Universität Erlangen-Nürnberg

Nickel oxide is an important catalyst for the cracking and partial oxidation of hydrocarbons. Under reaction conditions CO, $CO_2$ and water are frequently present in the gas phase. The formation of carbonates and the partial hydroxylation of the NiO surfaces, however, often leads to a reduction of the catalytic activity of NiO due to a blocking of available surface sites for the hydrocarbon reactions. To elucidate the nature and stability of the surface carbonates and hydroxyl groups we have used DFT+U calculations to study the adsorption of CO, $CO_2$ and water on different structural models of ideal and defective NiO surfaces. We find that undercoordinated Ni sites activate $CO_2$ and stable surface carbonates are formed which are bound in a tridentate configuration, similar as previously observed for ZnO [1]. Water adsorbs molecularly or dissociatively, depending on the surface sites with a similar binding energy as $CO_2$. Therefore, a strong competition between $CO_2$ and water for the low coordinated Ni surface sites can be expected. Finally, the influence of O vacancies on the adsorption of CO, $CO_2$ and water will be discussed.

[1] Y. Wang et al. *Angew. Chem. Int. Ed.* 46 (2007) 5624

O 41.29 Tue 18:30 Poster B1

**High-Dimensional Neural Network Potentials for Multicomponent Systems: First Applications to Zinc Oxide** — •Nongnuch Artrith, Tobias Morawietz, Marcus Maschke, and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Recently, artificial Neural Networks (NN) trained to first-principles data have shown to provide accurate potential energy surfaces for systems containing a single atomic species. In this work we present an extension of the NN approach to multicomponent systems by introducing physically motivated terms to deal with long-range interactions. This is a necessary condition for studying binary systems and general multicomponent systems with significant charge transfer. The capabilities of the method are demonstrated for crystal structures, amorphous structures, clusters, and surfaces of zinc oxide as a benchmark system. We show that the predicted energies and forces are in excellent agreement with reference density-functional theory calculations.

O 41.30 Tue 18:30 Poster B1

**A comparative Atomic Force Microscopy study on the preparation of the polished (111) and cleaved (100) surfaces of Magnesium Fluoride (MgF2).** — •Patrick Meisner, Enrico Barletta, and Klaus Wandelt — Inst. for phys. and theor. Chem., University of Bonn, Wegelerstr. 12 D-53115, Bonn, Germany

Alkaline earth fluorides are used for several applications in microelectronics, for example as protective coating and buffer layers for semiconductors. Because of its special optical attributes magnesium fluoride is also an important tool for the production of anti reflex coatings or for sealing Aluminium coated mirrors.Magnesium Fluoride is also used as catalyst in the chemical industry. Its birefringent effect makes it useful for non linear optics, and because of its wide transmitting window it is widely used for construction of high quality optical components. Consequently the finishing of the surface plays an important role on the performances of the final devices. The preparation of two different crystal faces, (111) and (100), was studied. Because of the low cleavage along the (111) surface, this surface orientation had to be prepared by cutting and polishing the crystal by abrasive submicrometer powders. On both surfaces, during cleaning of the fresh surface by thermal processes, morphological and structural effects were observed. Even during the molecular beam epitaxial growth, surfaces of different grade were achieved following different deposition conditions and post-deposition treatments. The achieved results point out to a big influence of the thermal treatments and to a better grade of the final surface after a reconstruction by MBE deposition of some mono-layers of fresh MgF2.

O 41.31 Tue 18:30 Poster B1

**Temperature dependent angle resolved photo-emission spectroscopy of quasi one-dimensional organic conductor tetrathiofulvalene tetracyanoquinodimethane (TTF-TCNQ) thin films** — •Martin Laux[1], Indranil Sarkar[1], Julia Demokritova[1], Jia Wei[1], Andreas Ruffing[1], Vita Solovyeva[2], Milan Rudloff[2], Michael Huth[2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Germany — [2]Physikalisches Institut, J. W. Goethe-Universität, Frankfurt am Main, Germany

The organic conductor TTF-TCNQ is known to form a classic quasi-one-dimensional metal that possibly can be used to test non-Fermi-liquid behavior in 1D Hubbard model systems [1]. Here we report on temperature dependent angle resolved photo-emission spectroscopy (ARPES) on TTF-TCNQ films deposited on KCl(100) substrate. The ARPES spectrum exhibits transfer of spectral weight near Fermi energy over a wide energy range of $\sim 0.2$ eV, comparable to bandwidth, for temperatures 80 K $< T <$ 300 K. Such a large spectral weight transfer compared to the thermal energy $k_BT$, indicates non-Fermi liquid behavior that cannot be explained by electron-phonon coupling and suggests the formation of 1D Hubbard model [2].

[1] N. Bulut et. al., Phys. Rev. B **74**, 113106 (2006)

[2] R. Claessen et. al., Phys. Rev. Lett. **88**, 096402 (2002)

O 41.32 Tue 18:30 Poster B1

**Effects of Electron Irradiation on the Composition, Energetics and Structure of the Calcium/Poly(3-Hexylthiophene) (P3HT) Interface** — •F. Bebensee[1], J. F. Zhu[2], J. H. Baricuatro[3], J. A. Farmer[3], H.-P. Steinrück[1], C. T. Campbell[3], and J. M. Gottfried[1] — [1]Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II — [2]University of Science and Technology of China — [3]University of Washington, Department of Chemistry

Energetics, composition and structure of Ca deposited on the $\pi$-conjugated polymer P3HT was studied with adsorption microcalorimetry, atomic beam/surface scattering, ion scattering spectroscopy and high-resolution XPS. Ca/P3HT is prototypical for interfaces between low work-function metals and semiconducting polymers, which are typically found in organic photovoltaic devices. The interface properties often play a crucial role with respect to the device performance, e.g. charge injection rates depend on the overlap of wave functions at the interface. Despite its outstanding importance, only little is known about the interface formation in these systems beyond their morphologies. Here, we extend our previous studies of Ca on pristine P3HT surfaces and present new results on the influence of electron irradiation ($E_{kin}$=100 eV) on the interface formation. While the adsorption energy of Ca remains unaltered, the sticking probability increases dramatically. This effect is related to changes in the C 1s XP spectra and, by comparison with results for pristine P3HT, provides a detailed mechanistic understanding of the impact of electron irradiation.

O 41.33 Tue 18:30 Poster B1

**Metal complexation and monolayer self-assembly of the bio-organic semiconductor Alizarin** — Neeti Uppal[1,5], Norbert Gast[1,3], Martin Bueno[4], Wolfgang M. Heckl[2,3], and •Frank Trixler[1,2,3] — [1]Dept. Earth and Environmental Sciences, Ludwig-Maximilians-Universität München (LMU) & Center for NanoSciences (CeNS), München, Germany — [2]Dept. of Physics, Technische Universität München (TUM), Garching, Germany — [3]Zentrum Neue Technologien, Deutsches Museum, München, Germany — [4]Fakultät Feinwerk- und Mikrotechnik, Physikalische Technik, Hochschule München, Germany — [5]Institut für Physik, Universität Augsburg, Germany

Organic Solid/Solid Wetting Deposition (OSWD) (Trixler et al.: Chem.Eur.J. 13 (2007), 7785) enables to deposit insoluble molecules such as organic pigments and semiconductors on substrate surfaces under ambient conditions. We explore the potential of OSWD to grow and manipulate monolayers of biomolecules and their chelates on graphite and use Alizarin as a model system - a natural organic compound which occurs mainly as an anthraquinone glycoside in plants.

Our investigations via Scanning Tunneling Microscopy (STM), Tunneling Spectroscopy (TS) and Molecular Modelling reveal that OSWD works also with bio-organic molecules and chelate complexes and show that the advantages of OSWD (self-assembly under ambient conditions in a non-solvent environment, nanomanipulation via molecular extraction) can all be tapped.

O 41.34 Tue 18:30 Poster B1

**Self-assembled monolayers on gold containing azobenzene ligands** — •Robert Ossig[1], Florian Vogel[1], Frauke Bretthauer[2], Ulrich Siemeling[2], and Frank Träger[1] — [1]Institut für Physik and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), Universität Kassel, Kassel, Germany — [2]Institut für Chemie and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), Universität Kassel, Kassel, Germany

Self-assembled monolayers (SAMs) of photoresponsive molecules yield a wide range of applications, for example, for optical devices. At present the SAMs usually consist of small anchor groups based on symmetric disulfids or thiols and large functional groups. However, the densely packed arrangement of these molecules on substrates causes a steric hindering for photoisomerisation. Hence, larger anchor groups or molecules with more than one anchor group are necessary to provide more space between the functional groups. For this purpose we have recently synthesised molecules consisting of a photoresponsive functional and two anchor groups. The functional group is based on azobenzene-derivatized 1,2-dithiolanes which can be switched between their *cis* and *trans* isomers. In this contribution we present fundamental adsorption studies of these molecules and the SAM formation, investigated by means of optical second harmonic generation. We demonstrate that for a concentration of 50 $\mu$mol/l the second order Langmuir kinetics describes the adsorption best. For a deeper insight of the involved processes concentration dependent measurements as well as ellipsometry and scanning-tunnelling microscopy have been conducted.

O 41.35 Tue 18:30 Poster B1

**Dominant spin-relaxation processes in the organic semiconductor CuPc determined by means of spin-resolved two-photon photoemission** — •Kathrin Koffler, Sabine Neuschwander, Jan-Peter Wüstenberg, Mirko Cinchetti, and Martin Aeschlimann — Department of Physics, University of Kaiserslautern, 67663 Kaiserslautern, Germany

Organic semiconductors (OSC) are considered as ideal materials for spintronic devices due to their chemical flexibility, their low production costs and the intrinsically low spin-orbit coupling [1]. A fundamental prerequisite for organic spintronic devices is an efficient spin injection from a ferromagnetic electrode into the OSC. With spin-resolved two-photon photoemission, a model system consisting of a thin cobalt film and the OSC copper phthalocyanine (CuPc) has been studied with focus on interfacial effects on spin injection and on the spin transport properties of CuPc [2]. In this contribution we extend the approach presented in [2] to determine the temperature dependence of the spin diffusion length in CuPc. This allows to draw conclucions about the spin relaxation mechanisms responsible for the polarization decay in the OSC CuPc.

[1] V.A. Dediu et al., Nature Mater. 8, 707-716 (2009)

[2] M. Cinchetti et al., Nature Mater. 8, 115-119 (2009)

O 41.36 Tue 18:30 Poster B1

**Characterization of the Interface Interaction of Cobalt on Top of Copper- and Iron-Phthalocyanine** — •Felix Schmitt, Jens Sauther, Yaou Smets, Stefan Lach, and Christiane Ziegler — Department of Physics, University of Kaiserslautern, D-67663 Kaiserslautern, Germany

A promising field of applications of organic semiconductors arises from the combination of organic materials and spintronics. In this field a deeper understanding of injection and transport as well as manipulation of spinpolarized charge carriers is necessary. The charge injection of organic semiconductor devices in general is co-determined by the geometric and the electronic structure of the specific interface and analogous behaviour is expected for the spin injection.

This motivates investigations of the interface between ferromagnetic metallic substrates and organic semiconductors. Here, a photoemission- (UPS, IPES and XPS) and IR-study of ferromagnetic cobalt on top of copper- and iron-phthalocyanine is presented. These measurements suggest chemical reactions in the interfacial region: For example, an oxidation of the Co atoms as well as a reduction of the Cu at the interface between Co and CuPc could be detected. Furthermore a diffusion of the Co into the layers of the organic substrate and the formation of Co clusters on the metal phthalocyanine surface occur.

O 41.37 Tue 18:30 Poster B1

**A Fast Model for Estimating Work-Function Modifications Induced by Organic Charge-Transfer (Sub)monolayers** — •Oliver T. Hofmann[1], Benjamin Bröker[2], Ralph-Peter

Blum[2], Ferdinand Rissner[1], Gerold M. Rangger[1], Ralph Rieger[3], Klaus Müllen[3], Norbert Koch[2], and Egbert Zojer[1] — [1]Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — [2]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstrasse 15, 12389 Berlin, Germany — [3]Max Planck Institute for Polymer Research, 55128 Mainz, Germany

Calculating work-function modifications for flat-lying conjugated molecules on extended metal surfaces using density functional theory (DFT) is an extremely resource intensive task. This prevents fast screening of new molecules for their potential to optimize metal work functions for good electron or hole injection in organic electronic devices. We present a semi-classical model, which avoids that problem. This is achieved by identifying the dominant processes occurring at the interface between metal and adsorbate in the pinning-regime, which are then parameterizing their description using band-structure DFT calculations for a small training set With the resulting interdependent equations at hand, only simple gas-phase calculations are needed to predict the work-function changes induced by new molecules. The model is tested for ten molecules on three different metal surfaces, where it shows excellent agreement with photoelectron spectroscopy data on these systems.

O 41.38 Tue 18:30 Poster B1

**Tuning surface properties via distributing dipoles in self-assembled monolayers on Au(111)** — •David A. Egger[1], Ferdinand Rissner[1], Gerold M. Rangger[1], Oliver T. Hofmann[1], Lukas Wittwer[1], Georg Heimel[2], and Egbert Zojer[1] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]Institut für Physik, Humboldt-Universität zu Berlin, Germany

Quantum-mechanical calculations are performed to study the interface between the Au(111) surface and self-assembled monolayers (SAMs) of $\pi$-conjugated molecules. Dipolar pyrimidine rings act as building units to tune the dipole moments of the SAMs in a systematic way via the number of rings in the molecular backbone. The resulting work-function modifications and the energetic alignment of the electronic states in the SAM with respect to the Fermi level are analyzed. Compared to SAMs, where strong dipole moments are introduced by end-group substitutions on otherwise non-polar molecules, an entirely different evolution of those two quantities with the backbone length is found for the present systems, where dipoles are built directly into the backbone. The distributed-dipole approach provides an additional handle for tuning surface properties and the achievable work-function modifcations can be huge. In fact, they are limited only by pinning of the metal Fermi-level at the frontier molecular states.

O 41.39 Tue 18:30 Poster B1

**Study of the electronic properties of cobalt phthalocyanine thin films on poly- and single crystalline gold substrate by photoemission spectroscopies** — •Fotini Petraki, Heiko Peisert, and Thomas Chassé — Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Auf der Morgenstelle 8, D-72076 Tübingen, Germany

Organic electronics is a new and fast developing sector of microelectronics which aims either to cover applications that are not accessible to conventional silicon semiconductor technology or to decrease the cost of the devices with the use of organic materials. In organic devices, the interfaces between the electrodes and the organic films play an important role, as they determine the injection efficiency by establishing barriers for carrier injection in the organic active layer. Therefore, interface studies contribute to the understanding and improvement of the device performance. In the present study, model experiments concerning the interface formation between Cobalt Phthalocyanine (CoPc) ultra thin films and gold substrate were carried out by X-ray and Ultra-Violet photoelectron spectroscopies (XPS, UPS) as well as Auger spectroscopy (XAES). The experimental data indicate a quite strong interaction between the organic molecules and the metallic substrate, which is confirmed by the presence of additional features at the characteristic Co2p and CoLVV peaks of the CoPc film at the very first steps of deposition. The valence band structure of CoPc is well resolved while new features are also present for monolayer coverage. Screening mechanisms in XPS and XAES are also discussed.

O 41.40 Tue 18:30 Poster B1

**Determination of Energy Levels in Organic Bulk-Heterojunction Systems** — •Holger Wetzstein[1], Stefan Krause[1], Moritz Liedtke[2], Julia Kern[2], Achim Schöll[1], Carsten Deibel[2], and Friedrich Reinert[1] — [1]Experimental Physics VII, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg

In order to improve the efficiency of electronic devices based on organic semiconducting materials the detailed knowledge about the exact position of the energy levels responsible for charge transport is crucial. The experimental determination is particularly complicated for bulk heterojunctions of p- and n-conducting materials in terms of sample preparation, film morphology and distinction of the different spectroscopic signatures. We investigated four promising materials for organic photovoltaic devices: the electron donor poly(3-hexylthiophene-2,5-diyl) (P3HT) and the three electron acceptors [6,6]-phenyl-$C_{61}$ butyric acid methyl ester ($PC_{60}BM$), its bisadduct analogue (bis-$PC_{60}BM$) and [6,6]-phenyl-$C_{71}$ butyric acid methyl ester ($PC_{70}BM$). Thin films of pristine materials as well as bulk heterojuction samples of P3HT:$PC_{60}BM$, P3HT:bis-$PC_{60}BM$ and P3HT:$PC_{70}BM$ were examined with respect to their valence levels using ultraviolet photoelectron spectroscopy (UPS).

O 41.41 Tue 18:30 Poster B1

**Preparation of $CuInS_2$ by sulfurization of CuIn samples** — •Alexandra Dombrowa, Carsten Lehmann, and Christian Pettenkofer — Helmholtz-Zentrum Berlin, Berlin, Deutschland

In search for a substitute for the heavy metal Cd in thin film solar cells based on p doped $CuInS_2$ and n doped ZnO it is proposed to use ZnS instead of CdS as buffer layer material [1,2]. By applying a MOMBE process based on diethylzinc and water a ZnS buffer layer formed on an $CuInS_2$(112) topped with CuS-segregations before epitaxial ZnO growth took place. This ZnO-ZnS-CIS interface yielded a very promising band aligment for photovoltaic applications [2]. For further band aligment investigations, which are presented in a separate talk entitled 'Band alignment studies of ZnO-ZnS-CIS interfaces', we studied polycristalline CIS films prepared in-situ by sulfurization of CuIn films. We present the results of our in-situ preparation and anaylsis of on various substrates. CuIn substrate films with a thickness of 10-100nm were prepared in-situ by MBE on Mo foil and epitaxial GaAs (111) and (100) substrates. Additionally, we used production-line quality CuIn films of 1-2 $\mu$m thickness prepared ex-situ by sputtering. The substrates and the sulfurized samples were investigated in-situ by XPS and UPS. Comparing the electrical and electronic properties of ZnS/ZnO interfaces prepared by MOMBE to epitaxially interfaces we discuss the implications with respect to an in-line process for the fabrication of the thin film solar cell devices. [1] M. Bär, et. al., Journal of Applied Physics 99 (2006) [2] S. Andres, et. al., Thin Solid Films 518 (2009)

O 41.42 Tue 18:30 Poster B1

**Tuning and Guiding Electron Current through Ag-SnPc-Ag Junctions** — •Yongfeng Wang[1], Jörg Kröger[1], Richard Berndt[1], Héctor Vázquez[2], Mads Brandbyge[2] und Magnus Paulsson[3] — [1]Institut für Experimentelle und Angewandte Physik,Christian-Albrechts-Universität zu Kiel,D-24098 Kiel,Germany — [2]Department of Micro and Nanotechnology, NanoDTU, Technical University of Denmark, DK-2800 Kongens Lyngby , Denmark — [3]Department of Physics, Kalmar University, Sweden

The transport of electrons through molecules is relevant for processes in many branches of science and has found applications in electrical engineering. Nevertheless, the understanding and, in particular, control of electron flow through metal-molecule-metal junctions on a (sub-)nanometre scale are still incomplete. Here, we report on guided electron transport through tin phthalocyanine (SnPc) contacted by silver electrodes, the tip of a cryogenic scanning tunneling microscope and a Ag(111) single crystal. By systematically modifying molecular orientations, molecule-substrate interactions, and the electrode atomic structure, the electron conductance of Ag-SnPc-Ag junctions is tuned from 1 to 25 microsiemens. Moreover, current flow through these junctions is directionally guided as visualized by supporting nonequilibrium Green's function calculations. Funding by the Deutsche Forschungsgemeinschaft through SFB 677 is acknowledged.

O 41.43 Tue 18:30 Poster B1

**Photoemission Study under Artificial Solar Irradiation: Interface Studies of the Systems Ag/$C_{60}$/CuPc and Ag/CuPc/$C_{60}$** — •Mathias Fingerle[1], Felix Schmitt[1], Ingmar Bruder[2], Stefan Lach[1], and Christiane Ziegler[1] — [1]Department of Physics, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]BASF, 67056 Ludwigshafen, Germany

During the last 3 decades research on organic solar cells has been performed and has gained increasing attention. This is due to the fact that devices can be produced at large scale and low cost. Most of today's prototype devices are of hybrid nature, i.e. the electrodes are made from inorganic materials whereas the active layers are composed by two or more organic thin films.

Here, fullerene ($C_{60}$) as n-type and copper phthalocyanine (CuPc) as p-type semiconductor were used as active organic materials. The electronic properties of the organic interfaces in layer structures composed of $Si/SiO_2/Ag/C_{60}/CuPc$ and $Si/SiO_2/Ag/CuPc/C_{60}$ were investigated by means of UPS and IPES. For the first time, UPS measurements were carried out under additional artificial solar irradiation. In particular for the interface $CuPc/C_{60}$, interesting changes in electron affinity and work function could be determined.

O 41.44 Tue 18:30 Poster B1

**Chemical trends in the metal-substrate interaction for the reactivity of 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. In this context, the so-called strong metal support interaction (SMSI) has been discussed intensively [1] which significantly influences the catalytic properties of group VIII metals. Using density functional theory, we have performed a systematic study of chemical trends in the metal-support interaction. As a first step, we considered up to four Pt atoms adsorbed on $TiO_2$, Si, Ru and Au substrates, thus making also contact to systems that are of interest in electrocatalysis. As a probe of the chemical reactivity, we determined the electronic structure of the adsorbed Pt atoms and evaluated CO adsorption energies on these metal-support systems. The results are compared to recent results of the local reactivity of surface alloy systems [1,2].

[1] S. Sakong, C. Mosch, and A Groß, Phys. Chem. Chem. Phys. **9**, 2216 (2007).

[2] Y. Gohda and A. Gross Surf. Sci. **601**, 3702 (2007).

O 41.45 Tue 18:30 Poster B1

**Non-equilibrium structures in Ultrathin V-Oxide films on Rh(111) under Reaction Conditions: The O2 + H2 reaction with and without alkali promotion** — •Martin Hesse, Florian Lovis, and Ronald Imbihl — Institut für Physikalische Chemie und Elektrochemie, Leibniz-Universität Hannover, Callinstr. 3-3a, D-30167 Hannover, Germany

As a model system for vanadium-oxide based catalysts we prepared ultrathin vanadium oxide films on a Rh(111) surface1. At 400°C 0.1, 0.25 and 2.4 ML of vanadium were evaporated in oxygen with p(O2)=2*10-7 mbar. After characterization with LEED and Auger electron spectroscopy the films were subjected to the O2 + H2 reaction using photoemission electron microscopy (PEEM) as spatially resolving method. After evaporation a large variety of differently ordered Rh(111)/V/O phases were identified in LEED. The O2 + H2 reaction was studied in the 10-8 - 10-5 mbar range at temperatures between 400 and 500°C. With PEEM we observe that under reaction conditions the film is no longer homogeneous but reaction fronts and stationary Turing-like patterns develop. In the evaporated V-film we find partially ordered patterns which are very stable and change only very slowly after turning off the gases. The patterns induced by the reaction are discussed in the context of the concept of reactive phase separation. When we promote the Rh(111)/V/O-system with alkali metals turbulent spatialtemporal patterns are found.

[1] Surnev, S., M.G. Ramsey, and F.P. Netzer, Progress in Surface Science, 2003. 73, 117.

O 41.46 Tue 18:30 Poster B1

**Ab initio molecular dynamics simulation of electronic energy dissipation: HCl/Al(111)** — •Michael Grotemeyer and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel, Germany

The scattering of vibrationally excited HCl molecules from Au(111) has been studied experimentally and interpreted in view of electronically nonadiabatic processes [1]. We present *ab initio* molecular dynamics simulations of the scattering of highly vibrationally excited HCl molecules at Al(111). The time-dependent Kohn-Sham equations are integrated numerically for the electrons, and the positions of the ions follow Ehrenfest dynamics. The electronic excitation along the trajectory is obtained from comparison of the time-dependent electronic structure with the electronic ground state at the respective frozen-in ionic positions. Reducing numerical expenses, the simulations are carried through for mass-scaled systems. Under the assumption of linear friction, the dissipation is extrapolated to the physical masses of the ions [2]. For not vibrating HCl molecules we obtain only a faint energy transfer into electron-hole pairs. Electronic energy dissipation is significant for a strongly vibrating HCl molecule in front of Al(111). Different geometries with either the H-or Cl-atom pointing towards the surface are compared. We note that electronic friction has turned out not to be enhanced for a situation where the H-atom points towards the surface and oscillates in the charge density tail of the metal.

[1] I. Rahinov *et al.*, J. Chem. Phys. **129**. 214708 (2008).

[2] M. Lindenblatt and E. Pehlke, Surf. Sci. **23**, 5068 (2006).

O 41.47 Tue 18:30 Poster B1

**Cluster-induced desorption of alkali halides from metals and insulators - influence of substrate and adsorbate configuration** — B.-J. Lee[1], C.R. Gebhardt[2], H. Schröder[3], K.L. Kompa[3], and •M. Dürr[1] — [1]Fakultät Angewandte Naturwissenschaften, Hochschule Esslingen, Esslingen — [2]Bruker Daltonik GmbH, Bremen — [3]Max-Planck-Institut für Quantenoptik, Garching

Cluster-induced desorption is a versatile tool for the investigation of surface adsorbates. During cluster surface collision, the system is heated to high temperatures on a very short time scale, thus activating reactions not accessible by means of conventional heating. As an example, fragmentation-free desorption of biomolecules as large as 6000 u from various surfaces has been demonstrated [1].

For surface adsorbates prepared wet-chemically from alkali halide solutions, we show that the surface configuration, especially the influence of water molecules, can be monitored by cluster-induced desorption. As long as the anions are effectively screened by a hydration shell, they are efficiently desorbed by means of cluster impact. To higher surface temperatures, the hydration shell is lost and a strong adsorbate-surface bond prevents desorption of the anions. Cations are seen to desorb from metals via a neutral desorption channel with subsequent charge separation in the cluster whereas only a positive signal is observed for desorption from insulators.

[1] Gebhardt *et al.*, Angew. Chem. Int. Ed. **48**, 4162 (2009).

O 41.48 Tue 18:30 Poster B1

**Adsorption and reactions of unsaturated hydrocarbon molecules on stepped Pt surfaces** — Erik Darlatt[1], Sandra Wickert[1], Michael P. A. Lorenz[2], Regine Streber[2], Christian Papp[2], Hans-Peter Steinrück[2], and •Reinhard Denecke[1] — [1]Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnestr. 2, 04103 Leipzig, Germany — [2]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany

Using in-situ high-resolution XPS at the synchrotron radiation source BESSY II, bonding configurations of ethylene and propylene have been investigated on stepped Pt surfaces. Ethylene adsorbs on Pt(355) with significant spectral changes in C 1s compared to Pt(111), resulting from a specific step related feature. The saturation coverage related to this more strongly bound species amounts to about 1/3 of the terrace population. For propylene, two different C 1s binding energies can be related to the three carbon atoms. On Pt(355), a structureless peak results from additional step contributions. For both adsorbates, the respective alkylidin species appears as the major dissociation intermediate. Differences in thermal reactivity between flat and stepped Pt are observed for both molecules in temperature-programmed (TP-) XPS experiments.

This work was supported by BMBF (05 ES3XBA/5).

O 41.49 Tue 18:30 Poster B1

**Locally resolved kinetics of catalytic CO oxidation on polycrystalline platinum** — •Diana Vogel[1,2], Christian Spiel[1], Yuri Suchorski[1], Wolfgang Drachsel[1], Robert Schlögl[2], and Günther Rupprechter[1] — [1]Institute of Materials Chemistry, Vienna University of Technology, Austria — [2]Fritz Haber Institute (Max-Planck-Gesellschaft), Berlin, Germany

In this contribution we present a microscopic study of the kinetics of the catalytic CO oxidation reaction on a polycrystalline Pt foil consisting of (100)-, (110)- and (111)-type domains (∼100 $\mu$m) under reaction conditions (reactants pressure $\sim 10^{-5}$ mbar ). The study was performed by combination of photoemission electron microscopy (PEEM) with mass-spectroscopy (MS). PEEM allows an *in situ* observation of the local kinetic phase transitions in the reaction, MS, in turn, provides the global kinetics. By combining the laterally resolved (PEEM) and global (MS) data we elucidate the role of the individual domains in the reaction and elaborate the contributions of the particular domains to the global kinetics. We show that the global kinetic phase diagram can be composed as a superposition of the local kinetic phase diagrams of the individual domains.

Furthermore, we compare the catalytic behaviour of the polycrystalline Pt foil with that of a Pt(111) single crystal and a sputtered Pt foil to show the influence of the surface morphology on the reaction kinetics. Increasing surface roughness shifts the kinetic phase diagram to lower temperature and higher partial CO pressure.

O 41.50 Tue 18:30 Poster B1

**In-situ XPS and reactivity studies on different Au/TiO2 catalyst systems** — •Martina Hank, Karif Dumbuya, Ole Lytken, Piotr Bobrowski, Bernhard Arnold, J. Michael Gottfried, and Hans-Peter Steinrück — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen, Germany

Nano-sized gold on oxidic substrates shows a high activity in heterogeneous catalysis which sharply contrasts the inertness of bulk gold. The origin of the catalytic activity and the nature of the active sites are still discussed controversially: Quantum size effects, low coordinated gold atoms, the substrate/gold perimeter interface or anionic as well as cationic gold species have been considered as possible candidates. We have studied surfaces of different gold-based catalysts using X-ray photoelectron spectroscopy (XPS) under ultra high vacuum conditions as well as with in-situ XPS in the presence of reactive gases (CO, $O_2$, propene and mixtures thereof) at pressures of up to 1mbar. These model systems include a Au/$TiO_2$ reference powder catalyst, a Au/$TiO_2$(110) planar model catalyst and a $TiO_2$/Au(111) inverse model catalyst. Comparison of the latter systems enables us to discriminate between cluster-size and interface related effects. Furthermore, we will discuss a novel reaction cell, which is used to study the activity of different model catalysts under ambient pressure conditions.

This work is supported by the DFG through grant GO 1812/1-1 and by the Cluster of Excellence "Engineering of Advanced Materials"

O 41.51 Tue 18:30 Poster B1

**Cluster Model Studies on Catalytic Sulfidation of $MoO_3$** — Xue-Rong Shi[1,2], Mathis Gruber[2], •Klaus Hermann[2], and Jianguo Wang[1] — [1]State Key Laboratory of Coal Conversion, Institute of Coal Chemistry, Chinese Academy of Sciences, Taiyuan, Shanxi 030001, P.R. China; — [2]Fritz-Haber-Institut der MPG, Faradayweg 4-6, D-14195 Berlin and Sfb 546 "Transition Metal Oxide Aggregates", Berlin (Germany).

$MoS_2$-based catalysts, initially prepared from $MoO_3$, are known to yield high activity and selectivity for the production of mixed alcohols. This makes research on the sulfidation of $MoO_3$ quite important. Here we apply density-functional theory (DFT) together with large surface clusters (cluster code StoBe) to study the sulfidation of the $MoO_3$(010) surface as well as hydrogen adsorption at an atomic level. Surface oxygen is always found to bind more strongly with its substrate than its sulfur substitute with binding distances that are shorter for oxygen than for sulfur. Sulfur-oxygen exchange reactions are energetically preferred over sulfur adsorption at $MoO_3$(010). Further, sulfur binding is found to be facilitated by the existence of surface oxygen vacancies where sulfur substitution takes place preferentially at the singly coordinated O(1) site. Hydrogen adsorption at the perfect and sulfidic surface leads to stable OH, $H_2O$ and SH, $H_2S$ groups which are quite weakly bound and may easily adsorb. Thus, the presence of pre-adsorbed hydrogen facilitates oxygen and sulfur removal from the $MoO_3$(010) surface which is in qualitative agreement with earlier findings.

O 41.52 Tue 18:30 Poster B1

**Homogeneity and catalytic activity of thin mesoporous Au/$TiO_2$ layers** — •Matthias Roos, Menhild Eyrich, Gabriela Kucerova, Joachim Bansmann, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

Structurally defined thin layers of homogeneous mesoporous Au/$TiO_2$ are investigated as model systems to bridge the gap between planar Au/$TiO_2$ model and powder catalysts. The dispersed mesoporous Au/$TiO_2$ catalysts were found to be significantly more active in the CO oxidation reaction [1] than catalysts based on non-porous $TiO_2$ powder (P25). Catalytically active thin Au/$TiO_2$ films are prepared by deposition of the Au/$TiO_2$ catalyst, e.g. via dip coating on planar oxide substrates. The structural integrity and the chemical properties of the obtained layers are characterized by electron microscopy methods and XPS, respectively. The local catalytic activity and homogeneity of the mesoporous Au/$TiO_2$ films for CO oxidation is studied by mass spectrometry, using a scanning mass spectrometer setup. Furthermore, IR measurements are planned in order to derive combined catalytic and in-situ spectroscopic information.

[1] Y. Denkwitz et al., *Appl.Catal.B* 91, **2009**, 470.
[2] M. Roos et al., *Rev.Sci.Instrum.* 78, **2007**, 084104.

O 41.53 Tue 18:30 Poster B1

**Methanol oxidation over ZnO and Au/ZnO nanoparticles studied by vibrational spectroscopy** — •Heshmat Noei[1], Martin Muhler[1], and Yuemin Wang[1,2] — [1]Lehrstuhl für Technische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, 44801 Bochum, Germany

Zinc oxide is one of the most studied materials due to its electrical, optical and catalytical properties and potential applications. The interaction of methanol with zinc oxide is a topic of fundamental and applied interest. In this work we report on the adsorption and oxidation of methanol over ZnO nanoparticles at a wide range of temperatures by employing a newly designed ultra-high vacuum infrared spectroscopy (UHV-FTIRS). Exposing the clean ZnO nanopowders to methanol at 110 K leads to the molecular adsorption, whereas at 300 K methanol is adsorbed dissociatively giving methoxy species. The FTIRS data further indicate the formation of two different methoxy species which are bound to the polar ZnO(000-1) and nonpolar ZnO(10-10) surfaces, respectively. During heating to higher temperatures, methoxy reacts partially with surface oxygen yielding formate species as confirmed by the appearance of formate-related IR bands. In addition, we could identify two different formate species, which are formed on ZnO(000-1) and ZnO(10-10) surfaces, respectively. Upon heating to 600 K, both formate species are decomposed completely. We have further studied methanol oxidation over Au/ZnO nanopartcles. The corresponding reaction mechanisms will be discussed in details.

O 41.54 Tue 18:30 Poster B1

**Interaction of propene with an oxygen-precovered Au(110)*(1x2) surface** — •Inga Spreine and Klaus Christmann — Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany

We have studied the interaction of propene with the $(1x2)$-reconstructed $Au(110)$ surface covered with well-defined amounts of reactive atomic oxygen species by means of thermal reaction mass spectrometry. The chemisorbed $O$ atoms were obtained by electron-bombarding an equilibrium coverage of physisorbed oxygen molecules at $T = 35$ K and $p(O_2) = 2 \cdot 10^{-8}$ mbar. The presence and amount of reactive $O$ was monitored and controlled by the well-known TD states appearing between 450 and 550 K [1]. After dosing defined amounts of propene at $T = 90$ K we looked for possible partial and total oxidation products and their fragments. Desorption of the total oxidation products $CO_2$ (m/z 44) and $H_2O$ (m/z 18) occurs between 170 and 520 K and represent the majority of the reaction products. Nevertheless, we were able to also detect minor amounts of partial oxidation products like propene oxide (m/z 58 and 31) and acrolein (m/z 55 and 56). The formation of acrylic acid (m/z 72) and acetone (m/z 43), however, could not be observed. Our results are discussed and compared with similar previous investigations on the $Au(111)$ [2] and the $Au(100)$ and $Au(111)$ surfaces [3].

[1] M. Gottfried et al., Surf. Sci. 511 (2002) 65 [2] X. Deng et al., J. Phys. Chem. B 110 (2006) 15982 [3] K.A. Davis and D.W. Goodman, J. Phys. Chem. B 104 (2000) 8557

O 41.55 Tue 18:30 Poster B1

**Femtosecond EUV photoelectron spectroscopy of phase transitions** — •Hatem Dachraoui[1], Christian Oberer[1], Günter Obermeier[2], Martin Michelswirth[1], Siegfried R. Horn[2], and Ulrich Heinzmann[1] — [1]Molecular and Surface Physics, Bielefeld University — [2]Experimental Physics II, Universität Augsburg

The thermo-induced insulator-metal phase transition in Vanadium dioxide (VO2) was investigated by use of a combination of a femtosecond EUV light source with time-of-flight (TOF) analysis of the emitted photoelectrons. The observed spectra give evidence of the changes in the electronic structure depending on temperature. Based on an analysis of the V3p- core level shift we get access to structural deviation of the VO2 and the changes of the density of states near the Fermi level responsible for the phase transition. The shift we obtained manifests this transition with its characteristic hysteresis.

O 41.56 Tue 18:30 Poster B1

**In-situ XRD studies on post deposition annealed iron oxide thin films** — •Florian Bertram[1], Carsten Deiter[1], Kathrin Pflaum[1], Oliver H. Seeck[1], Martin Suendorf[2], and Joachim Wollschläger[2] — [1]HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany — [2]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany

Because of their magnetic properties, iron oxide thin films are of interest for spintronic devices. Also, they can be used for model catalyst studies. Due to the small lattice mismatch to all iron oxide phases, MgO is a good choice as a substrate.

Here, we present studies on highly oxidized iron oxide films epitaxially grown on MgO(001), which have been annealed under vacuum conditions at beamlines BW2, W1 and P08 at DESY. For this purpose a UHV sample cell with heating and cooling capacity was developed.

Before annealing the sample it was analyzed by XRR and XRD. During the annealing process we performed CTR scans at the $(002)_{BULK}$ MgO peak, where all iron phases also have peaks. After cooling down the sample it was again analyzed by XRR and XRD.

Our analysis of the XRD measurements using kinematic diffraction theory shows a decrease in the iron oxide lattice constant pointing to a reduction of the iron oxide film.

O 41.57 Tue 18:30 Poster B1

**Deposition of Fe nanoparticles on thin Co(0001) films** — •Volker Hückelkamp[1], Wolfgang Rosellen[1], Christian Kleinhans[1], Furkan Bulut[1,2], Joachim Bansmann[2], Armin Kleibert[3], and Mathias Getzlaff[1] — [1]Institute of Applied Physics, University of Düsseldorf, Germany — [2]Department of Surface Chemistry, Ulm University, Germany — [3]Swiss Light Source at the Paul Scherrer Institute, Villigen, Switzerland

In recent years, 3d-metal nanoparticles are characterised by increasing importance, especially because of their magnetic properties which significantly differ from bulk behaviour. In this contribution we focus on Fe nanoparticles being deposited on thin Co films which are prepared on a W(110) crystal and exhibit a thickness between 1 and 15 ML. These films are acting as supporting material for the nanoparticles and are characterised by Auger electron spectroscopy (AES), low energy electron diffraction (LEED) and scanning tunneling microscopy (STM). Mass filtered Fe nanoparticles with a diameter ranging from 3 nm to 15 nm are produced by a continuously working arc cluster ion source (ACIS) and deposited on thin Co(0001) films under UHV condition in order to avoid any influence due to oxidation and contamination. We will discuss their structural properties and correlate them with their magnetic behaviour investigated by X-ray magnetic circular dichroism (XMCD)[J.Bansmann, A.Kleibert, Appl. Phys. A **80**, 957 (2005)].

O 41.58 Tue 18:30 Poster B1

**Influence of temperature on the shape of deposited nanoparticles** — •Wolfgang Rosellen[1], Georg Oeltzschner[1], Christian Kleinhans[1], Volker Hückelkamp[1], Furkan Bulut[1,2], Joachim Bansmann[2], Armin Kleibert[3], and Mathias Getzlaff[1] — [1]Institute of Applied Physics, University Düsseldorf — [2]Dep. of Surface Chemistry, Ulm University — [3]Paul Scherrer Institute, Switzerland

In this contribution we focus on the temperature behaviour of mass filtered Fe, Co and FeCo nanoparticles with diameters between 3 nm and 15 nm deposited on W(110). In RHEED experiments the orientation of mass filtered deposited Fe nanoparticles could be determined [1]. It was shown that small deposited Fe particles with diameter being less than 4 nm exhibit a spontaneously alignment, whereas larger particles with diameter of about 13 nm are randomly oriented on the W(110) surface. The temperature depending melting and orientation of deposited *3d*-metal nanoparticles produced by a continuously working arc cluster ion source (ACIS) will be discussed. The shape of the deposited nanoparticles is investigated in-situ by scanning tunneling microscopy (STM).

[1] A. Kleibert, A. Voitkans, and K. H. Meiwes-Broer, (submitted).

O 41.59 Tue 18:30 Poster B1

**STM-Study of Cu growth on ZnO and TiO$_2$ Surfaces** — •Martin Kroll[1], Abelhadi Chakir[1], Thomas Kuschel[1], Thomas Löber[1], Renate Wansing[1], Vadim Schott[2], Christof Wöll[2], and Ulrich Köhler[1] — [1]Experimental Physics IV, Ruhr-Universität Bochum, Germany — [2]Physical Chemistry I, Ruhr-Universität Bochum, Germany

The growth of Cu on ZnO(10$\bar{1}$0) and TiO$_2$(110) single crystal surfaces was studied as a first step to understand complex catalytically active systems often consisting of small metal clusters on metal oxide surfaces. For local STM studies flat and clean surfaces are needed. On ZnO(10$\bar{1}$0) the influence of the UHV preparation conditions and the substrate orientation (sample miscut) on the large scale morphology was studied [1].

Cu was deposited on ZnO(10$\bar{1}$0) by MOCVD. Thermal treatment resulted in a decreasing Cu coverage with increasing temperature up to 670K as already shown for Cu MBE depositon on ZnO(0001) [2]. Chemical analysis of the reaction of the Cu clusters with the ZnO substrate was done by XPS measurements.

Additionally, MBE Cu-growth with comparable coverage and similar thermal treatment on rutile TiO$_2$(110) was studied. In this case no decrease in Cu coverage up to annealing temperature of 670K was detected.

[1] M.Kroll et al., Surf. Sci. **603**, L49 (2009)

[2] M.Kroll, U. Köhler, Surf. Sci. **601**, 2182 (2007)

O 41.60 Tue 18:30 Poster B1

**Thermal Boundary Conductance of Bi/Si-Heterolayers: An Ultra-Fast Time-Resolved Electron Diffraction Study** — •Simone Möllenbeck, Anja Hanisch-Blicharski, Annika Kalus, Boris Krenzer, Martin Kammler, and Michael Horn-von Hoegen — Department of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE) Universität Duisburg-Essen, D-47057 Duisburg, Germany

The transient heating and cooling of hetero epitaxial thin film systems after fs-laser excitation with ps time resolution was studied by means of ultra fast time resolved electron diffraction in a grazing reflection geometry (RHEED). Diffraction patterns taken at different delays between pumping laser pulse and probing electron pulse are converted to the film temperature using the Debye-Waller effect. We present results on ultra thin epitaxial Bi(111) films on Si(001) and Si(111) substrates. For a 6 nm thin Bi-film a rapid increase of the surface temperature from 80 K up to 190 K upon laser excitation is followed by a slow exponential decay with a decay constant of 640 ps which is dominated by total internal reflection of the phonons at the hetero interface between film and substrate. A linear dependence, as predicted by the theoretical models, between film thickness and decay constant can be observed for the Bi-films on Si(111) down to 2.5 nm thickness. In contrast to this we observe a constant cooling rate for the Bi/Si(100) system for films thinner than 6 nm. The extreme low cooling rate for these thin films is determined not longer by the travel time through the film but by the mean free path of the phonons.

O 41.61 Tue 18:30 Poster B1

**DFT calculations on influence of co-adsorbed Cl on the self-diffusion on Au(100)** — •Mostafa Mesgar, Josef Anton, John A Keith, and Timo Jacob — Uni Ulm, Albert-Einstein-Allee 47

Adatom and vacancy diffusions play crucial roles in adsorption, desorption, crystal growth, and coarsening on metal surfaces. While several experimental and theoretical studies focused on the formation and diffusion of point defects on terraces, leading to a detailed understanding, much less is known about diffusion at steps and kink sites, even though this plays an important role in processes such as metal deposition and dissolution, Ostwald ripening, island and step fluctuations. Using *ab initio* density-functional theory, we investigated the self-diffusion behavior of adatoms on Au(100) surfaces with and without surface defects (e.g. steps, kinks, or vacancies) [1]. On terraced Au(100) surfaces, we find that exchange diffusion is the lowest energy mechanism while bridge diffusion is the next lowest. With surfaces in the presence of a perfect step edge, we find an even lower barrier for diffusion along the step-edge identifying that rearrangement of clusters will be faster than aggregation processes. This signifies that cluster edges might behave as catalysts. Afterwards we studied the influence of co-adsorbed Cl on the self-diffusion behavior, which turned out to have a drastic impact even on rather simple diffusion processes. Based on our present results the next aim is to perform large scale simulations, which then will provide macroscopic quantities readily comparable to experiments. [1] K. Pötting, T. Jacob, *et al.*, *High Performance Computing in Science and Engineering*, Springer-Verlag GmbH, Heidelberg, Germany (2006).

O 41.62 Tue 18:30 Poster B1

**Characterisation and setup of a noncollinear optical parametric amplifier and investigation of ultrafast dynamics of Na/Cu(111)** — •Daniel Wegkamp[1,3], Marcel Krenz[1,3], Uwe Bovensiepen[2,3], and Martin Wolf[1,3] — [1]Fritz Haber Institute of the MPG, Dept. of Physical Chemistry, Berlin, Germany — [2]Universität Duisburg-Essen, Dept. of Physics, Duisburg, Germany — [3]Freie Universität Berlin, Dept. of Physics, Berlin, Germany

To study ultrafast dynamics on a femtosecond timescale, laser pulses of comparable and shorter scale are used in this work in combination with 2-photon photoemission. Here, we report the principle, setup, and characterisation of a femtosecond light-source based on a noncollinear optical parametric amplifier (NOPA) and its application in studying the dynamics of Na/Cu(111) following [1]. Laser pulses with duration $<$ 20 fs have been generated in the visible spectral range using a 300 kHz regenerative amplifier. In a single color scheme ($h\nu = 2.3$ eV) the NOPA pulses are used to excite and photoemit hot electrons, which are detected with a time of flight (TOF) spectrometer. With time independent measurements the binding energy of the adsorbate-induced resonance at 2 eV is observed in agreement with [2]. As a function of pump-probe delay a time-dependent binding energy shift of the Na resonance with -2 meV/fs is observed. This shift is explained as a pump-induced movement of the sodium adsorbate away from the surface. All experiments were conducted at the Freie Universität Berlin.

[1] H. Petek et al., Science 288 (2000) 1402
[2] N. Fischer et al., Surf. Sci. 314 (1994) 89

O 41.63 Tue 18:30 Poster B1

**Ultra-Fast Time Resolved Electron Diffraction of Vibrational Dynamics in an Adsorbate Layer: ($\sqrt{3} \times \sqrt{3}$) Pb on Si(111)** — •Annika Kalus, Simone Möllenbeck, Paul Schneider, Anja Hanisch-Blicharski, Boris Krenzer, Martin Kammler, and Michael Horn-von Hoegen — Department of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE), Universität Duisburg-Essen, 47057 Duisburg, Germany

We use ultra-fast time resolved electron diffraction to analyze structural dynamics of adsorbates on surfaces on a ps-timescale upon excitation by fs-laser pulses. Surface sensitivity is obtained by a RHEED (reflection high energy electron diffraction)-geometry. Utilizing the Debye-Waller effect the damping of the vibrational amplitude of the adsorbate atoms could be followed as function of time in a pump probe set up. As an example we used the ($\sqrt{3}\times\sqrt{3}$) Pb/Si(111) system which was prepared by deposition of Pb on Si(111) - ($7\times7$) at 300 K followed by an annealing step to 500 K. As a result we obtained a Pb ($\sqrt{3}\times\sqrt{3}$) reconstruction with a coverage of one monolayer and a small number of large Pb islands. After excitation we measure a relaxation time constant of the hot adsorbate system of 150 ps. This low cooling rate is explained by the huge difference in mass of Si and Pb atoms which prevents effective coupling of the Pb vibrational modes to the phonon bath in Si substrate.

O 41.64 Tue 18:30 Poster B1

**Surface excitations of oxygen passivated Fe(001)** — •Pavel Ignatiev, Yu Zhang, Khalil Zakeri, Valery Stepanyuk, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Recent advances of spin polarized electron energy loss spectroscopy (SPEELS) [1] open up possibilities of simultaneous mapping of phonons and magnons on complex surfaces. This issues a challenge to reveal the properties of lattice dynamics, magnetic excitations and their couplings. We present a combined experimental and theoretical study of elementary excitations on the oxidized Fe(001) surface. Experimental measurements performed by means of SPEELS reveal 4 surface-related phonon branches and one magnon branch. Calculations of the force matrix from the ab initio input corroborate experimentally observed phonon dispersions. Special attention is paid to the phonons localized at oxygen atoms. Vertical vibrations of oxygen are accompanied by significant changes of the magnetic moment on the O atoms, which possibly can result in a magnon-phonon coupling.

[1] J. Prokop et al., Phys. Rev. Lett. 102, 177206 (2009).

O 41.65 Tue 18:30 Poster B1

**Mechanics at the molecular scale: Insight into the physical mechanisms** — •Olga A. Neucheva, Ruslan Temirov, and Stefan Tautz — Institut für Bio- und Nanosysteme (IBN-3) and JARA - Fundamental of Future Information Technology, Forschungszentrum Jülich, 52425 Jülich, Germany

The manipulation of atoms and molecules is one of the problems under investigation in a surface science. The first successful attempt to transfer an atom from a surface with use of a scanning tunneling microscope has been realized by Eigler et al [1]. An interest to understand the underlying physical mechanism from both experimental and theoretical points of view has led to investigations of many systems which can be used as atomic and molecular switches [2,3]. In our work the behaviour of a single PTCDA molecule on Ag(111) has been investigated with a LT-STM. Two level fluctuations of the conductance of the junction have been observed within a narrow range of the tip heights and bias voltages. The bistability is related to reversible switching of one of the carboxylic oxygen atoms between the surface and the STM-tip. The current passing through the junction induces vibrations of the molecule leading to weakening and breaking of a chemical bond with the surface and establishing a new one with the tip and vice versa. The switching frequency strongly depends on the bias voltages and tip heights, following a non-linear dependence on the current.

[1] D.M.Eigler, C.P. Lutz, and W.E. Rudge, Nature 352, 600 (1991)
[2] J.A. Stroscio, and R.J. Celotta, Science 306, 242 (2004)
[3] S. Gao, M. Persson, and B.I. Lundqvist, PRB 55, 7 (1997)

O 41.66 Tue 18:30 Poster B1

**Rate oscillations in the O2 + H2 reaction on a Rh(111) surface alloyed with nickel** — •Tim Smolinsky, Florian Lovis, and Ronald Imbihl — Institut für Physikalische Chemie und Elektrochemie, Leibniz-Universität Hannover, Callinstr. 3-3a, D-30167 Hannover, Germany

A Rh(111)/Ni surface with Ni in the submonolayer range was prepared by decomposing Ni(CO)4 at the Rh(111) surface. After characterization with low energy electron diffraction (LEED) and Auger electron spectroscopy the surface was subjected to the O2 + H2 reaction using photoemission electron microscopy (PEEM) as spatially resolving method. On a clean Rh(111) surface the O2 + H2 reaction is a bistable system. The alloying with nickel changes the system into an excitable medium. The reaction was studied in the 10-7 - 10-4 mbar range at temperatures between 300 and 700 °C. With PEEM chemical wave patterns involving simple reaction fronts have been observed. Under particular reaction conditions spiral waves and target patterns can be triggered. These spatiotemporal patterns were accompanied by rate oscillations observed with mass-spectrometry.

O 41.67 Tue 18:30 Poster B1

**Time-, energy-, and angle- resolved two-photon photoemission spectroscopy on Cu(1 1 11) with the Themis 1000** — •Jens Kopprasch[1,2], Martin Teichmann[1], Kristof Zielke[1,2], Oliver Schaff[3], Sven Mähl[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]SPECS GmbH, Voltastraße 5, 13355 Berlin, Germany

We present two-photon photoemission measurements with the angle-resolved time-of-flight spectrometer THEMIS 1000. The electrostatic lens system of the electron analyzer PHOIBOS (SPECS) in combination with a delay-line detector allows us to measure the kinetic energy ($E_{kin}$) and the wave vector parallel to the surface ($k_\|$) of the photoemitted electrons. Due to the axial symmetry of the spectrometer, $k_x$ and $k_y$ are detected without rotating the sample.

We present measurements on Cu(111), where we observe the first and second image-potential states. Furthermore, we measured the surface states at Cu(11 11), a vicinal surface with (001)-terraces. Depending on the $k_\|$-direction, we observe different dispersion of the surface states and lifetimes.

O 41.68 Tue 18:30 Poster B1

**Design and operation of a microscopy setup for optical second harmonic generation** — •Gerson Mette[1], Kristina Klass[1], Michael Dürr[1,2], Jens Güdde[1], and Ulrich Höfer[2] — [1]Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität Marburg, D-35032 Marburg — [2]Fakultät Angewandte Naturwissenschaften, Hochschule Esslingen, D-73728 Esslingen

Laser-induced processes like desorption or diffusion often show a strong non-linear dependence on laser fluence. As a consequence, the desorption- or diffusion-rates differ strongly for different areas of the excited surface because of the laser's beam profile.

We present a setup for spatially resolved optical second-harmonic generation (SHG), i.e. SHG-microscopy, and illustrate its operation on the basis of our time-domain study of laser-induced diffusion of oxygen on a vicinal Pt(111) surface at low substrate temperature. Femtosecond laser pulses excite not only the diffusion of oxygen on the surface itself but also generate the second-harmonic light which is detected spatially resolved by an intensified CCD camera. Magnification of the area of interest on the sample to the CCD chip is achieved by a commercial camera lens. The fluence dependence of the diffusion process can be measured in real space across the laser's beam profile. In combination with a two-pulse correlation experiment, the fluence dependence of the energy transfer time between electronic and adsorbate system can be investigated in the same way.

O 41.69 Tue 18:30 Poster B1

**Femtosecond VUV and Soft X-Ray Pulses for Surface Spectroscopy** — Robert Carley[1], Kristian Döbrich[1], Cornelius Gahl[1], •Matin Teichmann[1], Kai Godehusen[2], Olaf Schwarzkopf[2], Frank Noack[1], Philippe Wernet[2], and Martin Weinelt[1,3] — [1]Max-Born-Institut, Max-Born-Straße. 2A, 12489 Berlin, Germany — [2]Helmholtz-Zentrum für Materialien und Energie, Elektronenspeicherring BESSY II, Albert-Einstein-Straße 15, 12489 Berlin, Germany — [3]Fachbereich Physik der Freien Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

We present initial characterization results of a newly developed high-order harmonics (HHG) VUV beamline. It will be used to perform time-resolved studies of metal- and semiconductor surfaces, and of gas-phase molecular systems, and we show our first photoemission spectra from the W (110) surface. The HHG source is driven by the output of a commercial Ti-sapphire multipass laser amplifier generating 40 fs pulses at a repetition rate of 10 kHz, focused into an Ar-filled gas cell to create high-order harmonics. Following separation from the IR with an Al foil filter, a toroidal mirror images the HHG source onto the entrance slit of a toroidal grating monochromator, which selects a particular harmonic and the bandwidth of the transmitted radiation. A second toroidal mirror images the output slit of the monochromator onto the experimental sample housed in a custom-built UHV chamber equipped with a image-type hemispherical electron kinetic energy analyser. The VUV can be combined with a time-delayed IR pump beam from the driving laser in order to perform time-resolved measurements.

O 41.70 Tue 18:30 Poster B1

**Exploiting the quantum confinement of electrons for studying and engineering of magnetic properties of nanostructures at surfaces: an *ab Initio* study** — •Oleg O. Brovko and Valeri S. Stepanyuk — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

In the presented contribution we demonstrate, that the quantum confinement of electrons might just prove to be a universal tool for both studying and engineering magnetic properties of surface-bound nanostructures.

We demonstrate that it is possible to resolve magnetic properties and coupling of small clusters buried up to 1.5 nm deep beneath a metallic surface by studying the electrons confined between the nanostructure and the vacuum barrier [1]. We also demonstrate, that the exchange coupling of adatoms and addimers adsorbed at the surface to buried magnetic structures is strongly dependent on the local confinement of electrons in the host metal and can be manipulated by a deliberate variation of the nanostructure's burying depth [2]. Finally we point out the possibility to utilize the quantum confinement of electrons on nanoscale islands in order to tune the coupling of single spins [3].

[1] O. O. Brovko, V. S. Stepanyuk, W. Hergert, and P. Bruno, Phys. Rev. B **79**, 245417 (2009).

[2] O. O. Brovko, P. A. Ignatiev, V. S. Stepanyuk and P. Bruno, Phys. Rev. Lett. **101**, 036809 (2008).

[3] O. O. Brovko, W. Hergert, and V. S. Stepanyuk, Phys. Rev. B **79**, 205426 (2009).

O 41.71 Tue 18:30 Poster B1

**Oxidative properties of $Co_mPt_n$ clusters** — •Ivan Baev, Kai Chen, Steffen Fiedler, Michael Martins, and Wilfried Wurth — Universität Hamburg, Institut für Experimentalphysik

From investigations of the magnetic properties of $Co_mPt_n$ clusters with XMCD it could be seen that the presence of Pt in these clusters can enhance their probability to oxidize. Now these oxidative properties are studied systematically.

It is possible to create small, mass-selected clusters with the size of several atoms with the "ICARUS" cluster source. The created clusters are landed onto a Cu(100) surface with a surface coverage of approximately 5% and investigated with XPS. We measure the Co-2p photoemission lines of Co, $Co_2$, CoPt and $Co_2Pt$ clusters to gather information about their oxidative properties. The goal is to measure the change in shape and position of the 2p-lines if the clusters are exposed to a particular oxygen atmosphere and temperature. For comparison CoO and $Co_2O$ clusters can also be created directly with "ICARUS".

A proof of the oxidative properties of Pt in $Co_mPt_n$ clusters is a starting point to search for other reactions that are mediated by $Co_mPt_n$.

The small size of $Co_mPt_n$ clusters allows in principle to conduct in depth theoretical calculations. This can lead to new predictions of catalytic active clusters.

This work is supported by the DFG through the collaboration research center SFB 668.

O 41.72 Tue 18:30 Poster B1

**Ab initio investigations of Co and Ni adlayers on wide-band-gap semiconductors** — •Bernd Stärk, Peter Krüger, and Johannes Pollmann — Westfälische Wilhelms-Universität, Münster

Metal-semiconductor hybrid systems feature novel functionalities which are not feasible with metals or semiconductors alone, combining, e.g., the high conductivity and spin-polarization of ferromagnets with the controllability of semiconductors. In this contribution, we present the results of a comparative study of Co and Ni multilayers on diamond as well as SiC surfaces employing the generalized-gradient approximation of density-functional theory.

Adsorption of Co/Ni adlayers on the C(001)/C(111)-(1x1) surface is distinguished by a very small lattice mismatch. For one adlayer the metal adatoms are found to be located in a position where all surface dangling bonds are saturated. They form covalent *pd* bonds giving rise to characteristic bonding and antibonding bands which exhibit no significant spin splitting. These bonds markedly reduce the magnetic moment at the interface. Adding further adlayers reveals that this effect is very localized and does hardly affect neighboring metal layers. Spin polarization at the Fermi level is quite large amounting to about 50% which is a prerequisite to spintronic applications.

Furthermore, we compare this behaviour to Co/Ni-deposited 6H-SiC(0001) surfaces. They show complex $2\sqrt{3} \times 2\sqrt{3}$ reconstructions due to a large lattice mismatch between the substrate and the adlayers. We discuss implications on the structural and electronic properties and compare our results to experimental findings.

O 41.73 Tue 18:30 Poster B1

**Ab initio Insight on Magnetism and Electronic Properties of Fe(001)-p(1x1)O Surface** — •Corina Etz[1], Arthur Ernst[1], Serghei Ostanin[1], Wolfram Hergert[2], and Ingrid Mertig[2] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Martin Luther University, Halle, Germany

Besides the electronic structure changes and the enhanced magnetism, the surfaces can undergo further intriguing changes due to relaxations, impurities, oxidation etc.

In the present contribution we chose to present an *ab initio* study of the electronic structure and the magnetic properties of the bcc Fe(001) surface. In order to be able to correlate our results with the latest experimental observations, we have investigated the pure Fe(001) surface taking into account the effect of structural relaxations on its magnetic properties. Since Fe reacts strongly with oxygen, we also studied the iron surface in the presence of oxygen, i.e. Fe(001)-p(1×1)O. The comparison between the magnetic and electronic properties between the clean Fe surface and the oxygen covered one, revealed that the oxygen layer leads to a stabilization of the magnetism in the system. Furthermore, the Fe(001)-p(1×1)O presents a spin–filter capability, which provides the system a great potential for practical applications.

This first principles study was performed using a multi–code approach. The structural relaxations were investigated using VASP. While by means of the Korringa–Kohn–Rostocker Green's function method, including the self interaction corrections (KKR–SIC), the electronic and magnetic properties were studied.

O 41.74 Tue 18:30 Poster B1

**XMCD of ultrathin magnetite ($Fe_3O_4$) films on titanates ($BaTiO_3$, $SrTiO_3$)** — Remya Govind[1], •Martin Trautmann[1], Franziska Steudel[1], Michael Huth[1], Stephan Borek[1], Liudmilla Makhova[2], Joachim Gräfe[2], Daniel Wett[2], Vasili Hari Babu[2], Angelika Chassé[1], Karl-Michael Schindler[1], and Reinhard Denecke[2] — [1]Institute of Physics, Martin-Luther-University Halle-Wittenberg, Germany — [2]Wilhelm-Ostwald-Institute for Physical and Theoretical Chemistry, University Leipzig, Germany

Coupling ferromagnetism to ferroelectricity in multiferroic systems raises interesting fundamental and application related questions. Within the framework of the SFB 762 all-oxide systems (magnetite on titanates) have been investigated using x-ray absorption spectroscopy (XAS) and x-ray magnetic circular dichroism (XMCD) at BESSY II. Thin and ultrathin films of magnetite ($Fe_3O_4$) have been prepared by reactive metal evaporation of iron in an $O_2$ atmosphere and characterized using XAS. The controversy about published assignments of XAS spectra to $SrTiO_3$ and $BaTiO_3$ could be resolved on the basis of experimental O K-edge and Ti L-edge spectra and multiple scattering calculations. After in-plane magnetization the XMCD of the films has been determined in grazing incidence at room temperature. Thin films of $Fe_3O_4$ (30 ML on $SrTiO_3$ and 10 ML on $BaTiO_3$) exhibited an XMCD comparable to published data of bulk and bulk-like systems. However, an ultrathin film on $BaTiO_3$ with a thickness of 3 ML showed no XMCD. Obviously, remanent in-plane magnetization could no longer be achieved.

O 41.75 Tue 18:30 Poster B1

**Spin dynamics of Co nano-islands on Cu(111) from first principles** — •Danny Böttcher, Arthur Ernst, Ingrid Mertig, and Jürgen Henk — Max Planck Institute of Microstructure Physics, Halle, Germany

Co nano-islands on Cu(111) show a variety of interesting quantum phenomena. Concerning magnetism, the switching of the islands' magnetizations by an external magnetic field has been investigated experimentally by STM [1]. The findings of these experiments can hardly by interpreted satisfactorily in terms of the Stoner-Wohlfarth model because the latter gives disputable numbers (e. g., too large an anisotropy constant). Hence, a microscopic model, with exchange and anisotropy parameters computed reliably from first principles, seems to be necessary.

Here, we present detailed calculations on the spin dynamics of Co nano-islands on Cu(111) within the framework of the Landau-Lifshitz-Gilbert equation with Langevin dynamics. The Heisenberg exchange parameters and the magnetocrystalline anisotropy have been computed from first principles, using our scalar-relativistic and relativistic KKR codes. We address in particular the behaviour of the islands' spins under switching by an external magnetic field and the dependence of the switching fields on the island size.

[1] G. Rodary, S. Wedekind, D. Sander, and J. Kirschner, Jap. J. Appl. Phys. **47**, 9013 (2008).

O 41.76 Tue 18:30 Poster B1

**Ultrafast melting of a charge-ordered state in 1*T*-TaS$_2$ investigated with photoelectron spectroscopy at FLASH** — Kai Rossnagel[1], •Christian Sohrt[1], Stefan Hellmann[1], Martin Beye[2], Timm Rohwer[1], Florian Sorgenfrei[2], Michael Bauer[1], Alexander Föhlisch[2], Wilfried Wurth[2], and Lutz Kipp[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24118 Kiel, Germany — [2]Institut für Experimentalphysik, Universität Hamburg, 22761 Hamburg, Germany

The Free-Electron-Laser in Hamburg (FLASH) generates highly brilliant, ultrashort, and coherent pulses in the XUV regime enabling many fascinating experiments that are not possible at any other source. After various challenges concerning space-charge effects as well as timing and synchronization issues have recently been solved optical pump-XUV probe photoelectron spectroscopy on solid surfaces is now possible over a wide probing photon energy range (~24 - 570 eV) with time and energy resolutions of ~700 fs and ~300 meV, respectively. Our most recent experiments, performed on the correlated layer compound 1*T*-TaS$_2$ deep in the charge-density-wave (CDW) state, demonstrate that core-level dynamics on the femto-, pico- and nanosecond time scale can be investigated at FLASH. We find that long-range charge order in 1*T*-TaS$_2$ collapses promptly and that a domain-like CDW state is reached within about 1 ps. The results imply that the CDW and the accompanying periodic lattice distortion, which are strongly coupled in equilibrium, are decoupled after photoexcitation on the time scale for electron-phonon thermalization.

O 41.77 Tue 18:30 Poster B1

**Surface and Image-Potential States of Gadolinium Investigated with Spin- and Time-Resolved 2PPE** — •Beatrice Andres[1,2], Kristian Döbrich[1], Andreas Goris[1,2], 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

It is still an open question which microscopic processes are responsible for the laser-induced ultrafast demagnetization in ferromagnetic materials. Most of the experiments performed so far lack spin-resolution. Our first goal is to investigate the occupied majority and unoccupied minority $5d_{z^2}$ surface state (SS) of Gd, following the work of Ref. [1]. We will investigate exchange splitting $\Delta E_{ex}$, binding energy and spin polarisation of the SS and their dependence on the temperature. Here the fundamental of our Ti:Sa laser serves as IR pump and the frequency tripled UV as probe pulse (photon energies 1.5 and 4.5 eV, respectively, pulse durations ≈ 40 fs).

In a second step we will focus on the image-potential states which are also expected to show $\Delta E_{ex}$ and spin dependent lifetimes (frequency doubled photons at $h\nu = 3$ eV will serve as pump and 1.5-eV-photons as probe). As samples we use 100-Å-thick Gd(0001) films grown *in situ* on W(110).

[1] M. Lisowski *et. al.*, *Phys. Rev. Lett.* **95**, 137402 (2005).

O 41.78 Tue 18:30 Poster B1

**Influence of Neon Spacer Layers on Image-Potential States on Cu(100)** — •Nico Armbrust[1], Jens Güdde[1], Peter Feulner[2], and Ulrich Höfer[1] — [1]Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg — [2]Physik-Department E20, TU München, D-85748 Garching, Germany

The binding energy and lifetime of image-potential states on metal surfaces can be drastically altered by the presence of insulating spacer layers. Previous investigations of Xe, Kr or Ar on Cu(100) showed that the effect of the decoupling depends systematically on the electron affinity of the rare-gas. Here we present an investigation of the influence of Ne spacer layers on the image-potential states on Cu(100) using time-resolved two-photon photoemission (2PPE). Neon represents a particularly interesting case because its large negative electron affinity of −1.3 eV should result in a large tunneling barrier even for very thin Ne adlayers. Experimental challenges are posed by the requirement of a low sample temperature (≤ 7 K) in combination with the optical experiment which requires an unshielded sample. Furthermore the optical excitation leads to unwanted desorption of the Ne adlayers. We find that the binding energies of the first two image-potential states are reduced by about 30% to $E_1 = 438$ meV and $E_2 = 139$ meV and that the lifetime of the $n = 1$ state increases from 40 fs on the clean surface to 300 fs for only one monolayer of Ne coverage. This is an almost three times larger increase of the lifetime than that caused by one monolayer of Ar/Cu(100). With Kr or Xe layer thicknesses of more than 4 ML are required to achieve a similar degree of decoupling.

O 41.79 Tue 18:30 Poster B1

**Surface resistivity of Cu ultrathin films due to impurity scattering** — •Swantje Heers, Phivos Mavropoulos, Samir Lounis, and Stefan Blügel — Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich

In order to understand resistivity measurements on an atomic scale in ultrathin films, it is of crucial importance to investigate the influence of scattering at surface defects on the surface resistivity, especially in the presence of surface bands. Using the Korringa-Kohn-Rostoker Green function method [1] and solving the Boltzmann-equation self-consistently, the surface resistivity can be calculated for adatoms, impurities and vacancies in and below the surface. We have performed density-functional calculations for the Cu(111) surface of finite-thickness slabs with 3d and 4sp atoms as impurities. The thickness of the slab is varied, ranging from six to forty atomic layers. Our formalism allows us to separate the contribution by scattering to bulk states from the one by scattering to surface states. We show that trends are qualitatively different for adatoms, compared to impurities in the surface. This work was supported by the ESF EUROCORES Programme SONS under contract N. ERAS-CT-2003-980409 and the Priority Programme SPP1153 of the DFG grand Bl 444/8-1.

[1] N. Papanikolaou, R. Zeller, P. H. Dederichs *J. Phys.: Condens. Matter* **14**, 2799 (2002).

O 41.80 Tue 18:30 Poster B1

**Electronic structure and spin dynamics in Rashba-split quantum-well electron states** — •Sebastian Jakobs[1], Felix Jünger[1], Andreas Ruffing[1], Sabine Neuschwander[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

In the last few years, methods that allow manipulating and measuring the spin of electrons have received lot of attention. For instance, in a two-dimensional electron gas spin-split energy bands can appear, because of spin-orbit interaction and asymmetric confinement of the electron gas (Rashba splitting). Recently, we found quantum-size induced giant Rashba splitting for quantum-well states in Pb and Bi overlayers on Cu(111). These quantum-well systems present ideal model systems to further explore the electron and spin structure as a function of quantum-well film thickness. We carried out first time-, angle- and spin-dependent photoemission experiments, which will be presented in this contribution.

O 41.81 Tue 18:30 Poster B1

**Spin-resolved Inverse Photoemission on Rashba-Systems** — •Sune Wissing, Christian Eibl, Anke B. Schmidt, and Markus Donath — Physikalisches Institut, Westfaelische Wilhelms-Universitaet, Wilhelm-Klemm-Str. 10, 48149 Muenster, Germany

The possibility to create spin currents without using external magnetic fields could result in useful applications to spintronics. Therefore, the discovery of the spin-orbit splitting on a Au(111) surface by LaShell *et al.* [1] gave rise of a highly interesting and rapidly growing field of research. Many different systems have been investigated by using angle-resolved photoemission in order to find a "giant" Rashba splitting. Yet it was not possible to follow the splitting of the dispersion within the Brillouin zone above the Fermi level.

We present an experimental setup for spin and angle-resolved inverse photoemission for measurement of the Rashba spin splitting in the unoccupied states. In order to observe a Rashba splitting, it is necessary that the in plane wave vector of the electrons is perpendicular to their spin-quantization axis. Therefore we turned our spin-polarized electron source by 90 degrees with the result that the spin-quantization axis is parallel to the rotation axis of our sample. By measuring the Cu(111) L-gap surface state we can show that the angle and energy resolution of our experiment conforms to the requirements for measuring the Rashba splitting.

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

O 41.82 Tue 18:30 Poster B1

**Electron coincidence spectroscopy of the neutralization of slow Helium ions above metal surfaces** — •Christian Tusche and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

The neutralization of highly charged ions, scattered at a single-crystal metal surface with kinetic energies of a few 10 eV, is usually accompanied by a number of electrons ejected from the target or from the projectile. For instance, neutralization of ground state He$^{+}$ ions proceeds by Auger neutralization, emitting an Auger electron from the metal. In contrast, He$^{2+}$ neutralization can proceed along several paths. E. g. a double electron capture into the outer He-2s and -2p shells is followed by the emission of a He-KLL Auger electron.

The experimental observation that almost all of the scattered ions leave the surface in the neutral ground state requires that a couple of electron-capture and -emission processes take place on each scattering event. Using electron coincidence spectroscopy, we detect electrons emitted form two such steps in the neutralization cascade of 30 eV He$^{2+}$ ions. The experiment employs two separate electron analyzers. The first one triggers the detection, while the second analyzer records all electrons that arrive within a time window of a few ns. Our results suggest that each ion neutralized at the surface emits two electrons – one in the high energy part of the spectrum (20 eV - 40 eV) and one in the low energy part – with a high probability.

O 41.83 Tue 18:30 Poster B1

**Electronic structure of RScO$_3$ from x-ray spectroscopies and first–principles calculations** — •Christine Derks[1], Karsten Kuepper[2], Michael Raekers[1], Andree Postnikov[3], Reinhard Uecker[4], and Manfred Neumann[1] — [1]Department of Physics, University of Osnabrück, D-49069 Osnabrück — [2]Departement of Solid-state Physics, Univeristy 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 RScO3, where R represents a trivalent rare-earth metal, exhibit an enormous variety of physical properties and can be used for different applications. They 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 RScO3.

The electronic structures of a series of RScO3 single crystalls are investigated by means of x-ray photoelectron spectroscopy (XPS), x-ray emission spectroscopy (XES), x-ray absorption spectroscopy (XAS) and band structure calculations. By combining XES and XAS measurements together with theoretical calculations the band gaps of the compounds can be accurately determined. The presented results will broaden the complete experimental and theoretical picture of the valence bands of RScO3 series.

O 41.84 Tue 18:30 Poster B1

**Electronic structure of LaAg$_5$ alloy films on Ag(111)** — •Christoph Seibel[1], Hendrik Bentmann[1], Luca Moreschini[2], Gustav Bihlmayer[3], Frank Forster[1], and Friedrich Reinert[1,4] — [1]Universität Würzburg, Experimentelle Physik VII, Am Hubland, D-97074 Würzburg, Germany — [2]Ecole Polytechnique Fédérale de Lausanne (EPFL), Institut de Physique des Nanostructures, CH-1015 Lausanne, Switzerland — [3]Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany — [4]Forschungszentrum Karlsruhe, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe, Germany

We have characterized the growth of La on Ag(111) by UPS, XPS and LEED. At La coverages of about 4 ML or higher and subsequent annealing we observe an ordered (2x2) surface structure that is rotated by 30° with respect to the substrate. In analogy to the well-studied system CePt$_5$, we identify our system as a LaAg$_5$ alloy in a CaCu$_5$-type structure.

Employing angle-resolved photoelectron spectroscopy (ARPES) we measured the band structure along high symmetry lines and the Fermi surface (FS) of the LaAg$_5$ films. We find several sharp bands near the Fermi level and a high anisotropy in the FS. Our results are compared to ARPES results on CePt$_5$ and LaPt$_5$ as well as first-principles calculations. The system shall serve as a reference for iso-structural alloys composed of other lanthanoids, such as Ce or Gd, potentially showing Kondo physics or other magnetic effects.

O 41.85 Tue 18:30 Poster B1

**Momentum microscope mapping of electronic states at Cu(111) surfaces by two- and three-photon photoemission** — •Ahmet Akin Ünal, Christian Tusche, Cheng-Tien Chiang, Aimo Winkelmann, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

We investigate occupied and unoccupied electronic states of Cu(111) using multi-photon photoemission experiments. The frequency-doubled linear-polarized output of a Ti:sapphire oscillator with photon energy of $h\nu = 3.1$ eV is used as the excitation source. The electronic dispersions of the unoccupied Shockley surface state and n = 1 image potential state of Cu(111) are obtained by two- and three-photon photoemission using a momentum microscope, which comprises a photoelectron emission microscope (PEEM) in combination with two hemispherical imaging energy analyzers. In the case of three-photon photoemission, a one-photon resonance between the unoccupied surface and image-potential states is observed at $k_\parallel \approx \pm 0.66\,\text{Å}^{-1}$. We also investigate the space-charge effects in the momentum microscope as a function of laser intensity and electron optical conditions in the instrument. As a measure of the space-charge effects, the broadening in the energy and momentum distributions of the observed electronic transitions is analyzed.

O 41.86 Tue 18:30 Poster B1

**Electronic Properties of Gold Chains on Ge(001) by Angle-resolved Photoemission** — •Andreas Dollinger[1], Thorsten Umbach[1], Sebastian Meyer[1], Jörg Schäfer[1], Christian Blumenstein[1], Philipp Höpfner[1], Xiaoyu Cui[2], Luc Patthey[2], and Ralph Claessen[1] — [1]Experimentelle Physik 4, Universität Würzburg, 97074 Würzburg, Germany — [2]Swiss-Light-Source, Paul-Scherrer-Institut, 5232 Villigen, Switzerland

Metallic nanowires formed by adatom adsorption on semiconductor surfaces have established themselves as playground for studying phenomena in low dimensions. A key requisite is their spatial confinement where charge is mostly maintained within the chain architecture. Examples known are, e.g., Au and In on silicon surfaces, where a charge density wave (CDW) is discussed as the low-temperature ground state. Here finite interchain coupling stabilizes the Peierls state and seemingly hinders a stricter one-dimensional regime. In contrast, Au nanowires on Ge(001) are an alternative system where the chains are well separated by several substrate lattice constants. The electronic band structure from angle-resolved photoemission (ARPES) reveals metallic states, persisting down to low temperatures. No structural change, such as a CDW, is observed when cooling to liquid helium temperatures, which allows the search for deviations from the Fermi liquid picture. Variation of photon energies reveals a great variety of bands within the periodicity of the surface reconstruction. We will present high-resolution data on the band topology, as well as an analysis of the spectral properties near the Fermi level.

O 41.87 Tue 18:30 Poster B1

**(SP)VLEED: A spin-polarized very-low-energy electron-diffraction experiment** — •Kathrin Wulff, Ulrich Burgbacher, Anke B. Schmidt, and Markus Donath — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster

This poster has been withdrawn.

O 41.88 Tue 18:30 Poster B1

**Paramagnetic Y(0001) as a model for ferromagnetic Gd(0001)** — •Sebastian D. Stolwijk, Anke B. Schmidt, and Markus Donath — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Yttrium and gadolinium are isoelectronic elements with respect to their valence bands but differ in their magnetic properties due to the additional 4f electrons in Gd. Therefore, Y may be viewed as paramagnetic model for ferromagnetic Gd. A comparative study of the electronic structure of Y and Gd promises to reveal electronic properties that are directly linked to ferromagnetism.

We determined the surface electronic structure in the vicinity of the Fermi level $E_F$ by a combined direct (PE) and inverse photoemission (IPE) experiment. Our study on clean Y(0001) films on W(110) reveals a surface state right at $E_F$, which is observed both below and above the Fermi level. High-resolution IPE measurements and results on the stable $p(1 \times 1)$O/Y(0001) surface oxide expose an additional spectral feature at about 0.6 eV above $E_F$. Based on bulk-band structure calculations this emission is ascribed to the band edge of Y(0001). The possible observation of a band-edge emission for Gd(0001) sheds new light on the interpretation of its spin-dependent electronic structure [1]. Implications for the understanding of the ferromagnetic Gd(0001) surface will be discussed.

[1] M. Donath et al., Phys. Rev. Lett. 77, 5138 (1996).

O 41.89 Tue 18:30 Poster B1

**A Study of band-gap-engineering in $ZrS_2Se_{2-x}$ by means of ARPES** — •Alexander Paulheim, Stephan Thürmer, Mohamed Moustafa, Christoph Janowitz, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany

The layered Zirconium dichalcogenide semiconductors $ZrS_2Se_{2-x}$ allow to adjust the band gap depending on the parameter $x$ [1]. Therefore, they are candidates for third generation solar cell applications. The ternary compounds of $ZrS_xSe_{2-x}$ have been successfully grown with high control of the parameter $x$ by means of the chemical vapor transport technique (CVT) [2]. In an attempt to understand the mechanism of this band-gap-engineering and the underlying band structure variations, the electronic structure of various $ZrS_xSe_{2-x}$ crystals were measured by angle resolved photoemission spectroscopy (ARPES). In great detail the $x$-dependent behavior of the upper valence band has been studied along all high-symmetric directions of the Brillouin zone. The results reveal a smooth transition of the energetic positions and splitting of the bands from $ZrS_2$ to $ZrSe_2$.

[1] M. Moustafa, T. Zandt, C. Janowitz, and R. Manzke, Physical Review B 80, 35206 (2009)

[2] R. Nitsche, H.U. Bölsterli, and M. Lichtensteiger, J. Phys. and Chem. of Solids 21, S.199-205, (1961)

O 41.90 Tue 18:30 Poster B1

***In situ* real-time investigations during the formation of a magnetoelectric Fe/ZnO nanocomposite** — •Erik Kröger[1], Matthias Kalläne[1], Kai Rossnagel[1], Hendrik Bentmann[2], Frank Forster[2], Friedrich Th. Reinert[2], and Lutz Kipp[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24098 Kiel, Germany — [2]Experimentelle Physik II, Universität Würzburg, 97074 Würzburg, Germany

Magnetoelectric materials composed of piezoelectric and ferromagnetic substances have drawn significant interest in recent years due to their multifunctionality and potential technological applications. In order to investigate the geometric, chemical, and electronic structure of such complex materials, we have designed an experimental station for the new storage ring PETRA III in Hamburg for angle-resolved photoelectron spectroscopy. The instrument was used for *in situ* real-time investigations during the formation of the magnetoelectric Fe/ZnO interface. The ZnO substrate was sputtered and annealed under UHV conditions to guarantee high surface quality. LEED and EXAFS studies showed a relaxation of the hexagonal unit cell. Real-time XPS measurements were done on the polar oxygen surface of the ferroelectric ZnO compound during Fe deposition. A charge transfer from the iron adatoms to the ZnO substrate was observed and quantified. The resulting enhanced conductivity of the ZnO surface enabled very high resolution ARPES measurements of the electronic structure over the full 3D Brillouin zone. This work was supported by the BMBF.

O 41.91 Tue 18:30 Poster B1

**Electron-Phonon Coupling in a Thin Epitaxial Bi(111) Film on Si(111) studied by ARPES** — •Holger Schwab, Hendrik Bentmann, Frank Forster, and Friedrich Reinert — Universität Würzburg, Experimentelle Physik VII, Am Hubland, D-97074 Würzburg, Germany

Employing angle-resolved photoelectron spectroscopy (ARPES) we have studied the electronic structure in thin films of Bi(111) on the Si(111) substrate. The film growth was characterized by low energy electron diffraction (LEED). We present Fermi surfaces and band structures in the high symmetry directions for different film thicknesses. Quantum well states (QWS) as well as the Bi(111) surface state (SS) are observed. The variation of the line width of the SS was measured over a broad temperature range from 40K to 200K. This allows for the determination of the electron-phonon coupling constant $\lambda$. The result agrees with previous measurements for the bulk crystal.

O 41.92 Tue 18:30 Poster B1

**Comparison of topography and electronic structure of Gd/W(110) and Gd/Y(0001)** — •Karen Zumbrägel, Henry Wortelen, Anke B. Schmidt, and Markus Donath — Physikalisches Insitut, Westfälische Wilhelms-Universität Münster, Germany

In Gd the $4f$ electrons are the main carriers of the magnetic moment. In contrast to the $3d$ ferromagnets Fe, Co and Ni, whose ferromagnetic coupling occurs via direct exchange, in Gd the polarisation of the $5d$ and $6s$ valence electrons mediates the ferromagnetic coupling (RKKY interaction). Hence the investigation of Gd is of fundamental relevance for understanding the nature of ferromagnetism.

The electronic structure of thin Gd films is studied as a function of film thickness, topography and substrate. We compare Gd films grown on W(110), the substrate prevalent in literature, with films grown on Y(0001). The high lattice mismatch between W and Gd of up to 15% leads to layer-island growth, while Gd grows layer-by-layer on the well fitting Y (mismatch 0.4%). Combined with varying annealing temperatures, films with different degrees of roughness and impurity could be investigated. For characterising the film quality we employ low energy electron diffraction, Auger electron spectroscopy and scanning tunnelling microscopy. Spin- and angle-resolved direct and inverse photoemission provide information about the spin-dependent electronic structure below and above the Fermi level. The surface state close to the Fermi energy is used as criterion for the quality of the preparation.

O 41.93 Tue 18:30 Poster B1

**Splitting of quantum well states in Pb films induced by spin dependent confinement** — •yingshuang fu, germar hoffmann, and roland wiesendanger — Institute of Applied Physics, University of Hamburg

The electronic structure of Pb(111) quantum films epitaxially grown on Fe/W(110) substrate is investigated with a cryogenic scanning tunnelling microscope. Spin averaged scanning tunnelling spectroscopy (STS) measurements show that quantum well states are formed inside the nanometre thick Pb films. Interestingly, quantum well states (QWSs) of Pb films split into double peaks, and the splitting energy can be tuned by changing the quantum number of QWS and thickness of quantum films. The splitting is explained by spin dependent quantum confinement from the magnetic substrate which shifts the binding energy of supported QWSs and effectively removes their spin degeneracy. Thus, the Pb layer inherits the exchange splitting of the magnetic substrate and could provide spin-polarized two dimensional electron gases for both spin directions. Further investigations with spin resolved STS are underway to confirm the spin splitting of QWSs.

O 41.94 Tue 18:30 Poster B1

**The Two-Dimensional Electron System Sn/Si(111) Investigated by Scanning Tunneling Microscopy** — •Thomas Schramm, Philipp Höpfner, Maximilian Herpich, Jörg Schäfer, and Ralph Claessen — Experimentelle Physik 4, Universität Würzburg, 97074 Würzburg

The confinement of electrons to two dimensions may lead to strong electron correlation effects, including a Mott transition. Such two-dimensional electron systems (2DES) can be realized by adsorbing layers of metal adatoms with less than 1 monolayer thickness on (111) semiconductor surfaces. Examples include Pb and Sn on Ge(111) and Si(111) which form a $\sqrt{3} \times \sqrt{3}$-reconstruction upon deposition of 1/3 monolayer of metal. Recent results from scanning tunneling microscopy (STM) and angle-resolved photoelectron spectroscopy provide evidence of a phase transition to a Mott-insulating ground state [1]. Moreover, the triangular lattice in the presence of correlations leads to magnetic frustrations. We have studied the formation of the $\sqrt{3}\times\sqrt{3}$-Sn/Si(111) structure by (STM) and scanning tunneling spectroscopy experiments. Our refined surface preparation leads to perfectly $\sqrt{3} \times \sqrt{3}$-reconstructed surfaces with low defect densities and long range order. The understanding of defect formation is of foremost importance, as this may lead to unintentional doping effects that influence a potential Mott transition. Current studies are underway, and will give a more defined insight into the correlation effects at low temperature.

[1] Modesti *et al.*, Phys Rev. Lett. **98**, 126401 (2007).

O 41.95 Tue 18:30 Poster B1

**Liquid and solid lubrication for nanopositioning and nanomeasuring systems** — Thomas Haensel[1], Xiangjun Zhang[2], Xiaohao Zhang[2], Angela Keppler[1], Stefan Krischok[1], and •Syed Imad-Uddin Ahmed[1] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany — [2]State Key Laboratory of Tribology, Tsinghua University, P.O. Box 100084, Beijing, P.R. China

One of the biggest challenges in the $21^{st}$ century is to handle the decreasing structure sizes in the low nanometer range. A nanopositioning and nanomeasuring system developed at the TU Ilmenau is an enabling technology that makes this possible. For optimum operation of the positioning tool, it is necessary to have stable and controlled friction as well as low wear. This can be achieved by a combination of solid lubricants like diamond-like carbon (DLC) and liquid lubricants like ionic liquids (ILs). This contribution reports on friction and wear experiments made with tribometers. To implement this machine in vacuum, preliminary friction measurements in high vacuum were performed to ensure that a vacuum application is possible. Especially the liquid film lubrication with ILs might be very suitable as the IL vapor pressure is very low. The results show that in the combination of solid and liquid film lubrication, effects like polarity, viscosity and the force regime play an important role. The results and aspects, which are related with the achieved friction and wear, are discussed under the aspect of stable and low friction.

O 41.96 Tue 18:30 Poster B1

**Tribological self-repair mechanisms investigated under medium load conditions** — •Mathias Biester[1], Xinlei Gao[2], Jian Li[3], Syed Imad-Uddin Ahmed[1], and Matthias Scherge[1] — [1]Institut für Physik und Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany — [2]Department of Chemical and Environmental Engineering, Wuhan Polytechnic University, Wuhan, P.O. Box 430023, P. R. China — [3]Wuhan Research Institute of Materials Protection, Wuhan, P.O. Box 430030, P.R. China

Wear is the main effect for the limited life-time of most mechanical systems and causes very cost-intensive repair and replacement activities. Therefore, a lot of efforts are made to reduce wear and to increase the life-time of modern mechanical systems. Cu (II) chelate of bissalicylaldehyde-ethylenediamine was chosen as additive for liquid lubricants, which is investigated as it has a big self-repair potential. This Schiff base copper complex is a metal-organic chelate complex, which is able to create negative wear as well as to reduce friction due to the self-assembling of a protective layer. Under high temperatures and high contact pressures, which occur during the friction processes, the copper is released from the complex and attaches at the surface. This process is investigated using a micro-tribometer in the milli Newton range to create applicational friction conditions. Additional characterisations are performed with AFM, SEM and spectroscopic methods to analyse the self-repair effects and display tendencies for future applications.

O 41.97 Tue 18:30 Poster B1

**Velocity Dependence of the Kinetic Friction of Nanoparticles** — •Michael Feldmann, Dirk Dietzel, and André Schirmeisen — Institute of Physics and Center for Nanotechnology, University of Münster, Germany

The velocity dependence of interfacial friction is of high interest to unveil the fundamental processes in nanoscopic friction. So far, different forms of velocity dependence have been observed for contacts between friction force microscope (FFM) tips and a substrate surface. In this work we present velocity-dependent friction measurements performed by nanoparticle manipulation of antimony nanoparticles on atomically flat HOPG substrates under UHV conditions. This allows to analyze interfacial friction for very well defined and clean surface contacts. A novel approach to nanoparticle manipulation, the so called 'tip-on-top' technique [1], made it possible to manipulate the same particle many times while varying the velocity. The antimony particles exhibit a qualitatively different velocity dependence on friction in comparison to direct tip-HOPG contacts. A characteristic change in velocity dependence was observed when comparing freshly prepared particles to contaminated specimen, which were exposed to air before the manipulation experiments.

[1] Dietzel et al., Appl. Phys. Lett. 95, 53104 (2009)

O 41.98 Tue 18:30 Poster B1

**Dynamische Topographieveränderung einer Kupferoberfläche in einem geschmierten Tribosystem mittels eines neuartigen Tribometers** — •Spyridon Korres[1,2] und Martin Dienwiebel[1,2] — [1]Fraunhofer IWM, Joseph-von-Fraunhofer-Straße 7, 76327 Pfinztal, Deutschland — [2]Karlsruhe Institute of Technology - izbs, Kaiserstraße 12, 76131 Karlsruhe, Deutschland

In diesem Beitrag werden experimentelle Ergebnisse topographischer Veränderungen einer Kupferoberfläche in einem geschmierten Tribosystem gezeigt. Um dies zu erreichen, wurde ein neuer experimenteller Versuchsaufbau entwickelt. Dieser erlaubt eine gleichzeitige on-line Messung der Reibung, Topographie und des Verschleißes mit hoher Auflösung. Die Topographie der Kupferoberflächen wurde mittels Holographiemikroskopie aufgenommen, Sub-mikrometer Lateralauflösung wurde mit einem Rasterkraftmikroskop erreicht und eine Radionuklidtechnik-Anlage ermöglicht das Online Messen von Verschleißwerten.Die Änderungen der Topographie wurden mit den Reibkräften korreliert. In dem Versuch wurde ein Eisenstift als Gegenkörper und Poly-alpha Olefin als Schmierstoff eingesetzt. Für das vorliegende System konnte gezeigt werden, dass ein Großteil der Oberflächenstrukturen plastisch verformt bzw. an den Gegekörper transferiert wurde. Zusätzlich wurde die Änderung der Zusammensetzung beider Reibpartner mittels XPS nach der tribologischen Belastung durchgeführt.

O 41.99 Tue 18:30 Poster B1

**Energy Dissipation in Dynamic Force Microscopy: The Effect of Temperature** — •Gernot Langewisch, Harald Fuchs, and Andre Schirmeisen — CeNTech (Center for Nanotechnology) and Institute of Physics, University of Muenster, Germany

Since its development dynamic force microscopy has proven to be a powerful tool for surface imaging and mapping of tip-sample interactions down to the atomic scale. Conservative as well as dissipative tip-sample forces can be distinguished by dynamic force spectroscopy. Conservative tip-sample forces have been readily described by classical force laws. The exact origin of the dissipative forces is still under discussion, but current theories predict an explicit temperature dependence of the energy dissipation. Therefore, we performed systematic temperature dependent studies to better understand the interaction processes leading to dissipation in dynamic force microscopy. The dissipative tip-sample interactions were measured by dynamic force spectroscopy for silicon tips on NaCl(001) in ultrahigh vacuum in the attractive and repulsive force regimes. Force and dissipation versus distance curves were obtained for different surface temperatures ranging from 35 K to room temperature. Detailed comparison in different distance regimes shows that neither the force nor energy dissipation exhibits a systematic variation with sample temperature.

O 41.100 Tue 18:30 Poster B1

**Ab initio based simulations of atomic force and friction force microscopy of KBr(001)** — •Christine Broelemann, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster

Atomic force microscopy offers the capability to investigate surface structure with atomic resolution. In addition, it allows one to study frictional phenomena of single contacts. To analyse the information that can be extracted from such experimental studies theoretical explorations are essential.

We report on ab initio based simulations of noncontact AFM images, corresponding force fields and friction force line profiles. The short range part of the tip-sample interaction potential is calculated within the local-density approximation of density-functional theory and is supplemented by the long range van-der-Waals interaction due to the macroscopic part of the tip. The microscopic part is modeled by $K^+$ and $Br^-$ terminated tips.

We use an extended Tomlinson model employing the van-der-Waals interaction together with the DFT derived interaction potential to simulate the sliding friction on the surface. Solving the equations of motion within this framework, we obtain lateral force line profiles with typical stick-slip characteristics. The dependance of the results on different tip types as well as on the spring constant and loading force is discussed.

O 41.101 Tue 18:30 Poster B1

**Influence of adhesion interaction between rough surfaces on real contact area formation** — •Alexander Kovalev[1,2], Nikolai Myshkin[2], and Heinz Sturm[1] — [1]Federal Institute of Materials Research and Testing (BAM), D-12200 Berlin, Germany — [2]Metal-Polymer Research Institute (MPRI), 246050 Gomel, Belarus

Friction units used in the micromechanical systems have a very high surface to volume ratio, so there are high contact adhesion and friction, leading to low operational reliability. For reliable estimating of the adhesion effect is necessary to take into account the local physical-mechanical properties of the asperities and the real geometry of rough surfaces in micro- and nanoscale. The aim of work was to study formation of the real contact area (RCA) between rough surfaces taking into account the action of adhesion force. The contact simulation was carried out involving the well-known contact models of Hertz, JKR, and DMT at micro/nanoscale of forces and deformations level transformed to the Winkler foundation. The DLC coating used for this study was deposited on the silicon plate using a pulsed vacuum arc deposition system. The surface topography of DLC coating was measured with typical AFM. It was found the adhesion force has obvious action at the external load up to 100 *N. At the external load about 100 mN deformation is comparable with basic roughness and adhesion interaction has insignificant effect on RCA. Using the JKR theory has been shown that the dependence between the adhesion force and deformation has S-shaped pattern like the bearing surface curve.

O 41.102 Tue 18:30 Poster B1

**Ordered structure of viologen monolayers on a Copper electrode surface** — •Emilia Sak[1,3], Min Jiang[1], Knud Gentz[1], Ralf Troff[2], Christoph Schalley[2], Aleksander Krupski[3], 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,Taknstr.3, 14195 Berlin,Germany — [3]Institute of Experimental Physics, University of Wroclaw , pl.Maksa Borna 9 , 53-204 Wrocław, Poland

As a typical molecule in the redox-active viologen family, dibenzylviologens (DBV) has been studied by means of EC-STM on a Cu(100) electrode. DBV$^{2+}$ dications adsorb on a chloride modified Cu(100) electrode surface forming a laterally well ordered 2D array of supramolecular cavitand ensembles. Based on these observations we designed new molecules, such as dimetyl-DBV (DMDBV) and tetrametyl-DBV (TMDBV) in order to study in influence of extra substituents. So far, we found two redox peaks P1/P1'( P1 - 305 mV, P1' -240 mV) in the cyclic voltammogram of Cu(100) in a mixture of 10mM HCl and 0,1mM DMDBV for values of Ework $>$ - 420 mV vs RHE. STM images, show that DMDBV molecules form a stable and ordered adlayer structure which also looks like a chessboard with two kinds of mirror domains. When the applied potential is decreased to -400 mV, no obvious structural changes are visible.

O 41.103 Tue 18:30 Poster B1

**Structure of water-metal interfaces studied from first principles** — •Xiaohang Lin, Sebastian Schnur, and Axel Gross — Institute for Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

In spite of numerous studies, it is fair to say that the exact atomistic structure of water layers at metal surfaces is not fully clarified yet. We have used density functional theory calculations to address the structure of water layers on different flat and stepped metal substrates which is for example important for an understanding of processes in electrocatalysis and electrodeposition. In order to account for thermal effects, we have performed ab initio molecular dynamics (AIMD) simulations. The simulations indicate that at room temperature water becomes liquid-like on noble metal surfaces such as Au or Ag whereas on more strongly interacting substrates such as Pt and Ru an ice-like hexagonal structure persists, however, the orientation of the single water molecules is disordered [1]. Additional information on the water layers has been obtained by evaluating the vibrational spectra of the water molecules at the metal surface which reflect the water-metal interaction strength.

[1] S. Schnur, A. Groß, New J. Phys., in press.

O 41.104 Tue 18:30 Poster B1

**Surface electronic structure of imidazolium-based ionic liquid films on Au(111)/Mica** — •Marcel Marschewski[1], Tomonori Ikari[2,3,4], Angela Keppler[3], Oliver Höfft[4], Markus Reinmöller[3], Wichard J. D. Beenken[3], Wolfgang Maus-Friedrichs[1], Stefan Krischok[3], and Frank Endres[4] — [1]Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — [2]Ube National College of Technology, Department of Electrical Engineering 2-14-1 Tokiwadai, Ube, Yamaguchi 755-8555, Japan — [3]Institut für Physik and Institut für Mikro- und Nanotechnologien der TU Ilmenau, P.O. Box 100565, 98684 Ilmenau — [4]Institute of Particle Technology, TU Clausthal, Arnold-Sommerfeld-Str. 6, 38678 Clausthal-Zellerfeld

Room temperature Ionic Liquids (RT-ILs) are a class of materials, which has recently gained enormous interest. Here we present our results for the surface electronic structure of very thin imidazolium-based ionic liquid (ILs) films on Au(111)/Mica and thick IL films. This was studied by electron spectroscopy using ultraviolet photoelectron spectroscopy (UPS, HeI and HeII) and metastable induced electron spectroscopy (MIES). We have prepared monolayers of four different types of imidazolium-based ILs ([RMIm]Tf$_2$N; R stands for Ethyl-, Butyl-, Hexyl- and Octyl-chains) on Au(111)/Mica by vapour deposition. By comparing these results with our data for the thick IL films we find evidence for ordered growth of the ILs in the monolayer regime. For better understanding of the electronic structure of the ILs, we compare the experimental data with corresponding DFT calculations.

O 41.105 Tue 18:30 Poster B1

**Invetigatins on the self assembly process of Octacosan-1-ol and its derivates on artificial surfaces** — •Alexander Hommes and Klaus Wandelt — Institut für Theoretische und Physikalische Chemie, Wegelerstr. 12, 53115 Bonn

Waxes occur on the surfaces of all land plants. That the structure of epicuticular wax crystallites is predominantly a process of self-assembly, is now well established both from correlative and generic observations. The waxes are embedded into the 3D matrix of the cuticle and also cover the surface where they build plant specific microcrystalline structures. Dominant wax components are normally considered to be responsible for the formation of wax crystallites. In general, across a wide variety of waxy components like alkanes, alcohols, ketons and aldehyds, several different crystal structures on plant cuticles can be observed.

Long chained alkanes and alcohols were some of the first hydrocarbons to be imaged at solution/solid interface with AFM and STM since they form well ordered films on graphite near room temperature. Investigations on the physisorbed monolayers of Octacosan-1-ol, Hentricontan-16-on (Palmiton), Octacosanoicacid and Triacontan-1-ol at the solution/solid interface on HOPG, Mica and Siliconoxid show an order, e.g. strictly follow the hexagonal arrangement of the carbon atoms of the HOPG.(studied with STM and AFM) The good lattice match between the alkyl backbone and the graphite lattice favours commensurate packing of the hydrocarbon film with the underlying substrate.

O 41.106 Tue 18:30 Poster B1

**Self-Assembly of 3D-molecule: Benzene 1,3,5 Triphosphonic acid (BTP) studied by Scanning Tunneling Microscopy**

**(STM) at the Liquid-Solid Interface** — •Nguyen Thi Ngoc Ha[1], Michael Dieblich[1], Michael Mehring[2], and Michael Hietschold[1] — [1]Institute of Physics, Solid Surfaces Analysis Group, Chemnitz University of Technology, Chemnitz, Germany. — [2]Institute of Chemistry, Coordinations Chemistry Group, Chemnitz University of Technology, Chemnitz, Germany.

During the last two decades, there has been major effort toward metal phosphate chemistry due to their endearing properties and their potential for supramolecular assembly[1]. Crystal engineering is a relatively new field of chemical research used to control or predict types of metal phosphonate structure[1,5]. Surprisingly, the phosphonic acids have not been the subject of scanning tunneling microscopy (STM) to our knowledge so far. Here we report a very first STM studying of the benzene triphosphonic acid (BTP) [1,3,5-[(HO)2(O)P]3C6H3] dissolved in an alkanoic acid solvent (octanoic acid). The three-dimensional network formed by self-assembly of this triphosphonic acid on a HOPG(0001) substrate exhibits a ladder-like appearance and agrees very well with other crystallographic studies[2,4,5]. BTP in this structure adsorbed opposite to each other as viewed along an axis orthogonal to the plane defined by the aromatic rings. The brightest features in regular patterns should be reported phosphonic end-groups.

O 41.107 Tue 18:30 Poster B1

**Modification of graphene by ion irradiation** — •Hanna Bukowska[1], Sevilay Akcöltekin[1], Mourad El Kharrazi[1], Orkhan Osmani[1,2], and Marika Schleberger[1] — [1]Universität Duisburg-Essen, Fakultät für Physik, Lotherstraße 1, 47057 Duisburg, Germany — [2]Technische Universität Kaiserslautern, Fachbereich Physik, Gottlieb-Daimler-Straße, Gebäude 47, 67663 Kaiserslautern, Germany

Ion irradiation can be used to modify surfaces on the nanometer scale. We investigate graphene on different insulator ($SrTiO_3$, $TiO_2$, and $Al_2O_3$) and semiconductor ($SiO_2$) substrates. The bombardment of those target surfaces with swift heavy ions under grazing angle of incidence creates chains of nanodots on the substrate and folds graphene to typical origami-like structures. The shape of the folded graphene seems to depend on the length of the tracks. The length can be controlled by the angle of incidence. From the analysis of atomic force microscopy measurements, we classify the different types of modifications, with the aim to determine the relationship between chain length and origami shape. Further more we want to develop a theoretical understanding of the physical processes leading to the folding.

O 41.108 Tue 18:30 Poster B1

**Electronic structure of a monolayer graphene on Ir(111) probed by ARPES** — •Marko Kralj[1], Ivo Pletikosić[1], Milorad Milun[1], Petar Pervan[1], Alpha N'Diaye[2], Carsten Busse[2], Thomas Michely[2], Jun Fujii[3], Ivana Vobornik[3], and Tonica Valla[4] — [1]Institut za fiziku, Zagreb — [2]II. Physikalisches Institut, Köln — [3]TASC Laboratory, Trieste — [4]BNL, New York

Amongst realized examples of epitaxial growth on metal substrates, graphene on iridium is an exceptional case of long range structural quality and weak (electronic) bonding to a metal surface. These properties make this system very appealing for experimental studies of the electronic structure of graphene. Our recent ARPES study focused on the K point of graphene revealed that the weak electronic interaction of graphene with Ir(111) is reflected through the 0.1 eV hole doping and a minigap opening in the Dirac cone which is due to the 2.5 nm superperiodic potential originating from the about 10 % mismatched iridium and graphene [1]. In this work, ARPES is used to further investigate electronic properties and quality of graphene on Ir(111). For that purpose, we scan a wide portion of the Brillouin zone, use variable photon energy and different light polarization, and also perform photoemission of the adsorbed Xe.

[1] I. Pletikosić et al., Phys. Rev. Lett. 102, 056808 (2009).

O 41.109 Tue 18:30 Poster B1

**Theory of ultrafast carrier relaxation dynamics in graphene** — •Torben Winzer, Stefan Butscher, Frank Milde, Andreas Knorr, and Ermin Malić — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, 10623 Berlin, Germany

We present a microscopic calculation of the relaxation dynamics of photoexcited hot electrons and phonons in graphene.

Using a density matrix formalism, the combination with a tight binding approach for the band-structure and a Born-Markov approximation yields Boltzmann-like equations for interacting electrons and phonons.

In the case of electron-phonon coupling, we find an initial fast carrier cooling on the femtosecond timescale followed by slowed down relaxation dynamics due to the generation of non-equilibrium hot phonons.[1][2]

Even though the relaxation of excited carriers into thermal equilibrium occurs predominantly by energy dissipation through phonons, electron-electron scattering thermalizes the system at the time scale of the electron-phonon interaction.

[1] S. Butscher, F. Milde, M. Hirtschulz, E. Malić, and A. Knorr, Appl. Phys. Lett. 91, 203103 (2007). [2] T. Kampfrath, L. Perfetti, F.Schapper, C. Frischkorn, and M. Wolf, Phys. Rev. Lett. 95, 187403 (2005).

O 41.110 Tue 18:30 Poster B1

**Scanning tunneling microscopy (STM) studies of microsoldered graphene** — •Alexander Georgi[1], Anne Majerus[1], Viktor Geringer[1], Bart Szafranek[2], Daniel Neumaier[2], Marcus Liebmann[1], and Markus Morgenstern[1] — [1]II. Physikalisches Institut, RWTH Aachen and JARA-FIT, Otto-Blumenthal-Straße, 52074 Aachen — [2]Advanced Microelectronic Center Aachen (AMICA), Otto-Blumenthal-Straße 25, 52074 Aachen

Since STM is very susceptible to dirt, it is important to avoid contamination by prior processing. For graphene, we show that microsoldering [1] avoids dirt as resist, which has been found on lithographic samples. However, both samples show intrinsic corrugation with wavelength of 15 nm as previously reported for lithographically contacted graphene [2]. Ni deposition on the surface leads to clusters exhibiting spectroscopic features comparable to theoretical predictions [3]. Further measurements probing the properties of freely suspended graphene layers are presented.

[1] Ç. Ö. Girit and A. Zettl, Appl. Phys. Lett. 91, 193512 (2007).
[2] V. Geringer, M. Liebmann, T. Echtermeyer, S. Runte, M. Schmidt, R. Rückamp, M. C. Lemme and M. Morgenstern, Phys. Rev. Lett. 102, 76102 (2009).
[3] P. A. Khomyakov, G. Giovannetti, P. C. Rusu, G. Brocks, J. van den Brink, and P. J. Kelly, Phys. Rev. B 79, 195425 (2009).

O 41.111 Tue 18:30 Poster B1

**Adsorption of diatomic halogen molecules on graphene** — •Alexander N. Rudenko[1,2], Frerich J. Keil[1], and Alexander I. Lichtenstein[2] — [1]Technische Universität Hamburg-Harburg, Institut für Chemische Reaktionstechnik, Eißendorfer str. 38, 21073 Hamburg, Germany — [2]Universität Hamburg, Institut für Theoretische Physik, Jungiusstraße 9, 20355 Hamburg, Germany

We investigate the adsorption of fluorine, chlorine, bromine, and iodine diatomic molecules on graphene using density-functional theory taking into account nonlocal correlation effects by means of vdW-DF approach. It is shown that the van der Waals interactions play a crucial role in the formation of chemical bonding between graphene and halogen molecules, and therefore important for a proper description of adsorption in this system. Adsorption energies are found to be up to an order of magnitude larger than the values obtained using standard semilocal functionals without vdW corrections. In the cases of $F_2$ and $I_2$ we also found a considerable ionic contribution to the binding energy, slowly vanishing with the distance. The analysis of the electronic structure shows that ionic interaction arises due to the charge transfer from graphene to the molecules. In addition, graphite intercalation by halogen molecules have been investigated. It is found that the binding energy of graphite layers becomes significantly weaker in the presence of halogen molecules, which agrees with the results of recent experiments on sonochemical exfoliation of intercalated graphite.

O 41.112 Tue 18:30 Poster B1

**Gas permeation in graphenoid nanomembranes** — •Nils Mellech, Elina Oberländer, Xianghui Zhang, André Beyer, and Armin Gölzhäuser — Universität Bielefeld, Postfach 10 01 31, 33501 Bielefeld, Germany

Permeation and selectivity measurements with Helium and Argon were carried out on freestanding nanomembranes of crosslinked self-assembled biphenylthiol and nitrobiphenylthiol monolayers. An ultrahigh vacuum permeation measurement system based on a quadrupole mass spectrometer was used to determine the permeation properties. The monolayers of biphenylthiol and nitrobiphenylthiol are prepared on gold on mica and crosslinked by electron irradiation. After preparation the nanomembranes which have a thickness of approximately 1 nm are transferred onto a micron-sized opening in a silicon nitride window of a silicon substrate. The nanomembrane seals the UHV chamber from the high pressure feed gas side of the system. Despite its thinness, the membranes remain stable under pressures of up to 30 kPa, even for days. The permeability of nitrobiphenylthiol nanomembranes was found to be substantially lower as compared to biphenylthiol membranes. This is accompanied by a significant increase in the permeation selectivity of He to Ar gas.

O 41.113 Tue 18:30 Poster B1

**Graphite and multigraphene based Gas sensor** — •Ana Ballestar, Jose Barzola-Quiquia, and Pablo Esquinazi — Division of Superconductivity and Magnetism, Universität Leipzig, 04103 Leipzig

The research and development of solid state gas sensors have widely advanced in recent years. Sensing gas molecules is critical to environmental monitoring, control of chemical processes, space missions and medical applications. In order to judge whether or not a sensor is likely to be commercially successful, the sensitivity, selectivity, stability, speed of response and low cost manufacturing are the parameters to be taken into account. Graphite, considered a semi-metal or zero-gap semiconductor, is a good electrical conductor at 300K. The operational system proposed here is based on the changes of the electrical resistivity produced in mm- and $\mu$m-sized samples of graphite and multigraphene while being exposed to different gas molecules. By means of low noise measurements and high sensitivity concerning the variations in the resistivity of graphite samples, we are able to detect the adsorption and desorption of the gas molecules on graphite surface. Depending on the gas molecules we get different variations in the signal, so we have selectivity in the device as well.

O 41.114 Tue 18:30 Poster B1

**Automated preparation of high-quality epitaxial graphene on 6H-SiC(0001)** — •Markus Ostler, Florian Speck, Markus Gick, and Thomas Seyller — Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Germany

Thermal decomposition of silicon carbide is a viable route for preparing graphene films. In contrast to other methods it has the potential for upscaling graphene synthesis to a wafer scale and the advantage of providing an insulating substrate at the same time. In particular, graphenization of SiC(0001) surfaces in Ar atmosphere has been shown to yield graphene films superior to UHV-grown epitaxial graphene. In this contribution we present details on a recently installed hot-wall reactor for graphene growth on SiC in Ar. Both preparation steps, i.e. the preconditioning of the SiC substrate by hydrogen etching and the graphene growth are performed in this setup in a fully automated manner thus ensuring the preparation of high-quality graphene on an everyday basis. Samples prepared in the new setup were characterized by atomic force microscopy (AFM) and x-ray induced photoelectron spectroscopy (XPS). We present results on the optimization of the hydrogen etching procedure by varying gas flow and temperature. The thickness distribution of graphene samples grown in the automated process is Gaussian with a mean value of 1.1 monolayers and a standard deviation of 0.15 monolayers. This indicates a highly controlled process.

O 41.115 Tue 18:30 Poster B1

**Band structure engineering of mono- and bilayer Graphene on SiC(0001) via molecular functionalization** — •Camilla Coletti[1], Christian Riedl[1], Dong Su Lee[1], Luc Patthey[2], Benjamin Krauss[1], Klaus von Klitzing[1], Jurgen Smet[1], and Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [2]Paul-Scherrer-Institut, CH-5234 Villigen-PSI, Switzerland

Although epitaxial graphene on SiC(0001) is a realistic candidate for the implementation of graphene-based electronic devices a drawback might sensibly limit its perspectives. Epitaxial graphene on SiC is in fact electron doped and consequently displays a metallic nature. Hence, the need to tailor its electronic band structure in such a way that the excess of electrons is compensated precisely to the point of charge neutrality. Noncovalent functionalization of epitaxial graphene surfaces with the strong acceptor molecule tetrafluorotetracyanoquinodimethane (F4-TCNQ) allows for a fine tuning of the doping level. Charge neutrality can be achieved for mono- and bilayer graphene as shown from ARPES and Raman spectroscopy. On bilayer samples the magnitude of the existing bandgap can be increased up to more than double of its initial value. Core level analysis and valence band investigations are used to provide a structural characterization of the charge transfer complex. The molecules are stable to air exposure, temperature resistant and can be applied via wet chemistry. Hence surface functionalization via F4-TCNQ appears to be a technologically relevant method to successfully engineer the band structure of graphene.

O 41.116 Tue 18:30 Poster B1

**Preparation and characterization study of graphene on SiC(0001)** — •Thomas Druga, Martin Wenderoth, and Rainer G. Ulbrich — IV. Physikalisches Institut, Georg-August-Universität Göttingen

We present a preparation and characterisation study of graphene on the silicon-terminated 6H-SiC(0001) surface. The untreated crystals were electrically contacted and transferred in UHV. After annealing at base pressure of $1 * 10^{-10}$ mbar at 500°C for several hours the samples were graphitized between 1250 and 1300°C by direct current heating. The temperature during preparation was controlled by an optical pyrometer. The surfaces were investigated by low energy electron diffraction (LEED) and scanning tunnelling microscopy (STM) at room temperature. The graphitized surfaces show different step heights resulting from coexisting mono- and bilayer graphene films. Atomically resolved topographies show the typically honeycomb structure of the graphene layer and the $6 \times 6$ periodicity resulting from the underlying buffer layer. Lateral resolved scanning tunnelling spectroscopy data indicate finite conductivity around zero bias and lateral variations in the local density of states. This work was supported by the DFG as part of SFB 602 Tp A7.

O 41.117 Tue 18:30 Poster B1

**Growth and Chemical Modification of Graphene on Ni(111)** — •Wei Zhao, Oliver Höfert, Christian Papp, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

The outstanding electronic properties of graphene make it a promising candidate for future spintronic applications in electronic devices and setups as well as gas sensors. Therefore, we first studied the growth of graphene on Ni (111) under different temperatures (773-950 K) and with different carbon sources such as ethylene and propylene, by in situ X-ray photoelectron spectroscopy (XPS). After cooling to room temperature, a second contribution showed up in C 1s region of graphene on Ni (111), enabling a better understanding of the structure of graphene on this surface.

For potential use in chemical gas sensors, functionalized graphene needs to be. Doping with hetero atoms like N might be one way to introduce sensitivity towards different gases. Our approach to achieve what gentle sputtering chemical modification of the graphene sheets on Ni (111) with molecular nitrogen. To reveal changes in chemical properties due to the sputtering process, we used benzene as probe molecule and studied its interaction with pristine and modified graphene layers by XPS and TPD.

This work was supported by BMBF (05 ES3XBA / 5) and the DFG through the Cluster of Excellence"Engineering of Advanced Materials".

O 41.118 Tue 18:30 Poster B1

**Influence of charge on the Raman Spectrum of Epitaxial Graphene on Silicon Carbide** — •Stephan Wittmann[1], Jonas Röhrl[1], Daniel Waldmann[2], Johannes Jobst[2], Florian Speck[1], Markus Ostler[1], Heiko Weber[2], Martin Hundhausen[1], and Thomas Seyller[1] — [1]Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Germany — [2]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Germany

Epitaxial graphene prepared on the surface of SiC wafers might be mechanically strained and electrically charged due to doping from the substrate. Raman spectroscopy can be employed for characterization of graphene layers due to influence of strain and charge on the frequencies of the Raman-active phonons. In order to differentiate between both effects on the prominent features in the Raman spectra (G-peak and 2D-peak) we employ a 6H-SiC wafer with an integrated back gate. By varying the electric field, applied on the graphene layer via a back gate, we change the charge state and accordingly some phonon frequencies. We show, that the variation of the back gate voltage influences the zone-center optical phonon (G-peak).

O 41.119 Tue 18:30 Poster B1

**Electronic structure of graphene on SiC produced via low-**

**T synthesis** — •Martin Weser, Carsten Enderlein, Karsten Horn, and Yuriy Dedkov — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The graphitization of the SiC(0001)-surface, by annealing at temperatures above 1150° C under UHV conditions, has been known since a long time and became one of the dominating methods for graphene fabrication in the field of experimental physics in the last ten years. Here the LEED, core-level PES, and ARPES-results of a graphene layer produced by nickel diffusion on SiC are presented. The band maps show clear graphene $\pi$-bands with an unusual band splitting at the border of the Brillouin zone that is, up to our knowledge, not comparable to any graphene-based system known so far. This band splitting, as well as a number of unusual features in the spectral function, are ascribed to the formation of a $Ni_2Si$-interlayer that locally breaks the symmetry of the two sublatices, by hybridization of only one of them, which leads to an electronically separated second sublattice.

O 41.120 Tue 18:30 Poster B1

**Analysis of model interfaces for Li ion batteries** — •Andreas Seemayer, Aparna Pareek, Dirk Vogel, Michael Rohwerder, and Frank Renner — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Lithium ion batteries are the most promising power source for future electromobility applications. Therefore a better understanding of the basic processes in Lithium ion batteries is needed. Especially nowadays research projects aim to improve real systems in terms of higher rate capability, cycle life, safety and operating temperature.

Following the surface science approach we focus on the investigation of single crystal model systems of possible anode and cathode materials and electrode / solid electrolyte interfaces prepared by electrochemical deposition, molecular beam epitaxy or pulsed laser deposition.

## O 42: Invited talk (Rossnagel, Kai)

Time: Wednesday 9:30–10:15 Location: H36

**Invited Talk** O 42.1 Wed 9:30 H36

**Electrons in quasi two dimensions: Revelations from photoemission mapping, microscopy, and filming** — •Kai Rossnagel — Christian-Albrechts-Universität zu Kiel, D–24098 Kiel, Germany

Layered transition-metal dichalcogenides are quasi-two-dimensional solids—consisting of three-atom-thick hexagonal crystal sandwiches—that are particularly famous for three things: a strong electron-phonon coupling leading to various charge-density-wave phases as well as superconductivity, the intercalation by foreign atoms and molecules which enter the van der Waals gaps between the sandwiches, and the formation of misfit layer compounds which result from alternate stacking with cubic monochalcogenide slabs and lack full three-dimensional periodicity. All three phenomena are intimately connected to the electronic structure of the host dichalcogenide sandwiches and can result in profound changes of their electronic properties. In this talk, these changes will be explored for selected systems using synchrotron-based photoemission spectroscopy techniques with high momentum, position, and time resolution. The questions discussed include: Does angle-resolved photoemission spectroscopy measure bulk electronic properties for layered compounds? Why do charge-density waves occur, and how fast are they formed? How can the surface electronic properties be tuned in a controlled and non-destructive way? What binds the slabs together in misfit layer compounds?

## O 43: Graphene I

Time: Wednesday 10:30–12:45 Location: H31

O 43.1 Wed 10:30 H31

**Mechanical characterization of graphenoid nanomembranes from self-assembled monolayers** — •Xianghui Zhang, Christoph T. Nottbohm, André Beyer, Andrey Turchanin, and Armin Gölzhäuser — Fäkultät für Physik, Universität Bielefeld, Postfach 10 01 31, 33501, Germany

We report on the fabrication and mechanical characterization of novel graphenoid nanomembranes with a thickness of approximately 1 nm. The nanomembranes are prepared from electron cross-linked aromatic self-assembled monolayers (SAMs). After etching the support, the nanomembranes are transferred to window-structured substrates for mechanical characterization. Bulge testing within an atomic force microscope (AFM) is utilized to investigate their mechanical properties. A series of biphenyl-based molecules with different types of terminal groups and/or anchor groups were used to prepare the nanomembranes, such as carbonitrile-biphenyl-trimethoxysilyl (CBPS), biphenylthiol (BPT), nitro-biphenyl-thiol (NBPT) and biphenyl-propanethiol (BP3). Biphenyl-based nanomembranes display elastic moduli ranging from 6 to 12 GPa. Annealing of the cross-linked nanomembranes in ultra high vacuum (UHV) gives rise to a systematic increase of the Young's moduli from 10 GPa to ~45 GPa for an annealing temperature of ~1000 K. Strain relaxation lowers the residual strain from 0.9 % to ~0.35 % for temperatures of 800 K and above. This indicates that the relevant structural transformation is completed at that temperature.

O 43.2 Wed 10:45 H31

**Collective Excitations of Graphene in a Strong Magnetic Field** — Andrea Fischer[1], Alexander Dzyubenko[2,3], and •Rudolf Römer[1] — [1]University of Warwick, Coventry, UK — [2]California State University, Bakersfield, US — [3]Russian Academy of Science, Moscow, Russia

Graphene, a two-dimensional form of carbon, has become famous for its wide range of unusual properties, both fundamental and applicable. Both theory and experiment indicate the relevance of many body interactions to the magneto-optical response of graphene. Neutral collective excitations of pristine graphene in a strong perpendicular magnetic field have already been studied theoretically. In this work, we consider graphene with a low impurity density and determine the neutral magnetoplasmons, which become localised on an impurity. Two impurity types are considered: a screened Coulomb impurity and a $\delta$-function scatterer due, e.g., to a neutral foreign atom on one of the lattice sites. We assume Zeeman and valley splitting of Landau levels (LLs) $n$=0 and $n = \pm 1$, so that these LLs have four sublevels; we consider various integer fillings of the zeroth LL. For both impurity types, we predict the existence of optically active bound states above and below the magnetoplasmon continuum for high enough impurity strengths [1]. Our results indicate that polarisation-resolved magneto-optical spectroscopy can be an effective tool for discriminating between different types of impurities in graphene. [1] A. M. Fischer, A. B. Dzyubenko, and R. A. Römer, PRB **80**, 165410 (2009)

O 43.3 Wed 11:00 H31

**Absolute Raman Cross Section of Graphene** — •Philipp Klar[1], Robert Panknin[1], Elefterios Lidorikis[2], Andrea Carlo Ferrari[3], Stephanie Reich[1], and Cinzia Casiraghi[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin — [2]Engineering Department, University of Ioannina, Greece — [3]Engineering department, Cambridge University, UK

Raman spectroscopy in graphitic systems is extremely interesting because it involves resonant conditions, defect-induced processes and because of strong electron-phonon coupling effects [1-3]. However, measurements of the absolute scattering cross section of graphite are rather scarce [4-5]. Here we measured the first- and second-order Raman spectrum of graphene and graphite using excitation energies covering the visible range, from 1.96 eV to 2.7 eV. By using the substitutional method, we have found that the G peak Raman cross section is $\sim 2 \times 10^{-5} m^{-1} Sr^{-1}$ at 2.41 eV for both graphene and graphite, in agreement with Ref. 5. The 2D peak Raman cross section of graphene is $\sim 3 \times 10^{-5} m^{-1} Sr^{-1}$ at 2.41 eV, well comparable with the one of the first order G peak. This confirms the resonant nature of the 2D peak [1-2].

1. C. Thomsen, S. Reich, PRL 85, 5214 (2000)
2. D. M. Basko, PRB, 78, 125418 (2008)
3. S. Piscanec et al, PRL 93, 185503 (2004)
4. K. Sinha, J. Menendez, PRB 41, 10845 (1990)
5. N. Wada, S. A. Solin, Physica 105B, 353 (1981)

O 43.4 Wed 11:15 H31

**Electronic bound and scattering states in an integrable graphene quantum dot** — •George Pal, Walter Apel, and Ludwig Schweitzer — Physikalisch-Technische Bundesanstalt (PTB), Bundesalee 100, 38116 Braunschweig, Germany

We study theoretically the confinement of electrons in a graphene quantum dot created by an electrostatic gate potential applied to single-layer graphene. In the low-energy limit, the electronic properties of graphene are given by a two-dimensional Dirac-like equation for massless chiral electrons. The graphene quantum dot is described by a radially symmetric confining potential with a sharp boundary and that makes the problem analytically integrable. Also, couplings between the graphene layer and the substrate and atomic scale defects and impurities are taken into account by adding a sub-lattice anisotropy and an inter-valley scattering to the Hamiltonian. These terms open a gap in the energy spectrum and allow for the existence of true bound states, forbidden otherwise due to the Klein tunneling phenomenon in an ideal, clean graphene. Considering a wave function with four components (two valleys times two sub-lattice indices), we discuss the conditions for the existence of bound and scattering states for different regimes of the confinement potential. Furthermore, we calculate the energies of the bound states and the scattering matrix. The influence of disorder in the graphene sheet and in the quantum dot is also discussed.

O 43.5 Wed 11:30 H31

**Ab-initio determination of the electronic and optical properties of functionalized group IV monolayers for optoelectronic and photovoltaic devices.** — •Margherita Marsili — ETSF, Dipartimento di Fisica Università di Roma 'Tor Vergata' (Italy)

Graphene, one of the most intensively material studied recently, is well known as being metallic. The absence of an electronic gap limits its possible use in electronic and optoelectronic devices. A route to the opening of a gap is the functionalization of graphene through the absorption of molecules. In particular a reversible metal-insulator transition of graphene upon hydrogenization has been experimentally achieved, after it was theoretically predicted. Graphane, the fully hydrogenated graphene, has indeed a wide gap of almost 6 eV. The extent of the electronic gap of graphane limits its use in photovoltaic devices, one of the key technologies for the attainment of green energy. Possible solutions are either to functionalize graphene with other molecules, or to change the backbone material looking at the other group IV elements such as Si and Ge. Here we present results exploring both paths: the optical properties of different molecules on graphane and on polysilane and polygermyne (Si and Ge counterparts of graphane) monolayers are investigated also including many-body effects beyond density functional theory. Many-body effects are also crucial in the quantitative description of a material's electron affinity. Hydrogenated diamond surfaces are known to have negative electron affinity, therefore the effect of hydrogen on graphene's electron affinity is also determined taking into account self-energy effects.

O 43.6 Wed 11:45 H31

**Adsorption of water on graphene from first principles** — •Elena Voloshina[1], Krzysztof Rosciszewski[2,3], and Beate Paulus[1] — [1]Physikalische und Theoretische Chemie, Freie Universität Berlin, 14195 Berlin, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [3]Institute of Physics, Jagiellonian University, 30059 Krakow, Poland

Although current density functionals are able to describe quantitatively different systems at much lower computational cost than other first principles methods, they fail to do so for the consideration of van der Waals (vdW) interactions. The problem of restoring the vdW interactions in DFT methods has been addressed by a number of authors. However, all these works are based on approximations leaving the main lack of systematic improvability within the DFT framework. Furthermore, even in the case of investigation of similar systems under similar conditions DFT can predict quite different results, e.g., as in the case of adsorption of $H_2O$ on graphene [1]. Therefore ab initio wavefunction-based correlation methods are desirable. A possibility to apply them to extended systems is to use the so-called local correlation methods, e.g. method of increments [2]. Recently this method has been extended to the description of interaction between molecules and surface (see e.g. [3]). Here we present the results for the adsorption of $H_2O$ on a graphene layer using a CCSD(T) correlation treatment.

[1] D. W. Boukhvalov and M. I. Katsnelson, J. Phys.: Condens. Matter 21, 344205 (2009). [2] H. Stoll, J. Chem. Phys. 97, 8449 (1992). [3] B. Paulus and K. Rosciszewski, Int. J. Quant. Chem. 109, 3055 (2009).

O 43.7 Wed 12:00 H31

**Optical detection of single graphenes on mica with a contrast as high as 14%** — •Martin Dorn, Philipp Lange, Alexei Chekushin, Nicolai Severin, and Jürgen Rabe — Humboldt-Universität zu Berlin, Department of Physics, Newtonstr. 15, 12489 Berlin, Germany

Graphene is a one atom thick material with unique properties arising from its two dimensional crystal lattice. Most of graphene devices are fabricated on silicon wafers covered with a SiO2 layer necessary for optical detection of single graphenes. Graphene adhering to a SiO2 layer follows the intrinsic roughness of the latter and therefore cannot be considered strictly two dimensional. Mica is a natural crystal with perfect atomically flat cleavage planes. We demonstrate here a simple optical microscopy method for the detection of graphenes on mica with up to 14% of single graphene optical contrast. The experimental results are rationalized with a Fresnel-law based model. The contrast is only weakly wavelength dependent, i.e. white light contrast of single graphenes is sufficiently high for easy detection. The theory predicts also a high contrast for single graphenes on different transparent substrates with refractive indices close to that of mica, e.g. lime glass and ITO.

O 43.8 Wed 12:15 H31

**Local work function of defective graphene probed by Kelvin Probe Force Microscopy** — •Liang Yan[1], Sasa Vinaji[1], Christian Punckt[2], Ilhan Aksay[2], Hanna Bukowska[3], Marika Schleberger[3], Gerd Bacher[1], and Wolfgang Mertin[1] — [1]Werkstoffe der Elektrotechnik & CeNIDE, Universität Duisburg-Essen, Bismarckstr. 81, 47057 Duisburg, Germany — [2]Department of Chemical Engineering, Princeton University, Princeton, New Jersey, USA — [3]Fakultät für Physik & CeNIDE, Universität Duisburg-Essen, 47057 Duisburg, Germany

Graphene is currently one of the hottest topics in research due to its unique properties. In particular for electronic applications, the influence of defects on its electronic properties such as work function is of great interest since it might be possible to taylor these properties by changing the type and density of defects. In this work we demonstrate local work function measurements on thermally exfoliated graphene on HOPG and on mechanically exfoliated graphene on SrTiO3 and SiO2 using Kelvin Probe Force Microscopy, which allows us to correlate the electronic properties with the topography of the defective areas. We find that in case of thermally exfoliated graphene, where the presence of defects and functional groups leads to wrinkling of the sheets, the work function at defective areas is increased compared to non-defective regions. In mechanically exfoliated graphene, a partial overflipping of the graphene layer is achieved by swift heavy ion bombardment, which results in a pronounced change of the local work function and thus in the electrical properties as compared to the non defective areas.

O 43.9 Wed 12:30 H31

**Electrical transport measurements in graphene and graphenoids from pyrolized self-assembled monolayers** — •Andrey Turchanin[1], Dirk Weber[2], Matthias Büenfeld[1], Joachim Mayer[3], Christian Kisielowski[4], Thomas Weimann[3], and Armin Gölzhäuser[1] — [1]Physik supramolekularer Systeme, Fakultät für Physik, Universität Bielefeld — [2]Physikalisch-Technische Bundesanstalt, Braunschweig — [3]Gemeinschaftslabor für Elektronenmikroskopie, RWTH Aachen — [4]National Center for Electron Microscopy, Berkeley

We investigate the transition of insulating ultrathin (∼1 nm) carbon nanosheets (graphenoid sheets) to conducting graphene. Self-assembled monolayers (SAM) of aromatic biphenyl molecules are cross-linked by electrons. The cross-linking results in mechanically stable graphenoid sheets with the thickness of a single molecule and arbitrary sizes. The nanosheets can then be lifted from their surface and transferred to another solid substrate or holey structure, where the nanosheets become suspended free-standing nanomebranes [1]. Upon annealing (pyrolysis) at higher temperatures (up to ∼1300K) the nanosheets transform into a graphitic phase that consists of nano-size graphene patches. This transformation is accompanied by a drop of the sheet resistivity from $\sim 10^8$ to 10 kΩ/sq [2]. We characterize the insulator to conductor transition by complementary spectroscopic and microscopic techniques and electrical transport measurements.

[1] C. T. Nottbohm et al, Ultramicroscopy 108, 88 (2008)

[2] A. Turchanin et al, Adv. Mater. 21, 1233 (2009)

## O 44: Plasmonics and Nanooptics III

Time: Wednesday 10:30–13:15 Location: H32

O 44.1 Wed 10:30 H32

**3D optical Yagi-Uda nanoantenna array** — •Daniel Dregely, Richard Taubert, and Harald Giessen — University of Stuttgart, Germany

Optical nanoantennas have gained a lot of interest in the past few years [1,2]. They are able to link propagating radiation and confined optical fields. Only little work has been done on complex antenna geometries on the nanoscale. In our experiments, we investigate a 3D optical Yagi-Uda nanoantenna array. Due to the high directivity of the array structure the incoming light is received efficiently at resonant wavelengths in the near-infrared (around $\lambda = 1.3$ $\mu$m).

Our 3D gold nanoantenna structure was fabricated with electron beam lithography using layer-by-layer stacking. We measured the transmission and reflection spectra of the nanoantenna array from both directions in order to examine the directive behavior of the structure. FIT-calculations agree very well with our experimental findings and confirm the concentration of the incoming plane-wave radiation to the feeding points of the antenna array.

References: [1] P. Mühlschlegel, H.-J. Eisler, O. J. F. Martin, B. Hecht, and D. W. Pohl, Science 308, 1607 (2005). [2] T. H. Taminiau, F. D. Stefani, F. B. Segerink, and N. F. van Hulst, Nature Photon. 2, 234 (2008).

O 44.2 Wed 10:45 H32

**Few-cycle nonlinear optics of single plasmonic nanoantennae** — •Tobias Hanke, Günther Krauss, Daniel Träutlein, Barbara Wild, Rudolf Bratschitsch, and Alfred Leitenstorfer — Department of Physics and Center for Applied Photonics, University of Konstanz, D-78457 Konstanz, Germany

We have studied the nonlinear optical properties of single gold nanoantennae driven with few-cycle laser pulses in the near infrared [1]. Intense third harmonic emission is obtained when exciting with fundamental spectra below 1.1 eV. At higher photon energies frequency doubling and two-photon induced luminescence are observed. We relate these findings to the band structure of bulk gold, especially a two-photon resonance with the d-band transitions.

The intense third-harmonic emission enables precise detection of frequency-resolved interferometric autocorrelation traces of individual nanoantennae. We find an enhancement up to 3 orders of magnitude when driving on resonance with the fundamental plasmon mode. A sub-cycle dephasing time as short as 2 fs is measured directly in the time domain, highlighting the strong radiation coupling and ultra-broadband response of these efficient nanodevices.

[1] Hanke et al., Phys. Rev. Lett., accepted for publication.

O 44.3 Wed 11:00 H32

**plasmon-enhanced high-order harmonic generation in the vicinity of metal nanostructures** — •song-jin im, anton husakou, and joachim herrmann — Max-Born-Institute for Nonlinear Optics and Short Pulse Spectroscopy, Max-Born-Str. 2a, D-12489 Berlin, Germany

Generation of high harmonics in noble gases is one of key topics of nonlinear optics, which is of a critical importance in many disciplines, for example in attosecond physics. Recently, plasmon-enhanced high-order harmonic generation became possible in the vicinity of bow-tie shaped nanostructures by pulses directly from an oscillator with MHz repetition rate. In this contribution, we simulate high-order harmonic generation by sub-TW/cm$^2$ pulses using large plasmon field enhancement near metallic nanostructures such as bowtie-shaped antennas or nanocones. Our simulations using a commercial software JCMwave predict intensity enhancement of 3 orders of magnitude near the surface of silver nanocones. The generation of the high harmonics was modeled using a modified Lewenstein approach taking into account the inhomogeneity of the field and the electron absorption by the metal. Our results are consistent with experimental observations for bowtie elements. Considering the generation of high harmonics in argon in the vicinity of silver nanocones, we show that harmonics numbers up to 50, corresponding to 15 nm wavelength, can be achieved using relatively low input intensity of 300 GW/cm$^2$, characteristic for nJ laser pulses directly from a laser oscillator with MHz repetition rate.

O 44.4 Wed 11:15 H32

**Analytic photoemission localization and switching in plasmonic nanoantennas by laser pulse shaping** — Martin Aeschlimann[1], Michael Bauer[2], Daniela Bayer[1], Tobias Brixner[3], Stefan Cunovic[4], Alexander Fischer[1], Pascal Melchior[1], Walter Pfeiffer[4], Martin Rohmer[1], Christian Schneider[1], Christian Strüber[4], •Philip Tuchscherer[3], and Dmitri V. Voronine[3] — [1]Fachbereich Physik and Research Center OPTIMAS, Technische Universität Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — [2]Institut für Experimentelle und Angewandte Physik, Universität Kiel, Leibnizstr. 19, 24118 Kiel, Germany — [3]Institut für Physikalische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [4]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany

We experimentally achieve two-photon photoemission localization and switching on a subwavelength scale in plasmonic nanoantennas. Complex polarization-shaped laser pulses which are found in adaptive optimizations control the linear response of the nanostructure. We consider previous analytic investigations to identify the interference of two excited modes in the nanostructure as the main control mechanism. The optimal pulse shapes for switching are then found deterministically. Adaptive and analytic control schemes are compared, and agreement between both approaches is demonstrated.

O 44.5 Wed 11:30 H32

**Swichable Hot Spots in Bipyramid-Nanoresonators** — •Siji Wu, Calin Hrelescu, Frank Jäckel, and Jochen Feldmann — Photonics and Optoelectronics Group, Department of Physics and Center for Nano Science (CeNS), Ludwig-Maximilians-Universität München, Amalienstrasse 54, 80799 München, Germany

Highly enhanced and strongly localized electromagnetic fields, so-called hot spots, are attractive for imaging applications, based on raman scattering or fluorescence enhancement.[1,2] Hot spots can be provided by nonspherical gold nanoparticles or nanoparticles aggregates. Here, we report on nanoresonators consisting of two bipyramidal gold nanoparticles prepared by AFM manipulation. Applying a force with the AFM allows switching between the two possible adsorption geometries of an individual bipyramid on the substrate. The plasmonic coupling between two bipyramids is different in the two configurations. Consequently, the hot spot in the nanoresonator can be switched mechanically. Furthermore, the hot spot can be located within 1nm above the substrate surface in contrast to dimer nanoresonators from spheres, rods or ellipsoids.

[1] C. Hrelescu, T.K. Sau, A.L. Rogach, F. Jäckel, J. Feldmann Appl. Phys. Lett., 94, 153113 (2009)

[2] A. Bek, R. Jansen, M. Ringler, S. Mayilo, T. A. Klar, J. Feldmann Nano Lett., 8 (2), 485 (2008)

O 44.6 Wed 11:45 H32

**Near-field measurements on nanoscopic sphere-on-plane-systems by means of PEEM** — •Florian Schertz[1], Marcus Schmelzeisen[2], Hans-Joachim Elmers[1], Gerd Schönhense[1], and

Max Kreiter[2] — [1]Inst. f. Physik, Johannes Gutenberg-Universität, 55099 Mainz — [2]Max-Planck-Inst. f. Polymerforschung, 55128 Mainz

Surface immobilized gold nano-spheres above a gold surface with a gap distance in the order of a nanometer act as sphere-on-plane (SOP) optical resonator systems showing unique optical properties. In the vicinity of a flat metal surface, a second resonance band red-shifted with respect to the isolated particle resonance occurs, understandable on the basis of multipole interactions of the sphere with its own mirror image in the gold film. Several theoretical and optical far-field studies of SOP resonators were performed, investigating the dependence of the resonance wavelength on the resonator geometry and dielectric properties of the spacer material [1]. The optical near-field of the system under fs-laser-radiation causes highly non-linear (n=3-5) photoemission processes strongly varying depending on the particle properties. Photoelectron microscopy turned out to be a valuable tool for the investigation of the optical near-field of individual SOPs (cf.[2]). We present the gap-resonance-induced photoemission characteristics of several SOPs (individually characterized by SEM), excited by fs-laser radiation in the range from 750nm to 850nm. This work was supported by DFG (EL172-16) and MWFZ, Univ. Mainz. [1] A. Rueda et al., J. Phys. Chem. C 112 (2008) 14801, and Refs. therein. [2] M. Cinchetti et al., Phys. Rev. Lett. 95 (2005) 047601

O 44.7 Wed 12:00 H32

### Strong-field photoelectron emission from metal nanotips

•Max Gulde, Reiner Bormann, Alexander Weismann, Sergey Yalunin, and Claus Ropers — University of Göttingen, Courant Research Center Nano-Spectroscopy and X-Ray Imaging, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The generation of ultrashort, localized electron pulses is of fundamental interest for future applications in time-resolved electron imaging and diffraction. Femtosecond electron sources of great spatial coherence make use of a combination of local field enhancement at metal nanotips and nonlinear photoelectric effects. Previous studies have resulted in a controversial debate about the underlying physical processes.

Here, we present our most recent theoretical and experimental results regarding ultrafast photoelectron emission from nanometric gold tips. For the first time, we conclusively show the transition between the multiphoton and the optical field emission (i.e. tunneling) regimes. Direct evidence for this transition is found from both the power dependence of the total current and the spatial characteristics of the resulting electron beam. The results are supported by theoretical modeling.

O 44.8 Wed 12:15 H32

### Dark-Mode Plasmonic Nanorod Cavity

•Johannes Kern, Swen Grossmann, Jer-Shing Huang, Paolo Biagioni, and Bert Hecht — Experimental Physics 5, University of Würzburg, Germany

We report ultra-small nanoplasmonic cavities consisting of a self-assembled, side-by-side aligned gold nanorod dimer. The rods are 50-70 nm long and are separated by a 3 nm gap. The structure corresponds to a finite piece of a two-wire transmission line with two highly reflective open ends which supports a quasi-TE fundamental mode which propagates along the transmission line. Reflection at the end caps leads to length-dependent Eigenmodes, whose energies are determined by the cavity length and the phaseshift introduced upon reflection. Unlike the dipolar longitudinal and transverse plasmon resonances that are also supported by the structure, the fundamental cavity mode is a dark quadrupol mode.

Nevertheless the cavity mode is experimentally accessible by excitation of electron-hole pairs in the gold bandstructure, which act as local dipole sources. The ultra-small mode volume and comparatively high Q-factor leads to a high selectivity of the cavity and the electron-hole pairs preferentially decay into the cavity resonance. Therefore luminescence spectra of the cavities clearly show the peak of the cavity mode. The wavelength of the cavity mode depends on the cavity length and lies in the VIS region, consistent with FDTD simulations and analytical modeling.

The ultra-small mode volume and high Q-factor make our cavities promising candidates to study lasing and/or strong coupling effects.

O 44.9 Wed 12:30 H32

### Temperature related nanoantenna extinction in infrared range

•Chung Hoang, Frank Neubrech, Makus Klevenz, Robert Lovrincic, Olaf Skibbe, and Annemarie Pucci — Kirchhoff-Institut für Physik der Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

We present important progress in the experimental studies of single-crystalline lead nanorods grown on Si(557) vicinal surfaces by self-assembling process in ultra-high vacuum. The growth of such nanorod arrays is governed by four experimental parameters: substrate temperature, surface energy, deposition rate, and amount of deposited lead. Upon cooling, strong enhancement of the infrared signal at resonance is observed, indicating the increase of extinction-cross section. This scenario can be attributed to the reduction of electron scattering events where electron - phonon scattering is the main factor that is involved in this process. Below half of the Debye temperature, the maximum resonant antenna extinction is nearly temperature independent, indicating residual electron scattering at surfaces.

O 44.10 Wed 12:45 H32

### Polarization-independent chiral split-ring resonator arrays with colossal optical activity

•Max Wunderlich, Sebastian Engelbrecht, Alexey Shuvaev, and Andrei Pimenov — Experimentelle Physik IV, Universität Würzburg

We have studied the optical activity of bi-layered split-ring resonator arrays. They form chiral quasi-molecules due to inductive coupling. We have examined these structures with the instruments of quasioptical terahertz-spectroscopy. Our investigation shows that such systems can produce a colossal optical activity of 600 degree per wavelength. This results might lead to negative refraction due to chirality. Furthermore we present a way to effectively suppress polarization-dependent behavior of split-ring resonator arrays by introducing $C_n$ symmetries. Thus we have demonstrated a way to realize a ultra-thin orientation-independent polarization rotator.

O 44.11 Wed 13:00 H32

### Efficient surface-plasmon-polariton excitation on nanoparticle structures by inclined incident light

•Andreas Seidel, Wei Cheng, Andrey Evlyukhin, Carsten Reinhardt, and Boris Chichkov — Laser Zentrum Hannover e.V., Hollerithallee 8, 30419 Hannover

We study the features of local surface plasmon polariton (SPP) excitation on single and chains of gold nanoparticles positioned near a gold surface using a light beam under inclined incidence. It is shown that by tuning the incident angle and the parameters of the surface nanoparticle structure one could obtain symmetric or asymmetric excitations of SPP beams propagating along certain directions depending on the particle/chain distances. The reasons and conditions for this behaviour and efficiency of SPP excitation as a function of the incident angle are studied. It is demonstrate that the SPP excitation efficiency strongly depends on the incident angle. Adjusting the incident angle to the maximum field component perpendicular to the metal dielectric interface can lead to a large increase of SPP excitation efficiency. In the case of nanoparticle chains the symmetric or asymmetric patterns of the SPP distributions are the result of the interference of the scattered waves generated by each nanoparticle in a structure. The theoretical consideration is based on the Green*s function technique for the Maxwell equations of the total electric field and on the point-dipole approximation. Experimental investigation is realized by leakage radiation microscopy in real and reciprocal space.

# O 45: Electronic structure I

Time: Wednesday 10:30–12:45 Location: H33

O 45.1 Wed 10:30 H33

**Electronic structure and photoemission of ferromagnetic 3d-metals and related binary alloys** — •J. Braun[1], J. Minar[1], H. Ebert[1], H.A. Dürr[2], J. Fink[2], T. Allmers[3], and M. Donath[3] — [1]Dept. Chemie und Biochemie, LMU Universität München, Germany — [2]Helmholtz-Zentrum Berlin, Germany — [3]Physikalisches Institut, Universität Münster, Germany

We compare calculated spectral features of bcc Fe(110), fcc Co(100) and hcp Co(0001) for in-plane and out-of-plane configurations of the magnetization. Furthermore, it will be shown that life-time effects can be quantitatively explained in terms of electron-hole pair interactions. The influence of chemical disoder on the spectroscopical data is analysed, as an example, for the binary intermetallic $\mathrm{Co}_x\mathrm{Cu}_{1-x}$ alloy. The spectral distributions will be compared with corresponding experimental data. The calculations have been performed in the framework of the fully relativistic version of the one-step model of photoemission that is part of the upgraded version of the Munich SPR-KKR program package [1]. The electronic structure input is calculated self-consistently for ordered and disordered materials using the LSDA+DMFT approach in combination with the Coherent Potential Approximation (CPA) alloy theory. To guarantee for a quantitative description of the surface-sensitive spectral features special attention is payed to the image-potential behavior of the surface barrier, which is included as an additional layer in the photoemission formalism.

1. H. Ebert et al., The Munich SPR-KKR package, version 3.6, http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR (2008).

O 45.2 Wed 10:45 H33

**Valence band photoemission $Ni_xPd_{1-x}$ alloy films on $Cu_3Au(100)$** — •Matthias Gulik[1,2], Lukasz Plucinski[1], and Claus M. Schneider[1] — [1]Forschungszentrum Jülich GmbH, Wilhelm-Johnen-Straße, 52428 Jülich, Germany — [2]Technische Universität Dortmund, Maria-Goeppert-Mayer- Str. 2, D-44221 Dortmund, Germany

Spin and angle-resolved photoemission are important experimental methods to investigate the electronic band structure of crystalline materials. Spin-integrated measurements can be performed relatively fast with a high energy and momentum resolution, whereas spin-resolved measurements reveal further information about the band structure.

On the compound of $Ni_xPd_{1-x}/Cu_3Au(100)$ we will investigate the electronic and magnetic properties with regard to the thickness and the composition of the ultrathin $Ni_xPd_{1-x}$ layer. The composition differences should be reflected in an inverse spin-reorientation transition. Furthermore we will compare the measured spectra to the theoretical calculations of the band structure.

The measurement takes place at Beamline 5 at DELTA, Dortmund, with an unique detector setup. We can acquire 2-dimensional angle resolved data for band mapping and spin resolved one-dimensional data quasi-simultaneously. This will provide us with high resolution band structure spectra and images as well as spin resolved valence band spectra. Our samples are prepared in-situ by e-beam evaporation and characterized by LEED and Auger spectroscopy.

O 45.3 Wed 11:00 H33

**Fermi-surface mapping of graphene/Ni(111) and Ni/graphene/Ni(111)** — Martin Weser[1], Alexander Generalov[1,2], Carsten Enderlein[1], Stefan Böttcher[1], Karsten Horn[1], Mikhail Fonin[3], and •Yuriy Dedkov[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]St.-Petersburg State University, Russia — [3]Universität Konstanz, Germany

Recent ab initio spin-dependent transport calculations have suggested an application of graphene/graphite as a perfect spin filter in ferromagnet/graphene/ferromagnet sandwich-like structures. Due to the overlapping of the electronic structures of graphene layers and the ferromagnetic material for the minority spin only, one can expect a preferential transport of electrons of one kind of spins through this trilayer system. The Ni(111)/graphene/Ni(111) sandwich can be considered as a model system, due to the extremely small lattice mismatch, permitting to study in detail the effects of growth and interactions at interfaces without detrimental effects such as grain boundaries or the formation of Moiré patterns. Here, we present results of LEED, STM, and photoemission studies of the morphology and electronic structure of the graphene/Ni(111) and Ni/graphene/Ni(111) systems. We focus on the investigation of electronic structure of these systems in the vicinity of the Fermi level. These results are presented and discussed in the light of the available band structure calculations. The perspectives of these graphene/ferromagnet interfaces for future spintronics devices are debated.

O 45.4 Wed 11:15 H33

**Ni/GaAs(001): Looking for a bcc signature with spin-resolved inverse photoemission** — •Christian Eibl, Manuel Prätorius, André Berken, Anke B. Schmidt, and Markus Donath — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster

To understand the interplay between crystal structure, electronic states, and magnetism, it is worthwhile to compare the different ferromagnetic elements. Unfortunately, at room temperature the thermodynamically stable crystal structures of Ni, Fe, and Co are face-centered cubic (fcc), body-centered cubic (bcc), and hexagonal close-packed (hcp), respectively. Thus, a direct comparison is hampered and scientists endeavor to crystallize Fe, Co, and Ni in a non-native structure.

Recently, it was shown by Tian et al. that Ni can be stabilized in the bcc structure on a GaAs(001) substrate. In contrast to the fcc structure, it was found that bcc Ni exhibits different magnetic properties, e.g., Curie temperature and magnetic anisotropy [1].

A crystallographic change from fcc to bcc is known to be reflected in the electronic structure [2]. Therefore we used a spin-resolved inverse photoemission experiment to look for characteristic bcc type fingerprints. Furthermore, we compared our results with measurements taken on (bcc-)Fe/Pd(001) and (fcc-)Ni/Cu(001).

[1] C.S. Tian et *al.*, Phys. Rev. Lett. **94**, 137210 (2005)

[2] Donath et *al.*, J. Phys.: Condens. Matter **21**, 134004 (2009)

O 45.5 Wed 11:30 H33

**Temperature dependent quasiparticle renormalization in nickel and iron.** — •Ruslan Ovsyannikov, Setti Thirupathaiah, Jaime Sánchez-Barriga, Jörg Fink, and Hermann Dürr — Helmholtz Zentrum Berlin, BESSY II, Albert-Einstein-Strasse 15, D-12489 Berlin, Germany

One of the fundamental consequences of electron correlation effects is that the bare particles in solids become 'dressed' with an excitation cloud resulting in quasiparticles. Such a quasiparticle will carry the same spin and charge as the original particle, but will have a renormalized mass and a finite lifetime. The properties of many-body interactions are described with a complex function called self energy which is directly accessible to modern high-resolution angle resolved photoemission spectroscopy (ARPES). Ferromagnetic metals like nickel or iron offers the exciting possibility to study the spin dependence of quasiparticle coupling to bosonic modes. Utilizing the exchange split band structure as an intrinsic 'spin detector' it is possible to distinguish between electron-phonon and electron-magnon coupling phenomena. In this contribution we will report a systematic investigation of the $\boldsymbol{k}$– and temperature dependence of the electron-boson coupling in nickel and iron metals as well as discuss origin of earlier observed anomalous lifetime broadening of majority spin states of nickel at Fermi level.

O 45.6 Wed 11:45 H33

**Cobalt/nickel mixed oxides - cathode materials for Li-Ion-Batteries** — •Stephan Schmidt and Dieter Schmeisser — Brandenburgische Technische Universität 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 are interested in whether this replacement causes changes in the valence band (VB) and conduction band (CB) states or not.

Samples were prepared as thin films from nitrate solutions on metal substrates and annealed in air and UHV. The Co to Ni ratio was varied from 50/50 over 40/60 and 30/70 up to 20/80. The results are compared to the pure Co-oxide. Experiments were carried out at the

U49/2 beamline at BESSYII, Berlin.

XPS of the TM2p states reveals the existence of charge transfer ground states and different oxidation states. NEXAS at the Co2p, Ni2p and O1s edges projects the density of unoccupied states while resonant PES at these edges provides the related partial density of states (pDOS) and thus can be used to distinguish between the different contributions of TM3d and O2p states in the valence band region.

We find systematic variation of the VB structure, the valence band maximum and a shift at the O1s absorption edge while the TM2p XPS and absorption spectra do not seem to be affected by the mixing.

O 45.7 Wed 12:00 H33

**Neutral Excitations of Physisorbed Helium** — •Sarah Kossler[1], Reinhold Schneider[1], Peter Feulner[1], and Jean Pierre Gauyacq[2] — [1]TU München, Garching, Germany — [2]UMR CNRS-Université Paris Sud, Orsay, France

We study neutral excitations of He mono- and bilayers on Pt(111), Ru(001), Ag(111) and Cu(111) surfaces, and sandwich layers of He on well ordered Ne and Ar monolayers on these substrates. We apply narrow bandwidth undulator radiation of variable polarization (BESSY, UE-112-PGM-1) in combination with a Time-Of-Flight technique that enables us to detect electrons, ions, metastable atoms and fluorescence photons. Therewith we obtain comprehensive data sets on excitation and decay processes below the 1s ionization edges of these layers. Compared to the isolated atom, strong inter- and intralayer coupling is found that is well reproduced by calculations. We observe hybridization of s and p final states, and for higher principal quantum numbers also admixture of d states. We demonstrate that the comparison of data from different samples as indicated above is indispensable for a complete understanding of these processes.

Support by the Deutsche Forschungsgemeinschaft (Fe346/2-1), travel funding by the HZB, and help during the experiment by N.Armbrust, D.Heim and the staff of BESSY is gratefully acknowledged.

O 45.8 Wed 12:15 H33

**Rashba Type Spin-Splitting in the Two-Dimensional Electron System Au/Ge(111) Studied by Angle-Resolved Photoemission** — •Philipp Höpfner[1], Jörg Schäfer[1], Sebastian Meyer[1], Christian Blumenstein[1], Andrzej Fleszar[2], Xiaoyu Cui[3], Luc Patthey[3], Werner Hanke[2], and Ralph Claessen[1] — [1]Exp. Physik 4, Universität Würzburg — [2]Theor. Physik 1, Universität Würzburg — [3]Swiss Light Source, PSI, Villigen, Switzerland

The confinement of electrons in a single atomic adsorbate layer on a semiconductor surface presents an excellent playground for the study of electronic correlations in low dimensions. In this way, several intriguing two-dimensional electron systems (2DES) have been realized experimentally, such as e.g. the $\sqrt{3}$-reconstructions on (111) surfaces of Si and Ge. These systems are candidates for a spin-orbit splitting, due to the strong potential gradient at the surface, being in particular of the Rashba type.

In choosing heavy elements as adatoms, the spin-orbit interaction may play a significant role and one may ask what will happen to the Rashba splitting. We present results from angle-resolved photoelectron spectroscopy using synchrotron light of the metallic $\sqrt{3}$-Au/Ge(111) system. Two sets of metallic surface bands are observed, each of which appears to be split in pairs, originating from a Rashba type spin-splitting, as assigned by density functional theory calculations. Interestingly, the in-plane spin component varies across the Fermi surface. This metallic monolayer 2DES may represent a novel approach for spin injection into a semiconductor from a monolayer only.

O 45.9 Wed 12:30 H33

**Structure and Energetics of Si(111)$5\times2$−Au Atomic Chains** — •Ingo Barke[1], Steven C. Erwin[2], and F. J. Himpsel[3] — [1]Universität Rostock, Germany — [2]Naval Research Laboratory, Washington, DC — [3]University of Wisconsin-Madison, WI

We propose a structural model for the Si(111)5x2-Au reconstruction [1]. The model incorporates a revised experimental value of 0.6 monolayer for the coverage of gold atoms, equivalent to six gold atoms per $5\times2$ cell [2]. Results obtained from first-principles total-energy calculations are in excellent agreement with experimental observations: (1) In the presence of silicon adatoms the periodicity of the gold rows spontaneously doubles. (2) The dependence of the surface energy on the adatom coverage indicates that a uniformly covered phase is unstable and will phase separate into empty and covered regions. (3) High-resolution scanning tunneling microscopy images are precisely reproduced by theory. (4) The calculated band structure is consistent with angle-resolved photoemission spectra. (5) The calculated activation barrier for diffusion of silicon adatoms along the row direction is in excellent agreement with the experimentally measured barrier [3].

[1] S. C. Erwin et al., Phys. Rev. B 80, 155409 (2009)
[2] I. Barke et al., Phys. Rev. B 79, 155301 (2009)
[3] E. Bussmann et al., Phys. Rev. Lett. 101, 266101 (2008)

## O 46: Density functional theory and beyond for real materials I

Time: Wednesday 10:30–13:15 Location: H34

O 46.1 Wed 10:30 H34

**Structure and magnetism of clean and decorated grain boundaries in nickel** — Monika Všianská[1,2] and •Mojmír Šob[1,2] — [1]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic — [2]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic

With the help of density-functional theory, we have studied the structure and magnetism of the $\Sigma5(210)$ grain boundary (GB) in nickel as well as segregation and embrittling potency of sp-elements in the 3rd, 4th and 5th period (Al, Si, P, S, Ga, Ge, As, Se, In, Sn, Sb and Te) at this GB. For comparison, segregation of these impurities at the (210) free surface (FS) has also been investigated. Full relaxation of the geometric configuration of the GB and FS without and with impurities has been performed and the effect of impurities on the distribution of magnetic moments has been analysed. We determined the embrittling potency energy from the difference between the GB and FS binding energies on the basis of the Rice-Wang model; here a positive/negative value of this quantity means that the solute atom has the embrittling/strengthening effect on the GB. It turns out that all substitutionally segregated impurities studied are GB embrittlers in Ni.

O 46.2 Wed 10:45 H34

**Electron Correlation and the Ferromagnetic Behaviour of Chromium Oxide** — •Mallia Giuseppe[1], John Drain[1], and Nicholas M. Harrison[1,2] — [1]Imperial College London - Thomas Young Centre - Chemistry Department, London UK — [2]STFC, Daresbury Laboratory, Daresbury, Warrington WA4 4AD, UK

One might expect that the half-metallic ferromagnet CrO2 would provide an excellent spin injection material for use in spintronics applications. In practice this is not the case. CrO2 was first predicted to be a half-metallic ferromagnet on the basis of density functional theory calculations (Schwarz 1986). In the current work a more reliable treatment of electronic correlation that includes strong on-site Coulomb interactions is used to reexamine the bulk and surface electronic structure. It is demonstrated that strong electron correlation significantly reduces the density of states at the Fermi edge in the bulk phase and is sufficient to open an energy gap at the (110), (100) and (001) surfaces. This data is used to rationalise recent ultraviolet photoemission spectra and point contact Andreev spectroscopy measurements.

K. Schwarz J. Phys: F-Metal Physics 16(9):L211-L215 (1986)

O 46.3 Wed 11:00 H34

**Theory of angular resolved X-ray photoelectron spectroscopy in correlated magnetic solids** — •Jan Minar, J. Braun, and H. Ebert — Dept. Chemie und Biochemie, LMU University of Munich, Germany

The combination of local spin density approximation (LSDA) and the dynamical mean field theory (DMFT) provide a powerful basis to treat correlations beyond plain LSDA. The KKR or multiple scattering approach implemented on this basis allows among others to deal with surface systems as well as to study spectroscopic properties [1]. The latter feature is particularly interesting as a direct comparison with experiment reveals the impact of correlation effects unambiguously as matrix element effects are treated on the same level. This is demonstrated by results for the angle-integrated as well as angle-resolved photo emission of transition metal ferromagnets [2]. Special emphasis will be put on the spin-polarised relativistic mode allowing to deal with the spin-orbit coupling induced properties like orbital magnetic moment and magnetic dichroism. Applications of this formalism on the 3d-transition metal surfaces, Heusler alloys and transition metal oxides will be presented.

1. J. Minár et al., Phys. Rev. B 72, 0415125 (2005); S. Chadov et al., Europhys. Lett. 82, 37001 (2008)
2. J. Minar et al., Phys. Rev. Lett. 95, 166401 (2005); J. Braun et al., Phys. Rev. Lett. 97, 227601 (2006); M. Pickel et al., Phys. Rev. Lett. 101, 066402 (2008); J. Sanchez-Barriga et al., arXiv:0910.4360v1 (2009).

O 46.4 Wed 11:15 H34

**LDA+DMFT calculations of x-ray absorption and x-ray circular dichroism spectra: Role of valence-band correlations** — •Ondrej Sipr[1], Jan Minar[2], Antonin Simunek[1], and Hubert Ebert[2] — [1]Institute of Physics AS CR, Cukrovarnicka 10, Prague, Czech Republic — [2]Universitat Munchen, Butenandtstr. 5-13, Munchen, Germany

$L_{2,3}$-edge XAS and XMCD spectra of 3d elements are calculated via a self-consistent LDA+DMFT method (including thus valence-band correlations). It is found that the asymetry of the calculated XAS white lines increases upon inclusion of the correlations for Fe and Co but not for Ni. The change in the height of the $L_3$ and $L_2$ peaks in the XMCD spectra is in a good agreement with the change of the orbital magnetic moment caused by adding the valence-band correlations. As a whole, adding valence-band correlations improves the agreement between the theory and experiment but visible differences still remain. Therefore, a core hole is additionally accounted for via the final state approximation and the impact of such a procedure is assessed.

O 46.5 Wed 11:30 H34

**A strong correlation study: the paradigmatic case of $V_2O_3$** — •Federico Iori — Lsi - Ecole Polytechnique,Cnrs -Cea-Iramis Palaiseau, France

Aim of our work is to study through an ab initio theoretical approach the paramagnetic metallic (PM) and insulating (PI) phase of $V_2O_3$ in order to understand better the metal-insulator phase transition of this system. It has been shown that at DFT level it's not possible to describe properly the insulating paramagnetic phase because of a poor treatment of the strong electronic correlation for such systems with d- or f- incomplete shell within including many body effect such the ones arising from a direct photoemission spectroscopy. Hard x-ray inelastic x-ray scattering in the non resonant regime has indeed proven highly effective to measure low energy losses, especially dd excitations, when operating at high momentum transfer. The dynamical structure factor for PM and PI phase of the $V_2O_3$ has been thus evaluated through *ab initio* calculations of the loss function for large transferred momenta parallel and perpendicular to the *xy* plane. Experimental evindence shown in the energy region between 2-3 eV, non dipolar transitions which favor intraband excitations become increasingly allowed while the probing length $q^{-1}$ approaches typical d orbital spatial extension.

O 46.6 Wed 11:45 H34

**The calculations of the XANES L edges 3d compounds** — •Robert Laskowski and Peter Blaha — Vienna University of Technology, Institute of Materials Chemistry, Vienna, Austria

We report on the calculations of the x-ray absorption near-edge structure spectra focusing on the transition metals L edges. In our approach we solve Bethe-Salpeter equation (BSE) formulated in a basis of single particle states calculated within DFT. The presented method goes beyond the commonly used DFT electron-hole calculations and is an alternative to a relativistic Hartree-Fock configuration interaction method. The DFT core-hole method, cannot reproduce some features of the L edge spectra, usually interpreted as multiplet effects. For example in the single particle approximation, the branching ratio should be proportional to the occupancy of the corresponding core levels, for p3/2 and p1/2 branches it should be close to 2:1. However the measured branching ratio may be quite different, for example for 3d0 cations like K+, Ca 2+, Ti 4+ the p1/2 branch is enhanced such that a ratio closer to 1:1 is observed. We show that this is related to the interaction between elementary excitations from p3/2 and p1/2 core states in the BSE approach. Independent calculations performed for p3/2 and p1/2 branches result in a ratio close to 2:1 and only when the interaction between the p3/2 and p1/2 excitation is included the correct ratio is obtained.

O 46.7 Wed 12:00 H34

**Optical Absorption and Bound Excitons in MnO, FeO, CoO, and NiO** — •Claudia Rödl, Frank Fuchs, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik and European Theoretical Spectroscopy Facility (ETSF), Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Since magnetic materials gain more and more importance also for technological applications, we calculate the optical properties of the row of antiferromagnetic oxides from MnO to NiO from first principles.

We present optical absorption spectra solving the Bethe-Salpeter equation (BSE), thus including excitonic and local-field effects (LFE). It turns out that the main absorption peaks are due to *d*-*d* excitations which are dipole forbidden at the Γ point. It is shown that the influence of LFE is almost vanishing for the materials under investigation, while the electron-hole attraction leads to a significant redistribution of spectral weight to lower energies.

Besides the dipole allowed excitations which contribute to the absorption spectra, also optically forbidden excitations within the fundamental gap occur. The latter are related to Frenkel-like bound excitonic states. These excitons have their origin in transitions between the occupied and empty *d* states of the transition-metal cations. Due to the separation of the excitonic Hamiltonian into the independent subspaces of spin-allowed and spin-forbidden transitions, they can be split into two groups: excitons which involve a flip of the one-particle spin between valence and conduction bands and excitons without spin flip.

O 46.8 Wed 12:15 H34

**CO adsorption on transition metal surfaces applying the random phase approximation** — •Laurids Schimka[1], Judith Harl[1], Alessandro Stroppa[2], Andreas Grüneis[1], Martijn Marsman[1], Florian Mittendorfer[1], and Georg Kresse[1] — [1]Faculty of Physics, University of Vienna, Austria — [2]CNR-INFM-CASTI Regional Laboratory, University of L'Aquila, Italy

Most gradient corrected density functionals predict surfaces to be more stable than they are experimentally. This observation would suggest that adsorption energies on surfaces are too small, but the contrary is often found: chemisorption energies are usually overestimated within the generalized gradient approximation. By modifying the gradient correction either the adsorption or the surface energy can be improved, but never both at the same time [1]. We show that a computationally fairly efficient approach, the random phase approximation (RPA) [2] to the correlation energy, yields both: accurate surface and accurate adsorption energies for carbon monoxide (CO) on transition metal surfaces ((111)-Cu,Ru,Rh,Pd,Ag and Pt). In addition and contrary to most semi-local functionals, the RPA predicts in every single case the correct adsorption site of the CO molecule on the surface.

References

[1] Stroppa, A. & Kresse, G. New Journal of Physics 10, 063020 (2008).

[2] Nozieres, P. & Pines, D. Phys. Rev. 111, 442-454 (1958).

O 46.9 Wed 12:30 H34

**Time-dependent Kohn-Sham self-interaction correction** — •Dirk Hofmann, Thomas Körzdörfer, and Stephan Kümmel — Department of Physics, University of Bayreuth, 95440 Bayreuth

The self-interaction error of commonly used density functionals leads to a number of well-known problems in density functional theory (DFT). A particularly pronounced and practically important one is the serious overestimation of charge transfer in extended molecular systems.

Perdew and Zunger proposed an energy functional to overcome the selfinteraction problem (SIC), but their approach is not unitarily invariant and thus difficult to straightforwardly incorporate into Kohn-Sham theory. It has recently been shown, though, that the unitary invariance problem can systmatically be overcome by employing the generalized optimized effective potential (GOEP) formalism. However, in a time-dependent Kohn-Sham framework self-interaction correction is even more involved. The time-dependent optimized effective potential (TDOEP) equation is very demanding to solve and approximations to the TDOEP are not necessarily reliable.

Here, we extended the GOEP approach to the time-dependent case for a proper treatment of the unitary invariance problem. Furthermore, we implemented and tested this time-dependent Kohn-Sham SIC (TD-SIC) scheme in a real-time Kohn-Sham propagation code. First results indicate that orbital localization improves the stability of the TDSIC scheme, making it a possible candidate for dealing with the problem of charge-transfer excitations.

O 46.10 Wed 12:45 H34

**Electronic excitations in nanostructures: an empirical pseudopotential based approach** — •Gabriel Bester — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany

In this contribution we will outline the framework, based on empirical pseudopotentials and configuration interaction [1], to obtain quantitative predictions of the excited state properties of semiconductor nanostructures using their experimental sizes, compositions and shapes. The methodology can be used to describe colloidal nanostructure of few hundred atoms all the way to epitaxial structures requiring millions of atoms. The aim is to fill the gap existing between *ab initio* approaches and continuum descriptions. Based on the pseudopotential idea and the developments of empirical pseudopotentials for bulk materials in the early 60's, the method has evolved into a powerful tool, where the pseudopotential construction has lost some of its empirical character and is now based on density functional theory. We will present the construction of these potentials and the way the ensuing wave functions are used in a subsequent configuration interaction treatment of the excitation. We will illustrate the available capabilities by recent applications of the methodology to unveil new effects in the optics of nanostructures. We will close by an outlook on some envisionned improvements of the method.
[1] G. Bester, J. Phys.: Condens. Matter.**21** 023202 (2009).

O 46.11 Wed 13:00 H34

**Time dependent hybrid density functional calculations on semiconductor nanocrystallites** — Marton Voros and •Adam Gali — Budapest University of Technology and Economics

Recent technological developments allow the preparation of nanometer sized semiconductor nanocrystals [1-2]. Due to the small size, these nanocrystals exhibit several special features [2-4], therefore understanding the electronic and optical properties at the molecular level is crucial for applications. We show that by using a hybrid functional based TDDFT approach the calculated absorption spectrum of small diamond nanocrystals (diamondoids) near quantitatively agrees with recent experiments [5-6]. We show that Rydberg transititions rule the low energy part of the absorption spectra even in relatively large diamondoids [6] which is not common in other group IV type semiconductor nanocrystals. This property makes it computationally hard to get a well-converged result using supercell based methods. Applying the same technique we show that the low energy part of the absorption spectrum of biologically inert silicon carbide nanocrystals strongly depends on the actual type of surface reconstruction. This would allow the identification of surface reconstruction by comparing the experimental and calculated absorption spectra.

[1] J. E. Dahl et al., Science 299, 96 (2003) [2] X. L. Wu et al., Phys. Rev. Lett. 94, 026102 (2005) [3] Jiyang Fan et al., Small 4, No. 8, 1058 (2008) [4] W. L. Yang et al., Science 316, 1460 (2007) [5] Lasse Landt et al., Phys. Rev. Lett. 103, 047402 (2009) [6] Márton Vörös and Adam Gali, Phys. Rev. B 80, 161411(R)(2009)

## O 47: Metal substrates: Adsorption of organic / bio molecules V

Time: Wednesday 10:30–13:00 Location: H36

O 47.1 Wed 10:30 H36

**Adsorption behaviour of Phthalocyanine molecules on a Au(1 1 0) surface** — •Tobias Pertram[1], Jan-Markus Essen[1], Séverine Le Moal[2], Marco Moors[1], Michael Peintinger[1], Conrad Becker[2], Thomas Bredow[1] und Klaus Wandelt[1] — [1]Institute of Physical and Theoretical Chemistry, Wegelerstr. 12, D-53115 Bonn, Germany — [2]CINAM - CNRS - UPR 3118, Campus de Luminy - Case 913, F-13288 Marseille, France

The {1 1 0} surfaces of fcc metals contain an intrinsic anisotropy due to their rectangular surface unit cell. This anisotropy is even more pronounced in case of the $(1 \times 2)$ missing row reconstruction, which is typical for the Au(1 1 0) surface. We have used this reconstructed surface as a substrate for the deposition of phthalocyanine molecules. In our STM and LEED study we found the formation of molecular double rows which are aligned with the closed packed rows of the reconstructed Au(1 1 0) surface. In addition to a coverage dependence of the length of the double rows, we found that the presence of these rows also influences the type of the reconstruction of the Au(1 1 0) surface. Whereas at uncovered regions the $(1 \times 2)$ reconstruction could be observed, at regions covered with phthalocyanine double rows a $(1 \times 3)$ reconstruction was found. The formation of double rows on the $(1 \times 3)$ reconstructed Au(1 1 0) surface is triggered by both a strong molecule–molecule interaction and a strong molecule–substrate interaction. In contrast only a weak interaction between adjacent dimmers along the rows could be observed, the closest distance between them equals six times the Au lattice constant.

O 47.2 Wed 10:45 H36

**Diffusion of phthalocyanine on Ag(100) investigated by STM** — •Grazyna Antczak[1,2] and Karina Morgenstern[1] — [1]Leibniz University, Hannover, Germany — [2]University of Wroclaw, Wroclaw, Poland

Information about the thermal stability of phthalocyanine as well as how the molecule binds to surfaces are crucial in a bottom up approach to build molecular electronics. Phthalocyanine is already widely used in technology, for example in laser printers, CDs, colorants and so on. How do these organic molecules move over a surface? In contrast to the well studied diffusion of individual atoms, molecules exhibit more motional degrees of freedom that make their movement much more complicated. It is likely that concerted mechanisms will play an important role in their diffusion. Such concerted movements were already proven to be present for movement of close-packed metallic clusters. We have carried out a study of phthalocyanine motion on the Ag(100) surface in low-temperature scanning tunneling microscopy in the temperature range 50-80 K. We will show that phthalocyanine starts thermal movement over the surface at 55 K and follows an Arrhenius relation at least up to 80 K. From the Arrhenius plot of diffusivity the activation energy of 116 meV for the movement of single molecules was obtained. The prefactor of diffusivity will also be discussed.

O 47.3 Wed 11:00 H36

**XSW experiments on Copper(II)-Phthalocyanine submonolayer films on noble metal surfaces** — •Ingo Kröger[1], Christoph Stadler[2], Benjamin Stadtmüller[1], Christoph Kleimann[1], Giuseppe Mercurio[1], Patrick Bayersdorfer[2], Florian Pollinger[2], and Christian Kumpf[1] — [1]Institute of Bio- and Nanosystems 3 (IBN-3), Forschungszentrum Jülich & JARA-FIT — [2]Experimentelle Physik II, Universität Würzburg

The adsorption of large pi-conjugated molecules on noble metal surfaces is in the focus of recent experimental and theoretical investigations. The basic bonding mechanisms are of particular interest, as well as their influence on crucial parameters like workfunctions and the alignment of molecular levels with respect to the substrate Fermi level. Geometric parameters are also of high interest. However, the most prominent and fundamental parameter, the adsorption height, is generally overestimated in state of the art DFT calculations. We present a series of X-ray standing wave measurements of the bonding distances for the model system Copper(II)-Phthalocyanine in different submonolayer phases on Ag(111), Au(111) and Cu(111). It is shown that the adsorption height does not only depend on the substrate, but also on the lateral structure of the molecular thin film which is very sensitive to small changes in the coverage [1]. The data are compared with the results of other techniques (see also contributions of C. Kleimann and B. Stadtmüller) and discussed in terms of the interaction strength.

[1] Stadler et al., Nature Physics 5, 153 (2009)

O 47.4 Wed 11:15 H36

**Sub-monolayer growth of CuPc on Cu(111)** — •Benjamin Stadtmüller[1,2], Ingo Kröger[1], Friedrich Reinert[2], and Christian Kumpf[1] — [1]Forschungszentrum Jülich (IBN-3) & JARA-FIT — [2]Exp. Physik II, Univ. Würzburg

The geometric arrangement of organic molecules within the first monolayer adsorbed on a metal surface has crucial influence on the interface properties as well as on the growth behavior of the following molecular layers. We studied the sub-monolayer growth of the model system copper-II-phthalocyanine (CuPc) on the Cu(111) surface using high resolution low energy electron diffraction (SPA-LEED) and photoelectron spectroscopy (UPS). This system is of highest interest since phthalocyanine molecules show an unusual intermolecular repulsion upon adsorption on the Ag(111) surface [1]. This is also discussed in the contributions of I. Kröger and C. Kleimann. On Cu(111), however, the alignment of the molecules indicates an attractive intermolecular interaction at sub-monolayer coverages. At low coverages the molecules align in linear chains of different length. At higher coverages they start to form islands having a commensurate structure. UPS-measurements show a new electronic state close to the Fermi level which indicates charge transfer (i.e. chemical interaction) between the molecules and the substrate. This breaks the 4-fold symmetry of the molecule and consequently influences the molecular order. From the comparison of results found for CuPc on Cu(111), Ag(111) and Au(111) we gain insight the influence of the substrate on the intermolecular interaction.

[1] Stadler et al., Nature Physics 5, 153 (2009)

O 47.5 Wed 11:30 H36

**Selective bonding and apparent symmetry of single Cobalt-Phthalocyanine on a Cu(111) surface** — •Deung-Jang Choi[1], Benjamin W. Heinrich[1], Cristian Iacovita[1], Thomas Brumme[2,3], Laurent Limot[1], Mircea V. Rastei[1], Jens Kortus[2], Werner A. Hofer[4], and Jean-Pierre Bucher[1] — [1]IPCMS(CNRS), UMR 7504, Université de Strasbourg, France — [2]Institut für Theoretische Physik, TU Bergakademie Freiberg, Germany — [3]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, Germany — [4]Surface Science Research Centre, University of Liverpool, United Kingdom

Low-temperature scanning tunneling microscopy and spectroscopy are combined with *ab initio* calculations to study isolated CoPc molecules on a Cu(111) surface. Tip-assisted manipulation and constant-height scans are employed to resolve the adsorption geometry of the molecule and to obtain high-resolution maps of the intramolecular conductance. We show that nitrogen atoms play a central role in the adsorption and the conductance of the molecule on Cu(111). The preferential adsorption of nitrogen on top of surface atoms centers CoPc on a bridge site of the Cu lattice and anchors the molecule to the surface with an adsorption energy estimated at 6.9 eV. Furthermore, we show that the $p$-orbitals of the nitrogen atoms along with the $d$-orbitals of cobalt govern the molecular conductance, the former contribution being responsible for the symmetry of CoPc on the surface. The symmetry is seen to change at selected biases due to electronic effects, which are discussed in detail.

O 47.6 Wed 11:45 H36

**Modification of magnetic properties of a manganese phthalocyanine by axial coordination of CO molecule** — •Anna Strozecka and Jose Ignacio Pascual — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

The coordintation of small molecules, like NO, CO or $O_2$, to transition metal phthalocyanines can substantially modify properties of these complexes and their interaction with the underlying substrate. We investigated the effect of coadsorption of CO molecules on magnetic properties of manganese phthalocyanines (MnPc) adsorbed on Bi(110) surface. STM experiments reveal that the Kondo resonance observed for unligated MnPc molecules changes upon bonding of CO to a central metal ion. The increase in the Kondo temperature of the complex indicates the enhancement of spin-electron coupling. The original magnetic state of MnPc is recovered after selective desorption of CO molecules.

O 47.7 Wed 12:00 H36

**Effect of fluorination on the adsorption geometry and electronic structure of Zn-phthalocyanine molecules** — •A. Gerlach[1], T. Hosokai[1], F. Schreiber[1], S. Duhm[2], N. Koch[2], H. Yamane[3], Y. Tanaka[3], Y. Mi[4], and J. Zegenhagen.[4] — [1]Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany — [2]Institut für Physik, Humboldt-Universität, Berlin, Germany — [3]Institute for Molecular Science, Okazaki, Japan — [4]European Synchrotron Radiation Facility, Grenoble, France

Using the X-ray standing wave (XSW) technique and angle-resolved UPS (ARUPS) we studied the structural and electronic properties of Zn-phthalocyanine (ZnPc) and perflurinated Zn-phthalocyanine ($F_{16}$ZnPc) molecules on Cu(111).

The element specific bonding distances of ZnPc and $F_{16}$ZnPc derived by XSW show that the molecule-substrate interaction depends significantly on the chemical structure of the adsorbate. Compared to its perfuorinated derivative ZnPc shows a surprisingly small bonding distance ($d(C) = 2.49\,\text{Å}$), which reflects the strong interaction of the molecules with the copper substrate. Moreover, the XSW data reveal different distortions of these molecules that can be related to their specific bonding mechanism: Relative to the molecular plane the central zinc atom of ZnPc is pulled 0.25 Å towards the substrate, whereas the fluorine atoms of $F_{16}$ZnPc are pushed 0.15 Å towards the vacuum side. We show that these adsorption induced changes of the molecular geometry are reflected in electronic structure of both systems.

O 47.8 Wed 12:15 H36

**SnPc on Ag(111) investigated by STM** — •Christoph Kleimann, Ingo Kröger, Christian Weiss, Christa Elsaesser, and Christian Kumpf — Institut für Bio- und Nanosysteme (IBN3), FZ Jülich & JARA-FIT

The investigation of interfaces between thin organic films and metal surfaces is a field of highest interest because it represents the basis for future applications of organic electronic devices. In this context, phtalocyanines are of particular interest since repulsive intermolecular interaction was found recently for this group of organic molecules [1]. Tin(II)-phtalocyanine (SnPc) is non-planar and can adsorb in two different geometries: with the Sn atom pointing downwards (Sn down) or upwards (Sn up). In our group different Pc molecules have previously been studied using several experimental techniques like SPA-LEED or XSW (see also contributions by I. Kröger and B. Stadtmüller). Here we present STM studies of SnPc on Ag(111), taken at different coverages and temperatures, and discuss the results in the context of our previous findings. At low coverages the formation of chains can be observed for Sn down molecules while Sn up molecules tend to stay separated. This originates from a strong interaction with the substrate which leads to a broken symmetry of the SnPc molecules. Measurements at higher coverages show large ordered areas of Sn down molecules which are oriented along the different domains of the silver surface. The combination of STM and LEED in our setup allows to precisely correct the STM images for distortions and therefore enables a quantitative analysis of the adsorption geometry. [1] Nat. Phys. 5, pp 153-158 (2009)

O 47.9 Wed 12:30 H36

**STM and STS study at the organic-metal interface: Adsorption of CoPc on Ag(111) surface** — •Marius Toader, Pavel Shukrynau, and Michael Hietschold — Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany

In this work, we have studied the interface effects which arise upon adsorption of cobalt(II)-phthalocyanine (CoPc) on a silver (111) surface, in terms of morphology and electronic properties. The organic ultra-thin film corresponding to a slightly sub-monolayer coverage has been prepared using OMBD and investigated with an UHV VT-STM from Omicron. A strong molecule-substrate coupling is emphasized by template-guided molecular arrangements of single molecules, molecular nanochains and extended molecular domains. Therefore, the reported highly-oriented adlayer structures, like pseudo-square and superstructures with different molecular appearance, have to be discussed. The electronic properties at the organic-metal interface, are discussed based on voltage polarity-dependent STM imaging and tip-sample distance-dependent scanning tunneling spectroscopy. A molecular HOMO-LUMO gap narrowing has been reported with decreasing tip-sample distance. Moreover, the features in the superstructure exhibit slightly different electronic properties. For a better understanding of the interface effects, single molecule DFT calculations were also employed and compared with STS data.

O 47.10 Wed 12:45 H36

**Electronic structure of ultra thin organic hetero-interfaces - SnPc/PTCDA/Ag(111)** — •Achim Schöll[1], Marc Häming[1], Michael Greif[1], Michael Wiessner[1], and Friedrich Reinert[1,2] — [1]Universität Würzburg, Experimentelle Physik VII, D-97074 Würzburg, Germany — [2]Karlsruhe Institute of Technology, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe, Germany

While the interfaces of molecules to a substrate have been studied extensively, knowledge about the interface between different molecular compounds is still relatively scarce. This is to some extend caused by the fact that these interfaces, which are of great relevance for optoelectronic devices consisting out of multiple organic compounds, are more complicated to access experimentally. Structurally well defined model systems, which allow for a systematic and detailed investigation of the interface characteristics, are thus of great importance. In this work we provide data from x-ray absorption and photoelectron spectroscopy on the organic heterolayer system tin-phthalocyanine (SnPc) / perylen-tetracarboxylicacid dianhydride (PTCDA). We show, that SnPc, prepared on a Ag(111) surface precovered by a monolayer of PTCDA, forms a well defined interface with a closed first layer of flat lying molecules. Moreover, the bonding of the SnPc molecules to the PTCDA interlayer is clearly non-covalent and a detailed inspection of the valence spectra shows that the respective molecular signatures can be distinguished well. The SnPc/PTCDA/Ag(111) system is thus well-suited for further investigations employing complicated techniques.

## O 48: Surface dynamics I

Time: Wednesday 10:30–12:45 Location: H40

O 48.1 Wed 10:30 H40

**Probing the Momentum-Dependent Response of the Charge Density Wave Phase in $TbTe_3$ by Ultrafast Time- and Angle-Resolved Photoemission** — •P.S. Kirchmann[1,2], F.T. Schmitt[1], U. Bovensiepen[2,3], R.G. Moore[1], L. Rettig[2], M. Krenz[2], J.-H. Chu[1], N. Ru[1], L. Perfetti[2,4], M. Wolf[2,5], I.R. Fisher[1], and Z.-X. Shen[1] — [1]Department of Applied Physics, Stanford University, Stanford, CA 94305, USA — [2]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — [3]Universität Duisburg-Essen, Institut für Experimentelle Physik, 47048 Duisburg, Germany — [4]Ecole Polytechnique, 91128 Palaiseau cedex, France — [5]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany

Charge density wave (CDW) systems such as $TbTe_3$ offer fascinating options for studying the correlation of electrons and the lattice. We investigate the ultrafast response of the charge density wave (CDW) phase in $TbTe_3$ [1] after femtosecond IR excitation using time- and angle-resolved photoemission [2]. The time-dependent photoemission intensity at the Fermi level yields a characteristic time for the closing of the CDW bandgap. With increasing laser fluence the bandgap closes faster, pointing to an increasing slope of the excited potential energy surface. As function of electron momentum the amplitude of the response increases strongly at the position of the Fermi wave vector $k_F$. These results vividly demonstrate that the CDW system is most susceptible to electronic excitations near $k_F$ and that these electronic perturbations drive collective excitations of the coupled electron-lattice system. [1] Phys. Rev. B **77** (2008) 235104. [2] Science **321** (2008) 1649.

O 48.2 Wed 10:45 H40

**Fluence-dependent two-pulse correlation for electronically induced diffusion of O/Pt(111)** — •Kristina Klass[1], Gerson Mette[1], Jens Güdde[1], Michael Dürr[1,2], and Ulrich Höfer[1] — [1]Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg — [2]Fakultät Angewandte Naturwissenschaften, Hochschule Esslingen, D-73728 Esslingen

We present results of a time-domain study of electronically induced diffusion of atomic oxygen on a vicinal Pt(111) surface. At low substrate temperatures, hot electrons are excited by femtosecond laser pulses and result in a hopping of O atoms from the O-saturated steps onto the terraces. Optical second-harmonic generation (SHG) was used to observe this process via monitoring the occupation of the step sites. The strong fluence dependence of the diffusion process was detected via SHG microscopy by analyzing the signal across the laser beam profile. In combination with two-pulse correlation measurements this techniques was used to study the dynamics of energy flow from the initial excited substrate electrons to the adsorbate degree of freedom at different laser fluences. The widths of the two-pulse-correlations are in the picosecond range and increase with increasing laser fluence. The results are qualitatively similar to those obtained recently for CO/Pt(111) [1]. They are discussed on the basis of an empirical friction model using an electronic friction coefficient that depends on excitation density.

O 48.3 Wed 11:00 H40

**Ultrafast electron transfer across polar molecule-metal interfaces: strong coupling vs. molecular screening** — •Julia Stähler[1,2], Michael Meyer[1], Uwe Bovensiepen[1,3], and Martin Wolf[1,2] — [1]Freie Universität Berlin, FB Physik, Berlin, Germany — [2]Fritz-Haber-Institut der MPG, Abt. Phys. Chemie, Berlin, Germany — [3]Universität Duisburg-Essen, FB Physik, Duisburg, Germany

Heterogeneous charge transfer plays a crucial role for the development of molecular electronics such as, for example, OLEDs. The screening properties of the involved molecules hereby play an important role as they determine the timescales on which electron transfer (ET) occurs. However, also the substrate's electronic band structure significantly influences the ET dynamics. We use amorphous $D_2O$ and $NH_3$ layers on Cu(111) and Ru(001) surfaces as model systems for systematic investigation of the ultrafast ET dynamics at polar molecule-metal interfaces by means of time-resolved two-photon photoelectron (2PPE) spectroscopy. With a $1^{st}$ laser pulse, electrons are excited in the metal and injected into the adsorbate layer where they localize at favorable sites. The subsequent electron (back) transfer to the substrate is monitored with a $2^{nd}$, time-delayed laser pulse. The study unveils that (i) molecular screening is observed for $t > 200$ fs after electron injection, (ii) before, ET is dominated by the strong coupling to the substrate states. Our results strongly suggest that this transition from the *substrate-dominated* to the *barrier-determined* regime of ET is a general characteristic of ET across (polar) molecule-metal interfaces.

O 48.4 Wed 11:15 H40

**Neutral hydrogen desorption from graphite induced by ultra short laser pulses** — •Robert Frigge[1], Tim Hoger[1], Björn Siemer[1], Helmut Zacharias[2], Thomas Olsen[2], and Jakob Schiøtz[1] — [1]Physikalisches Institut, Universität Münster, Germany — [2]CINF, Technical University of Denmark, Denmark

The desorption of hydrogen from HOPG is an important issue in the understanding of molecular hydrogen formation on durst particles upon irradiation. Surface mediated processes lead to H atom desorption. The velocity distribution of atomic hydrogen from HOPG is examined after surface excitation with fs pulses at $\lambda = 400\,\mathrm{nm}$ using a Ti:sapphire laser. Desorbing neutral H atoms are ionized using (2+1) REMPI via the 2s ← 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 desorbing hydrogen atoms.

Electron scattering calculations are performed employing a repulsive electronic state and the H-graphite adsorption potentials appropriate for different adsorption sites[1]. Besides populating different vibrationally excited states in multiple scattering events, velocity distributions for desorption out of different adsorption sites are obtained. A good agreement with the experimentally observed velocities is obtained, not only for the fast but also for the very slow atoms. [1]L. Hornekær et al., Phy. Rev. Lett., **96**, 156104 (2006)

O 48.5 Wed 11:30 H40

**Momentum dependent electron and hole relaxation dynamics in $EuFe_2As_2$** — •L. Rettig[1], R. Cortes[1], S. Thirupathaiah[2], U. Bovensiepen[1,3], M. Wolf[1], H. A. Duerr[2], P. Gegenwart[4], T. Wolf[5], and J. Fink[2,6] — [1]Freie Universität Berlin, D-14195 Berlin — [2]Helmholtz-Zentrum Berlin, D-12489 Berlin — [3]Universität Duisburg-Essen, D-47048 Duisburg — [4]Georg-August-Universität Göttingen, D-37077 Göttingen — [5]Karlsruhe Institute of Technology, D-76021 Karlsruhe — [6]Leibniz-Institute for Solid State and Materials Research Dresden, D-01171 Dresden

The influence of the electronic bandstructure on the fundamental relaxation processes of excited carriers leading to intra- and interband scattering is of fundamental interest in solid state physics. Here, we report on fs time- and angle-resolved photoemission spectroscopy (trARPES) on the parent compound $EuFe_2As_2$ of the new class of FeAs based high-$T_c$ superconductors. Using intense fs laser pulses ($h\nu = 1.5\,\mathrm{eV}$), part of the electronic population is excited to states above the Fermi level. The transient evolution of both occupied and unoccupied states is probed by energy- and angle-resolved photoelectron spectroscopy using a time-delayed ultraviolet pulse ($h\nu = 6.0\,\mathrm{eV}$). Upon excitation, occupied states around the hole-pocket at the Γ-point of the Brillouin zone become partially depopulated by excited holes, whereas electrons are filling the empty states within the hole-pocket. The timescales of electron and hole dynamics within this band differ drastically and cannot be explained solely by intraband e-h pair generation, but an additional interband excitation channel has to be considered.

O 48.6 Wed 11:45 H40

**Relaxation dynamics and bulk-to-surface-recombination of hot electrons 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

We have studied the relaxation of hot carriers excited to the conduction band minimum (CBM) on the Si(001) surface. Two-photon photoemission combined with an electron analyzer equipped with a 2D-CCD-imaging detector allows us to follow the relaxation dynamics of photoexcited carriers in energy and momentum space simultaneously on a femtosecond timescale. With a pump fluence of 570 $\mu J/cm^2$ an electron density of $\approx 10^{18}$ $cm^{-3}$ is created 1 eV above the CBM, leading to an ultrafast cooling of initially excited electrons within the laser pulse width of 70 fs. After 350 fs the hot carriers can be described by a Fermi-distribution with a temperature of several thousand Kelvin. This temperature initially decreases on a fast time scale of 1 ps to 350 K, the same time scale on which the observed intensity from the normally unoccupied surface state $D_{down}$ shows a strong increase. On a second time scale the remaining occupation in the CBM decreases within several hundred picoseconds. We conclude that electron-electron-scattering, which becomes important in semiconductors for excited carrier densities $> 10^{17}$ $cm^{-3}$, is the main mechanism behind efficient bulk-to-surface-recombination in the first picosecond after excitation.

O 48.7 Wed 12:00 H40

**Ultrafast electron dynamics at alkali-ice interfaces probed with two-photon photoemission** — •Michael Meyer[1], Mathieu Bertin[2], Uwe Bovensiepen[3], and Martin Wolf[1] — [1]Freie Universität Berlin, FB Physik, 14195 Berlin, Germany — [2]LPMAA, Université Pierre et Marie Curie, 75252 Paris cedex 05, France — [3]Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany

An excess charge in a polar environment, i.e. an electron or an ion, is known to form a charge-solvent complex. This process involves a re-orientation of the molecules surrounding the charge, resulting in the screening of the extra charge and in the increase of its binding energy. Following earlier work, which investigated the dynamics of such solvated electrons in amorphous $D_2O$/Cu(111) by time-resolved two-photon photoemission, we analyze here the influence of coadsorbed sodium ions. In amorphous ice multilayers these electrons are located in the bulk of the ice film. After adsorption of sub-monolayer coverages of sodium ions a new species of solvated electrons is observed. By titration experiments using Xe overlayers we can demonstrate that the binding site of these electrons is located at the ice/vacuum-interface. Depending on the sodium coverage the lifetime of the excited electrons in this state is up to ten picoseconds, which is more than one order of magnitude longer compared to solvated electrons in amorphous water ice on Cu(111). The energetic stabilization rate of around 800 meV/ps is almost three times higher than in the case without sodium. The observed state can be attributed to excess electrons located at the alkali ions residing at the ice/vacuum-interface.

O 48.8 Wed 12:15 H40

**Two-dimensional Fano resonances on Si(100)** — •Martin Teichmann[1], Christian Eickhoff[1,2], Jens Kopprasch[1,2], Cornelius Gahl[1], and Martin Weinelt[1,2] — [1]Max-Born-Institut, Max-Born-Straße 2a, 12489 Berlin — [2]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

Fano resonances have enabled the understanding of many systems, from atomic to nuclear physics, and in the solid state. We present a two-dimensional extension of Fano's theory for the description of a transition between two discrete states both degenerate with a continuum. As a model system, we have studied the surface- and image potential states on Si(100) using two-photon photoemisson. These states are degenerate with the bulk continuum. Tuning the photon energy reveals Fano line shapes of the intensity. This allows us to deduce couplings between surface and bulk states, and to estimate the lifetime of single hole excitations in an inhomogeneously broadened system.

O 48.9 Wed 12:30 H40

**Electronic structure and charge carriers dynamics in 6T absorbed on Au(111).** — •Erwan Varene, Isabel Martin, Martin Wolf, and Petra Tegeder — Freie Universitaet Berlin, Fachbereich Physik, Arnimallee 14, 14195

Two-photon photoemission (2PPE) spectroscopy is employed to gain insight into the electronic structure as well as the charge carriers dynamics at the sexithiophene (6T)/Au(111) interface. This oligothiophene was chosen because it serves as a model system for the more structurally disordered polythiophene. These materials are used as electron donors in organic photovoltaic cells and organic field effect transistors. We observed the formation of an interface dipole of -0.8 eV and we found the highest occupied molecular orbital (HOMO) to be located 1.5 eV below the Fermi level (EF). In addition, we resolved two unoccupied states at 1.2 eV and 3 eV with respect to EF. The state 1.2 eV exhibiting a long lifetime of 500 fs can be assigned to an exciton. The state at 3 eV originates from the LUMO+1, possessing a lifetime of about 150 fs.

## O 49: Surface chemical reactions I

Time: Wednesday 10:30–12:45 Location: H42

O 49.1 Wed 10:30 H42

**Temperature programmed desorption from surfaces of electronic devices** — Andreas Peckhaus, Kevin Stella, •Detlef Diesing, and Eckart Hasselbrink — Institut für Physikalische Chemie, Universität Duisburg Essen

Surface chemical reactions depend crucially on the cleanliness and morphology of the surface. Usual cleaning procedures as sputtering and annealing can be well applied to single crystal surfaces. But thin film electronic devices can be hardly exposed to such kind of procedures since either the thermal stability of the devices is too low or the devices internal interfaces may be damaged be sputtering ions. We present first experiments on temperature programmed desorption of CO on the platinum surface of thin film platinum-silicon oxide-(n-type)-silicon devices. Problems as damages in the platinum films due to electromigration and degradation of the oxide films in the high temperature range $> 600$ K are discussed. We show that heating rates up to 3 K/s from 150 K to 600 K can be established with reproducible desorption peaks indicating an activation energy of desorption of 90 - 120 kJ/mol for CO adsorbed on the device surface.

O 49.2 Wed 10:45 H42

**Functionalization of AlGaN/GaN heterostructures with TFAAD** — •Stefan Udo Schwarz[1], Volker Cimalla[2], Christoph Nebel[2], and Oliver Ambacher[2] — [1]Institute of Microsystem Technology (IMTEK), University of Freiburg, Georges-Köhler-Allee 106, 79110 Freiburg, Germany — [2]Fraunhofer Institute for Applied Solid State Physics, Tullastraße 72, 79108 Freiburg, Germany

AlGaN/GaN high electron mobility transistors (HEMTs) show great promise for the realization of sensors for biomolecular, pharmaceutical and medical purposes. The high sensitivity and the stability in biological solutions are great advantages of this principle. The transduction is based on the AlGaN/GaN heterostructure. Charges on its surface influence the electron density in the 2-dimensional electron gas (2DEG) near the interface of the heterostructure. For a specific sensor, biological recognition methods shall be used. Therefore biomolecules need to be covalently linked to the semiconductor. The surface must be functionalized with a single layer of molecules that form covalent bonds to the surface and present functional groups for the connection with the biomolecule. In this work we investigate the functionalization of AlGaN/GaN heterostructures with 10-Trifluoroacetamiddec-1-ene

(TFAAD), a molecule that can bond to GaN in a photochemical reaction and has a protected Amino group for the further procedure. The focus is on the influence of the illumination spectrum and surface pretreatments on the reaction kinetics and the resulting layer morphology with respect to the designated application.

O 49.3 Wed 11:00 H42

**Adsorption and thermal behaviour of ethane and ethene on oxygen precovered Ni(111)** — •Michael Peter Andreas Lorenz[1], Thomas Fuhrmann[1], Karin Gotterbarm[1], Regine Streber[1], Fabian Bebensee[1], Christian Papp[1], Reinhard Denecke[2], and Hans-Peter Steinrück[1] — [1]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen — [2]Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnéstr. 2, 04103 Leipzig

Ni as well as NiO are widely-used catalysts in chemical industry. To understand the adsorption and reaction properties of small hydrocarbons on such surfaces we studied ethane and ethene on clean and oxygen precovered Ni(111) by means of XPS using synchrotron radiation at BESSY II. The gases were dosed using a supersonic molecular beam; for $C_2H_6$ this provided the kinetic energy required for the activated adsorption yielding adsorbed $C_2H_5$. On clean Ni(111) both $C_2H_5$ and $C_2H_4$ give rise to two separate C 1s peaks, indicative of a different local environment for the two C atoms in both cases. In contrast, on oxygen precovered Ni(111) only one C 1s peak is observed after exposing the surface to $C_2H_4$, and for $C_2H_5$ the peak separation is strongly reduced, indicating major changes in the adsorption geometries. Furthermore, we also studied the thermal evolution of the adsorbed hydrocarbons and found significant differences between oxygen free and oxygen precovered Ni(111).

This work was supported by BMBF (05 ES3XBA/5) and the DFG through the Cluster of Excellence "Engineering of Advanced Materials".

O 49.4 Wed 11:15 H42

**Switching Single Azopyridine Supramolecules in Ordered Array on Au(111)** — •Yongfeng Wang[1], Xin Ge[1], Guillaume Schull[1], Richard Berndt[1], Hao Tang[2], Claudia Bornholdt[3], Felix Koehler[3], and Rainer Herges[3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität, D-24098 Kiel, Germany — [2]CEMES/CNRS, France — [3]Institut für Organische Chemie, Christian-Albrechts-Universität, D-24098 Kiel, Germany

Understanding and controlling molecular switches on surfaces is of interest in both fundamental science and functional device at the single molecule level. Single molecular switches have been realized by modifying covalent bonds or ionic bonds. Decoupling of the reactive component of the molecule from a metal substrate by an insulating layer can be necessary as reversible switching is usually quenched on metals for the rather high barrier to overcome and the short lifetime of excitations. In contrast to molecules, supramolecules are connected through weak noncovalent interactions like hydrogen bonding. Lower energy barriers to switching may be expected for these weaker bonds. Here we report on supramolecular switches of 4,4-azopyridine trimers and 4-phenylazopyridine dimers in ordered array on Au(111). During switching, a single weak C-H...N hydrogen bond breaks and reforms. For 4,4-azopyridine, the switching mechanism occurs via electron attachment. 4-phenylazopyridine dimer, however, can be switched by electric fields, too. Funding by the Deutsche Forschungsgemeinschaft through SFB 677 is acknowledged.

O 49.5 Wed 11:30 H42

**Atomistic modelling of the oxidation of Co, Cr and CoCr alloy surfaces** — •Janina Zimmermann[1,2] and Lucio Colombi Ciacchi[2,3] — [1]Fraunhofer IWM, Freiburg, Deutschland — [2]Fachbereich Produktionstechnik, Universität Bremen, Deutschland — [3]Fraunhofer IFAM, Bremen, Deutschland

In this work, first-principles molecular dynamics based on density-functional theory is employed to investigate the early oxidation stages of the Co(0001), Cr(110) and CoCr(0001) surfaces. Oxide nucleation on cobalt follows a metastable path, with the place-exchange of metal and oxygen atoms leading to the growth of an open, pseudo-amorphous oxide structure with evident $Co_3O_4$-like features. Instead, the oxidation of Cr(110) occurs along an energy path close to thermodynamic equilibrium and limited by Cr-ion diffusion already in the earliest oxidation stages. The initial formation of highly oxidized chromate-like structures seems to be precursory for the subsequent growth of $Cr_2O_3$ thin films. The oxidation of CoCr alloys occurs via selective oxidation of chromium, which leads to vacancy formation and enables the diffusion of oxygen atoms into inner atomic layers. The outward diffusion of chromium is strongly facilitated by the matrix of amorphous cobalt oxide. These results suggest that superficial oxidation may proceed along two distinct possible pathways: a thermodynamically stable path along the potential energy minimum surface and a metastable, kinetically driven path that results from the high heat release during the dissociation of $O_2$.

O 49.6 Wed 11:45 H42

**'QM/Me' - a novel embedding approach for adsorbate dynamics on metal surfaces** — •Jörg Meyer[1] and Karsten Reuter[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin (Germany) — [2]Technische Universität München (Germany)

The dissociative adsorption of oxygen molecules on metal surfaces is a commonly known, highly exothermic reaction and in its slow or fast form of great importance for corrosion or oxidation catalysis, respectively. However, knowledge about atomistic details of the heat dissipation, a central conceptual concern, is very limited at best. Even on the level of Born-Oppenheimer potential energy surfaces, accurate dynamical *ab-initio* descriptions of such reactions are quite challenging from a computational point of view: Modeling the excitations of substrate phonons within periodic boundary conditions requires huge supercells, whereas traditional 'QM/MM' embedding schemes do demand unfeasibly large metal clusters. In the novel 'QM/Me' approach presented here, the adsorbate-substrate interaction is obtained from periodic first-principles calculations in convenient supercells and combined with the description of a 'bath-like' substrate based on classical potentials, which are parametrized to seamlessly fit the first-principles data. We apply our approach to dissociative adsorption of $O_2$ and $H_2$ on Pd(100) using density-functional theory and a modified embedded atom potential. In both cases, we observe a dominant fraction of the released chemisorption energy to be dissipated into the bulk already on a femtosecond time scale. Implications for the adsorbate dynamics will be discussed.

O 49.7 Wed 12:00 H42

**Material and Orientation dependent activity for heterogeneously catalyzed carbon-bromine bond homolysis** — •Hermann Walch, Rico Gutzler, Thomas Sirtl, Georg Eder, and Markus Lackinger — LMU Munich, Section Crystallography

Adsorption of the organic molecule 1,3,5-tris(4-bromophenyl)benzene on different metallic substrates, namely Cu(111), Ag(111) and Ag(110) has been studied by variable temperature Scanning Tunneling Microscopy (STM). Depending on substrate temperature, material and orientation, we observe a surface-catalyzed dehalogenation reaction. Deposition onto the catalytically active substrates Cu(111) and Ag(110) held at room temperature leads to cleavage of the carbon-bromine bonds and subsequent formation of protopolymers, i.e radical metal coordination complexes. However upon deposition on Ag(111) no such reaction has been observed. Instead, various self-assembled ordered structures based on intact molecules could be identified. Also sublimation onto either substrate held at 80 K did not result in any dehalogenation, thereby exemplifying that the dehalogenation reaction is thermally activated. We explain the differences in catalytic activity by charge transfer into unoccupied molecular orbitals and subsequent destabilization of the C-Br bond, whereby enhanced molecule-substrate interaction leads to an increasing magnitude of charge transfer. The interaction strength follows the general reactivity order Cu $>$ Ag $>$ Au for (111) faces and is generally enhanced on higher corrugated surfaces as the (110) facet in case of fcc substrates.

O 49.8 Wed 12:15 H42

**High pressure behavior of Au/$TiO_x$/Pt(111) model catalysts** — Luca Artiglia[1], Gaetano Granozzi[1], •Heinrich Hartmann[2], Thomas Diemant[2], Joachim Bansmann[2], and R. Jürgen Behm[2] — [1]Department of Chemical Sciences, via Marzolo 1, University of Padova, Italy — [2]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

In an effort to bridge the pressure gap between model and realistic catalytic processes, three different ultrathin $TiO_x$ on Pt(111) films have been prepared and investigated in-situ using XPS, LEED and IRAS to determine their stability in pure CO and $CO/O_2$ (1:1) at pressures up to 100 mbar. Two of the $TiO_x$ films consist of reduced phases with and without a long range order of defects, the third film is a fully oxidized

$TiO_2$ phase.

All three $TiO_x$ phases were stable in a reducing CO atmosphere at RT. In a $CO/O_2$ (1:1) mixture, only the fully oxidized phase showed no structural and electronic changes. The reduced phases underwent a process of oxidative surface restructuring with a partial dewetting of the Pt(111) substrate.

The $TiO_x$/Pt(111) films were used as substrates to deposit Au nanoparticles (1-6 nm) with surface morphologies particular to each $TiO_x$ phase. IRAS measurements on these Au/$TiO_x$/Pt(111) model catalysts showed, that the size of the Au nanoparticles (itself dependent on the morphology of the underlying $TiO_x$ phase) plays a major role for the adsorption of CO, while the oxidation state of the oxide support is less relevant.

O 49.9 Wed 12:30 H42

**Adsorption and reaction of $SO_2$ on clean and oxygen precovered Pt surfaces** — •Regine Streber[1], Christian Papp[1], Michael Peter Andreas Lorenz[1], Andreas Bayer[1], Oliver Höfert[1], Wei Zhao[1], Sandra Wickert[2], Erik Darlatt[2], Reinhard Denecke[2], and Hans-Peter Steinrück[1] — [1]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen — [2]Willhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnéstr. 2, 04103 Leipzig

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 clean and oxygen precovered Pt surfaces by in-situ high-resolution XPS applying synchrotron radiation at BESSY II. The comparison of spectra obtained on flat and stepped Platinum allows to elucidate the role of steps for the thermal stability of different $SO_2$ species, and in particular for their disproportionation to S and $SO_3$ upon heating. On the oxygen precovered surfaces a fraction of $SO_2$ reacts to $SO_3$ immediately upon adsorption, even at temperatures as low as 100 K. Heating of the resulting mixed adsorbate layers first results in the reaction of all remaining $SO_2$ species to $SO_3$, followed by subsequent oxidation to $SO_4$ above 300 K.

## O 50: [CPP] Organic Electronics and Photovoltaics III (Joint Session DS/CPP/HL/O)

Time: Wednesday 9:30–12:45 Location: H37

O 50.1 Wed 9:30 H37

**High-resolution spectroscopic mapping of P3HT:PCBM organic blend films for solar-cell applications** — •Xiao Wang[1], Dai Zhang[1], Kai Braun[1], Hans-Joachim Egelhaaf[2], Christoph J. Brabec[2], and Alfred J. Meixner[1] — [1]Institute of Physical and Theoretical Chemistry, University of Tübingen — [2]Konarka Technologies GmbH, Nürnberg

We present a high resolution near-field spectroscopic mapping of the poly(3-hexylthiophene) and [6, 6]-penyl-C61 butyric acid methyl ester (P3HT:PCBM) blend film upon different thermal annealing.[1] From the simultaneously recorded morphology and spectroscopic information, the interplay among the blend film morphology, the local P3HT:PCBM molecular distribution, and the P3HT photoluminescence (PL) quenching efficiency were discussed. The PL and Raman signals of the electron donor (P3HT) and acceptor (PCBM) have been probed at an optical resolution of approximately 10 nm which allow the direct identification of the chemical nature of the different domains. Moreover, we were able to reveal and quantify local quenching, which is related to the electron transfer from P3HT to PCBM. Based on the experimental results, it is proposed that high resolution near-field spectroscopic imaging proves its clear capability of mapping the local chemical composition and photophysics of the P3HT:PCBM blends on a length of a few nanometers.

[1] X. Wang, et al. Advanced Functional Materials (in press)

O 50.2 Wed 9:45 H37

**Investigations on thickness dependence of electrical characteristics and stability of self-assembled monolayers** — •Dana Habich — FAU Erlangen-Nürnberg, Institute of Polymer Materials

We investigated the influence of the molecular chain length (n) of aliphatic Cn-phosphonic acids on the electrical characteristics of self-assembled monolayers (SAMs) based on these molecules. SAMs prepared on aluminium/aluminium oxide (Al/AlOx) and conductive indium tin oxide (ITO) substrates behave as molecular dielectric layer. In integrated devices (e.g. capacitors) with activated Al-bottom electrode, the dielectric layer is created from a double-layer AlOx/SAM. Capacitance and breakdown voltage correlates monotonically with the SAM thickness, the current density at low voltage does not follow the expected correlations in detail. We address this behavior to morphological changes of the SAMs on AlOx, from an amorphous structure for short chains to a crystalline state for longer alkyl chains. To decouple the relative contributions of the AlOx and the SAM to the insulation, an independent analytical approach to characterize the SAM was chosen: cyclic voltammetry on SAM decorated ITO. The faradic current of a redox active compound in solution is indirect proportional to the molecular chain length. Qualitatively, this observation proofs the conclusions from the capacitor measurements. The system ITO/SAM, further provide an approach for functional coatings on ITO with the possibility to tune addressability and stability of the electrodes. Stability was investigated by static contact angle and STM measurements before and after electrical stress. Ref.: Org. Electron. 10 (2009) 1442.

O 50.3 Wed 10:00 H37

**2D mapping of the Electron Beam Induced Current (EBIC) in organic solar cells** — •Piet Reuter[1], Thomas Rath[2], Gregor Trimmel[2], and Peter Hadley[1] — [1]Institute of Solid State Physics, TU Graz, A-8010 Graz, Austria — [2]Institute for Chemistry and Technology of Materials & Christian Doppler Laboratory for Nanocomposite Solar Cells, TU Graz, A-8010 Graz, Austria

Electron Beam Induced Current (EBIC) measurements were used to produce 2D nanoscale maps for investigating the homogeneity of solar cells. These maps are acquired by putting the electron beam of a scanning electron microscope (SEM) in spot mode and using a programmable sample stage to move the solar cell under the stationary beam. The electron beam generates electron-hole pairs in the solar cell much like light does in normal operation. The variations in the EBIC signal can be attributed to changes in the morphology. By comparing these measurements with morphological information of the devices, one can identify the cause of inferior performance which should then lead to an improvement of further devices. It should be mentioned that long time exposures to an electron beam destroys the organic semiconductors. Studies were performed to determine the acceptable electron dose during the measurement.

O 50.4 Wed 10:15 H37

**Analysis of Metallic Conduction at the Interface of TTF and TCNQ Crystals.** — •Viktor Atalla, Mina Yoon, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, Germany

Organic materials are promising candidates for a next generation of electronic devices, since they offer a variety of new intriguing electronic phenomena while being environmentally friendly, low cost, and mechanically flexible. Here we study the interface of tetrathiofulvalene (TTF) and 7,7,8,8-tetracyanoquinodimethane (TCNQ) organic molecular crystals which was found to exhibit metallic conduction [1] whereas the individual crystals are large band-gap semiconductors. Using quantum mechanical first-principles approaches employing the FHI-aims code [2] basic properties of monomers, dimers, and individual crystals are investigated. We construct interfaces between the two types of crystals and study the electronic band structures of the interface-induced states, which are relevant to the charge transport properties of the material. Depending on the relative orientation of the crystals the band structures were found to indicate metallic conduction at the interface. Furthermore the energetics of the polaron is investigated by calculating the geometry relaxation energy. For monomers of TTF and TCNQ this is found to be in the order of 0.1 eV, indicating that the electron-lattice interaction is an important parameter for charge transport in this system. [1] H. Alves et al., Nat. Mat. 7, 574 (2008). [2] V. Blum et al., Comp. Phys. Comm. 180, 2175 (2009).

O 50.5 Wed 10:30 H37

**Structural analysis of photoactive polymer blend films on textured polymeric and inorganic substrates** — •Robert Meier[1], Matthias A. Ruderer[1], Gunar Kaune[1], Alexander Diethert[1], Fabian Markl[1], Volker Körstgens[1], Johannes Wiedersich[1],

Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department LS E13, James-Franck-Straße 1, 85747 Garching — [2]HASYLAB at DESY, Notkestraße 85, 22603 Hamburg

Due to their large chemical variety photoactive conducting polymers are of great interest for versatile applications such as organic photovoltaics. In order to improve the device characteristics not only the polymer film but also the rest of the device has to be optimized regarding light absorption and charge carrier separation. Therefore the focus of this work is put on the use of structured substrates in order to improve the light absorption and the overall device performance. A new route based on solution casting is introduced to structure the electron blocking PEDOT:PSS layer. Absorption spectra of polymer blend films spincoated on such structured substrates show promising aspects for their suitability for organic photovolatics. In addition the inner film morphology of a polymer blend based on M3EH-PPV and F8BT spincoated on structured channel-like substrates is investigated using GISAXS measurements. The obtained results show a dependence of the film morphology and the topographic shape on the etched depth of the channels. The study is complemented with atomic force and scanning electron microscopy measurements.

**15 min. break**

O 50.6 Wed 11:00 H37

**Structural and morphological changes in P3HT thin film transistors applying an electric field** — •Deepak kumar Tiwari[1], Souren Grigorian[1], Ullrich Pietsch[1], Heinz Flesch[1,2], and Roland Resel[1,2] — [1]University of siegen, siegen, Germany — [2]Graz University of technology

We report on electric field dependent crystalline structure and morphological changes of drop casting and spin coated poly(3-hexyltheiopine) (P3HT) thin films. In order to probe the morphological changes induced by an applied electric field the samples were covered with thin source/drain electrodes separated by a small channel of 2 mm width. A series of x-ray reflectivity, X-ray grazing incidence out-of-plane and in-plane scans have been performed as function of the applied electric voltage. The (100) peak shows a decrease in intensity with increase of the applied electric field. This might be caused by Joule heating and the creation of current induced defects in the P3HT film. On other hand the (020) peak intensity shows much stronger changes with applied field. Considering the *-* stacking direction the measured effect can be directly related to a change in the electric transport. The observed changes in structure are reversible and the current-voltage cycle can be repeated several times. For X-ray reflectivity major changes have been found close to critical angle of total external reflection indicating the film becomes less dense and increases in surface roughness with increase of the voltage. This change in surface behaviour could be confirmed by in-situ AFM measurements.

O 50.7 Wed 11:15 H37

**Thickness dependent structural order in P3HT films - a key parameter for high OFET mobility** — •Benedikt Gburek, Richa Sharma, Torsten Balster, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Applications of organic electronics require cheap and fast production methods on flexible substrates. Following these goals, top-gate OFETs on PET foils were used to analyze the dependence of the device characteristics on the crucial parameter of semiconductor layer thickness. The organic semiconductor, regio-regular P3HT, and the gate insulator were deposited by spin-coating under atmospheric conditions.

The charge carrier mobility was found to be rather low for extremely thin layers of several nanometers only. However, with increasing layer thickness, mobility increases by two orders of magnitude until a "saturation thickness" of 50 nm, above which it remains constant.

Further details of the ordering were extracted according to the Vissenberg-Matters model with gate-voltage dependent mobility $\mu = \mu_0\ \left(\left(V_{GS} - V_{th}\right)/1V\right)^{\gamma}$, where $\gamma$ is directly related to the width of the density of states. The analysis reveals that the disorder parameter $\gamma$ decreases from 3.1 to 1.0 over the examined thickness range, which explains the low mobility of thinner films by higher energetic disorder.

This analysis proves to be highly advantageous as it represents the whole transfer curve, gives better comparability and offers more physical insight. Our study demonstrates the crucial role of layer thickness tuning for improved film structure and optimum material performance.

O 50.8 Wed 11:30 H37

**Deposition of P3HT via dip coating onto transistors with channel lengths below 1 $\mu$m** — •Silviu Botnarash, Steve Pittner, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, D-28759, Germany

A high quality interface between the organic semiconductor and the oxide is crucial for the high performance of an OFET. A good surface treatment is imperative, but it will lower the surface energy of the oxide, making it difficult to spin coat on it uniform semiconductor layers from solvents like chloroform or toluene. We report on the usage of the dip coating technique to achieve highly ordered layers of regioregular poly(3-hexylthiophene) (rr-P3HT). By varying the removal speed of the silicon substrate from solution, the concentration of the solution or both, one can achieve ultrathin layers of rr-P3HT which permit to analyze OFET properties in the sub-monolayer regime. Decreasing the channel length of the transistors down to the range of the contour length of the rr-P3HT is expected to improve the characteristics of the OFET's. An additionally applied electric field between the source and drain electrodes during dip coating facilitates the trapping of P3HT molecules on the electrodes increasing the performance of the device. We used rr-P3HT with an average contour length of 80-100 nm. Compared to previously reported results for chloroform based solutions, the same concentration range of rr-P3HT in toluene displayed better characteristics, which is believed to be due to lower evaporation rate of toluene. Subsequent drying in a nitrogen rich atmosphere over a period of up to 24 h positively influences the performance of the OFET's.

O 50.9 Wed 11:45 H37

**Semitransparent small-molecule organic solar cells** — •Jan Meiss[1], Christian Uhrich[2], Stefan Sonntag[2], Wolf-Michael Gnehr[2], Martin Pfeiffer[2], Karl Leo[1], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]heliatek GmbH, Liebigstraße 26, 01187 Dresden, Germany

Semitransparent, colourful solar cells are of interest for a wide range of applications, e.g. sun shading of residential and office buildings or cars. Previously, among organics-containing devices, only semitransparent dye-sensitized solar cells showed power conversion efficiencies (PCE) that allowed first meaningful applications, whereas semi-transparent small-molecule organic solar cells (OSC) were limited to PCE well below 1%.

We present small-molecule semitransparent OSC deposited by thermal vacuum evaporation on ITO-coated glass. The organic materials include absorber materials and doped dedicated charge transport layers. Due to our unique device architecture, the top electrode is ITO-free, consisting only of an ultra-thin multi-layer metal film.

The OSC exhibit light transmission in the visible range of 30-50% with PCE of over 2%. Organic capping layers are used to significantly lower reflection and increase transmission without significant loss of PCE. Furthermore, we have achieved first large-area semitransparent tandem OSC with 3.5% PCE at 20-40% transmission in the visible range on 4cm$^2$, which show the potential of this type of device for large-scale building integration.

O 50.10 Wed 12:00 H37

**Stability optimisation of small molecule organic solar cells** — •Martin Hermenau, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, George-Bähr-Str. 1, 01069 Dresden

In addition to high efficiency and low cost, a long device lifetime is a crucially important factor for the commercialisation of small molecule organic solar cells. Previous results mostly covered unencapsulated devices and showed low lifetimes under 1000 hours even without permanent illumination.

Here, we present results on improving the intrinsic stability of glass-glass-encapsulated p-i-n solar cells containing small molecules. Zinc-Phthalocyanine and the fullerene $C_{60}$ are used as photoactive materials. Doped layers of wide gap materials and $C_{60}$ are used as hole and electron transport layer, respectively. All devices are illuminated with monochromatic or white LEDs and IV characteristics are automatically recorded during the entire measuring period.

In contrast to polymer solar cells, we do not observe an influence of different types of top contact materials on the lifetime. All variations of Gold, Silver and Aluminium lead to stable cells for about 1500 hours of continued illumination.

However, by changing the type and even the thickness of the hole transport material we are able to enhance the extrapolated lifetime (t80) from about 1100 hours with 30nm PV-TPD up to more than 5000 hours with 60nm Di-NPB. These results are achieved with encapsulated devices and illumination intensitites up to 840 mW/cm$^2$ from high-power white LEDs at controlled temperatures of 50°C.

O 50.11 Wed 12:15 H37

**Self organized molecular electronic junctions using two phase liquid structures in microfluidic channels** — •Shashi Thutupalli[1], Mark Elbing[2], Matthias Fischer[2], David Muñoz[3], Ralf Seemann[1,4], Marcel Mayor[2,3], and Stephan Herminghaus[1] — [1]MPI for Dynamics and Self Organization, Göttingen, Germany — [2]Forschungszentrum Karlsruhe GmbH, Institute for Nanotechnology, Karlsruhe, Germany — [3]University of Basel, Department of Chemistry, Basel, Switzerland — [4]Experimental Physics, Saarland University, Saarbrücken, Germany

Using a combination of microfluidics and molecular design, we demonstrate self assembled, reconfigurable molecular electronic junctions. To construct metal-molecule-metal junctions, we employ liquid mercury as the electrode contact in crossed microfluidic channels. Self assembled monolayers (SAM's) of conducting molecular rods are created on the surface of the mercury, which are then bridged to the other mercury electrode via microfluidic control. By precise flow control, we create rectifying molecular junctions using asymmetric molecules. We report on the electrical properties of these microfluidic metal-molecule-metal junctions. Also, we use surfactant stabilized foam-like water-in-oil emulsions to form variable molecular junctions. Here, molecules synthesized with hydrophobic conducting cores and hydrophilic ends self-insert into the lamellae between aqueous droplets. Using the aqueous droplets then as the molecular contacts, we report on the conducting properties of the inserted molecules and demonstrate the possibility of reconfigurable circuits using topological droplet rearrangements.

O 50.12 Wed 12:30 H37

**DNA Based Molecular Electronics Using Mercury Droplets in Microfluidic Channels** — •Shuang Hou, Shashi Thutupalli, and Stephan Herminghaus — Max Planck Institute for Dynamics and Self Organization, D-37073, Göttingen, Germany

Mercury droplets in microfluidic channels are used as electrodes to investigate the electronic properties of single strand DNA (ssDNA) molecules. In this system, a self assembled monolayer (SAM) of thiolated DNA oligomers (~ 5 nm length) of specific base sequences is formed on the surface of mercury droplets. Two such droplets are then brought together by microfluidic manipulation to form a mercury-ssDNA-mercury electrical junction. We identified single SAMs of ssDNA oligos, double SAMs of ssDNA oligos of the same composition, and complementary binding DNA composed junctions. Here, we report the influence of base pair type and DNA sequence length to the electronic characteristics. On the basis of these results, the design of DNA based molecular electronic elements (such as diodes) seems possible.

## O 51: Gaede-Prize talk (Linden, Stefan)

Time: Wednesday 14:00–14:45 Location: H36

**Prize Talk** O 51.1 Wed 14:00 H36

**Photonic Metamaterials: Novel Optics with Artificial Atoms** — •Stefan Linden — Institut für Nanotechnologie, Karlsruher Institut für Technologie (KIT)

At optical frequencies, electromagnetic waves interact with natural materials via the electronic polarizability of the materials. By contrast, the corresponding magnetizability is negligible. As a result, we can only directly manipulate the electric component of light while we have no immediate handle on the magnetic component. Photonic metamaterials open up a way to overcome this constraint. The basic idea is to create an artificial crystal with sub-wavelength periods. Analogous to an ordinary optical material, such a photonic metamaterial can be treated as an effective medium. However, proper design of the elementary building blocks ("artificial atoms") of the photonic metamaterial allows for a non-vanishing magnetic response at optical frequencies - despite the fact that photonic metamaterial consist of non-magnetic constituents. This artificial magnetism can even lead to a negative index of refraction. In this presentation, I will review our results and present new developments in this interesting field.

## O 52: Graphene II

Time: Wednesday 15:00–17:15 Location: H31

O 52.1 Wed 15:00 H31

**Direct writing of 1 nm thin graphenoid nanoribbons and nanosieves** — •Mark Schnietz[1], Andrey Turchanin[1], Christoph Nottbohm[1], André Beyer[1], Harun Solak[2], Peter Hinze[3], Thomas Weimann[3], and Armin Gölzhäuser[1] — [1]Physik supramolekularer Systeme, Fakultät für Physik, Universität Bielefeld — [2]Laboratory for Micro and Nanotechnology, Paul Scherrer Insitute, Villigen — [3]Physikalisch-Technische Bundesanstalt, Braunschweig

Graphenoid nanosheets are fabricated by electron/photon induced cross-linking of aromatic self-assembled monolayers (SAMs). The cross-linking results in mechanically stable carbon nanosheets with the thickness of a single molecule ($\sim$1 nm) and with a distinct chemical functionality. The nanosheets can be lifted from the substrate and transferred onto another solid substrate or holey structure, where they become free-standing membranes.[1] By vacuum annealing the electrical conductivity of nanosheets can be tuned introducing an insulator to conductor transition.[2] The sizes and shapes of the graphenoid nanosheets are flexibly adjusted by electron beam/EUV interference lithography. In this contribution we demonstrate the fabrication of large area graphenoid nanoribbons and suspended nanosieves with lateral dimensions of the periodic features down to $\sim$30 nm.[3, 4]

[1] C. T. Nottbohm et al, Ultramicroscopy 108, 88 (2008)
[2] A. Turchanin et al, Adv. Mater. 21, 1233 (2009)
[3] M. Schnietz et al, Small DOI: 10.1002/smll.200901283
[4] C. T. Nottbohm et al, J. Vac. Sci. Technol. B (2009) in press

O 52.2 Wed 15:15 H31

**Decoupling epitaxial graphene from SiC(0001) surface by a germanium buffer layer** — •Konstantin Emtsev and Ulrich Starke — Max-Planck Institute for Solid State Research, Stuttgart, Germany

Epitaxial graphene layers formed on SiC surfaces are currently intensively investigated with respect to their electronic, structural, and electrical transport properties [1]. On the SiC(0001) surface graphene layers are separated from the substrate by an interfacial carbon layer. The latter has a graphene-like atomic arrangement with complex ($6\sqrt{3} \times 6\sqrt{3}$)R30° periodicity but lacks characteristic $\pi$-bands due to strong hybridization with the substrate [2]. In this work we demonstrate that the interfacial layer can be converted into quasi-freestanding graphene upon intercalation of Ge atoms at the interface. The electronic properties of the surface and the atomic structures of the newly formed interfaces were characterized by ARPES, XPS, and LEED. Deposition of germanium on the $6\sqrt{3}$ reconstructed SiC(0001) surface and subsequent annealing steps were carried out in UHV following Kubler et al. [3]. Decoupling of the interface layer by intercalating Ge atoms begins at temperature of about 700°C as evident by the development of the electronic band structure characteristic of graphene. Depending on the amount of Ge deposited as well as on the annealing temperature the graphene layer exhibits electron or hole doping.

[1] Th. Seyller et al., Phys. Stat. Sol.(b), 245, 1436 (2008).
[2] K. V. Emtsev et al., Phys. Rev. B, 77, 155303 (2008).
[3] L. Kubler et al., Phys. Rev. B, 72, 115319 (2005).

O 52.3 Wed 15:30 H31

**SPM on epitaxial graphene on SiC** — •Markus Duschl and Franz J. Giessibl — Insitute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg

For some years, graphene has been of wide interest due to its extraordinary properties. First measurements done on exfoliated graphene in ambient conditions indicate that it might be possible to determine the number of graphite layers by force spectroscopy [1]. The stiffness increases with a decreasing number of layers, down to graphene. We compare these measurements to data taken with a combined STM and AFM in UHV at room temperature on epitaxial graphene grown on SiC [2].

[1] Hiermaier, V. Diploma Thesis, July 2009
[2] Seyller, T. et al. Nature Mater. 8, 203-207 (2009)

O 52.4 Wed 15:45 H31

**Defect-induced electron scattering and metal-insulator transition in graphene** — Aaron Bostwick[1], Jessica McChesney[1,2], Konstantin Emtsev[3], Thomas Seyller[3], •Karsten Horn[2], Stephen D. Kevan[4], and Eli Rotenberg[1] — [1]Advanced Light Source, Lawrence Berkeley Lab, California USA — [2]Fritz-Haber-Institut der MPG, Berlin — [3]Institut für Physik der Kondensierten Materie, Universität Erlangen — [4]Department of Physics, University of Oregon, USA

The influence of adsorbate-induced defects on the electronic properties of graphene are of great current interest. Here we show, using angle-resolved photoemission and conductivity measurements, that potassium and hydrogen adsorption on graphene induce very different types of defects in graphene prepared on SiC(0001). Whereas potassium acts as an electron donor, but causes only weak defect scattering, hydrogen locally saturates a carbon bond. This acts as a lattice defect, leading to a sharp reduction in conductivity, by several orders of magnitude even for coverages below 1 % of a monolayer. Angle-resolved photoemission spectra reveal a concomitant change in the electron scattering rate and the dispersion of the graphene bands near the Fermi level. These changes are interpreted in terms of a breakdown of the quasiparticle picture and strong charge carrier localization through the hydrogen-induced defects.

O 52.5 Wed 16:00 H31

**Quasi-free Standing Epitaxial Graphene on SiC by Hydrogen Intercalation** — •Camilla Coletti[1], Christian Riedl[1], Takayuki Iwasaki[1], Alexei A. Zakharov[2], and Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [2]MAX-Lab, Lund University, Box 118, Lund, S-22100, Sweden

Epitaxial graphene grown on silicon carbide (SiC) is an appealing material for future electronic applications. It combines most of the exciting properties of free standing graphene to a manufacturing friendly planar structure. Most of the remaining skepticism towards this material is related to the the strong interaction with the SiC substrate. The SiC surface is covalently bound to the first carbon layer, which act as a buffer-layer and therefore fails in displaying graphene properties. The undesired effects originating from this strong coupling, such as intrinsic n-type doping and degraded transport properties, affect the overlying graphene layers. Annealing the samples in molecular hydrogen offers an elegant solution to the problem of graphene-SiC coupling. ARPES, CLPES and LEEM demonstrate that hydrogen atoms migrate through the graphene layers, intercalate between the SiC substrate and the buffer-layer and bind to the Si atoms of the SiC(0001) surface. Thus the buffer-layer, decoupled from the SiC substrate, is turned into a quasi-free standing graphene monolayer. Similarly, epitaxial monolayer graphene turns into a decoupled bilayer. The intercalation process represents a highly promising route towards epitaxial graphene based nanoelectronics.

O 52.6 Wed 16:15 H31

**X-ray absorption and magnetic circular dichroism of graphene/Ni(111)** — Martin Weser[1], Yvonne Rehder[1], Karsten Horn[1], Muriel Sicot[2], Mikhail Fonin[2], Aleksej Preobrajenski[3], Elena Voloshina[4], and •Yuriy Dedkov[1] — [1]Fritz-Haber Institut der Max-Planck Gesellschaft, Berlin, Germany — [2]Universität Konstanz, Germany — [3]MAX-lab, Lund, Sweden — [4]Freie Universität Berlin, Germany

A long electronic mean free path and negligible spin-orbit coupling in graphene render this material ideal for applications based on ballistic transport like the spin filed effect transistor and the perfect spin-filtering device. The model system, graphene/Ni(111), is of special interest, providing an ideal interface between graphene and ferromagnetic material, from a structural point of view. Here we present the studies of the electronic and magnetic properties of the lattice-matched graphene/Ni(111) interface which were performed by means of angle-resolved x-ray absorption spectroscopy (XAS) and x-ray magnetic circular dichroism (XMCD) at the Ni $L_{2,3}$ and C $K$ absorption edges. The XAS C $1s \to \pi^*, \sigma^*$ spectra show pronounced changes as the angle, $\alpha$, between the electrical vector of the light and surface normal is varied, reflecting the symmetry of the final state. XMCD reveals an induced magnetic moment of the carbon atoms in the graphene layer aligned parallel to the Ni $3d$ magnetization. Our experimental results are discussed in the light of recent density-functional theory calculations and previous results on the observation of induced magnetism in non-magnetic materials. (See M. Weser *et al.*, arXiv:0907.4344v1).

O 52.7 Wed 16:30 H31

**An ab initio study of graphenen nanoribbons doped with boron clusters** — Cem Özdogan[1], •Jens Kunstmann[2], Alexander Quandt[3], and Holger Fehske[3] — [1]Department of Computer Engineering, Cankaya University, Ankara, Turkey — [2]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, Germany — [3]Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, Germany

We present results from an ab initio study of graphene and graphene nanoribbons (GNR) doped with $B_7$ clusters. We already showed that this system might serve as a blueprint for the controlled layout of graphene based nanodevices, where the semiconducting properties are supplemented by parts of the graphene matrix and the metallic wiring is provided by chains of boron clusters [1,2]. We study how the $B_7$ clusters alter the physical properties of GNRs. A special focus is put on the magnetic properties of zigzag GNRs. [1] A. Quandt, C. Özdoğan, J. Kunstmann, and H. Fehske, Nanotechnology **19**, 335707 (2008). [2] A. Quandt, C. Özdoğan, J. Kunstmann, and H. Fehske, phys. stat. solidi (b) **245**, 2077 (2008).

O 52.8 Wed 16:45 H31

**Effect of Noble-Metal Contacts on the Electronic Structure of Graphene** — •Andrei Varykhalov[1], Markus R. Scholz[1], Timur K. Kim[2], and Oliver Rader[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie — [2]Institute for Solid State Research, IFW Dresden

Graphene-metal contacts are crucial for a future planar bipolar nanoelectronics. We investigated these contacts by angle-resolved photoemission at high resolution using noble-metal intercalation. We observe that doping level and band gap depend strongly on which noble metal is intercalated. As predicted from first principles, strong electron doping is provided by Cu ($\Delta E_\mathrm{F} \sim -310$ meV) and Ag ($\sim -560$ meV) but also unexpected large gaps appear ($E_g = 180$ and 320 meV, respectively). Au affects the neutral state of graphene much less than predicted moving the Dirac point $E_\mathrm{D}$ by only $\Delta E_\mathrm{F} \sim +55$ meV above the Fermi level. In order to investigate whether or not graphene/Au is gapless also above $E_\mathrm{D}$, we adsorbed potassium and gadolinium on top of the graphene. Both act as efficient donors but potassium opens a substantial band gap due to symmetry breaking while $E_\mathrm{D}$ is well below $E_\mathrm{F}$ and gapless after doping by gadolinium. We propose that the large $9 \times 9$ unit cell of the graphene/Au interface amplifies via quantum interference the decoupling of the graphene from its substrate which leads to the quasifreestanding electronic structure of graphene.

O 52.9 Wed 17:00 H31

**Resonant Raman scattering of chemically functionalized graphene** — •Nils Scheuschner[1], Dimitrios Tasis[2], Kostas Papagelis[2], and Janina Maultzsch[1] — [1]Institut für Festkörperphysik, TU Berlin, Germany — [2]Materials Science Department, University of Patras, 26504 Patras, Greece

We present resonant Raman scattering of graphene functionalized with polyvinylalcohol (PVA). Raman spectroscopy is a powerful tool for characterization of carbon nanostructures. Functionalization of graphene is a promising way to modify its electronic structure, for example in order to open a band gap. To study the interaction between PVA and graphene with respect to their electronic and vibrational structure, we analyse the Raman spectra of the G mode and the double resonant defect mode. Furthermore, we use tip-enhanced Raman spectroscopy (TERS) for structural and spectroscopic information with high spatial resolution of the sample.

# O 53: Plasmonics and Nanooptics IV

Time: Wednesday 15:00–17:45 Location: H32

O 53.1 Wed 15:00 H32

**Raman and Luminescence Enhancement Produced in Gap-mode Near-field Optical Microscopy** — •Dai Zhang, Marcus Sakrow, Kai Braun, and Alfred J. Meixner — Institute of Physical and Theoretical Chemistry, University Tübingen, Auf der Morgenstelle 8, Tübingen

Tip-enhanced near-field optical microscopy can produce spectroscopic images of molecular layers deposited on smooth Au-surfaces, of single molecules and of organic semi-conductor films with an optical resolution on the order of 10 nm. This is made possible by a sharp laser-illuminated Au-tip approaching as close as a few nanometers to the sample surface. The system behaves as an optical antenna for confining and enhancing 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 this way the signal emitted from the gap can be enhanced by several orders of magnitude with respect to the diffraction limited background signal by enhancing the excitation efficiency and the emission yield. In this contribution, a variety of enhancement mechanisms will be discussed.

O 53.2 Wed 15:15 H32

**Quantifying Excitation and Radiation Rate Enhancement Provided by Near-field Optical Antennas** — •Miriam Böhmler, Nicolai Hartmann, Carsten Georgi, and Achim Hartschuh — Department Chemie und Biochemie & CENS, Ludwig-Maximilians-Universität, 81377 München

Tip-enhanced near-field optical microscopy provides nanoscale optical resolution beyond the diffraction limit [1]. This is due to the highly confined enhancement of the optical fields at the tip apex, which locally increases both excitation and radiation rates. In our experiments we use sharp gold tips to probe the photoluminescence (PL) of individual single-walled carbon nanotubes. We show that excitation and emission enhancement can be distinguished by imaging the radiation pattern in the back focal plane of the microscope objective. The analysis is based on the characteristic radiation patterns generated by single dipoles with a particular orientation in 3D [2]. We first find that the PL emission of a nanotube can be described by an in-plane oriented dipole. In the presence of our tip, the radiation pattern is strongly modified and dominated by the signatures of a vertical dipole corresponding to the tip axis. This observation illustrates the spatial redirection of the emission by the tip acting as an optical antenna [3]. By comparing radiation patterns with and without the influence of our tip, we estimate excitation and radiation rate enhancement quantitatively.

[1] A. Hartschuh, Angew. Chem. Int. Ed. 47, 8178 (2008)
[2] M. A. Lieb, J. Opt. Soc. Am. B 21, 1210 (2004)
[3] T. H. Taminiau, Nat. Photon. 2, 234 (2008)

O 53.3 Wed 15:30 H32

**Pseudo-heterodyne scanning near-field optical microscope for surface plasmon detection with actively stabilized phase** — •Stefan Griesing, Andreas Englisch, and Uwe Hartmann — Experimental Physics, Saarland University, D-66123 Saarbrücken

Amplitude and phase of the evanescent surface plasmon field were detected by a pseudo-heterodyne scanning near-field optical microscope (SNOM). Light from a HeNe laser (l = 633nm) and an argon ion (Ar) laser (l = 488nm) was combinied in a fiber coupler. One output channel of the coupler served as reference branch of an interferometer. A piezoelectric fiber stretcher in that branch was used for sinusoidal phase modulation. The other output of the coupler was linked to another coupler. By using different color filters, the two wavelengths were separated at the output channels. The HeNe laser was used for surface plasmon excitation under attenuated total internal reflection. The light from the Ar laser illuminated the sample under normal incidence, so that during the scanning process a constant phase from the Ar laser was detected. The SNOM tip detects both, surface plasmons excited by the HeNe laser and the spot from the Ar laser. The signal is combined in a third fiber coupler with the signal from the reference branch. At the output, the interference signal was wavelength- selectively detected by Si photodiodes and lock-in amplifiers. The signal from the Ar laser was used as input for a feedback- loop which modifies the drive signal of the fiber stretcher. In this way, the phase fluctuations due to thermal and mechanical disturbances were compensated.

O 53.4 Wed 15:45 H32

**Scattering near-field microscopy in the THz with a free-electron laser** — •Hans-Georg von Ribbeck[1,2], 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, Forschungszentrum Dresden - Rossendorf, 01314 Dresden

We present scattering-type scanning near-field optical microspectroscopy (s-SNOM) invstigations, successfully operated in the THz range with a wavelength independent spatial resolution of 150 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 Forschungszentrum Dresden-Rossendorf. This laser provides tunability from 30 - 250 um. We were able to record, for the first time ever, s-SNOM signatures with a FEL at wavelengths ranging from 30 um to 180 um (10 - 1.67 THz). In addition to the near-field dependent optical signals we also demonstrate the imaging 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 such samples, topography independent strong optical material contrast could be demonstrated at 150 um wavelength. We achieve a resolution of better than 150 nm corresponding to better than l/1000.

O 53.5 Wed 16:00 H32

**Ultrahigh temporal and spatial resolution imaging of second harmonic fields in random zinc oxide nanostructure arrays** — •Manfred Mascheck[1], Slawa Schmidt[1], Martin Silies[1], Takashi Yatsui[2], Motoichi Ohtsu[2], David Leipold[3], Erich Runge[3], and Christoph Lienau[1] — [1]Carl-von-Ossietzky-Universität, Oldenburg — [2]University of Tokyo — [3]Technische Universität Ilmenau

Among the most prominent signatures of the weak (Anderson) localization of light in random dielectric media are an enhanced coherent backscattering and the localization of electromagnetic fields in both space and time. Light localization is particulary relevant in nanophotonic materials, where it can give rise to strong field localization and greatly enhanced optical nonlinearities.

Here, we explore this light localization in densely packed, random arrays of ZnO nanoneedles with tip diameters of less than 20 nm. A phase-stabilized pair of 6 fs laser pulses is focused to its diffraction limit of $1\,\mu m^2$ onto the ZnO needles.

The generated surface second harmonic (SH) spectra are detected as a function of the lateral position of the laser focus and the delay between the two pulses. We observed a pronounced spatial localization of the SH signal in hot spots of less than 300 nm dimension. We show, by retrieving the time structure of the localized electric field from interferometric FROG traces, that light is stored in these hot spots for more than 100 fs. Such nanoneedle arrays therefore present a highly interesting new model system for exploring the rich physics of weakly localized light fields.

O 53.6 Wed 16:15 H32

**Second Harmonic Imaging of Gold Nanocones with a Parabolic Mirror Microscope** — •Anke Horneber[1], Dai Zhang[1], Monika Fleischer[2], Marcus Sackrow[1], Kai Braun[1], Dieter P. Kern[2], and Alfred J. Meixner[1] — [1]Institute of Physical Chemistry, Eberhard Karls University Tübingen, Germany — [2]Institute of Applied Physics, Eberhard Karls University Tübingen, Germany

Second harmonic generation (SHG) is a valuable technique for the visualization of surfaces. Our confocal optical microscope uses a parabolic mirror with a smaller focus than objective lenses in air and the largest possible signal collection angle. We use higher order laser modes which are often called cylindrical vector beams for the investigation of complex plasmonic structures. The longitudinal polarization component in a radially polarized laser beam focus can excite the longitudinal plasmon of a gold cone most efficiently[1]. We present first SHG images of gold nanocones with an optical resolution below 300 nm. We are developing a flexible setup that will allow non-linear experiments as well as near-field measurements. Such a setup will provide further opportunities like non-linear near-field investigations and the combination of a high spatial resolution with ultrafast dynamics.

[1] M. Fleischer et al., APL, 93 (2008) 111114.

O 53.7 Wed 16:30 H32

**Nanosphere Lithography of Sub-50 nm Plasmonic Structures** — •Jun Zhao, Bettina Frank, and Harald Giessen — Universität Stuttgart, Deutschland

Nanosphere lithography is a powerful and fast fabrication technique for periodic large-area metallic nanostructures of different and complex shapes [1]. We use tilted-angle-rotation thermal evaporation onto the monolayers of close-packed polystyrene nanospheres to fabricate metamaterial samples of up to $1cm^2$.

With this fabrication technique we can prepare sub-50 nm plasmonic structures such as pentamers, hexamers, and also ring structures with a centered or off-centered disk in the middle, which is useful for investigation of Fano-type plasmon resonances and future sensors.

The optical response of our structures was measured in reflectance geometry with FTIR-microscopy. The measurements show good agreement with our simulations. We also performed stacking experiments of split-ring resonators, which can be arranged in an ordered or twisted stereometamaterial fashion [2].

[1] . M. C. Gwinner, E. Koroknay, L. Fu, P. Patoka, W. Kandulski, M. Giersig, and H. Giessen, Small 5, 400 (2009) [2]. N. Liu, H. Liu, S. Zhu, and H. Giessen, Nature Photonics 3, 157 (2009)

O 53.8 Wed 16:45 H32

**Gold nanocone probes for near-field scanning optical microscopy** — •Bastian Zeeb, Christian Schäfer, Peter Nill, Monika Fleischer, and Dieter P. Kern — Institute of Applied Physics, University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen

Apertureless near-field scanning optical microscopy (ANSOM) provides the possibility to collect simultaneously high-resolution topographical and sub-diffraction limited optical information from a surface. When optically excited, the scanning probes act as optical antennae with a strong near-field enhancement near the tip apex. Spatial resolution and optical near-field enhancement depend strongly on the properties and geometry of the scanning probe - in particular on very sharp tip radii. Various possibilities for fabricating good antennae have been pursued. Most commonly, scanning probes consist of electrochemically etched gold wires which are sharp but not well-defined in geometry.

We present two different approaches for ultra sharp and well-defined antennae based upon fabricating gold nanocones with a tip radius smaller than 10 nm which can be used in ANSOM [e.g. *M. Fleischer et al., Appl. Phys. Lett.* ***93****, 111114 (2008)*]. A transfer process is presented that can be used to attach single gold nanocones to non-metallic probes such as sharp glass fiber tips. Alternatively, new processes are presented to fabricate cones directly on pillars of different materials such as silicon or bismuth, which can be applied to cantilever tips for ANSOM scanning applications.

O 53.9 Wed 17:00 H32

**Space Charge Effects in Photoemission Electron Microscopy** — •Jan Vanis, Niemma M. Buckanie, Ping Zhou, Dietrich von der Linde, Michael Horn-von Hoegen, and Frank-J. Meyer zu Heringdorf — University Duisburg-Essen, Germany

We use the combination of a spectroscopic Photoemission Electron Microscope (PEEM) with femtosecond (fs) laser pulses to investigate samples with high spatial and temporal resolution. For proper imaging, the laser pulses must have sufficiently low intensity to minimize the space charge. Here, we report on experiments with a regenerative Ti:sapphire amplifier system. The laser setup generates fs-pulses ($\lambda = 800\ nm$, i.e., a photon energy of $E = 1.55\ eV$). The system has a variable repetition rate up to 250 kHz. We studied Ag islands which have been grown *in-situ* by self-assembly on Si(111) surfaces. We used the fundamental and the 4th harmonic ($E = 6.2\ eV$) of the amplifier system to evaluate space charge effects in PEEM. The space charge effect is reflected in an energetic broadening of the electron distribution and, at higher laser fluence, in a loss of focus. Insertion of apertures into the electron path provides a way to change the electron density in different areas of the microscope and locate in which section of the PEEM the space charge effect is dominant. The influence of the laser energy, wavelength, and repetition rate on the energy spectra and the image distortions will be discussed.

O 53.10 Wed 17:15 H32

**Characterization of Single Gold Nanoparticles Using Confocal Interference Microscopy in Combination with Higher Order Laser Modes** — •Frank Wackenhut[1], Tina Züchner[1], Antonio Virgilio Failla[1,2], and Alfred J. Meixner[1] — [1]Eberhard-Karls-Universität Tübingen, Institut für Physikalische und Theoretische Chemie, Tübingen, Germany — [2]Max-Planck-Institut für Entwicklungsbiologie, Tübingen, Germany

By using confocal interference microscpoy in combination with higher order laser modes it is possible to directly image the orientation and to detect the shape of single metal nanoparticles, with sizes well beyond the diffraction limit [1,2]. Metal nanoparticles can be imaged by detecting both their luminesence or the elastically scattered light. In the scattering detection mode the visualized pattern strongly depends on the local environment, e.g. the refractive index of the surrounding medium [3]. With this technique we are also able to observe and quantify dynamics in the motion of single nanoparticles [4]. Ongoing measurements show that this technique might be utilized for studying the wavelength dependence of the polarizability tensor of a single gold nanorod.

[1] A.V. Failla, H. Qian, H. Qian, A. Hartschuh, A. J. Meixner (2006), Nano Lett. 6, 1374. [2] T. Züchner, A. V. Failla, A. J. Meixner (2008), J. Microsc. 229, 337. [3] T. Züchner, A. V. Failla, M. Steiner, A. J. Meixner (2008), Opt. Expr. 16, 14635. [4] T. Züchner, F. Wackenhut, A. V. Failla, A. J. Meixner (2009), Appl. Surf. Sci. 255, 5391.

O 53.11 Wed 17:30 H32

**Polarization dependence of the optical response of individual metallic nanostructures and arrays** — •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 of Micro and Nanotechnology, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland

The optical response of designed metallic nanostructures depends strongly on the properties of the exciting light beam, and especially on the polarization relative to the characteristic axis of the nanostructures. To address this dependence, we established an experimental setup in the visible wavelength range that allows us to measure the optical response of individual metallic nanostructures and arrays with varying incident wave vectors and polarization. The possible excitation covers the whole range from normal excitation (relative to the surface of the substrate) to parallel excitation. The latter is realized using objective-based TIRF. In this presentation, we explain the principle of our setup and the optical response of various Au-nanostructures, such as pillars and dimers under varying wave vectors and polarization.

## O 54: Electronic structure II

Time: Wednesday 15:00–17:15 Location: H33

O 54.1 Wed 15:00 H33

**Momentum resolved imaging of the surface electronic structure of Cu(111) in multi-photon photoemission** — •Christian Tusche, Cheng-Tien Chiang, Ahmet Akin Ünal, Aimo Winkelmann, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

We use a Photoelectron Emission Microscope (PEEM), combined with an imaging energy filter, to map the distribution of photoelectrons in energy and momentum space. In this “momentum microscope”, the angular distribution of electrons leaving the sample is transferred from the back focal plane of the objective lens into two hemispherical analyzers. [1] The projected images directly show the parallel momentum component of the photoelectrons at a constant energy, and maps of the band structure are obtained as a series of parallel cuts through the Brillouin zone.

Combined with multi-photon photoemission (mPPE), using ultra short laser pulses ($h\nu$=3.1 eV), unoccupied electronic states situated in between the vacuum level and the Fermi energy can also be mapped. For instance, for the adsorption system Cs/Cu(111), 2PPE takes place resonantly through an unoccupied Cs-induced state located ≈2 eV below the vacuum level. This resonant photoemission channel is absent in a 1PPE experiment, using 6 eV photon energy. Using 3PPE, our experiments can be extended to the unoccupied part of the Cu(111) Shockley surface state and the image potential states.

[1] Krömker, Escher, Funnemann, Hartung, Engelhard, Kirschner: Rev. Sci. Instrum. **79**, 053702 (2008)

O 54.2 Wed 15:15 H33

**One-dimensional Electron System of Au/Ge(001) Revealed by Angle-resolved Photoemission** — •Sebastian Meyer[1], Jörg Schäfer[1], Christian Blumenstein[1], Aaron Bostwick[2], Eli Rotenberg[2], and Ralph Claessen[1] — [1]Experimentelle Physik 4, Universität Würzburg, 97074 Würzburg, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley 94720, California, USA

Self-organized atomic nanowires of noble metals on semiconductor surfaces are characterized by strict spatial separation and a high degree of charge confinement [1]. The ultimate width of single-atom dimension seems to be reached with gold chains on Ge(001).Thus they might offer the possibility to observe exotic properties, like a charge density wave (CDW), or, alternatively, a Luttinger liquid phase. Insight is gained by angle-resolved photoelectron spectroscopy (ARPES). We find that two shallow electron pockets disperse along the wire direction within the surface Brillouin zone, while a dispersion perpendicular to the wires is absent. This is confirmed by mapping the full Fermi surface (FS) topology, where sheets are found to be perfectly 1D without any interchain coupling. This is indicative of the virtual absence of coupling to the second dimension. Interestingly, while various nesting conditions are offered from the FS topology, no band back-folding from a CDW superstructure or energy gap opening is found, which opens a pathway for non-Fermi liquid physics. Thus the system emerges as a prototypical 1D electron system.

[1] J. Schäfer *et al.*, Phys. Rev. Lett. **101**, 236802 (2008).

O 54.3 Wed 15:30 H33

**Angle-resolved photoemission in the multi-keV regime: first experimental data and theory for W and GaAs** — •C. Papp[1,2,3], A. Gray[2,3], S. Ueda[4,5], J. Minar[6], L. Plucinski[7], C. Sakai[5], H. Yoshikawa[4], Y. Yamashita[4], S.-L. He[4], B. Balke[2,3,8], K. Kobayashi[4,5], C. Schneider[7], J. Braun[6], H. Ebert[6], and C. S. Fadley[2,3] — [1]Physical Chemistry II, Uni Erlangen — [2]Materials Science Division, LBNL — [3]Physics, UC Davis — [4]SPring 8 — [5]National Institute for Materials Science — [6]Physical Chemistry, Uni Munich — [7]Solid State Physics, Juelich Research Center — [8]Inorganic and Analytical Chemistry, Uni Mainz

ARPES is the technique of choice for studying the electronic structure of solids and surfaces. However, the measurements are very surface sensitive, probing only about 1 nm into the material. In order to study bulk properties, the use of highenergy photons in the multi-keV regime is suggested. ARPES in the multi-keV regime is now possible via hard x-ray undulator beamlines, together with angle-resolving spectrometers. We will present first hard x-ray ARPES experiments on a tungsten (110)and a GaAs(001) crystal at energies of up to 6 keV. Data obtained at 30 K clearly show band structure effects for both materials, as well as photoelectron diffraction effects for corelevels and more localized valence-band states. The data will be compared with the results of both free-electron final-state theory and one-step theory including matrix element effects. Methods for correcting low-temperature data for residual phonon effects will be considered. Funded by the Humboldt foundation and the DOE (DEAC02-05CH11231).

O 54.4 Wed 15:45 H33

**Stabilization of bulk-like $\alpha$-Mn on W(110): LEED, PES, and DFT studies** — •Elena Voloshina[1], Yuriy Dedkov[2], and Manuel Richter[3] — [1]Freie Universität Berlin, Germany — [2]Fritz-Haber Institut der Max-Planck Gesellschaft, Berlin, Germany — [3]IFW Dresden, Germany

Manganese can be considered as the most complex of all metallic elements from the crystallographic point of view. Assuming regular structural trends as in the series of the 4*d* and 5*d* transition metals, one would expect crystallization of Mn in a hcp structure. Being a member of the 3*d*-row where elements crystallize in bcc, fcc, or hcp structures, Mn behaves in a completely different way. Depending on temperature and pressure, it exists in five allotropic forms [1]. $\alpha$-Mn, the stable phase below 1000K, has an exotic bcc crystal structure containing 58 atoms in the conventional cubic unit cell. Here we demonstrate a successful stabilization of bulk-like $\alpha$-Mn films with (110) orientation on W(110). The (3 x 3) overstructure observed for the Mn film with respect to the original W(110) LEED pattern is consistent with the suggested structural model. Density functional total energy calculations confirm that this structure, a strained $\alpha$-Mn phase, is close in energy to the ground state phase and thus can be prepared under carefully controlled conditions. It is metastable, though, and can be destroyed by annealing at 300°C. Angle-resolved PE spectra show weak but distinct dispersions of the electronic states in the valence band that confirm a high quality of the studied Mn films.

[1] J. Hafner *et al.* PRB **68**, 014407 (2003); PRB **68**, 014408 (2003).

O 54.5 Wed 16:00 H33

**Electronic structures of thin NaCl (100) films grown on a Ag (111) surface** — •Sarah-Charlotta Heidorn, André Sabellek Sabellek, and Karina Morgenstern — Institut für Festkörperphysik, Abteilung ATMOS, Hannover, Deutschland

In nanoelectronics, ultrathin epitaxical insulating films are needed to separate conducting material in electronic devices of the future. NaCl is a prototype wide bandgap insulator and its electronic interactions with metals are of great interest. We present a quantitative low-temperature scanning tunnelling spectroscopy study of the interface state of nanoscale NaCl(100)-islands on Ag(111) and of the surface state on Ag(111) close to NaCl(100)-islands. The interface state energy of NaCl(100) on Ag(111) depends on island-size and -geometry. Additionally, indications for size quantization on islands are observed. The surface state on the Ag(111) shifts close to the polar edges of NaCl(100)-islands. Details of the spatially resolved dI/dV-spectra will be discussed in the presentation.

O 54.6 Wed 16:15 H33

**Field Emission Resonances on Au Atomic Chains: Periodic Energy Variations on a sub-nm Scale** — •Stefan Polei, Ingo Barke, Kristian Sell, Viola von Oeynhausen, and Karl-Heinz Meiwes-Broer — Institut für Physik, Universität Rostock, Universitätsplatz 3, D-18051 Rostock

We present scanning tunneling spectroscopy (STS) data of field emission resonances (FER) on the quasi one-dimensional Si(111)5x2-Au structure. The image-state derived FER are investigated by dI/dV measurements in the energy range near the vacuum energy and above. A distinct splitting of the first peak in dI/dV curves is observed when varying the location perpendicular to the chains. The effect appears on a length-scale of less than one nanometer. We assign the splitting to variations of the local work function [1].

[1] H. C. Ploigt, C. Brun, M. Pivetta, F. Patthey, and W. D. Schneider, Phys. Rev. B 76, 195404 (2007).

O 54.7 Wed 16:30 H33

**The Interplay of Conductance, Force, and Structure Change in Metallic Point Contacts** — •Markus Ternes[1,2], César González Pascual[3], Chris P. Lutz[1], Franz J. Giessibl[4], Pavel Jelńek[5], and Andreas J. Heinrich[1] — [1]IBM Research Division, Almaden Research Center, San Jose, California — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [3]Instituto Ciencia de Materiales de Madrid, Spain — [4]Institute of Experimental and Applied Physics, University of Regensburg, Germany — [5]Institute of Physics, Academy of Sciences of the Czech Republic, Prague

A combined scanning tunneling and atomic force microscope was used to measure simultaneously the conductance and the short-range force between an atomically sharp tip and a single metal adsorbate on a metal surface. We found that in the tunneling regime the conductance as well as the attractive short-range force increased exponentially as the tip approached the adsorbate. In the transition regime between tunneling and point-contact a stronger than exponential increase in the conductance was found for a Cu atom on a Cu(111) surface probed with a Cu tip but not for a Pt atom on a Pt(111) surface. To explain the subtle details of the experimental findings, extensive density functional calculations where performed showing that both studied systems show a profound structural change when the transition between tunneling and point-contact occurs. The structural change strongly influences the conductance and forces between tip and sample. The experimental and numerical results are in excellent agreement and give new detailed inside into the transition and formation of metallic point-contacts.

O 54.8 Wed 16:45 H33

**Electronic structure of carboxylate molecules on Cu(110) surface: An experimental and theoretical investigation** — •Vasile Caciuc, Christina Lennartz, Nicolae Atodiresei, Silvia Karthäuser, Rainer Waser, and Stefan Blügel — Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

In the present contribution we report on a combined experimental and theoretical study focused on the electronic structure of aromatic organic molecules like benzoic acid ($C_7H_6O_2$) and pyridine-2-carboxylic acid ($C_6H_5NO_2$) adsorbed on the Cu(110) surface. A special focus of our study is to investigate the role of the substitution of an $CH$ functional group by an $N$ atom or by the addition of a second carboxylic group on the electronic properties of the adsorbate-substrate system. In particular, the electronic structure of the molecule-Cu(110) surface was analyzed by recording the differential conductance $dI/dV$ curves, whose shape show a significant dependence on the tip-molecule distance. A clear picture of the nature of the molecule-substrate states that lead to the observed shape of the $dI/dV$ curves was achieved by comparing the experimental differential conductance with the calculated density of states for the carboxylate-surface systems under consideration.

O 54.9 Wed 17:00 H33

**Nanoporous supramolecular networks: From quantum confinement to caged rotators** — •Florian Klappenberger — Physik Department E20, TU München, Germany

Making use of molecular self-assembly of dicarbonitrile-sexiphenyl (NC2Ph6) molecules, we confine the surface state of the Ag(111) surface with various nanoporous networks and investigate their properties by means of low-temperature scanning tunneling microscopy/spectroscopy and electronic structure calculation. The case of a hydrogen-bonded chiral Kagome superstructure induces a complex dichotomous electronic tessellation. An analysis employing a boundary element method based on Greens functions indicates a uniform repulsive scattering potential for the molecular building blocks. In a Co-directed metal-organic honeycomb network employing the same molecules, Co atoms scatter clearly different from the organic linkers with slight attractive potential for electrons at the Fermi energy, thus with strongly altered character than isolated Co adatoms. Further evaporation of NC2Ph6, acting as guest molecules, leads to the self-assembly of three-winged supramolecular units within the honeycomb pores and to further confinement of the surface state electrons. Thermal activation induces rotation of the trimeric unit and thus produces a dynamic quantum confinement. A temperature-dependent study yields the rate of the motion of the self-assembled rotor and shows various modes of motion.

## O 55: Density functional theory and beyond for real materials II

Time: Wednesday 15:00–17:15 Location: H34

O 55.1 Wed 15:00 H34

**Accurate band gaps of semiconductors and insulators with a semilocal exchange-correlation potential** — •Fabien Tran and Peter Blaha — Institute of Materials Chemistry, Vienna University of Technology, Vienna, Austria

Recently, Becke and Johnson [1] proposed a semilocal exchange potential which reproduces very well the shape of the exact exchange potential constructed from the optimized effective potential. We showed that this semilocal potential improves (albeit moderately) over the LDA and PBE potentials for the band gap of solids [2]. In order to have further improvement in the results for band gaps, we modified the Becke-Johnson potential (MBJ) [3]. This new potential leads to agreement with experiment which is very good for all types of solids we considered (e.g., wide band gap insulators, sp semiconductors, and strongly correlated 3d transition-metal oxides) and is of the same order as the agreement obtained with the hybrid functionals (e.g., HSE) or the GW methods. This semilocal exchange potential, which recovers the LDA for a constant electron density, mimics very well the behavior of orbital-dependent potentials and leads to calculations which are barely more expensive than LDA calculations. Therefore, it can be applied to very large systems in an efficient way.

[1] A. D. Becke and E. R. Johnson, J. Chem. Phys. **124**, 221101 (2006). [2] F. Tran, P. Blaha, and K. Schwarz,J. Phys.: Condens. Matter **19**, 196208 (2007). [3] F. Tran and P. Blaha, Phys. Rev. Lett. **102**, 226401 (2009).

O 55.2 Wed 15:15 H34

**Spectral properties of actinide materials: Charge density self-consistent LDA+Hubbard I method in FP-LAPW basis** — •Jindrich Kolorenc[1,2], Alexander B. Shick[1], Ladislav Havela[3], and Alexander I. Lichtenstein[2] — [1]Institute of Physics ASCR, Prague, Czech Republic — [2]University of Hamburg, Hamburg, Germany — [3]Charles University, Prague, Czech Republic

We provide a numerically efficient procedure to perform LDA + Hubbard I calculations including self-consistency over the charge density in the FP-LAPW basis [1]. The method is applied to Pu, Am, and PuAm and PuCe alloys. Our results for valence photoemission spectra (PES) agree with experimental data and with previous LDA+DMFT calculations [2]. Analysis of the J=5/2 and J=7/2 contributions to the f-occupation supports the intermediate-coupling picture of f-states in heavy actinides. The electronic specific heat coefficient is calculated for PuAm and PuCe alloys in reasonable agreement with recent experiments. We show that Pu atoms keep their mixed-valence character in these alloys. Next, we study electronic and spectral properties of Pu-based superconductor PuCoGa5 and obtain good agreement with experimental PES [3]. Finally, we analyze surface effects. In Pu monolayer, we find substantial modification of PES due to 5f-electron localization consistent with experimental observations [4].

[1] A. B. Shick et al., Phys. Rev. B 80, 085106 (2009).
[2] J. H. Shim et al., Phys. Rev. Lett. 101, 126403 (2008).
[3] J. L. Sarrao et al., Nature (London) 420, 297 (2002).
[4] L. Havela et al., Phys. Rev. B 65, 235118 (2002).

O 55.3 Wed 15:30 H34

**Self-doping Effects at a 45° Grain Boundary in $YBa_2Cu_3O_7$** — •U. Schwingenschlögl[1] and C. Schuster[2] — [1]KAUST, PCSE Division, P.O. Box 55455, Jeddah 21534, Saudi Arabia — [2]Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

The charge redistribution at grain boundaries determines the applicability of high-$T_c$ superconductors in electronic devices because the transport across the grains can be hindered considerably. We investigate the local charge transfer and the modification of the electronic states in the vicinity of the grain-grain interface by ab-initio calculations for a normal-state 45° [001] grain boundary in $YBa_2Cu_3O_7$. Our results explain the suppressed interface transport and the influence of grain boundary doping in a quantitative manner, in accordance with the experimental situation. The charge redistribution is found to be strongly inhomogeneous, which has a substantial effect on transport properties since it gives rise to a self-doping of 0.10±0.02 holes per Cu atom. Reference: Phys. Rev. Lett. **102**, 227002 (2009).

O 55.4 Wed 15:45 H34

**All-electron *GW* calculations for perovskite 3d transition-metal oxides La*TM*O$_3$** — •Andreas Gierlich, Christoph Friedrich, and Stefan Blügel — Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

The La$TM$O$_3$ family of compounds, where $TM$ is a 3d transition metal, shows a large variety of electronic and magnetic properties. It comprises Mott and band insulators, antiferromagnets, and metals. The rich diversity of properties originates from the interplay between the localization of the 3d electrons and their hybridization with O 2p states in the presence of crystal fields and Hund's rule physics. Standard density-functional calculations within the local-spin-density approximation often fail even qualitatively in describing the electronic structure of these correlated materials. To treat the band structure and electronic correlation on the same footing from first principles we employ the $GW$ approximation for the electronic self-energy. We use our recently developed implementation (http://www.flapw.de/spex) in the all-electron full-potential linearized-augmented-planewave (FLAPW) method. Within this method a large variety of materials can be treated, including d- and f-electron systems, oxides and magnetic systems, and thus it is particularly suited for the La$TM$O$_3$ family. We present and discuss first results.

O 55.5 Wed 16:00 H34

**Bridging rare-earth physics and chemistry: a hybrid functional study for Ce** — •Marco Casadei[1], Xinguo Ren[1], Angel Rubio[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, 14195 Berlin, Germany — [2]Dpt. Fisica Materiales, UPV/EHU, San Sebastian Spain

The presence of localized, partially occupied $f$ electronic states is responsible for many peculiar physical properties of rare-earth materials. Of particular interest is the $\alpha$-$\gamma$ phase transition in Ce metal, which poses a big challenge to first principles approaches based on local/semilocal (LDA/GGA) approximations to density functional theory (DFT). Within LDA and GGA, the $f$ electrons tend to be more delocalized than they should, and thus the $\gamma$ phase with localized $f$ electrons can not be described.

Hybrid functionals provide a way of improving the exchange-correlation functionals climbing the so-called Jacob's ladder in Perdew's sense to the fourth rung. By incorporating a fraction of exact exchange, hybrid functionals reduce the self-interaction error considerably which is the main reason for the failure of LDA/GGA in this case. It is highly interesting to see how quantitatively hybrid functionals work for this renowned problem. To this end we calculated the cohesive energies of the Ce clusters of increased size, cut from Ce bulk, as a function of the lattice constant. For these clusters, we establish that there exists multi-solution behavior at the hybrid functional (here PBE0) level, which is absent for LDA/GGA. We analyze the implication of this behavior to the $\alpha$-$\gamma$ phase in Ce bulk.

O 55.6 Wed 16:15 H34

**Nonadiabatic electron dynamics in time-dependent reduced-density-matrix functional theory** — •Ryan Requist and Oleg Pankratov — University of Erlangen-Nuremberg, Erlangen, Germany

Numerical simulation of real-time electron dynamics in strongly-driven molecules and confined environments remains a challenging problem for *ab initio* electronic structure methods. One of the most widely used methods is the adiabatic extension of the local density approximation (ALDA) in TD DFT. Although it often works well in linear response calculations, it performs poorly for charge transfer excitations and is unable to account for excitations of doubly-excited character. Progress toward describing these excitations has been made in time-dependent reduced-density-matrix functional theory, which uses the one-body reduced density matrix as the basic variable. This theory might have advantages for real-time dynamics as well. However, a nontrivial obstacle to applying the adiabatic extension approximation has been identified. Namely, the adiabatic extension of the available ground-state functionals leads incorrectly to time-independent occupation numbers (the eigenvalues of the one-body reduced density matrix). In this talk, we describe an adiabatic approximation [arXiv:0911.0945] that generates time-dependent occupation numbers. Tests for a model system demonstrate that it captures quite well Landau-Zener transitions and Stueckelberg oscillations, which are canonical nonadiabatic effects in real-time dynamics. Electron correlation is found to play a crucial role.

O 55.7 Wed 16:30 H34

**Is there a physical meaning of the natural orbitals? Analysis of exactly solvable models** — •Nicole Helbig[1], Ilya V. Tokatly[1,2], Johanna I. Fuks[1], and Angel Rubio[1,3] — [1]Nano-Bio Spectroscopy group and ETSF Scientific Development Centre, Dpto. Física de Materiales, 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

Reduced density matrix functional theory provides a set of orbitals, namely the natural orbitals, which are originally defined mathematically as the eigenfunctions of the one-body density matrix. We investigate the suitability of these orbitals as a basis for describing many-body excitations. We analyze to which extend the natural orbitals describe both bound as well as ionized excited states and show that depending on the specifics of the excited state the ground-state natural orbitals yield a good approximation or not.

O 55.8 Wed 16:45 H34

**On the way to exact-exchange quality from a semi-local functional** — •Andreas Karolewski and Stephan Kümmel — Theoretische Physik, Universität Bayreuth, 95440 Bayreuth, Germany

In this talk we discuss an approach for constructing a semi-local "ab initio" exchange functional that promises to incorporate many of the attractive features of exact exchange at low computational cost. A particularly relevant example is predicting the polarizabilities of extended systems. This has been a long-standing problem in density functional theory. We show that the new approach predicts the polarizabilities of extended conjugated molecules with much better accuracy than typical semi-local functionals.

The common approach of functional development is starting with an expression for the exchange correlation energy and calculating the exchange correlation potential via the functional derivative. In contrast, we start with an effective approximation for the exchange potential and show that it predicts the polarizabilities with much better accuracy than typical semi-local functionals. Furthermore we discuss a way of finding a corresponding energy functional.

O 55.9 Wed 17:00 H34

**Exchange an Correlation effects in the electronic properties of transition metal oxides: the example of NiO** — •Matteo Guzzo[1,3], Matteo Gatti[2,3], and Lucia Reining[1,3] — [1]LSI - ETSF, Ecole Polytechnique, Palaiseau CEDEX 91128, France — [2]Nano-bio group - ETSF, Universidad del Pais Vasco, San Sebastian, Spain — [3]European Theoretical Spectroscopy Facility (ETSF)

The original contributions O 55.9 "Insights in the T-matrix formalism" by Pina Romaniello and O 55.10 "GW without emipty states" by Arjan Berger have been withdrawn. Instead, this talk by Matteo Guzzo has been rescheduled from O 10.7 to this slot.

NiO, as a prototype for strongly-correlated materials, has been extensively studied experimentally and theoretically. Its Antiferromagnetic phase is reasonably well described in GW (a many-body approximated approach), but self-consistency is needed to obtain proper wavefunctions for the system. Still, agreement with experiment is not perfect. In particular, the unoccupied d-states result too high in energy by about 1 eV. In the present work we investigate the effects of vertex corrections derived from time-dependent density-functional theory on this result, starting from a simple LDA correction and going to more complex vertices including non-locality.

## O 56: Metal substrates: Adsorption of organic / bio molecules VI

Time: Wednesday 15:00–17:30 Location: H36

O 56.1 Wed 15:00 H36

**Electron induced conformational changes of imine-based molecular switches on a Au(111) surface** — •Christian Lotze[1], Ying Luo[2], Rainer Haag[2], and Jose Ignacio Pascual[1] — [1]Inst. f. Experimentalphysik, Freie Universität Berlin — [2]Inst. f. organische Chemie, Freie Universität Berlin

Organic molecules exhibiting controllable reversible transitions between isomeric states on surfaces promise an enormous potential in the field of molecular electronics. The reversible cis-trans isomerization of azobenzene-like molecules is often hindered by a strong interaction of the nitrogen lone-pair electrons of the di-azo bridge (-N=N-) with the substrate. In order to improve the isomerization capabilities, the di-azo bridge is substituted by an imine-group (-N=CH-).

Here, we use low-temperature scanning tunneling microscopy to investigate a sub-monolayer of the newly designed imine-based molecular switch NPCI on a Au(111) surface. Its carboxylic termination mediates the formation of hydrogen-bonded dimers, which align in rows along the herringbone reconstruction. We were able to induce reversible conformational changes with the tunneling electrons from the STM tip and determine its efficiency as a function of electron energy.

O 56.2 Wed 15:15 H36

**Optical Isomerization of tetra(*tert*-butyl)azobenzene (TBA) on Gold (111) and Coverage Dependent Conformation of the Corresponding Imine** — •Daniel Brete[1], Roland Schmidt[1], Cornelius Gahl[1], Robert Carley[1], Sebastian Hagen[2], Petra Tegeder[2], and Martin Weinelt[1,2] — [1]Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin — [2]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

NEXAFS and XPS have been used to investigate optically induced conformational changes of 3,3',5,5'-tetra(*tert*-butyl)azobenzene (TBA) monolayers and the influence of coverage and temperature on the conformation of the analogue imine 3,5-di-*tert*-butylbenzaldehyde-(3,5-di-*tert*-butyl-phenylimine)(TBI) on gold (111) surfaces.

Monolayers of TBA adsorb flat on the surface. Upon illumination with blue light TBA is transformed into a non-planar configuration. This change is thermally reversible. The photoisomerization cross section of TBA is reduced by two orders of magnitude compared to solution suggesting a substrate induced photoisomerization mechanism.

In contrast the monolayer of TBI exhibits a non-planar configuration, while submonolayers obtained by partial desorption exhibit a planar adsorbtion geometry. Both are very similar to the non-planar and planar species of TBA. We conclude that the energy gained by a higher packing density favours the non-planar configuration in the case of TBI.

O 56.3 Wed 15:30 H36

**Single enantiomorphism and chiral conflict in 2D crystals** — •Christian Roth, Leo Merz, Manfred Parschau, and Karl-Heinz Ernst — Nanoscale Materials Science, Empa, Swiss Federal Laboratories for Materials Testing and Research, Dübendorf, Switzerland

In order to investigate chiral recognition on the molecular level, we investigated the effect of chiral doping of monolayers of tartaric acid (TA), malic acid (MA) and succinic acid (SU) with STM and LEED. We reported earlier that doping achiral SU with a small amount of chiral TA leads to single chirality (sergeants-and-soldiers effect) [1]. Here we present results of cross-contamination experiments of TA and MA. The mixture of left and right handed TA (rac-TA) shows a superposition of the two enantiomorphs in LEED that are observed for the pure enantiomers. Adding one enantiomer of MA to the mixture suppresses formation of the two enantiomorphs. (R)-MA allows thereby only the formation of the structure known for pure (R,R)-TA, while (S)-MA leads to the (S,S)-enantiomorph. Mixing chiral (R,R)-TA into rac-MA leads indeed to single enantiomorphism as well, however, this time the structure is a completely new polymorph that has not been observed for pure MA. Two different mechanisms are proposed for the observed results: an entropy driven effect in the rac-TA / MA experiment and a chiral conflict in the rac-MA / TA case.

References

[1] M. Parschau, S. Romer and K.-H. Ernst 2004 J. Am. Chem. Soc.126 15398

O 56.4 Wed 15:45 H36

**The Role of Functional Groups for the Switching Efficiency of Surface-Adsorbed Molecular Switches** — •Erik R. McNellis[1] and Karsten Reuter[1,2] — [1]Fritz-Haber-Institut Berlin (Germany) — [2]Technische Universität München (Germany)

Azobenzene ($C_6H_5$-N=N-$C_6H_5$) adsorbed at coinage metal surfaces has transformed into an increasingly studied prototype system for a surface-adsorbed molecular switch. With photo-induced switching between the cis and trans configuration suppressed for bare azobenzene, controlled decoupling from the surface through bulky functional groups appears as a promising strategy. In particular, tetra-tert-butyl azobenzene (TBA), in which groups of three butyl ($CH_3$) groups are added to both meta positions of each phenyl ring, can be efficiently switched at Au(111), albeit not at Ag(111). In order to shed more light on the role of the functional groups and surface electronic structure for the different switching efficiency we perform density-functional theory calculations, accounting for van der Waals interactions on the level of semi-empirical dispersion correction schemes. The thereby obtained structural and vibrational properties of both bare azobenzene and TBA at Ag(111) and Au(111) compare favorably with existing experimental data. In the analysis of the electronic structure we focus on the hybridization of the molecular frontier orbitals with the substrate states, and discuss this in the context of previously published hypotheses concerning the switching mechanism of surface-adsorbed TBA.

O 56.5 Wed 16:00 H36

**Reversible photoisomerization of an azobenzene-functionalized self-assembled monolayer probed by sum-frequency generation vibrational spectroscopy** — •Felix Leyssner[1], Steffen Wagner[1], Christian Kördel[1], Sebastian Zarwell[2], Karola Rück-Braun[2], Martin Wolf[1], and Petra Tegeder[1] — [1]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, D-14195 Berlin — [2]Technische Universität Berlin, Institut für Chemie, Strasse des 17. Juni 135, D-10623 Berlin

We studied the reversible photoinduced *trans/cis*-isomerization of an azobenzene-functionalized self-assembled monolayer on a gold substrate using sum-frequency generation (SFG) vibrational spectroscopy. A cyano-group in *para*-position at the outer phenyl-ring is utilized as a marker to directly investigate the molecular orientation and therefore the switching state. The azobenzene unit is connected to a tripodal linker system with an adamantane core. This linker system provides: i) an adequate free volume to prevent steric hindrance and ii) sufficient decoupling from the metallic substrate to enable the isomerization process. Light exposure at a wavelength of 405 nm induces the *trans* → *cis* isomerization whereas illumination at 470 nm leads to the back reaction. The effective cross section for the photoinduced *trans* → *cis* reaction at 405 nm is $\sigma_{eff}(cis) = 4 \pm 1 \times 10^{-18} cm^2$, while for the back reaction (*cis* → *trans*) at 470 nm we obtain $\sigma_{eff}(trans) = 2.5 \pm 0.9 \times 10^{-19} cm^2$. Our study demonstrates that SFG vibrational spectroscopy is a highly suitable technique to analyze the molecular structure of functional surfaces.

O 56.6 Wed 16:15 H36

**Structure and energetics of azobenzene on Ag(111)** — •Giuseppe Mercurio[1,2], Erik McNellis[3], Isabel Martin[4], Sebastian Hagen[4], Felix Leyssner[4], Sergey Soubatch[1,2], Jörg Meyer[3], Martin Wolf[3,4], Petra Tegeder[4], Frank Stefan Tautz[1,2], and Karsten Reuter[3] — [1]Institut für Bio- und Nanosysteme 3, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany — [4]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany

Normal Incidence X-ray Standing Wave (NIXSW) and Temperature Programmed Desorption experiments have been performed in order to determine the adsorption geometry of azobenzene on Ag(111), i.e. to define the following key parameters: vertical adsorption height of N=N bridge, tilt angle of the phenyl rings, and adsorption energy. Experimental results suggest nearly planar adsorption geometry of the azobenzene molecule, with the nitrogen atoms at a height of 3.07 Å. Adsorption energy was found to be 1.08 eV. The determined geometry is in good agreement with the theoretically predicted values (2.98 Å and 3°) obtained by DFT with semi-empirical dispersion corrections, validating therefore this calculation method. Discrepancy between experimental and theoretical adsorption energy was attributed to electronic screening of dispersive interactions at the metallic surface.

O 56.7 Wed 16:30 H36

**Studies of azobenzene-containing triazatriangulenium adlayers on Au(111) surfaces** — •Ulrich Jung[1], Sonja Kuhn[1], Mathias Müller[1], Olena Filinova[1], Belinda Baisch[1], Jens Kubitschke[2], Rainer Herges[2], and Olaf Magnussen[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Leibnizstraße 19, 24118 Kiel, Germany — [2]Otto-Diels-Institut für Organische Chemie, Christian-Albrechts-Universität zu Kiel, Otto-Hahn-Platz 3, 24098 Kiel, Germany

The attachment of molecular functions such as photoswitches to metal surfaces is of major interest in nanotechnology. One of the most frequently studied class of photoswitches are azobenzenes, which exhibit trans-cis isomerism. The typical method to attach azobenzene to surfaces is self-assembly of thiols on Au. However, in such adlayers the photoisomerization is often totally quenched because of steric effects. To overcome the problems of conventional azobenzene adlayers, we were employing a novel approach using customizable triazatriangulenium (TATA) platforms [1]. Here, we will present the structure and photoswitching properties of azobenzene-containing TATA adlayers on Au(111), obtained by structure-sensitive, spectroscopic, and electrochemical methods. Functionalized TATA molecules exhibit a strong tendency to form bilayers. We will demonstrate, that it is possible to suppress bilayer formation and thus to form highly-ordered functionalized TATA monolayers. Furthermore, the photoswitching processes in these adlayers obey first order kinetics with quantum efficiencies of < 10-3. [1] Baisch et al., J. Am. Chem. Soc. (2009), 131, 442

O 56.8 Wed 16:45 H36

**Surface mounted molecular rotors with variable functional groups and rotation radii** — •Dingyong Zhong[1], Tobias Blömker[2], Katrin Wedeking[2], Lifeng Chi[1], Gerhard Erker[2], and Harald Fuchs[1,3] — [1]Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany & Center for Nanotechnology (CeNTech), Universität Münster, Heisenbergstr. 11 , 48149 Münster, Germany — [2]Organisch-Chemisches Institut, Universität Münster, Corresstr. 40, 48149 Münster, Germany — [3]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany

A strategy for designing and activating surface-mounted molecular rotors with variable rotation radii and functional groups is proposed and demonstrated. The key point of the strategy is to separate the anchor and the rotating functional group from each other by using a connector of adjustable length. The three independent parts of the molecule are responsible for different functions to support the rotating movement of the molecule as a whole. In this way, one can easily change each part to obtain molecular rotors with different sizes, anchors, and functional rotating groups.

O 56.9 Wed 17:00 H36

**Repulsion Between Molecules on a Metal: (Sub-) Monolayers of Hexa-*peri*-hexabenzocoronene on Au(111)** — •Christian Wagner[1,3], Daniel Kasemann[1], Roman Forker[1,2], and Torsten Fritz[1,2] — [1]Inst. für Angewandte Photophysik, TU Dresden — [2]Inst. für Festkörperphysik, FSU Jena — [3]Inst. für Bio- und Nanosysteme 3, FZ Jülich, JARA Fundamentals of Future Information Technology

We investigate the growth of hexa-*peri*-hexabenzocoronene (HBC) on Au(111) for monolayer (ML) and sub-ML coverage by scanning tunneling microscopy (STM) and low energy electron diffraction (LEED). A transition from a disordered isotropic phase at low coverage to a highly ordered phase with a coverage-dependent lattice constant at higher coverage is found and attributed to a repulsive intermolecular force. To deduce the origin of this repulsion a model is developed, containing the Coulomb and van der Waals interaction between the molecules. The metal substrate is accounted for by the inclusion of mirror charges and a dipole created by the pushback effect, while the van der Waals interaction is modeled on a force field level. The Coulomb repulsion is caused by the partially positively charged hydrogen atoms. The effect can, however, only be explained under the postulate of a screening of the attractive London forces by the metal substrate as a result of the non-additivity of dispersion forces. As the mechanisms described are rather universal they should be able to explain a similar repulsion observed for other hydrocarbons [1,2].

[1] C. Seidel et al., *Phys. Rev. B* **64**, 195418 (2001)

[2] S. Müllegger and A. Winkler, *Surf. Sci.* **600**, 1290 (2006)

O 56.10 Wed 17:15 H36

**Nanojoule Calorimetry of Surface Reactions: Cyclohexene on Pt(111)** — •Ole Lytken[1,2], Wanda Lew[1], Jonathan J.W. Harris[1], Ebbe K. Vestergaard[1], J. Michael Gottfried[2], and Charles T. Campbell[1] — [1]Department of Chemistry, University of Washington, Seattle, WA, USA — [2]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Erlangen, Germany

Platinum is an excellent hydrogenation/dehydrogenation catalyst. Many hydrocarbons therefore readily dehydrogenate on platinum instead of desorbing. This severely limits the usefulness of traditional desorption based techniques for measuring heats of adsorption, such as temperature programmed desorption (TPD). Cyclohexene on Pt(111) is a typical such system where reaction prevails over desorption. At 100 K cyclohexene adsorbs intact, but with increasing temperature, it dehydrogenates, forming first a partially dehydrogenated 1-cyclohexenyl species, then benzene and eventually graphite. However, unlike TPD, single-crystal microcalorimetry does not rely upon desorption and can therefore directly measure the heats of adsorption and reaction of the wealth of species formed as hydrocarbons adsorb on platinum. We have used microcalorimetry to successfully measure the heat of adsorption of cyclohexene on Pt(111) at 100 - 300 K and determined the heats of formation as a function of coverage of two adsorbed intermediates in the hydrogenation of benzene to cyclohexane, namely cyclohexene and 1-cyclohexenyl.

## O 57: Surface dynamics II

Time: Wednesday 15:00–17:30 Location: H40

O 57.1 Wed 15:00 H40

**Time-Resolved XUV pump probe measurements on Surfaces using High Harmonic Radiation** — •Thorben Haarlammert[1], Carsten Winter[1], Luca Bignardi[2], Petra Rudolf[2], and Helmut Zacharias[1] — [1]Physikalisches Institut, Westfälische Wilhelms Universität, Münster — [2]Zernike Institute for Advanced Materials, University of Groningen

We have developed an experimental set-up for time-resolved photoelectron spectroscopy at surfaces using High Order Harmonics of a Ti:Sapphire laser. By employing a $LN_2$ cooled laser amplifier system operating with repetition rates of up to 10 kHz fast and stable delay scans can be collected. The set-up allows for time-resolved pump and probe measurements with ultra-short pump pulses in the IR, visible or UV spectral range and ultra-short XUV probe pulses at the 25th harmonic order at 39 eV. The duration of the XUV pulses was estimated using the laser assisted photoelectric effect (LAPE). Measurements were performed on single layer Graphene on a Ni (111) crystal surface. First time-resolved results will be presented. In addition, a combination of a toroidal grating and the mirror monochromator allows for conventional angle resolved photoelectron measurements (ARUPS) at different photon energies in the spectral range between 20 eV and 110 eV by applying different Harmonic Orders.

O 57.2 Wed 15:15 H40

**Dependence of thermal CO diffusion on Cu(111) on local coverage** — •Christopher Zaum, Kastur Meyer-auf-der-Heide, and Karina Morgenstern — Institut für Festkörperphysik, Abteilung ATMOS, Gottfried Wilhelm Leibniz Universität, Appelstr. 2, D-30167 Hannover, Germany

Because of its importance as reactant in several catalytic reactions, carbon monoxide is often used in exemplary surface science studies. In order to investigate the diffusion of this molecule, we deposited CO molecules on a clean Cu(111) surface held at 22K and recorded several image series for dynamic analysis in a temperature range from 40K to 60K with a low-temperature scanning tunneling microscope. The diffusion of single CO molecules at low local coverages follows an Arrhenius law. At higher local coverages next-neighbor interactions influence the diffusion by increasing the local diffusion rates. We will discuss quantitatively the dependence of the diffusivity of single CO molecules on their local environment.

O 57.3 Wed 15:30 H40

**Desorption of ionic species from ice/graphite by femtosecond XUV free electron laser pulses** — •Björn Siemer[1], Tim Hoger[1], Robert Frigge[1], Sebastian Roling[1], Rolf Mitzner[2], Rolf Treusch[3], Stefan Düsterer[3], and Helmut Zacharias[1] — [1]Westfälische Wilhelms-Universität, Münster,Germany — [2]Helmholtz Zentrum Berlin, Berlin,Germany — [3]DESY, Hamburg, Germany

The interaction of high-energy photons in the soft x-ray regime with surface systems may lead to new and unexpected results due to the large number of accessible product states. In the past this photon energy regime has mainly been investigated using synchrotron radiation sources. The development of the Free Electron Laser at Hamburg (FLASH) now opens a new area in this spectral range. It provides pulsed radiation in the photon energy range from 20 to 200 eV, with pulse energies of tens of microjoule and a pulse duration of 20 to 50 fs.

We want to present first results from our recent measurement session. Highly-oriented pyrolytic graphite (HOPG) surfaces covered with $D_2O$ are irradiated and desorbing products are analyzed. Ionic species are formed by the FEL radiation on the surface and directly emitted from the graphite. The $O_2^+$ yield shows a highly nonlinear dependence on the FEL intensity. This opens the way to non-linear correlation measurements with an autocorrelator using two FEL pulses synchronized on a femtosecond time scale. First results from these two-pulse correlation measurements in the soft x-ray regime are reported.

O 57.4 Wed 15:45 H40

**ZEITAUFGELÖSTE ELEKTRONENBEUGUNG AN DÜNNEN METALLFILMEN** — •Manuel Ligges, Carla Streubühr, Thorsten Brazda, Ping Zhou und Dietrich von der Linde — Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Deutschland

Bei der Bestrahlung von Festkörpern mit ultrakurzen (fs) Laserimpulsen wird primär das elektronische System angeregt, währen das Gitter zunächst kalt bleibt. Die Elektron-Phonon-Wechselwirkung bewirkt einen Energiübertrag an das Gitter, so dass dieses sich aufheizt. Diese Aufheizung erfolgt typischerweise innerhalb von einigen Pikosekunden. Die zeitliche Entwicklung der Gitteranregung lässt sich durch Beugungsexperimente mit Hilfe des Debye-Waller-Effektes verfolgen.

Wir haben in zeitaufgelösten Elektronenbeugungsexperimenten die schnelle Gitteraufheizung in dünnen Gold-, Silber- und Kupferfilmen nachgewiesen [1]. Die aus den experimentellen Daten ermittelten Zeiten für den energetischen Austausch stimmen mit theoretischen Rechnungen [2] im Rahmen eines einfachen Zwei-Temperatur-Modelles [3] überein.

[1] M. Ligges, I. Rajkovic, P.Zhou, O. Posth, C. Hassel, G. Dumpich, and D. von der Linde, Appl. Phys. Lett 94, 101910 (2009) [2] Z. Lin, L. V. Zhigilei, and V. Celli, Phys. Rev. B. 77, 075133 (2008) [3] S. I. Anisimov, B. L. Kapeliovich, and T. L. Perelman, Sov. Phys. JETP 39, 375 (1974)

O 57.5 Wed 16:00 H40

**Ultrafast melting of orbital and charge order in magnetite** — •Niko Pontius[1], Torsten Kachel[1], Hermann A. Dürr[1], Christian Schüssler-Langeheine[2], Bill Schlotter[3], Martin Beye[3], Florian Sorgenfrei[3], Alexander Föhlisch[1,3], and Wilfried Wurth[3] — [1]Helmholtz-Zentrum Berlin, BESSY II, 12489 Berlin — [2]Physikalisches Institut, Universität zu Köln, 50937 Köln — [3]Institut für Experimentalphysik, Universität Hamburg, 22761 Hamburg

At 120K magnetite ($Fe_3O_4$) undergoes a metal-to-insulator transition (the famous Verwey transition [1]) which is accompanied by a transition from a charge and orbital ordered state below the transition temperature to a state without electronic order [2]. Until today the question whether this transition is driven by the lattice or by electronic degrees of freedom remains unanswered. We studied this transition using time-resolved resonant soft x-ray diffraction (RSXD) at the free electron laser FLASH in Hamburg. Thus we get direct insight into the "melting" of charge and orbital order after selectively exciting the electronic system by an infrared fs-laser pulse from below the transition temperature. The experimental data reveal an unexpectedly slow melting on a time scale of $\approx$ 500 fs. This suggests that the melting process is limited by a rearrangement of the lattice. Moreover, by performing time-resolved spectroscopy on the RSXD-reflection peak at the oxygen K-edge we observe the narrowing of the band gap during the melting process.

[1] E.J.W. Verwey, Nature 144, 327-328 (1939)

[2] J. Schlappa et al. , Phys. Rev. Lett. 100, 026406 (2008)

O 57.6 Wed 16:15 H40

**Investigation of thin Cu films on Fe/Pd and their dynamics with Positron annihilation induced Auger electron spectroscopy** — •Jakob Mayer[1,2], Klaus Schreckenbach[1,2], and Christoph Hugenschmidt[1,2] — [1]TU München, Lehrstuhl E21, James-Franck Straße, 85748 Garching — [2]ZWE FRM-II, Lichtenbergstr. 1, 85747 Garching

**P**ositron annihilation induced **A**uger **E**lectron **S**pectroscopy (PAES) is a powerful technique to investigate the topmost atomic layer of a sample. This is due to the different hole creation process by positron electron annihilation and due to the trapping of the positron at the surface of the sample. With conventional positron beam setups the measurement time for one PAES-spectrum amounted to several days. Now, with the highly intense positron beam NEPOMUC at the FRM-II in Munich ($9 \cdot 10^8 \frac{e^+}{s}$), it is possible to record a PAES spectrum within less than one hour. For the first time we succeeded to observe dynamic processes at the surface with PAES. Measurements of thin Cu layers (0.3-4ML) on Fe and Pd samples will be presented and the higher surface selectivity of PAES compared to conventional EAES will be shown. Furthermore, diffusion of Cu into the bulk of Pd was observed.

O 57.7 Wed 16:30 H40

**Vibrational Spectroscopy of Copper on Cu(111)** — •Olaf Skibbe, Heiner Maslosz, Jan Pischel, Diana Vogel, and Annemarie Pucci — Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, D-69120 Heideberg

It is known from literature that on some stepped copper surfaces vibrations exist at energies significantly above that of the bulk phonon band [1]. By use of high-resolution electron energy loss spectroscopy (HREELS) we found for sub-monolayer amounts of copper evaporated to the cooled Cu(111) surface vibrations at even higher energies (50% above the highest bulk phonon energy). It could be shown that the vibration is polarized perpendicularly to the surface. The vibrational energy shifts slightly upon annealing, and the peak disappears at temperatures above 200 K. Additional measurements of the work function change upon annealing have been performed.

In addition, to clarify data analysis, we examine the interaction of typical molecules from the residual gas (such as CO and $O_2$) with the roughened surface.

Since it is known that roughened surfaces provide a higher chemical activity than pristine single crystal surfaces, we hope to gain deeper insight in the interaction of molecules with defect-rich surfaces via the observation of the extra-ordinary high energy vibrational mode.

[1] A. Kara, P. Staikov, T.S. Rahman, J. Radnik, R. Biagi, and H.-J. Ernst. Phys. Rev. B 61(8):5714-5718, 2000.

O 57.8 Wed 16:45 H40

**Vanadium Oxide on Rh(111): Formation of stripe patterns under reaction conditions** — •Florian Lovis[1], Ronald Imbihl[1], Benjamin Borkenhagen[2], and Gerhard Lilienkamp[2] — [1]Institut f. Physikalische Chemie u. Elektrochemie, Leibniz-Universität Hannover, Callinstr. 3-3A, 30167 Hannover — [2]Institut f. Energieforschung u. Physikalische Technologien, Technische Universität Clausthal, Leibniz-Str. 4, 38678 Clausthal-Zellerfeld

Ultrathin films (< 1 ML) of vanadium oxide ($VO_x$) have been deposited on Rh(111). When subjected to the $H_2 + O_2$ reaction at 500°C in the $10^{-4}$ mbar range, stripe patterns on a micrometer scale form on the surface, consisting of $VO_x$-covered metal with bare Rh(111) in between. These are investigated under reaction conditions employing PEEM (PhotoEmission Electron Microscopy) and LEEM (Low Energy Electron Microscopy) as spatially resolving methods. The characteristic lenght depends on p and T, while the direction of the stripes on the isotropic Rh(111) surface is controlled by the step direction: While the stripes are initially formed perpendicular to the step direction, certain reaction conditions may also enforce a stripe direction parallel to the step edges. Since the stripe patterns have an intrinsic wavelenght and only form under reaction conditions, they are considered as a Turing-like non-equilibrium structure.

O 57.9 Wed 17:00 H40

**Mechanically induced grain boundary motion in Al-bicrystalls** — •Tatiana Gorkaya, Dmitri A. Molodov, and Günter Gottstein — Institut für Metallkunde und Metallphysik der RWTH Aachen, Aachen, Deutschland,

The mechanically induced migration of planar grain boundaries in Al-bicrystals was experimentally measured. The novel tensile/compression module for scanning electron microscope was utilized for in-situ measurements of grain boundary motion at elevated temperatures. From the measured temperature dependence of boundary mobility the migration activation parameters for investigated boundaries were determined. Normal boundary motion was observed to be coupled to a shear of the crystal in the region traversed by the grain boundary during its motion. The measured ratios of the normal grain boundary motion to the lateral translation of grains were compared with geometrical models of stress induced boundary migration.

O 57.10 Wed 17:15 H40

**Stochastic field equation for pattern formation on ion-beam eroded surfaces** — •Karsten Dreimann and Stefan Linz — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Straße 9, 48149 Münster

A recently proposed continuum model [1] for the formation of surface patterns on semiconductor surfaces generated by low-energy ion-beam erosion under normal ion incidence is studied in numerical detail. After transformation, this model takes on the form of a stochastic damped isotropic Kuramoto-Sivashinsky equation. Primary focus of our investigation [2] is the theoretical analysis of the impact of stochastic fluctuations on the competition of flat, rough and hexagonal surface structures observed in the deterministic case. In particular for the dependence of the surface roughness on the fluctuation strength, we identify distinct regimes with different scaling behavior that reflect different surface patterns.

[1] S. Vogel, S.J. Linz, Europhys.Lett. **76**, 884-890 (2006)
[2] K. Dreimann, S.J. Linz, unpublished

## O 58: Surface chemical reactions II

Time: Wednesday 15:00–17:30 Location: H42

O 58.1 Wed 15:00 H42

**Photoinduced substrate-mediated $N_2O$ reduction on MgO/Ag(001) surfaces** — •Harald Kirsch[1], Philipp Giese[1], Christian Frischkorn[1,2], and Martin Wolf[1,2] — [1]Institut für Experimentalphysik, FU Berlin, Arnimallee 14, 14195 Berlin — [2]Fritz-Haber-Institut, Abt. Physikalische Chemie, Faradayweg 4-6, 14195 Berlin

We investigate the photochemistry of $N_2O$ on in-situ prepeared thin MgO films, grown on an Ag(001) crystal. Structure and growth of the MgO films were characterized by means of LEED and Auger spectroscopy. Our goal is to study if defects are responsible for the photoinduced decomposition of $N_2O$ and the subsequent creation of reactive $O^-$ sites. After irradiation with a KrF laser (248 nm), we observe an increasing $N_2$ signal together with a decrease of the $N_2O$ mass in postirradiation thermal desorption spectra. From the increase of the $N_2$ signal with photon dose we determine a crossection of $3 \times 10^{-18}$ cm$^2$. We propose a mechanism where UV photons create electron-hole pairs at defect sites, which are responsible for the reaction. After several cycles of UV induced $N_2O$ reduction without subsequent annealing, the observed $N_2$ formation is dramatically reduced, which we interpret as a passivation of the reactive sites via occupation with oxygen.

O 58.2 Wed 15:15 H42

**Single-molecule synthesis and characterization of metal ligand complexes by low-temperature STM** — •Ingmar Swart[1,2], Peter Liljeroth[2,3], Sami Paavilainen[4], Jascha Repp[1,3], and Gerhard Meyer[3] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Condensed Matter and Interfaces, Debye Institute for Nanomaterials Science, PO Box 80000, 3508 TA Utrecht, the Netherlands. — [3]IBM Research - Zurich, 8803 Rüschlikon, Switzerland — [4]Institute of Physics, Tampere University of Technology, 33720 Tampere, Finland

The use of ultrathin insulating films facilitates the study of the unperturbed electronic structure of molecules by STM. This opens up the possibility of using the STM as a single-molecule laboratory where the molecules are both synthesized and electronically characterized in-situ.

Here, we present the STM-based synthesis of metal-ligand complexes, starting from individual metal atoms (iron and nickel) and organic molecules (dicyanoanthracene, DCA) deposited on an ultrathin insulating film. Lateral manipulation is used to form linear M(DCA)2 complexes. We directly visualize the frontier molecular orbitals by STM orbital imaging and characterize their spatial symmetries. In addition, we show how their order can be controlled by changing the nature of the metal atom. This is the first example of a synthesis and electronic characterization of a metal-ligand coordination complex on an ultrathin insulating film.

O 58.3 Wed 15:30 H42

**Oxidation of CO over $RuO_2$(110): a Reflection-Absorption IR Spectroscopy study** — •Attila Farkas, Georg Christoph Mellau, and Herbert Over — Physikalisch-Chemisches Institut, Justus-Liebig-Universitaet Giessen, Germany

Kinetic Monte Carlo (kMC) simulations [1,2] of heterogeneously catalyzed reactions present a powerful potential for unraveling the reaction mechanism at molecular level. The spatial distribution of the reactants at the catalyst surface can be computed even for pressures which fall outside the scope of standard ultra-high vacuum (UHV) experimental methods.

Reflection-Absorption IR Spectroscopy (RAIRS) has been used to study the oxidation of CO over the model catalyst $RuO_2$(110), under experimental conditions entailing a variation by four orders of magnitude in the reactant pressure (from $10^{-7}$ to $10^{-3}$ mbar) [3]. A careful analysis of high pressure RAIRS spectra has led to a rather complete picture of the steady state at the catalyst surface under reaction conditions at 350 K. While an elementary kMC approach of the type of Ref. [1] has been found satisfactory in accounting for the experimental results, more elaborated first principles (ab initio) kMC tretments [3] have failed to do so. The sources of discrepancy between experiment and first principles theory will be critically discussed.

1. R.M. Ziff, E. Gulari, Y. Barshad, Phys. Rev. Lett., 56, 2553 (1986)
2. K. Reuter, M. Scheffler, Phys. Rev. B, 73, 045433, (2006)
3. A. Farkas, G.Ch. Mellau, H. Over, J. Phys. Chem. C,113, 14341-14355, (2009)

O 58.4 Wed 15:45 H42

**High pressure XPS on supported planar model and powder Au/$TiO_2$ catalysts in the presence of reactive gases** — •Joachim Bansmann[1], Yvonne Denkwitz[1], Stefan Kielbassa[1], Birgit Schumacher[1], R. Jürgen Behm[1], Peter Schnörch[2], Elaine Vass[2], Michael Hävecker[2], Axel Knop-Gericke[2], and Robert Schlögl[2] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm — [2]Dept. Inorganic Chemistry, Fritz-Haber-Institut, D-14195 Berlin

The interaction of pre-conditioned, planar Au/$TiO_2$(110) model and dispersed Au/$TiO_2$ catalysts with $O_2$, CO and CO/$O_2$ atmospheres at sub-millibar pressures was investigated by in-situ X-ray photoelectron spectroscopy at BESSY. Measurements in different reaction atmospheres showed that Au is present as metallic Au nanoparticles on both types of catalysts. There was no evidence for positively charged $Au^{\delta+}$ species, neither during nor after exposure to the respective atmospheres. The $TiO_2$(110) substrate, on the other hand, changed its chemical, electronic and electric properties during these treatments, which results in variable shift of the substrate-related binding energy of the valence band and the Ti(2p) core levels. Whereas a detailed analysis in the case of powder catalysts was largely limited by severe charging effects, we could follow the chemically-induced variations in the electronic states of the planar Au/$TiO_2$(110) model catalysts.

O 58.5 Wed 16:00 H42

**Electronic valence band structure of $V_2O_5$** — •Torsten Stemmler, Eric Meyer, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin

We present high-resolution ARPES measurements of $V_2O_5$ single crystals carried out with synchrotron radiation and He I resonance lamp. The obtained experimentally band structure in k parallel is compared with calculations, e.g.[1] and [2]. The aging behavior of different bands with time is studied. The degradation of the surface due to the high reactivity is discussed referring to the previous reported experimental work, e.g. [3] and [4].

[1] A.Chakrabarti et al., Phys. Rev. B59, 10583 (1999)
[2] V.Eyert et al., Phys. Rev. B57, 12727 (1998)
[3] S.Shin, Phys. Rev. B41, 4993 (1990)
[4] Q.Wu, Chem. Phys. Let. 430, 309 (2006)

O 58.6 Wed 16:15 H42

**Reactions of Methanol on pseudomorphic Cu/Ru(0001) and O/Cu/Ru(0001)** — •Pawel Gazdzicki and Peter Jakob — Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany

The adsorption and reactions of methanol on pseudomorphic Cu/Ru(0001) and oxygen precovered Cu/Ru(0001) surfaces have been studied in UHV by IRAS and TDS. In contrast to the clean Cu(111) surface (reversible adsorption), a variety of reaction intermediates have been observed on the laterally expanded Cu/Ru(0001) monolayer. The reaction scheme with perpendicularly oriented methoxy ($CH_3O$) as the most prominent species proceeds very similar to Ru(0001). Interestingly, the Cu monolayer enhances the stability range of methoxy (with respect to decay into CO + 3H) considerably, which is attributed to a lower hydrogen binding energy on Cu/Ru(0001) as compared to Ru(0001).

Inspired by the possibility to enhance the reactivity of Cu(111) by the coadsorption of oxygen, the methanol decomposition has been investigated for Cu/Ru(0001) with preadsorbed oxygen as well. In fact, a completely new reaction pathway could be identified, with the methoxy species being present at 200-350 K and getting oxidized to produce formate (HCOO), as identified by characteristic bands in IRAS in the temperature range 380-460 K. As the dominant desorption product $CO_2$ is detected, which is in contrast to the non-oxidized surfaces which predominantly produce CO and $H_2$.

O 58.7 Wed 16:30 H42

**Interaction of methanol with the O-terminated ZnO(000-1) surface** — •Lanying Jin, Hengshan Qiu, and Yuemin Wang — Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, 44801 Bochum, Germany

Zinc oxide has attracted much research interest due to its particular electronic, optical and catalytic properties [1]. In catalysis, Cu/ZnO is the standard heterogeneous catalyst for the industrial methanol synthesis and its stream reforming. Therefore, studies of the interaction of methanol with ZnO are of fundamental importance in understanding the relevant catalytic processes on the atomic scale. In this work, the adsorption of methanol on O-ZnO(000-1) was studied by high resolution electron energy loss spectroscopy (HREELS) and thermal desorption spectroscopy (TDS). The clean, adsorbate-free O-ZnO(000-1) surface is electrostatically unstable and exhibits a (1x3) reconstruction with the presence of abundance of oxygen vacancies. It was found that exposing ZnO(000-1) to methanol at room temperature leads to the dissociative adsorption forming methoxy species at oxygen vacancies. After heating to higher temperatures the adsorbed methoxy species undergo further decomposition at 590 and 660 K releasing $CH_2O$, $H_2$, CO, and $CO_2$. The formation of formate species, which has been observed in methanol oxidation over ZnO powder samples, could be clearly ruled out based on the present results on ZnO(000-1). [1] Ch. Wöll, Prog, Surf. Sci. 82(2007) 55.

O 58.8 Wed 16:45 H42

**First-principles assessment of UBI-QEP derived rate constants for chemical kinetics** — •Matteo Maestri[1,2] and Karsten Reuter[1,3] — [1]Fritz-Haber-Institut Berlin, Germany — [2]Politecnico di Milano, Italy — [3]TU München, Germany

An accurate description of the elementary steps involved in a catalytic process is the basis for a reliable microkinetic modeling of the surface chemistry. Though desirable, a first-principles calculation of the reaction parameters is presently unfeasible but for models involving a small number of reactions. For complex catalytic systems, semi-empirical approaches, such as the UBI-QEP method [1], are therefore often employed to estimate reaction barriers and coverage effects. While computationally less demanding, the accuracy of UBI-QEP is uncertain and one has to question whether the corresponding energetics are mere artifacts of the employed effective modeling. At this scope and using the water-gas shift reacting system on Rh(111) as a showcase, we perform a density-functional theory based assessment of the UBI-QEP derived rate constants for specific classes of reactions (namely, dissociation/recombination and disproportionation). This comprises in particular the explicit coverage dependence of the reaction barriers predicted within the UBI-QEP framework. In doing so we aim at an increased awareness of the limitations of UBI-QEP methodology and the demonstration of possible strategies to overcome them. [1] E. Shustorovich and H. Sellers, Surface Science Reports, 31 (1998) 5.

O 58.9 Wed 17:00 H42

**Theoretical investigation of the mass-scaling of chemicurrents** — •Matthias Timmer and Peter Kratzer — Faculty of Physics and Centre for Nanointegration (CeNIDE), University Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

In recent years electronically nonadiabatic effects in adsorption on metal surfaces have been investigated. The chemicurrents detected by adsorption on a Schottky diode are of particular interest to our work. Utilizing our approach to calculate these currents [1], we investigate the electronic excitation spectra generated by adsorbates as function of their mass. Specifically, we study H isotopes on K(110) and Al(111) surfaces. From the insight gained in these calculations, we predict that the decay of the detectable current with increasing adsorbate mass should be weaker than expected from simple chemicurrent models used previously. We compare our predictions to recent experiments on Mg/Mg(0001) adsorption, and to calculations of this system.

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

O 58.10 Wed 17:15 H42

**Structure-Sensitivity in Catalytic Reactions on Ir(210) Surfaces** — •Payam Kaghazchi[1], Wenhua Chen[2], and Timo Jacob[1] — [1]Universität Ulm, Albert-Einstein-Allee 47, D-89069 Ulm, Germany — [2]Rutgers University, NJ 08854, USA

The formation of facets on single-crystal surfaces provides a reproducible basis and model systems for studying catalytic reactions. In this context, recent experiments on the adsorption and decomposition of NO on O-covered planar and nano-faceted Ir(210) with variable facet sizes showed pronounced structure-sensitivity and an unexpectedly high reactivity for NO decomposition. Using density functional theory we studied the adsorption of NO, O, and (NO+O) on Ir(210), as well as on Ir(311) and Ir(110), the surfaces which are exposed after facet formation. In agreement with TPD and HREELS data, we find that NO adsorbs on atop sites of planar Ir(210) but on both bridge and atop sites of Ir(311) and (110) faces of faceted Ir(210) [1]. Coadsorption of O does not influence adsorption sites of NO but reduces the Ir–NO bond strength on Ir(210), Ir(110) and Ir(311). In contrast, coadsorption of NO (on O-covered Ir surfaces) indeed influences adsorption sites of O and reduces Ir-O bond strength on Ir(110) and Ir(311) significantly [2]. Our findings should be of importance for the development of Ir-based catalysts for NO decomposition under oxygen-rich conditions. [1] W. Chen, T. E. Madey, A. L. Stottlemyer, J. G. Chen, P. Kaghazchi, T. Jacob, *J. Phys. Chem. C*, **112**, 19113, (2008), [2] W. Chen a, A. L. Stottlemyer, J. G. Chen, P. Kaghazchi, T. Jacob, T. E. Madey, R. A. Bartynski, *Surf. Sci.*, **603**, 3136, (2009).

## O 59: Poster Session II (Nanostructures at surfaces: Dots, particles, clusters; Nanostructures at surfaces: arrays; Nanostructures at surfaces: Wires, tubes; Nanostructures at surfaces: Other; Plasmonics and nanooptics; Metal substrates: Epitaxy and growth; Metal substrates: Solid-liquid interfaces; Metal substrates: Adsoprtion of organic / bio molecules; Metal substrates: Adsoprtion of inorganic molecules; Metal substrates: Adsoprtion of O and/or H; Metal substrates: Clean surfaces; Density functional theory and beyond for real materials)

Time: Wednesday 17:45–20:30 Location: Poster B1

O 59.1 Wed 17:45 Poster B1

**Monte Carlo simulations of nucleation processes on prepatterned surfaces** — •Stefan Frieder Hopp and Andreas Heuer — Institut für Physikalische Chemie, Universität Münster, 48149 Münster, Germany

The properties of template-directed nucleation are studied on a microscopic level by applying the kinetic Monte Carlo method. In this context, the conditions for full nucleation control as well as the progression of cluster growth with increasing coverage are investigated. The shape and the height of the clusters are discussed for 1D and 2D patterns with reference to the experimental observations.

It is shown that the simulation results of a continuous Monte Carlo algorithm can be approximated quite well using a discrete Monte Carlo technique based on the lattice gas model. In the course of this approach the latter algorithm is modified by the introduction of barriers depending on the particular diffusion process on the surface. Furthermore, the underlying discrete pair potential is adjusted to the Lennard-Jones potential. The application of the discrete method leads to a dramatic reduction of simulation time and thus allows in particular a more detailed comparison with experimental data.

O 59.2 Wed 17:45 Poster B1

**Analysis of surface nucleation processes with a coarse-grained Monte Carlo (CGMC) method** — •Tanja Mues and Andreas Heuer — Institut für physikalische Chemie, WWU Münster, 48149 Münster, Germany

The properties of template-directed growth on surfaces are the topic of this work. The theoretical study of the nucleation process has been performed via a particle based method (Monte Carlo (MC)) and with the help of a concentration field (finite-difference scheme (FD)) in our working group. We introduce a new CGMC method, combining four sites of a square lattice to one coarse-grained cell. Thereby we connect the MC method with the FD method, which differ in time and length scale. In other CGMC methods [1] boundary effects, which are necessary in the simulation of nucleation processes, are neglected. Therefore, we use fine-grid simulations to compute the average jump rate between two neighbouring cells by numerical sampling (before the MC-simulation) regarding boundary effects of every cell. With this new method, we analyse the nucleation behaviour via the radial distribution function g(r) and the nucleation density.

[1] Markos A. Katsoulakis and Dionisios G. Vlachos. Coarse-grained stochastic processes and kinetic monte carlo simulators for the diffusion of interacting particles. The Journal of Chemical Physics, 119(18):9412-9427, 2003.

O 59.3 Wed 17:45 Poster B1

**The height of size selected Ag clusters on C$_{60}$ films** — •Natalie Miroslawski[1], Niklas Grönhagen[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. We observed extremely narrow cluster height distributions. 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. A remarkable change in height occurs between Ag$^+_{80}$ and Ag$^+_{88}$ clusters. An additional monolayer formed at the top cluster facet might be responsible. Ag$^+_{88}$ and Ag$^+_{95}$ have the same height, Ag$^+_{138\pm2}$ is larger and corresponds to the height of the closed shell icosahedral cluster Ag$^+_{147\pm2}$. It was possible to deposit different cluster masses onto one sample. Although the deposition spots were deposited in close proximity, we were able to separate them clearly. Experiments with scanning tunnelling spectroscopy (STS) at 5 K hint to notable differences between our measurements on C$_{60}$/Au(111) and previous measurements on C$_{60}$/HOPG.

O 59.4 Wed 17:45 Poster B1

**Deposition of silver nanoparticles on to thin films of ionic liquid on SiO2** — •E. Pachomow[1], O. Höfft[2], M. Marschewski[1], W. Maus-Friedrichs[1], and F. Endres[2] — [1]Intitut für Physik und Physikalischen Technologien, Technische Universität Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — [2]Institut für Mechanische Verfahrenstechnik, Technische Universität Clausthal, Arnold-Sommerfeld-Str. 6, 38678 Clausthal-Zellerfeld

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 vapor pressure ionic liquids can be used in UHV. In this work the influences of ionic liquid films on the growth of silver nanoparticles on SiO2 were investigated. Here, monolayers of 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide [EMIM]Tf2N on SiO2 were produced by vapor deposition. On these layers silver was evaporeted. The chemical composition and electronic strucrure of the silver-IL-SiO2 interface was characterized by metastable induced electron spectroscopy(MIES) and photoelectron spectroscopy(XPS, UPS(HeI)). The particles size distribution was determined with AFM. We compare these resultes with measurements on silver deposited on pure SiO2. We find that due to the ionic liquid films the particles size is increased. [1] F. Endres, S. Zein El Abedin, Phys. Chem. Chem. Phys., 8(2006)2101

O 59.5 Wed 17:45 Poster B1

**THECLA - Setup of a THErmal CLuster Apparatus** — •Sabrina Hennes, Stefanie Duffe, and Heinz Hövel — TU Dortmund, Experimentelle Physik I, Otto-Hahn-Str. 4, 44221 Dortmund, Germany

THECLA is a THErmal CLuster Apparatus which produces clusters by supersonic nozzle expansion [1,2]. It enables optical spectroscopy of clusters in a free jet and of the same clusters deposited on substrates or in a matrix material. A hot-cathode plasma ionisation [3] and a moveable Faraday cup for ion-current measurement are installed for an in-situ determination of the cluster mass. Using the cluster velocity of the supersonic expansion, the ion-displacement by an electric field perpendicular to the cluster beam can be used to determine the cluster mass. In addition time-of-flight measurements can be used to analyse the cluster velocity and mass [1]. In first experiments we studied the plasmon resonance of Ag clusters deposited on SiO$_2$ in vacuum and exposed to air. Using the same samples it is planned to perform XANES measurements of the L-absorption edge at the synchrotron radiation source DELTA to gain detailed information about the structure, the chemical environment and changes of the unoccupied density of states of those clusters [4,5].

[1] O. F. Hagena, Z. Phys. D 20, 425 (1991). [2] H. Hövel et al., Phys. Rev. B 48, 18178 (1993). [3] I. M. Goldby et al., Rev. Sci. Instrum. 68, 3327 (1997). [4] O. Sipr et al., J. Synchrotron Rad. 6, 770 (1999). [5] A. Bzowski et al., Phys. Rev. B 49, 13776 (1994).

O 59.6 Wed 17:45 Poster B1

**Photoconductivity of metal nanoparticle ensembles supported by localized surface plasmon polariton resonances (LSPPRs)** — •Elena Vashchenko[1], Tigran Vartanyan[2], Frank Träger[1], and Frank Hubenthal[1] — [1]Universität Kassel, 34132 Kassel, Germany — [2]SPbSU ITMO, 197101 Saint-Petersburg, Russia

Owing to their specific properties, various kinds of dispersive systems attract great interest of researchers. Intriguing examples of such systems are metal nanoparticle ensembles (MNEs), which exhibit superior optical properties. Recently, the electric properties of such MNEs have found increasing attention. MNEs represent interlinked systems, which can be used as light driven electric devices.

In this contribution we demonstrate a LSPPR driven photoconductivity in silver and sodium nanoparticle ensembles. For this purpose MNEs were prepared on dielectric substrates and afterwards characterized by extinction spectroscopy and atomic force microscopy. The extinction spectra of the MNEs showed pronounced LSPPRs at wavelengths below the threshold of the external photo effect in the corresponding bulk metal. Subsequently a voltage has been applied to the MNEs and the current has been measured. We found that the current through the illuminated MNEs is more than one order of magnitude higher compared to the current without illumination. The strongest increase is obtained for wavelengths that are in resonance with the LSPPR of the MNEs. A theoretical interpretation of the observed phenomena based on the reduction of the tunneling barrier for the photoexcited electrons is provided.

O 59.7 Wed 17:45 Poster B1

**Photochemical particle growth in ordered two-dimensional arrays** — •Axel Seidenstücker[1], Thomas Härtling[2], Alfred Plettl[1], Phillip Olk[2], Paul Ziemann[1], and Lukas Eng[2] — [1]Universität Ulm, Institut für Festkörperphysik, 89069 Ulm (Germany) — [2]TU Dresden, Institut für Angewandte Photophysik, 01062 Dresden (Germany)

A novel procedure is reported which allows the controlled manipulation of the size of metal nanoparticles. The technique is demonstrated here on two-dimensional particle arrays of gold nanoparticles (diameter 10 nm), fabricated by means of diblock copolymer micelle lithography (BCML), but can in principle be applied to any kind of ordered structures. The particles are used as nucleation centers in seed-mediated photochemical metal deposition, whereby the particle diameter increases. Repeatedly combining photochemical growth with annealing steps facilitates controlling the particle shape as well as their uniformity.

O 59.8 Wed 17:45 Poster B1

**Characterization of Fe$_2$O$_3$-Nanotubes prepared by ALD** — •Markus Sproll[1], Ulf Wiedwald[1], Christian Pfahler[1], Alfred Plettl[1], Paul Ziemann[1], and Julien Bachmann[2] — [1]Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm — [2]Institut für Angewandte Physik, Universität Hamburg, D-20355 Hamburg

Metallic nanoparticles from a micellar technique or colloidal polystyrene (PS) particles with diameters of 100 nm are used to generate nanomasks on Si and $SiO_2$. Dip-coating the latter ones onto a pre-treated substrate permits the deposition of monolayers over areas up to 20 mm$^2$. Anisotropic separation and subsequent isotropic etching in an oxygen plasma reduces the size of the PS-particles down to the desired diameter. In case of the metallic Nanoparticles, the diameter can be varied by photoseeding [1]. Using both types of particles as a mask for anisotropic reactive ion etching (RIE), arrays of nano-pores can be fabricated with variable depth and diameter [2].
An Atomic Layer Deposition (ALD) process with ferrocene is used to refill the pores. After removing the top layer on the substrate, the remaining magnetic nanotubes can be investigated. In a furnace or a hydrogen plasma the $Fe_2O_3$ tubes are reduced to $Fe_3O_4$ or even metallic Fe. SQUID measurements of all these states will be presented.

[1] A. Seidenstücker - poster at this conference,
[2] A. Plettl et al., Adv. Funct. Mater. **19**, 3279 (2009).

O 59.9 Wed 17:45 Poster B1

**Enhanced LED emission by ordered metallic nanoparticle arrays** — •Tino Göhler[1], David Gottwald[1], Stefan Grafström[1], Jürgen Moosburger[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden — [2]OSRAM Opto Semiconductors GmbH, D-93055 Regensburg

The external quantum efficiency of light-emitting diodes (LEDs) based on AlGaAs is limited by the total internal reflection because of the high refractive index (typically between 3 and 4) of the semiconductor. Metal nanoparticles (MNPs) can be used as dipole scatterers in order to enhance this LED emission. We investigated arrays of MNPs, produced by Fischer pattern nanolithography [1] on top of both high-index substrates and on the LED itself. Light that would otherwise remain trapped inside the substrate is coupled out by both grating coupling and resonant plasmonic scattering. Here, we present 2D and 3D calculations based on the multiple-multipole method [2] of the light output produced by an array of MNPs of different sizes and distances, and then compare these findings with our experimental results.

[1] U.Ch. Fischer and H.P. Zingsheim, J. Vac. Sci. Technol. 19 (1981) 881

[2] C. Haffner, Post-modern Electrodynamics: Using Intelligent MaXwell Solvers. Wiley, (1999)

O 59.10 Wed 17:45 Poster B1

**Exploring the CoPc@HOPG interface: STM and STS study** — •Lars Smykalla, Marius Toader, Pavel Shukrynau, and Michael Hietschold — Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany

Using an UHV VT-STM, we report results obtained on a submonolayer of cobalt(II)-phthalocyanine (CoPc) grown on Highly Oriented Pyrolytic Graphite (HOPG) by OMBD. The very low deposition rate has allowed the formation of large defect-free self-assembled organic domains, mainly governed by the molecule-molecule interaction, where sometimes different orientation of the molecules with respect to each other leads to the development of relatively new type of structure. Nevertheless, the reported coexistence of molecular multi-phases has to be discussed in terms of the epitaxial relation between the organic adlayer structure and substrate surface orientation. Tip-sample distance-dependent scanning tunneling spectroscopy studies have been addressed in order to understand the electronic properties at the organic-inorganic interface. The observed shift in the molecular levels induced by the current set point variation is discussed and compared with the energy level diagram obtained by single molecule DFT calculations.

O 59.11 Wed 17:45 Poster B1

**Exploration of critical parameters in production of nano structures with Focused Ion Beams** — •Stefan Balk[1], Lukas Patryarcha[1], Karl Bauer[1], Axel Rudzinski[2], Lars Bruchhaus[2], and Heinz Hövel[1] — [1]TU Dortmund, Experimentelle Physik I — [2]Raith GmbH, Dortmund

Surface defects on highly orientated polycrystalline graphite (HOPG) were produced with Focused Ion Beams (FIB) in a pattern of squares with varying ion doses using the ionLiNE FIB-Tool (Raith GmbH). Thereafter the sample was oxidized at 500 °C for a duration of 200 minutes with 2% $O_2$. Only defect-rich areas oxidize completely and form nanocavities, which are nanopits deeper than 10 mono layers (ML). The gallium ions have a dose independent maximum penetration depth of about 50 nm at 25 keV. STM and AFM measurements show the existence of a critical ion dose at 20 $\mu As/cm^2$ where the transition from nanopit to nanocavity appears. Below 20 $\mu As/cm^2$ only a few ML deep nanopits are formed. Above 20 $\mu As/cm^2$ nanocavities with an increasing depth up to 50 nm were detected. The results have a good match with TRIM simulations of the produced defect density. The critical defect density is $6,25 \cdot 10^{-3}$ defects/$\AA^3$. We plan to use these results to realize isolated nano structures of HOPG by treatment of thin films of HOPG on insulator materials.

O 59.12 Wed 17:45 Poster B1

**Electrodeposition of free-standing regular arrays of metallic nanowires using template synthesizing technique** — •Nina Winkler, Yong Lei, and Gerhard Wilde — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

The fabrication of free-standing metallic nanowires with a template synthesizing method is investigated.

Magnetic nanowires may serve as high density perpendicular recording hard disks to avoid the superparamagnetic limit of nanometer-sized metallic structures.

Due to the high pore regularity of porous anodic alumina membranes, they serve as templates for the electrochemical growth of metallic nanowires. The alumina membranes were fabricated by a two-step anodization process of aluminum foils in oxalic and sulfuric acids. The insulating alumina barrier layer should be removed for electrodeposition of metallic nanowires. A method for perforating this barrier layer is presented in this work. A voltage pulse profile is applied for the electrodeposition processes with a potentiostat to achieve regular nanowires. The total time for the deposition is depending on the desired length of the nanowires.

After the deposition of the metals, the alumina membranes are removed by acidic etching to realize free-standing metallic nanowires. Their magnetic properties are investigated.

O 59.13 Wed 17:45 Poster B1

**One-dimensional ZnO nanostructures and their property investigation** — •Peter Hess, Yong Lei, and Gerhard Wilde — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster

One-dimensional (1-D) ZnO nanostructures were systematically investigated concerning their micro-structures and properties. The main focus of this work is on the assembly of thin and well-aligned nanowires to investigate their optical properties. The ZnO 1-D structures were prepared using a Chemical Vapour Deposition (CVD) system with ZnO/C mixtures as sources, Au-coated silicon or sapphire as substrates, and an argon and oxygen gas flow as a distributor and oxidation source. Depending on the conditions during the CVD process, different kinds of ZnO nanostructures were obtained. The morphology of the ZnO nanostructures was checked by SEM while the optical properties (photoluminescence) were investigated using a spectrometer. Additionally, the crystalline structures, the growth direction, and the lattice spacing of ZnO nanostructures were characterized using TEM. First experiments were also conducted using porous alumina membranes as templates to obtain very thin and well-aligned ZnO nanowires.

O 59.14 Wed 17:45 Poster B1

**Growth and photoluminescence of carbon-nanotubes laying on silicon substrates** — •Peter Löptien[1,2], Shigeru Moritsubo[1], Tomoaki Murai[1], and Yuichiro K. Kato[1] — [1]Institute of Engineering Innovation, University of Tokyo, Tokyo 113-8656, Japan — [2]Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, 20355 Hamburg, Germany

Carbon nanotubes are self-assembled one-dimensional systems with exceptional electronic properties. Depending on their structure they are either metallic or semiconducting. In this project, semiconducting carbon nanotubes were investigated with photoluminescence spectroscopy. Starting with a bare silicon wafer, islands were defined by e-beam-lithography. Cobalt acetate with silica nanoparticles were deposited as islands acting as catalysts in the chemical vapor deposition growth process. The obtained nanotubes on and in between the islands were revealed by scanning electron microscope images and Raman spectroscopy. According to our photoluminescence data and previous results, there is a signal from air-suspended carbon nanotubes, but no signal from carbon nanotubes laying on the wafer in between the islands. The samples were treated with surfactants in an attempt to obtain micelle-encapsulated nanotubes showing photoluminescence even when they are in contact with the surface.

O 59.15 Wed 17:45 Poster B1

**Structural and electronic properties of Au induced nanowires on Ge(001)** — •Tijs Mocking, Daan Kockmann, Arie van Houselt, Bene Poelsema, and Harold Zandvliet — MESA+ instute for Nanotechnology and University of Twente, Enschede, The Netherlands

The structural and electronic properties of Au induced self-organized nanowires on Ge(001), prepared by different procedures, are investigated with scanning tunnelling microscopy and spectroscopy at room temperature and 77 K [1]. The Au induced nanowires are comprised of dimers that have their bond aligned in a direction perpendicular to the nanowire. The dimers are buckled, leading to a 2x periodicity along the nanowires. Dimers located at anti-phase boundaries are dynamic and flip back and forth between two buckled configurations. The troughs between the nanowires have a depth of several atomic layers. Finally, the differential conductivities of the nanowires and the troughs are very comparable in magnitude.

[1]. D. Kockmann, A. van Houselt, T.F. Mocking, B. Poelsema and H.J.W. Zandvliet, Journal of Physical Chemistry C 113, 17156 (2009).

O 59.16 Wed 17:45 Poster B1

**Investigation of the geometric structure of one-dimensional Au nanowires on the Ge(001) surface with STM and LEED** — •Sebastian Mietke[1], Melanie Klinke[1], Tatjana Podlich[1], René Matzdorf[1], Christian Blumenstein[2], Jörg Schäfer[2], Sebastian Meyer[2], and Ralph Claessen[2] — [1]Fachbereich Naturwissenschaften, Experimentalphysik II, Universität Kassel, 34132 Kassel, Germany — [2]Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany

The deposition of Au on a clean Ge(001) surface yields one-dimensional (1D) structures, so-called nanowires. Using the techniques of low-temperature scanning tunneling microscopy (LT-STM) and low-energy electron diffraction (LEED), it could be demonstrated that the resulting surface reconstruction exhibits excellent $c(8 \times 2)$ long-range order. Since the wires are confined to atomic dimension, this system renders an ideal playground for the study of 1D physics, such as the charge density wave (CDW) or a Luttinger liquid. Experimentally, we find in addition to the $c(8 \times 2)$ structure that a fourfold superstructure along the wire direction exists over a wide temperature range. As the origin of the superstructure, the appearance of a CDW could be excluded by using scanning tunneling spectroscopy. By studying occupied and unoccupied states with the STM it could be shown that the nanowires consist of Au chains of single atom dimension.

O 59.17 Wed 17:45 Poster B1

**Micromanipulation of individual InAs nanowires** — Kilian Flöhr[1], •Marcus Liebmann[1], Kamil Sladek[2], Hilde Hardtdegen[2], Thomas Schäpers[2], Detlev Grützmacher[2], and Markus Morgenstern[1] — [1]II. Institute of Physics, RWTH-Aachen University and JARA-FIT, 52074 Aachen, Germany — [2]Institute of Bio- und Nanosystems (IBN-1), Jülich Aachen Research Alliance (JARA), Forschungszentrum Jülich, 52425 Jülich, Germany

We investigated methods to manipulate InAs nanowires using micromanipulators, an optical microscope as well as atomic force microscopy with the goal to produce InAs tips for scanning tunneling microscopy. Within the optical microscope, the InAs wires with diameters of approximately 100 nm and length up to 12 $\mu$m can be identified as colored stripes (1000 magnification) due to the diffraction of light. The wires, which have been grown by metalorganic vapor phase epitaxy (MOVPE) on a GaAs wafer without catalyst, could be picked up individually using the sharp corner of a doubly cleaved wafer exploiting adhesion forces. Later, the wires are placed onto a desired position at the edge of another wafer. Contacting of the wires is accomplished using indium microsoldering [1], which leads to a two-point resistance down to 1.5 k$\Omega$. First STM measurements, however, did not reveal a tunneling current probably due to oxidation of the tip. Different etching procedures have been tested in order to remove the oxide of the wire.

[1] C. Ö. Girit and A. Zettl, Appl. Phys. Lett. 91, 193512 (2007).

O 59.18 Wed 17:45 Poster B1

**Nanoline templates for single atom wires on Si(001)** — •Sigrun A. Köster[1], James H. G. Owen[1], François Bianco[1], Daniel Mazur[1], Alvaro Rodriguez-Prieto[2], David R. Bowler[2], and Chrisoph Renner[1] — [1]Université de Genève, Section Physique/DPMC, Quai Ernest-Ansermet 24, 1211 Genève 4, CH — [2]London Centre for Nanotechnology (LCN), University College London, UCL 17-19 Gordon Street, WC1H 0AH, London, UK

Low dimensional structures are of wide scientific and technological interest. The physics of single atom metallic wires is already described in detail by theory, but a more systematic experimental verification is still desirable. The experimental problems are mainly caused by the difficulties of growing electronically isolated wires which is necessary to test the expected properties from existing theories. Here we introduce templates on a Si(001) surface which enable the growth of self-assembled single atom wires on top of them. The main template consists of a Si reconstruction called the Haiku structure[1] which develops underneath self-assembled Bi nanowires[2]. By hydrogenation the Si surface can be passivated and additionally the Bi dimers are stripped off while the underlying reconstruction of the Si surface remains intact. In addition the Bi nanowire by itself can be considered as a template[3].

[1] J.H.G.Owen, K.Miki, H.Koh, H.W.Yeom and D.R.Bowler, Phys. Rev. Lett. 88, 226104 (2002) [2] J. H. G. Owen, K. Miki, and D. R. Bowler, J. Mater. Sci. 41, 4568 (2006) [3] J. H. G. Owen and K. Miki, Nanotechnology 17, 430 (2006)

O 59.19 Wed 17:45 Poster B1

**Iron-Induced Reconstructions on the Ge(001) Surface: a Scanning Tunneling Microscopy Study** — •Michael Lochner[1,2], Christian Blumenstein[1], Jörg Schäfer[1], and Ralph Claessen[1] — [1]Physikalisches Institut, Universität Würzburg, 97074 Würzburg — [2]Fachbereich Naturwissenschaften, Universität Kassel, 23132 Kassel

Low-dimensional systems can be realized by self-organized arrays of adatoms on semiconductor surfaces. In the last years, significant advances have been made in the growth and spectroscopy of nanowire systems, especially on Ge(001). A fascinating and still open question is whether one can grow such structures with magnetic atoms, which might lead to spin-ordered chains.

Here we study the growth of Fe atoms on Ge(001) by scanning tunneling microscopy (STM). Deposition of Fe at $\sim 400^\circ$C substrate temperature leads to formation of two different Fe-induced reconstructions: A (2×1) reconstruction exhibiting chain-like character, and a c(4×2) reconstruction that shows a two-dimensional architecture. The structural features for both phases as seen in STM, as well as their occurence in the phase diagram will be discussed in detail.

O 59.20 Wed 17:45 Poster B1

**Conductive AFM on Supramolecular Assemblies** — •Carsten Hentschel[1], Daniel Ebeling[1], Lin Jiang[1,2], Harald Fuchs[1], and Lifeng Chi[1] — [1]Center for Nanotechnology (CeNTech) and Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [2]present address: School of Materials Science and Engineering, Nanyang Technological University, Singapore

Based on the continuous reduction of electronic device sizes there is an increasing interest in conductors of molecular dimensions. As a result of these molecular dimensions the atomic force microscope (AFM) has developed for a suitable standard tool for surface analysis in this range.

However, among the mechanical characterisation it is possible to measure electrical properties of samples by this technique. Therefore, a conductive cantilever tip is scanned over a sample surface while a bias voltage is applied between tip and sample. With an external current amplifier the local current between tip and surface is measurable [1-2].

Here we will present a method to perform conductivity measurements with nanoscopic resolution on supramolecular assemblies. Therefore, the topographical images and current maps are simultaneously recorded in order to study the electrically behaviour on a length of about several micrometers.

[1] H. Dai, E. W. Wong, C. M. Liebert, Science 272 (1996)

[2] P. J de Pablo et al., Phys. Rev. Lett. 88 (2002) 036804

O 59.21 Wed 17:45 Poster B1

**Pentacene on insulators and the growth of nanocrystals: an STM study with submolecular resolution** — •Alexander Kabakchiev[1], Klaus Kuhnke[1], Theresa Lutz[1], and Klaus Kern[1,2] — [1]Max Planck Institut für Festkörperforschung, Stuttgart, Germany — [2]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Pentacene has become the drosophila of single molecule imaging. Molecular orbital maps in conjunction with tunneling spectroscopy provide new insight in the local electronic structures of model adsorbates. We use the dewetting of Pentacene films on thin insulating layers to grow nanocrystals a few nm high and base dimensions of several 100 square nanometers. Scanning tunneling microscopic (STM) topography reveals steep crystal edges reaching down to the bare insulator. Submolecular spatial resolution allows to image molecular orbitals on top of the crystal and to determine the local molecular structure. We demonstrate that in contrast to thin film structures so far found on insulators, the crystallites forming on KCl layers below room temperature exhibit a bulk-like phase with the long molecular axis oriented parallel to the surface. Comparison of scanning tunneling spectroscopy for the crystal phase with isolated molecules on the insulator layer indicates a shift of the molecular orbitals to lower binding energies.

O 59.22 Wed 17:45 Poster B1

**Ion induced surface topography evolution of Cu** — •Maria Lenius[1], Reiner Kree[2], and Cynthia A. Volkert[1] — [1]Institut für Materialphysik, Georg-August-Universität Göttingen — [2]Institut für Theoretische Physik, Georg-August-Universität Göttingen

Ion beam sputtered surfaces develop complex patterns that depend on crystal and ion beam parameters. The patterns are controlled by the interplay of various mechanisms such as surface curvature dependent sputtering, channelling effects, anisotropic and temperature dependent diffusion as well as ion induced diffusion processes and are not fully understood.

This work systematically considers the influence of crystal orientation dependent surface energy as a driving force. The sputter erosion profiles of Cu grains with various crystal orientations have therefore been investigated as a function of dose and ion beam incidence using a focused ion beam microscope. The resulting patterns with amplitudes up to 150 nm and wavelengths of about 0.5 um were characterized using SEM, AFM, and EBSD. Those investigations provide indications that surface energy minimization has an impact on pattern formation.

O 59.23 Wed 17:45 Poster B1

**Focused electron beam induced processing in UHV: "nanowriting" with an electron-beam as a pen and precursor molecules as ink** — Florian Vollnhals, Marie-Madeleine Walz, Michael Schirmer, Thomas Lukasczyk, Hans-Peter Steinrück, and •Hubertus Marbach — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Friedrich-Alexander-University Erlangen-Nuremberg, Egerlandstr. 3, 91058 Erlangen

In this contribution we aim towards the generation of arbitrarily shaped naonostructures with well defined chemical composition by focused electron beam induced processing (FEBIP) of either adsorbed precursor molecules or the substrate itself. The electron beam irradiation of adsorbed precursor molecules results in the local decomposition and thus the deposition of non-volatile fragments (electron beam induced deposition, EBID). In our distinct "surface science approach" to EBID we could show that working in an ultra clean environment, i.e. in ultra high vacuum (UHV), is advantageous in terms of cleanliness and partially size of the generated deposits. Recently we could also explore the localized activation of an oxide surface by an focused electron beam, such that $Fe(CO)_5$ dosed after the exposure is decomposed at the irradiated area, resulting in clean iron deposits. Results and principles of the described techniques will be presented and discussed as an engineering tool to generate or modify nanosized objects. This work was supported by the Deutsche Forschungsgemeinschaft under grant MA 4246/1-1.

O 59.24 Wed 17:45 Poster B1

**Characterization of Plasmonic Nanoantennas for Enhanced High Harmonic Generation by 2P-TOF-PEEM** — •Soo Hoon Chew[1], Adrian Wirth[2], Frederik Süssmann[2], Nils Weber[3], Matthias Escher[3], Sergey Zherebtsov[2], Jürgen Schmidt[1], Michael Hofstetter[2], Matthias Kling[2], Mark Stockman[4], Ferenc Krausz[1,2], and Ulf Kleineberg[1] — [1]Department of Physics, University of Ludwig-Maximilians, Garching, Germany — [2]Max Planck Institute of Quantum Optics, Garching, Germany — [3]Focus GmbH, Hünstetten Kasselbach, Germany — [4]Georgia State University, Altanta, USA

Metallic bowtie nanostructures have recently been demonstrated to enhance high harmonic generation from noble gases attributing to resonant plasmon field enhancement in the vicinity of nanostructures driven by femtosecond laser pulse excitation. Two-photon photoelectron emission microscopy (2P-PEEM) is a powerful tool to image the near field enhancement and "hot spot" photoemission from plasmonic nanostructures. Besides imaging the spatial electron distribution, the photoelectrons kinetic energy distribution within the nanostructures can be mapped using a time-of-flight (TOF) detector coupled to the 2P-PEEM. We have characterized various plasmonic nanoantennas by means of 2P-TOF-PEEM using a ps diode laser. Our ultimate goal is to characterize the nanoplasmonic fields not only on a nm spatial scale but also on ∼100 as temporal scale. Therefore, the concept of as field microscope utilizing a TOF-PEEM in combination with fs optical-pump/as XUV-probe experiment will be discussed.

O 59.25 Wed 17:45 Poster B1

**Excitation of plasmonic gap waveguides by nano antennas** — •Jing Wen[1,2], Peter Banzer[1,2,3], Daniel Ploss[1,2], Arian Kriesch[1,2], and Ulf Peschel[1,2,3] — [1]Institute of Optics, Information and Photonics, University Erlangen-Nuremberg — [2]Max Planck Institute for the Science of Light — [3]Cluster of Excellence 'Engineering of Advanced Materials' at the University of Erlangen-Nuremberg

We experimentally demonstrate the excitation of plasmonic gap waveguides by nano antennas. The excitation is shown to be both spatially and spectrally dependent which can potentially be used for the selective excitation of plasmonic nanostructures. Due to its small size the antenna can be easily integrated into plasmonic circuits.

The simulated optimized coupling efficiency of exciting with antenna is 10.6% which is 129 times as large as the case without antenna. In experiments, the coupling of the far field to the plasmonic waveguide can only be successfully achieved when the optical beam is on the antenna and at resonant wavelength with the right polarization direction. The measured sum of the coupling efficiency and antenna absorption reaches up to 20% compared to the simulated optimum value of coupling efficiency of 10%. The offset between the simulated coupling efficiency and the experimentally determined lack of power is quite likely due to absorption in the antenna or a higher coupling efficiency than expected.

O 59.26 Wed 17:45 Poster B1

**Near field and far field excitation of plasmonic waveguide arrays** — •Arian Kriesch[1,2,3], Jing Wen[1,2], and Ulf Peschel[2,3,4] — [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) — [4]Cluster of Excellence Engineering of Advanced Materials (EAM)

Recently it was demonstrated that highly birefringent materials can show negative refraction and self-imaging with sub-wavelength resolution. An array of metallic stripes with sub-wavelength periodicity can serve as such kind of metamaterial. It provides a negative permittivity for electric fields pointing along the stripes and a positive polarisability perpendicular to the lines. It also forms a system of coupled plasmonic waveguides thus transferring the concept of optical discreteness to the nano-world. Here we report results on the pointwise excitation of nanoscale plasmonic waveguide arrays with nanoantennas. We fabricated respective structures, using nanostructuring techniques. We found much stronger coupling between the waveguides than it is achievable and reported for arrays made from dielectrics, thus allowing for a much faster energy transport. Using a scanning near field optical microscope (SNOM) and highly focused beams propagating, waves were excited in the arrays. The experimental examination of coupling between neighbouring waveguides promises new insights into the processes of discrete diffraction and negative refraction on previously unmatched small spatial scales. A further goal is to achieve the formation of discrete spatial solitons in such a nanoarray.

O 59.27 Wed 17:45 Poster B1

**Interactions in electrically and magnetically coupled stereometamaterials** — •Lutz Langguth[1], Ralf Vogelgesang[2], and Harald Giessen[1] — [1]4th Physics Institute, University of Stuttgart, Germany — [2]Max Planck Institut für Festkörperforschung, Stuttgart, Germany

We consider metallic metamaterials which consist of stacked split-ring resonators. Upon twisting of two vertically adjacent split rings, the resonance frequencies of the coupled system change [1]. In split-ring resonators, both electric as well as magnetic interactions are present. Besides dipole interactions, also higher-order modes such as quadrupoles or octupoles play a significant role. We take an analytical model for the electric and magnetic dipole interactions and analyze the spatial dependence of both interactions in the quasistatic limit as well as in the dynamic case. We investigate the distance and the angle dependence of the coupled split-ring modes and find an intriguing behavior, especially at points in space where one or both of the dipole interactions are extremal. Our work explains this behavior in a dipole approximation, points out how to evaluate the strength of higher-order modes and will lead to a better theoretical modelling of the optical properties of stereometamaterials. [1] N. Liu et al., Stereometamaterials, Nat. Phot. 3, 157 (2009)

O 59.28 Wed 17:45 Poster B1

**Nanoparticle-based Photothermal Control of the Catalytic Activity of the Enzyme HRP** — Jan Bretschneider[1], Maximilian Reismann[2], •Malte Linn[2], Gero von Plessen[2], and Ulrich Simon[1] — [1]Institute of Inorganic Chemistry, RWTH Aachen University, Germany — [2]I. Inst. of Physics (IA), RWTH Aachen University, Germany

The optical excitation of particle plasmons in a gold nanoparticle by laser irradiation induces a temperature rise in the nanoparticle and its immediate surroundings. This effect can be exploited to control temperature-sensitive chemical reactions in a contactless and highly localized manner. In this work, this photothermal effect is utilized to control the catalytic activity of an enzyme. For this purpose, the enzyme horseradish peroxidase (HRP) is bound to the surface of gold nanoparticles which are suspended in water. The HRP catalyses the oxidation of the diazonium compound ABTS to ABTS$^{+}$. A resonant excitation of the HRP-functionalized nanoparticles by cw-laser light with a wavelength of 532 nm leads to a heating of the nanoparticle environment.

We show that this photothermal heating reduces the rate of the catalytic conversion process. For this purpose, the reaction kinetics is spectroscopically monitored via a color change of the colorless reactant (ABTS) transformed into the greenish product (ABTS$^{+}$).

O 59.29 Wed 17:45 Poster B1

**Optical Properties of Plasmonic Planar Septamer Nanostructures** — •Mario Hentschel[1,2], Na Liu[1], and Harald Giessen[1] — [1]4. Physikalisches Institut, Universität Stuttgart — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart

Planar septamer nanostructures are supposed to show interesting coupling effects. Mirin et al. [1] predicted a plethora of symmetry-dependent spectral features. For instance, the symmetric mode takes in-phase oscillations of all particle plasmons into account, whereas the antisymmetric mode allows for phase shifts of pi.

We fabricated a variety of septamer structures by high-resolution electron beam lithography and varied coupling as well as symmetry parameters. Coupling distances as small as 12 nm have been achieved.

We are going to discuss the optical spectra as a function of structure sizes, geometry, and neighbor-neighbor distance and find interesting coupling effects. A simple dipole-dipole coupling picture between the electric dipole moment of particle plasmons can be utilized to visualize the energy levels as well as the oscillator strength of the optical spectra.

[1] Nikolay A. Mirin et al., J. Phys. Chem. A 113, 4028-4034 (2009)

O 59.30 Wed 17:45 Poster B1

**Calculation of the up-conversion efficiency of $\mathrm{Er}^{3+}$ ions near noble-metal nanoparticles** — Florian Hallermann[1], Jan Christoph Goldschmidt[2], Stefan Fischer[2], Philipp Löper[2], •Christian Maasem[1], and Gero von Plessen[1] — [1]Institute of Physics (1A), RWTH Aachen University, 52056 Aachen, Germany — [2]Fraunhofer Institute for Solar Energy Systems, Heidenhofstr. 2, 79110 Freiburg, Germany

In conventional silicon solar cells, the near-infrared part of the solar spectrum could possibly be exploited by making use of up-conversion processes. For instance, electrons could be excited from the ground state to a final state via intermediate states through sequential absorption of infrared photons. The radiative relaxation of the electrons from the final state generates 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 efficiency of $\mathrm{Er}^{3+}$ ions can be enhanced using spherical gold nanoparticles. The changes of the excitation rate in the vicinity of nanoparticles are computed for $\mathrm{Er}^{3+}$ ions homogeneously distributed around a single gold nanoparticle using Mie theory and a rate equation system. In addition, the relaxation rates of all involved excited states of the ions are changed due to additional radiative and nonradiative decay channels provided by the metallic nanoparticle. Using experimentally accessible transition rates of $\mathrm{Er}^{3+}$ ions, we semi-analytically calculate the effects these changes have on the up-conversion efficiency.

O 59.31 Wed 17:45 Poster B1

**Near-field phase and flux controllability in the near-field** — •Giovanni Piredda, Caroline Gollub, Regina de Vivie-Riedle, and Achim Hartschuh — Physikalische Chemie, Department Chemie und Biochemie, Ludwig-Maximilians-Universität München

Ultrafast nanooptics is an emerging field that combines the concepts and tools of ultrafast spectroscopy with those of near-field optics [1]. A basic form of coherent control in the near-field is the ability to concentrate the linear optical flux at a desired location with sub-diffraction resolution. This task requires polarization pulse shaping of the incident electric field [2]. We show, using simple examples, that the presence of quick spatial variations of the phase ("near-field phase") is an essential ingredient for the controllability of linear flux in the near-field. The near-field phase, that does not depend on propagation, is almost always present when light interacts with a nanostructure [3]. We analyze a nanoparticle and incident field configuration in which near-field spatial variations of the phase are almost completely absent to highlight the fact that without them control of flux localization cannot succeed. In addition we present our first results of control of second-harmonic generation from rough gold films in a near-field optical setup.

[1] M.I. Stockman et al., Phys. Rev. Lett., **88**, 067402 (2002).
[2] T. Brixner et al., Phys. Rev. B, **73**, 125437 (2006).
[3] R. Carminati, Phys. Rev. E **55**, R4901 (1997).

O 59.32 Wed 17:45 Poster B1

**Acousto-Plasmonic Properties of Single Metal Nanoparticles** — •Kai Kratzer[1,2], Thorsten Schumacher[1,2], and Markus Lippitz[1,2] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart — [2]4. Physikalisches Institut, Universität Stuttgart

Acoustic vibrations of a single metal nanoparticle are detectable via the particle's plasmonic properties because mechanical oscillations cause a periodical variation of the electron density and thus a periodically changing plasmon resonance. Ultrafast pump-probe spectroscopy allows us to measure these small variations and to characterize a single nanoparticle by analyzing the acoustic breathing mode on a picosecond timescale.

Metal nanoparticles show a diverse behavior as they vary in shape, size and coupling to the substrate. To overcome this inhomogeneity it is necessary to measure single particles. We demonstrate these variations by a series of experiments on the single particle level and show the influence of deviations from spherical shape and the coupling to the substrate.

O 59.33 Wed 17:45 Poster B1

**Temperature dependence of antenna-like plasmon resonances of gold nanowires in the Infrared** — •Jörg Bochterle[1], Frank Neubrech[1], Hoang Vu Chung[1], Dominik Enders[2], Tadaaki Nagao[2], and Annemarie Pucci[1] — [1]Kirchhoff-Institute for Physics, Heidelberg University, Germany — [2]National Institute for Material Science, Tsukuba, Japan

Quantitative knowledge about conductivity parameters in metal nanostructures is of high practical interest in nanotechnology. Since contacts for direct current measurements mostly are problematic, contact-free spectroscopic measurements would be preferable. In fact, plasmonic resonance spectra are determined by the conductivity parameters. Unfortunately, except few special cases, the relation between metal conductivity and plasmonic particle resonance is complicated and it is important to get systematic experimental data.

We therefore study infrared plasmonic excitation of lithographic gold nanowires at various temperatures between 30 K and 600 K. The experiments were performed under UHV conditions to realize LHe cooling down to 30 K without formation of thick adsorbate layers. Electron impact heating was used to control the amount of energy transferred to the sample holder, thus being able to approach various temperatures in the desired range. With decreasing temperature a decreasing number of phonons in the gold nanowires is expected and therefore a lower relaxation rate of conducting electrons and accordingly a change in the plasmonic resonance curve.

O 59.34 Wed 17:45 Poster B1

**Third harmonic generation from gold nanostructures using a femtosecond laser scanning microscope** — •Siegfried

Weisenburger[1,2], Tobias Utikal[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

There are different competing mechanisms of third harmonic generation from gold nanostructures on a dielectric substrate: First of all third harmonic light generated at the dielectric-air interface is Rayleigh scattered at the metal structure. Furthermore the strong field enhancement in the vicinity of the plasmonic nanostructure increases the dielectric bulk third harmonic generation. Last but not least there is third harmonic generation from the particle itself due to a nonlinear potential of the metal's conduction electrons caused by the finite size of the structure. We look into the question, which of these mechanisms dominates in which size regime the third harmonic generation from the nanostructures.

We use a titanium-sapphire laser system producing 8 fs pulses that are strongly focussed onto the samples by a reflective Cassegrain objective. The third harmonic signal at 4.6 eV is collimated by an immersion glycerin quartz objective and detected by an UV photomultiplier. The focussing properties of the Cassegrain objective and the influence of the Cassegrain on the ultrashort laser pulses are investigated experimentally and by numerical simulations. We will show the principle of a femtosecond laser scanning microscope setup as well as first experimental results on the third harmonic generation from gold nanostructures.

O 59.35 Wed 17:45 Poster B1

**Second-harmonic generation at thin gold films: Comparison of experiment and theory** — •Philipp Reichenbach, Andreas Hille, Stefan Grafström, and Lukas M. Eng — Technische Universität Dresden, Institut für Angewandte Photophysik, George-Bähr-Str. 1, 01062 Dresden

The existence of optical second-harmonic generation (SHG) at metallic surfaces has been well known for a many years in experiment [1] as well as in theory, where several electron gas models exist [2-4]. Further investigations have dealt with SHG at thin metallic films [5, 6], for which these models have been compared with experimental measurements. In our work the SHG signal from thin gold films of various thicknesses was measured. The experimental results are compared with a simple and fundamental classical model: an extended Lorentz model taking second-order corrections into account. The model was implemented into a discontinuous Galerkin algorithm [7], which provides higher spatial resolution in time domain than other common methods such as FDTD and FVTD.

[1] F. Brown et al., Phys. Rev. Lett. 14, 1029 (1965)
[2] S. S. Jha, Phys. Rev. 140, A2020 (1965)
[4] J. E. Sipe et al., Phys. Rev. B 21, 4389 (1980)
[5] J. C. Quail and H. J. Simon, Phys. Rev. B 31, 4900 (1985)
[6] C. S. Chang and J. T. Lue, Surf. Sci. 393, 231 (1997)
[7] J. S. Hesthaven and T. Warburton,
*Nodal Discontinuous Galerkin Methods*, Springer (2008)

O 59.36 Wed 17:45 Poster B1

**Controlling the Third-Harmonic Generation in a Metallic Photonic Crystal Coupled to a Waveguide** — •Reinold Podzimski[1], Matthias Reichelt[1], Torsten Meier[1], Tobias Utikal[2], and Harald Giessen[2] — [1]Department Physik und CeOPP, Universität Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany — [2]Physikalisches Institut, Universität Stuttgart, D-70550 Stuttgart, Germany

The behavior of waveguide plasmon polaritons is studied employing ultrafast coherent control like schemes for a gold lattice coupled to a photonic waveguide, see Ref. [1] for the structure. Different models to describe the third-harmonic generation are presented and the resulting equations are solved numerically. [2] The calculations are compared to recent experimental data and show good agreement for the most prominent features in the time-integrated third order intensity. [3]

[1] T. Utikal *et al.*, Phys. Rev. B. **76** , 245107 (2007).
[2] T. Meier, P. Thomas, and S.W. Koch, *Coherent Semiconductor Optics*, Springer (2007).
[3] R. Podzimski, *Modellrechnungen zur Erzeugung und Kontrolle der dritten Harmonischen*, Bachelor Thesis, University of Paderborn (2009).

O 59.37 Wed 17:45 Poster B1

**Coupled surface plasmon polariton - exciton modes for absorbing and pumped excitons** — •Stephan Schwieger, David Leipold, and Erich Runge — Institut für Physik and Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, 98693 Ilmenau, Germany

The coupling of surface plasmon polaritons (SPPs) at metal gratings and excitons in optically excitable media can potentially be used to compensate the large SPP-losses found at metal gratings [1,2]. This coupling leads to very much increased propagation lengths and new device concepts such as SPASERS proposed by Bergman and Stockman [3]. The coupled modes are investigated theoretically for a model system that consists of a gold-nanowire array and a semiconductor quantum-well (QW) structure. Properties of the coupled modes as, e.g., their dispersion relations, their group velocities, and the coupling to propagating far-field modes are discussed. The cases of absorbing QW and optically pumped QW are compared.

[1] P. Vasa, R. Pomraenke, S. Schwieger, Yu. I. Mazur, Vas. Kunets, P. Srinivasan, E. Johnson, J. E. Kihm, D. S. Kim, E. Runge, G. Salamo, and C. Lienau, *Phys. Rev. Lett.* **101**, 116801 (2008).
[2] S. Schwieger, P. Vasa, and E. Runge, *Phys. Stat. Sol. (b)* **245**, 1071(2008).
[3] D. J. Bergman and M. I. Stockman, *Phys. Rev. Lett.* **90**, 027402 (2003).

O 59.38 Wed 17:45 Poster B1

**Surface plasmon polaritons in a gold double-grating structure** — •Steve Lenk, Stephan Schwieger, and Erich Runge — Institut für Physik und Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, 98693 Ilmenau, Germany

We investigated theoretically the near- and the far-field distribution of a gold double-grating structure with two overlapping lattice periods. Under illumination by a plane wave, surface plasmon polaritons (SPPs) can be excited at the resonance angle and the resonance frequency. For single-grating structures, the detection signal is a mixture of directly reflected and re-radiated light from the SPPs. The double-grating structure allows the detection of the SPPs at novel angles compared to the angles of the single-grating. Thus, detection angles may be found where the SPP character dominates the signal and information on the SPP (lifetime, intensity, ...) can be obtained in the far field. For our calculation, we solved Maxwells equations in time-domain (FDTD) and frequency-domain (FEM). We compared our results with recent experimental studies.

O 59.39 Wed 17:45 Poster B1

**Simulation of the behaviour of surface plasmon polaritons on $C_3$ symmetric nano-holes arranged as $C_4$ symmetric arrays** — •David Leipold, Stephan Schwieger, and Erich Runge — Institut für Physik und Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau

Surface plasmon polaritons (SPPs) can couple to propagating light, e.g., via a grating. We perform FDTD simulations to obtain insight into the coupling via arrays of nano-holes cut into a silver film. In particular, we investigate the influence of nano-holes with three-fold symmetry, which is incompatible with the four-fold symmetry of the whole array. These studies are motivated by earlier experiments[1] that revealed unexpected dependencies of the reflectivity on the direction and the polariziation of the incident light. Our simulations reproduce many aspects of these findings and give insight into the behaviour of the near fields and, in particular, their relation to the excitation of SPPs.

[1] B. Ashall, M. Berndt, and D. Zerulla, *App. Phys. Lett.* **91**, 203109 (2007)

O 59.40 Wed 17:45 Poster B1

**Goos-Hänchen-Effect for a SPP** — •Felix Huerkamp[1,2], Alexei Maradudin[2], and Tamara Leskova[2] — [1]Westfälische Wilhelms-Universität, Münster — [2]Univerity of California, Irvine

When a beam of finite cross section is incident from an optically more dense medium on its planar interface with an optically less dense medium,and the angle of incidence is greater than the critical angle for total internal reflection, the reflected beam undergoes a lateral displacement, as if it is being reflected from a plane in the optically less dense medium parallel to the physical interface. This lateral displacement of the reflected beam is the *Goos-Hänchen effect* .

We show that a surface plasmon polariton beam can also display a Goos-Hänchen effect. The system we consider consists of vacuum in the region $x_3 > 0$, a metal whose dielectric function is $\epsilon_1(\omega)$ in the regions $x_1 < 0$ , $x_3 < 0$,and $x_1 > L$ , $x_3 < 0$, and a metal whose dielectric function is $\epsilon_2(\omega)$ in the region $0 < x_1 < L$, $x_3 < 0$ ($|\epsilon_1(\omega)| < |\epsilon_2(\omega)|$). By means of an impedance boundary condition, and solution of the integral equations for the scattering amplitudes to which its use gives rise, by a purely numerical approach and by the *Wiener-Hopf method*, we determine the reflected surface plasmon polariton beam when a surface plasmon polariton beam is incident from the region $x_1 < 0$ on the interface $x_1 = 0$ at an angle that is greater than the critical angle for total internal reflection. The system where $L$ tends to infinity is also studied in this way. In both of these systems the reflected beam undergoes a lateral shift along the $x_2$ direction whose magnitude is a few times the wavelength of the incident beam.

O 59.41 Wed 17:45 Poster B1

**Influence of $C_{60}$-Adsorption on Surface Plasmon Polariton Properties** — •Pierre Kirschbaum, Niemma M. Buckanie, Michael Horn-von Hoegen, and Frank-J. Meyer zu Heringdorf — Universität Duisburg-Essen, Fakultät für Physik, Lotharstraße 1, 47057 Duisburg

Surface Plasmon Polaritons (SPP) are collective excitations of the free electron gas in metallic systems that propagate along nanoparticle surfaces. In our experiments, SPPs are optically excited at the edges of Ag-Islands. These SPPs can be imaged by nonlinear Photoemissions Electron Microscopy (PEEM), using ultra short femtosecond laser pulses for illumination. The observed periodic pattern in PEEM relates to a time integrated superposition of the exciting laser pulse and the excited SPP-wave (beating pattern). Defects and adsorbates manipulate the observed pattern.

Here, the influence of $C_{60}$-adsorption on the properties of surface plasmon polaritons is discussed. Under illumination with femtosecond laser pulses we observe a decrease of the photoemission yield with increasing coverage. Furthermore, the beating pattern wavelength changes because of a modified effective surface dielectric function. Our findings imply that the SPP-wavelength becomes shorter as a result. Finally, we observe a decrease of the intensity of the beating pattern maxima compared with the intensity of the first maximum with increasing $C_{60}$ coverage. Accordingly the damping becomes stronger, which means the propagation length decreases.

O 59.42 Wed 17:45 Poster B1

**Acoustic surface plasmons on Au(111) and Au(788)** — •U. Krieg[1], L. Vattuone[2], M. Smerieri[2], M. Rocca[2], H. Pfnür[1], and C. Tegenkamp[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover, Germany — [2]Dipartimento di Fisica and IMEM-CNR, Università di Genova, I-16146 Genova, Italy

The Acoustic Surface Plasmon (ASP), was predicted theoretically long ago but due to its relatively low cross section it eluded observation until it was firstly observed on Be(0001) and eventually also on Cu(111). We show here that the ASP exists also on Au(111) and on its vicinal surface Au(788). The experiment was performed using ELS-LEED which allows for a high momentum resolution and easy investigation of azimuthal anisotropy of Plasmon dispersion. Interestingly, we find for Au(111) two dispersion branches for ASP. One is nearly isotropic in k-space with slope of 3.8 eVÅ, whereas the other has roughly twice the slope and is visible only along the $\Gamma M$ direction. Although Au(788) exhibits a quasi one-dimensional partially occupied surface state, the plasmonic dispersion for ASP measured here is two-dimensional and even nearly isotropic. The periodic step structure, however, leads to strong Umklapp scattering so that the multiple branches seen here can actually all be derived from only one dispersing ASP. These results will be discussed taking into account the Rashba split surface bands as well as the role of the reconstruction on flat and regularly stepped Au surfaces. Theoretical ab initio calculations are needed to achieve a full understanding of this complex behaviour.

O 59.43 Wed 17:45 Poster B1

**Probing Exciton Propagation and Localization in Single-Walled Carbon Nanotubes** — •Carsten Georgi, Miriam Böhmler, and Achim Hartschuh — Department Chemie und Biochemie & CeNS, Ludwig-Maximilians-Universität München, Germany

Tip-enhanced near-field photoluminescence (PL) microscopy providing nanoscale spatial resolution has been mainly used to image localized emitters, such as single molecules [1,2]. Semiconducting single-walled carbon nanotubes are photoluminescent 1D-nanostructures with highly mobile excited states (excitons). We study exciton propagation by combining near-field PL measurements and numerical simulations describing exciton diffusion and the imaging process. Hereby, we can extract e.g. the exciton diffusion range [3]. In some cases, highly confined and exceptionally bright PL is observed and attributed to exciton localization. This localization results from strong exciton energy gradients exceeding 2 meV/nm, evidenced by energy-resolved PL imaging. Numerical simulations of exciton diffusion in the presence of energy variations support this interpretation predicting strongly enhanced PL at local energy minima. Our results indicate that the PL intensity along a single nanotube is determined by the complex interplay between exciton mobility, localization and quenching sites.

[1] A. Hartschuh, Angew. Chem. Int. Ed. 47, 8178 (2008)
[2] T. Taminiau et al., Nature Photon. 2, 234 (2008)
[3] C. Georgi et al., phys. stat. sol. (b) 246, 2683 (2009)

O 59.44 Wed 17:45 Poster B1

**FDTD Simulations of Near-field Mediated Semiconductor Molecular Optical Properties** — Dai Zhang, Marcus Sakrow, •Josip Mihaljevic, and Alfred J. Meixner — Institute of Physical and Theoretical Chemistry, University Tübingen, Auf der Morgenstelle 8, Tübingen

The optical properties of molecules can be dramatically altered when they are in a close proximity of an excited metal antenna. In order to get insight into how the antenna generated near-field influences the optical properties of low quantum yield molecules, we carried out FDTD simulations of a sharp laser-illuminated Au tip approaching to a semiconductor thin film. The time-averaged field distribution between the semiconductor thin film and the tip antenna is calculated regarding to different distances. Our calculation demonstrates that the coupling between the localized plamon at the tip apex and semiconductor polariton can be achieved building up a distance-dependent high field enhancement. Our experimental results show that such a high field strength enhances not only the excitation process by a factor of 104, but alters the radiative : non-radiative decay rate giving approx. 15 times stronger photoluminescence emission.

O 59.45 Wed 17:45 Poster B1

**One-dimensional analytical model for strong-field photoelectron emission from metal nanostructures** — •Sergey Yalunin, Reiner Bormann, Alexander Weismann, Max Gulde, and Claus Ropers — University of Göttingen, Courant Research Center Nano-Spectroscopy and X-Ray Imaging, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Ultrashort electron pulse generation from nanostructures has attracted significant interest, due to its potential for time-resolved electron experimentation. Alongside numerical models of the associated nonlinear emission processes, an analytical model can provide important insight in the physical principles.

Here, we present an analytical quantum mechanical model for nonlinear photoelectron emission that takes into account multiple emission channels. The model describes both multiphoton and optical field (i.e. tunneling) emission in the presence of arbitrary static and laser fields. Several limiting cases are correctly reproduced. In the multiphoton regime and without a static field, the model yields the usual power law for the emission current. In the absence of a laser field, the Fowler-Nordheim equation is obtained. For the optical tunnel regime, the results coincide with the adiabatic approximation.

O 59.46 Wed 17:45 Poster B1

**Modeling the Optical Response of Metallic Nanostructures in the Discontinuous Galerkin Time-Domain Method** — •Christopher Prohm[1], Michael König[1,2], Jens Niegemann[1,2], and Kurt Busch[1,2] — [1]Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie — [2]DFG Forschungszentrum Center for Functional Nanostructures (CFN), Karlsruher Institut für Technologie

The discontinuous Galerkin time-domain method (DGTD) combines the highly flexible spatial discretization of finite-element methods with the possibility to investigate nanophotonic systems in the time-domain. Here, we investigate the interaction of three-dimensional metallic nanostructures with an incoming light field. In particular, we discuss the linear modeling of the dielectric function of metals via a combination of Drude and Lorentz terms. Furthermore, we present some results on the nonlinear modeling of the metallic response by using a hydrodynamic model.

O 59.47 Wed 17:45 Poster B1

**Ultrafast optical response of metal surfaces** — •Mathias Wand,

Arno Schindlmayr, Yevgen Grynko, Torsten Meier, and Jens Förstner — Department Physik and CeOPP, Universität Paderborn, 33098 Paderborn, Germany

We present a numerical method for calculating the dynamics of surface electrons in metals. This will enable us to simulate the linear or nonlinear response of complex plasmonic nanostructures, e.g., metamaterials built from split-ring resonators. As shown by Rudnick and Stern [Phys. Rev. B 4, 12 (1971)], the motion of electrons perpendicular to the surface requires a quantum-mechanical treatment due to nonlocal effects. As we aim to incorporate the ultrafast material response into a Maxwell solver, it is highly desireable to have a time-domain description of the surface electron dynamics. This can be achieved by using the time-dependent density-functional theory (TDDFT), which is able to describe the time evolution of the charge density of a quantum-mechanical many-body system. The charge density along the normal direction of the metal surface is resolved on an Ångström scale and propagated in time on a secondary grid. The current density can be extracted from the TDDFT simulation and incorporated into Maxwell's equations as a nonlinear source current. To illustrate the capabilities of TDDFT we further present optical conductivities of selected simple and noble metals extracted from ab initio calculations of the linear response function.

O 59.48 Wed 17:45 Poster B1

**Time-Domain Simulations of Semiclassical Radiation Dynamics in Photonic Nanostructures** — •Paolo Longo, Jens Niegemann, and Kurt Busch — Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology

Versatile numerical techniques have become indispensable in the field of photonics. In particular, the Discontinuous Galerkin Time-Domain Method (DGTD) [1] combines key benefits from both classical finite element and finite-difference approaches such as adaptive meshing, a local coupling of neighboring elements and an explicit time-stepping scheme.

Within this framework, we go beyond the widely spread purely classical models of light-matter-interaction and investigate radiation dynamics in photonic systems by simultaneously evolving Maxwell's equations and quantum mechanical equations of motion in time. In a first step, matter is modeled as an ensemble of two-level systems which results in the well-known Maxwell-Bloch equations [2]. Such semiclassical models automatically incorporate back-action effects, e.g., the non-Markovian radiation dynamics of emitters in photonic band-gap media.

[1] Niegemann et al., Photonics and Nanostructures: Fundamentals and Applications 7, 2 (2009)

[2] L. Allen and J. H. Eberly: Optical Resonance and Two-Level Atoms, Dover Publications (1987)

O 59.49 Wed 17:45 Poster B1

**Cantilever based Scanning Near Field Optical Microscopy probes as platform for optical antenna sensors** — •Bernhard Schaaf[1], Marc Salomo[1], Jennifer Linden[1], Daniela Bayer[1], Jens Niegemann[2], Michael König[2], Christopher Prohm[2], Martin Aeschlimann[1], Kurt Busch[2], and Egbert Oesterschulze[1] — [1]Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany

Scanning Nearfield Optical Microscopy (SNOM) is a powerful tool to investigate the electron dynamics in metallic nanostructures. An AFM cantilever based SNOM probe is presented exploiting a hollow pyramidal tip as platform for the integration of an nano-antenna onto the very tip. As a prerequisite, various types of antennas were fabricated on planar substrates to investigate their spectral resonance behavior. In the next step antennas are placed onto the pyramidal tips using FIB milling as well as e-beam lithography as high precision fabrication tools. The probes aim at the investigation of the excitation of e.g. collective electron oscillations like localized surface plasmons (LSPs). For this purpose, metallic nanostructures are prepared on planar glass or silica substrates. Measurements on the farfield and nearfield performance of the probes and samples as well as coupling of both regimes are presented as function of the impinging field amplitude distribution and the polarization state. Simulations of the spatial as well as temporal field distribution were conducted to get insight in the probe performance and in future also into the coupling of probe and sample.

O 59.50 Wed 17:45 Poster B1

**Lateral manipulation of surface plasmons by hollow structures** — •Michael Lutz, Stephen Riedel, Paul Leiderer, and Johannes Boneberg — Universität Konstanz

A frequency doubled Nd:YAG pulse (10ns,532nm) is splitted into three beams of equal intensity. The beams are recombined on a thin goldfilm under specific angles which define the periodicity of the resulting interference pattern. We observe the formation of hollow structures with diameters between few microns and few hundred nanometers.

The structures originate from thermal expansion upon melting of the surface which occurs only in regions of high intensity. This generates a shift of the centre of mass off the surface. The motion of the centre of mass causes the liquid lamella to lift off. After resolidification a nanostructured surface with hollow bumps has formed.

We show how these structures can be used to manipulate surface plasmons laterally.

O 59.51 Wed 17:45 Poster B1

**Golden Nanocones for Near-Field Optical Applications** — •Christian Schäfer[1], Bastian Zeeb[1], Peter Nill[1], Alexander F. F. Weber-Bargioni[2], Stefano Cabrini[2], Monika Fleischer[1], and Dieter P. Kern[1] — [1]University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen — [2]Molecular Foundry, 1 Cyclotron Road, Berkeley, CA94720, USA

Manipulating light by means of the enhanced electromagnetic field of metallic nanoparticles has become an interesting and well developed method for microscopic imaging in several branches of study. Through external electromagnetic excitation particle plasmons can be generated, and the resulting field enhancement can be used for near-field imaging as well as for tip enhanced Raman-Spectroscopy. Here two different processes for the fabrication of sharp-tipped golden nanocones are presented. In the first process we use electron beam lithography to structure a layer of hydrogen silsesquioxane (HSQ) coated on a gold surface, which can be evaporated thermally on different kinds of substrates. The structured layer of HSQ is then used as mask in the following Argon-ion etch step which forms the golden nanocones. In this way fields of nanocones with tip radii of less than 10 nanometers can be produced in parallel. In the second method, which is particularly useful for non-planar surfaces, we use electron beam induced deposition to structure an etch mask. For that purpose the precursor tetra-ethyl-ortho silicate is brought next to the gold surface. Silicon oxide is deposited via decomposition by the focused electron beam and serves as etch mask in the following Argon-ion etch step.

O 59.52 Wed 17:45 Poster B1

**Signal-to-background ratio in scattering-type Scanning Near-Field Microscopy (s-SNOM)** — •Jón Mattis Hoffmann[1], Jon Schuller[2], Mark Brongersma[2], Stefanie Bensmann[3], and Thomas Taubner[1,3] — [1]I. Physikalisches Institut (IA), RWTH Aachen — [2]Stanford University — [3]Fraunhofer-Institut für Lasertechnik

The scattering-type Scanning Near-Field Optical Microscopy (s-SNOM) surpasses the diffraction-limit and provides the possibility of non-destructive microscopy and the analysis of material properties at the nanometer scale [1]. This allows, for example, the identification of different polymers [2] or the analysis of viruses [3]. Furthermore, the combination of s-SNOM with a broadband light source gives the possibility to record a full spectrum with a single measurement [4].

One limiting factor of the s-SNOM is the signal-to-background ratio. This is getting more crucial for the probing of weakly-absorbing samples and especially for the the use of broadband lasers, which offer less power. In our current research project, the possibility of increasing the sensitivity of s-SNOM by using resonant probing-tips will be worked out. Therefore, as a first step, commercially available tips will be characterized with respect to their scattering properties, in the far-field and the near-field.

[1] F. Keilmann et al., Phil. Trans. R. Soc. Lond. A, 787 (2004)

[2] T. Taubner et al., Appl. Phys. Lett. 85, (2004)

[3] M. Brehm et al., Nano Lett. 6, 1307-1310 (2006)

[4] S. Amarie et al., Opt. Express 17, 21794-21801 (2009)

O 59.53 Wed 17:45 Poster B1

**Shadow nanosphere lithography of nanospirals** — •Bettina Frank, Jun Zhao, and Harald Giessen — Universität Stuttgart, Deutschland

We fabricated a hexagonal densely packed monolayer of polystyrene nanospheres (Langmuir-Blodgett film) with 450$nm$ diameter. Coating a 1$cm^2$ glass substrate with such a monolayer resulted in a good evaporation mask for nanopinhole lithography [1] of high quality. We deposited planar gold nanospirals inbetween the nanosphere mask by polar and azimuthally stepper-motor controlled sample rotation during the evaporation process. Large-area samples of very high quality were obtained. Measuring reflectance spectra by FTIR-spectroscopy yields good agreement with FDTD simulations. We modified gap width and wire length of the spiral structure and studied the dependence of the optical spectra on these parameters. Such structures are useful for broadband optical nanoantennas that radiate preferentially into the third dimension.

[1] M. C. Gwinner, E. Koroknay, L. Fu, P. Patoka, W. Kandulski, M. Giersig, and H. Giessen, Small 5, 400 (2009).

O 59.54 Wed 17:45 Poster B1

**Pump-probe apertureless near-field microscopy - a Tool for time resolved Nanooptics** — •Marcus Rommel[1,2], Stephanie Essig[1,3], Ralf Vogelgesang[1], and Markus Lippitz[1,3] — [1]Planck Institute for Solid State Research, Stuttgart, Germany — [2]Department of Experimental Physics 5, University of Würzburg, Würzburg, Germany — [3]4th Physics Institute, University of Stuttgart, Stuttgart, Germany

We develop a pump-probe apertureless scanning near-field optical microscope (PPaSNOM) to analyze plasmonic structures. This setup allows us to detect the temporal and spatial dependence of localized surface plasmon resonances (LSPR) as well as propagating SPRs. One of the first applications of this instrument will be the investigation of acoustic vibrations in single plasmonic particles of different shape.

As LSPR's depend sensitively on the electron density, the changes in volume due to GHz acoustic oscillations can be tracked with time-resolving pump-probe experiments [1]. The optical near-field indirectly contains information on the structure's acoustic oscillation. This allow us to extract nanoscale Chladni figures, i.e., maps of the acoustic vibration amplitude on the particle surface.

[1]M. A. van Dijk, M. Lippitz, M. Orrit, Detection of acoustic oscillations of single gold nanospheres by timeresolved interferometry, Phys. Rev. Lett. 2005, 95, 267 406.

O 59.55 Wed 17:45 Poster B1

**LEEM/LEED investigation of $Fe_3O_4$ thin film growth on a Pt(111) substrate: morphology, growth and atomic termination** — •Alessandro Sala, Helder Marchetto, Thomas Schmidt, and Hans-Joachim Freund — Fritz Haber Institut der Max Planck Gesellschaft, Berlin, Germany

Iron oxide is widely used as a catalyst and as a support for catalytically active systems. Although the system has been intensively studied with various techniques, controversies arise in the literature regarding the surface termination and structural inhomogeneities. This clearly hinders the direct linking of surface electronic and structural properties to chemical properties. Our aim is therefore a comprehensive and consistent characterization of the $Fe_3O_4$ film growth on a Pt(111) substrate with well defined preparation conditions by using the unique SMART instrument. This Low Energy and Photo-Emission Electron Microscope (LEEM/PEEM) is specially designed to obtain chemical and structural information with high lateral resolution.

O 59.56 Wed 17:45 Poster B1

**Growth of nanostructures on fcc(110) metal surfaces at the atomic scale** — •Oleg V. Stepanyuk[1,2,3], Nikolay N. Negulyaev[2], Pavel A. Ignatiev[3], Wolfram Hergert[2], and Alexander M. Saletsky[1] — [1]Faculty of Physics, Moscow State University, 119899 Moscow, Russia — [2]Fachbereich Physik, Martin-Luther-Universität, D06099 Halle, Germany — [3]Max-Planck-Institut für Mikrostrukturphysik, D06120 Halle, Germany

We report on an unusual mechanism of atomic-scale structures growth on fcc(110) metal surfaces, which is promoted by interface intermixing of deposited and substrate atoms. We investigate a self-assembly of 1D and 2D nanostructures during thermal deposition of 3d atoms on Pd(110) [1] and Cu(110) [2] surfaces at different temperatures. Diffusion barriers of basic atomic events are calculated by means of density functional theory. Incorporation of deposited 3d atoms into the topmost substrate layer is found to be energetically and kinetically feasible in the examined interval of temperatures (120-350 K). Kinetic Monte Carlo model for atomic self-organization demonstrates that surface nanostructures consist mainly of expelled substrate atoms, while deposited 3d magnetic atoms are embedded into the topmost surface layer [1, 2]. Recently our theoretical predictions have been confirmed by experiments [3]. Magnetic properties of novel nanostructures are also discussed.

[1] Stepanyuk O.V., et al., Phys. Rev. B 78, 113406 (2008). [2] Stepanyuk O.V., et al., Phys. Rev. B 79, 155410 (2009). [3] Wei D.H., et al., Phys. Rev. Lett. 103, 225504 (2009).

O 59.57 Wed 17:45 Poster B1

**Adatoms with character: Co and Pt atoms on Pt (111)** — •Andreas Garhofer[1,2], Zuzana Bortlova[1], Michael Schmid[1], Peter Varga[1], and Josef Redinger[1,2] — [1]Institut f. Angewandte Physik, TU Wien — [2]Center for Computational Materials Science, TU Wien

Surface diffusion of Co adatoms on Pt(111) has been studied by first principles DFT methods, implemented in the program package VASP and STM. A diffusing Co adatom jumps over bridge sites between two surface Pt atoms from stable fcc to hcp sites and vice versa. The calculated barrier of 0.194 eV is in good agreement with recent experiments (0.200 eV) [1]. Adding a second Co adatom at the largest separation possible on a (5x5) surface unit cell reveals a repulsive interaction between the Co adatoms, presumably due to unfavorable relaxations imposed on the Pt substrate, while magnetic interactions could be ruled out. Only if the two Co atoms come close together a stable dimer is formed. Both theoretical findings agree well with our STM observations. Mimicking the onset of growth of Co layers, calculations for three Co adatoms confirm our STM experiments by predicting a triangular Co adatom configuration to be most stable. Surprisingly, the results for three (four) Pt adatoms on Pt(111) are different. In contrast to Co, Pt adatoms behave "strange" and prefer linear configurations instead of maximizing the number of nearest neighbor bonds.

[1] P. Buluschek, thesis No. 3944, Ecole Polytechnique federale de Lausanne (2007)

O 59.58 Wed 17:45 Poster B1

**Ultrathin Epitaxial Molecular $C_{60}$ Layers on Bi(111): Morphology, Strain State, and Order-Disorder Phase Transition** — •Hichem Hattab, Dennis Meyer, Giriraj Jnawali, and Michael Horn-von Hoegen — Faculty of Physics, University of Duisburg-Essen, Lotharstr.1, 47048 Duisburg, Germany

Using Spot Profile Analyzing Low Energy Electron Diffraction (SPA-LEED) we have studied the order-disorder structural phase transition [1] of $C_{60}$(111) films on a Bi(111) surface. Initially a smooth Bi(111) base film was prepared on Si(001) [2]. Sub-monolayer coverages of $C_{60}$ were adsorbed at 80 K and annealed to 450 K. These molecular adsorbate layers exhibit a moiré pattern with a periodicity of 5 nm which is determined by the lattice mismatch of the $C_{60}$ adlayer and the Bi(111) virtual substrate. The coverage of the $C_{60}$ film was subsequently increased by additional deposition of $C_{60}$ at 450 K. For each step LEED spot profiles were recorded at 80 K. Comparing these profiles, we conclude that the initial (1×1) phase changes into the disordered (2×2) phase as soon as the coverage is increased beyond a single layer of $C_{60}$. The formation of the second molecular $C_{60}$ layer is accompanied by a sudden relaxation of the lateral lattice parameter of the $C_{60}$ adlayer. We have additionally confirmed that $C_{60}$ films thicker than 1 BL show the temperature dependent surface orientational-disordering phase transition from (2×2) to (1×1) at 235 K in analogy to previous studies [1].

[1] A. Goldoni *et al.*, Phys. Rev. B **54**, 2890 (1996)
[2] G. Jnawali *et al.*, Phys. Rev. B **74**, 195340 (2006)

O 59.59 Wed 17:45 Poster B1

**Properties of ultrathin In layers on the Ni(001) face** — •Aleksander Krupski, Maciej Góral, and Wojciech Pawłowski — Institute of Experimental Physics, University of Wroclaw, pl. Maksa Borna 9, 50-204 Wroclaw, Poland

The atomic structure and morphology of ultrathin In layers on the Ni(001) face deposited in ultrahigh vacuum at the substrate temperature ranging from 145 K to 900 K were investigated with the use of Auger electron spectroscopy (AES) and low-energy electron diffraction (LEED).

O 59.60 Wed 17:45 Poster B1

**Properties of Ultrathin Pb Layers on the Ni(001) Face** — •Katarzyna Miśków, Maciej Góral, Wojciech Pawłowski, Tomasz Kraśnicki, Tomasz Kosmala, Zbigniew Jankowski, and Aleksander Krupski — Institute of Experimental Physics, University of Wroclaw, PL.Maksa Borna 9, Pl 50-204 Wroclaw, Poland

The atomic structure and morphology of ultrathin Pb layers deposited on the Ni(001) face in ultrahigh vacuum at the substrate temperature ranging from 145 K to 900 K were investigated with the use of Auger Electron Spectroscopy (AES) and Low-Energy Electron Diffraction (LEED). AES results indicate that the growth of lead layer on the Ni(001) face depends on substrate temperature. The analysis of AES measurements shows that the two-dimensional growth of the first Pb monolayer takes place for the substrate temperature from 145 K to 900 K. After the completion of the first lead monolayer, the three-dimensional growth of Pb is observed. Over the range the Stransky - Krastanov growth was observed. The Pb-Ni alloy formation was not observed. Above T > 600K, desorption of lead atoms is observed. The ordered LEED patterns corresponding to p(1x1) and c(2x2) structures have been observed.

O 59.61 Wed 17:45 Poster B1

**General aspects of surface alloy formation** — •Andreas Bergbreiter[1], András Berkó[2], Albert K. Engstfeld[1], Ralf T. Rötter[1], Harry E. Hoster[1], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — [2]Permanent address: Institute of Nanochemistry and Catalysis, of CRC-HAS, University of Szeged, H-6720 Szeged, Hungary

Surface confined alloys are excellent model systems for studies of structure-property relationships of bimetallic surfaces. They are formed by deposition of a guest metal B onto a substrate A, followed by annealing to a temperature, where place exchange between adatoms and atoms from the underlying surface layer becomes possible and diffusion into the bulk is sufficiently slow. We exemplarily confirmed by scanning tunneling microscopy and Auger electron spectroscopy for PtRu/Ru(0001) [2], PdRu/Ru(0001) [3,4], AuPt/Pt(111), AgPt/Pt(111), and AgPd/Pd(111), surface alloys are obtained for systems where metal B has a negative surface segregation energy within metal A [1]. By exchanging A and B, however, AB surface alloys are most likely overgrown by metal B, which we will demonstrate for RuPt/Pt(111) [5,6] in comparison to PtRu/Ru(0001) [2].

[1] A. Christensen et al., *Phys.Rev.B* 56(10), **1997**, 5822.
[2] H.E. Hoster et al., *Phys.Chem.Chem.Phys.* 10, **2008**, 3812.
[3] H. Hartmann et al., *Surf.Sci.* 603, **2009**, 1439.
[4] N. Rougemaille et al., *Phys.Rev.Lett.* 99, **2007**, 106101.
[5] A. Bergbreiter et al., *Vacuum* 84(1), **2009**, 13.
[6] A. Berkó et al., *Surf.Sci.* 603, **2009**, 2556.

O 59.62 Wed 17:45 Poster B1

**Temperature-induced modifications of PdZn surface alloys on Pd(111) and first results for Ga on Pd(111)** — •Werner Stadlmayr, Christoph Rameshan, Simon Penner, Berhard Klötzer, and Norbert Memmel — Institut für Physikalische Chemie, Universität Innsbruck, Innrain 52a, 6020 Innbruck, Austria

Pd-Zn and Pd-Ga alloy films on Pd(111) are model systems aiming for a microscopic understanding of the mechanisms in Pd-Zn and Pd-Ga based catalysis for methanol steam reforming. The temperature-induced compositional and structural changes of these films are investigated in the catalytically relevant temperature range. We find that upon heating from 550 K to 630 K the alloy films change from a multilayer PdZn system to a "monolayer" situation due to diffusion of subsurface Zn into the Pd bulk. The change in subsurface stoichiometry triggers an inversion of the surface corrugation from Zn-out/Pd-in to Pd-out/Zn-in. This modification in surface geometric (and electronic) structure provides an explanation for the recently observed drastic changes in catalytic selectivity.

Furthermore, first results for Ga on Pd(111) are presented. Similar to Zn/Pd(111) we observe, that in the temperature window around 500 K an alloy with a 1:1 surface composition is formed. However in contrast to the Zn/Pd system no long-range order is observed in the alloyed state, while the short range order is preserved.

O 59.63 Wed 17:45 Poster B1

**Transport-measurements of electro-chemically fabricated metallic contacts under laser illumination** — •Bastian Kopp[1], Markus Schmotz[1], Daniel Benner[1], Christian Obermair[2], Fangqing Xie[2], Thomas Schimmel[2], Paul Leiderer[1], and Elke Scheer[1] — [1]Universität Konstanz — [2]Universität Karlsruhe

Aim of this work is to study the effects of laser illumination on metallic point contacts. So far lithographically fabricated Mechanically Controllable Breakjunctions (MCBs) [E. Scheer, Phys. Rev. Lett. **78**, 3535 (1997)] as well as Gate-Controlled Atomic Quantum Switches (GQS) [F.-Q. Xie, Phys. Rev. Lett. **93**, 128303 (2004)] were used to create atomic point-contacts. MCBs operate at ambient conditions whereas GQS use the electrochemical deposition and dissolution of metal atoms to create these contacts.

Previous work on illumination effects on MCBs showed dependences on the wavelength, the position, the size of the contacts [D. C. Guhr, Phys. Rev. Lett. **99**, 086801 (2007)] and the optical properties of the substrate material [unpublished]. The latter result points to the possible influence of thermal expansion besides the photo-assisted transport due to the excitation of high-energy quasiparticles [J.K. Viljas, Phys. Rev. **B 75**, 075406 (2007)] and the excitation of surface plasmons.

In order to minimize the influence of thermal expansion we now investigate the effect of light on GQS. We will present first results obtained under light irradiation on GQS and discuss possible mechanisms including photochemical reactions.

O 59.64 Wed 17:45 Poster B1

**Dealloying below the critical potential: Cu-Au and Cu-Pd** — Frank Uwe Renner, •Shilan Meimandi, and Aparna Pareek — MPI Eisenforschung, Düsseldorf

Corrosion causes a loss of more than 3% of GDP to society. Dealloying is an important corrosion process occurring at alloy surfaces immersed in electrolyte, and which are composed of elements with a large difference in Nernst potentials. The dealloying behaviour of the model system Cu3Au in 0.1M H2SO4 was previously investigated using in-situ X-ray diffraction [1] and we will present here recent ex-situ measurements using scanning Auger electron spectroscopy with a lateral resolution of less than 10 nm. We reported the formation of an ultra-thin epitaxial passive Au layer at lower overpotentials with a reversed stacking sequence, which transforms to thicker Au islands and finally to porous Au at higher overpotentials (critical potential for dealloying). For the in-situ X-ray diffraction studies we developed recently an UHV compatible electrochemical chamber in order to study more reactive samples and electrolytes which we recently adapted for use with ionic liquids as electrolytes [2]. The research on dealloying is now extended to the system of Cu-Pd alloys and we will present first results by in-situ XRD, scanning Auger electron spectroscopy and atomic force microscopy (AFM).

[1] Renner et al., Phys. Rev. B 77 (2008) 235433 [2] Borrisov et al., submitted to PCCP

O 59.65 Wed 17:45 Poster B1

**Atomic structures of absorbed Zn(ll) phthalocyanine on an iodide modified Cu(1 0 0) electrode** — •Thanhhai Phan[1], Hahn Uwe[2], Thomas Torres[2], and Klaus Wandelt[1] — [1]Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr.12, 53115 Bonn, Germany — [2]Departamento de Quimica Organica c-i-305, Universidad Autonoma de Madrid, Campus de Canoblanco, 28049 Madrid, Spain

Combined Voltammetric and in-situ STM studies were employed to gain information about the structures of partially water-soluble ZnPcPyMe molecules covered on an iodide template. The flat-lying molecules form a square-lattice on a $c(p \times 2)$–I superstructure modified Cu(1 0 0) within the double layer regime. The distance between molecules was estimated to be $(1.95 \pm 0.2)$ nm based on line-profile measurements. This molecular lattice is rotated by $(62 \pm 2)^\circ$ with respect to the [0 1 1] direction of the substrate, i.e. the commensurate direction of the iodide under layer. This clearly excludes a template effect of the substrate surface, but rather hints to a molecular self-assembly. Detailed molecular models are also proposed for two phases obtained in perfect agreement with the experimental observation.

O 59.66 Wed 17:45 Poster B1

**Competitive Adsorption of Viologen Species on a Chloride Modified Copper (100) Surface** — •Martino Saracino[1], Nguyen Thi Minh Hai[2], Peter Broekmann[2], and Klaus Wandelt[1] — [1]Institut of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, 53115 Bonn, Germany — [2]Interfacial Electrochemistry Group, Department of Chemistry and Biochemistry, University of Berne, Freiestr. 3, 3012 Berne, Switzerland

A number of technological relevant processes involve charge transfer reactions at electrified solid\liquid-interfaces. Their microscopic understanding requires the study of the electrode surface under in situ reactive conditions, for instance STM and cyclic voltammetry. The competitive adsorption of Diphenyl- (DPV) and Dibenzylviologen (DBV) on a $Cl^-$ modified Cu(100) surface was chosen as model system for similar N-containing aromatic molecules, which play a significant role as additives in metal plating. Upon adsorption $DPV^{2+}$ is reduced even at most anodic potentials to the monocationic radical $DPV^{+*}$ and forms a full monolayer of a hydrophobic $\pi$-stacked stripe phase which, however, does not prevent further redox reactions to take place. Lowering the electrode potential to the $DBV^{2+}$ reduction potential at -250mV [RHE] leads to the replacement of the $DPV^{+*}$ phase by a $\pi$-stacked stripe phase consisting of the produced monocationic $DBV^{+*}$. Conversely, returning to the $DPV^{+*}$ oxidation potential at -100mV [RHE] leads to a re-substitution of the $DBV^{+*}$- by the initial $DPV^{+*}$-stripe phase. In contrast to mono-viologen systems no stable dicationic phases have been observed at all.

O 59.67 Wed 17:45 Poster B1

**Deposition of thin films of Ionic Liquids - Access to the IL/Solid-interface** — •Michael Stark[1], Till Cremer[1], Claudia Kolbeck[1], Florian Maier[1], Peter Wasserscheid[2], and Hans-Peter Steinrück[1] — [1]Lehrstuhl für Physikalische Chemie II — [2]Lehrstuhl für Chemische Reaktionstechnik, University of Erlangen-Nuremberg, Egerlandstr. 3, 91058 Erlangen

Ionic Liquids (ILs), salts with melting points below 100° C, have attracted a great deal of interest in the last few years due to their promising physico-chemical properties. Important phenomena such as surface passivation, charge transfer and wetting behavior are determined by the IL/solid interface.

To access such interfaces by means of XPS, ultra thin IL films are prepared by physical vapor deposition (PVD) under ultra high vacuum conditions, as has been shown earlier.[1]

In this study, thin layers of selected ILs were deposited on well defined Au (111) single crystal surfaces in order to obtain a more detailed understanding of IL/substrate interactions. The main aspects thereby are the electronic interactions between the gold surface and the IL and the growth behavior of the films.

This work was supported by the DFG through SPP 1191 "Ionic Liquids" and by the "Cluster of Excellence 'Engineering of Advanced Materials'".

Literature: [1] T. Cremer, ChemPhysChem, 2008, 9, 2185-2190

O 59.68 Wed 17:45 Poster B1

**Structural transitions of heptyl viologen adlayers on Cu(1 0 0) – an electrochemical and in situ STM study** — •Min Jiang, Knud Gentz, and Klaus Wandelt — Institute for Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, 53115 Bonn

The redox behaviour and potential dependent adsorption structure of heptyl viologen (abbreviated as $DHV^{2+}$) on a Cu(1 0 0) electrode have been investigated in a chloride-containing electrolyte solution by in situ electrochemical scanning tunneling microscopy (EC-STM). After injecting $DHV^{2+}$ molecules into the KCl electrolyte solution, a highly ordered 2D dot-array structure in STM images emerges on a $c(2 \times 2)$ chloride modified Cu(1 0 0) electrode surface. $DHV^{2+}$ molecules spontaneously arrange themselves with their molecular planes facing to the electrode surface and their long molecular axis parallel to a step edge. Such adsorption structure can be described by mirror domains and rotational domains which stably exist between 200mV and −100mV. One-electron reduction of dication $DHV^{2+}$ around −150mV causes a phase transition from a dot-array assembly to a stripe pattern in STM images which has a bilayer structure. With a decrease of the applied electrode potential, the structure of $DHV^{\bullet+}$ adlayer undergoes a change from a loose stripe phase to a more compact stripe phase, and a subsequent decay of the compact structure, and then a formation of new dimer phase. A further electron transfer reaction at −400mV causes the appearance of an amorphous phase on the electrode surface.

O 59.69 Wed 17:45 Poster B1

**Chemical Charaterization of Porphyrin Adsorbed on Anion Modified Copper Electrodes: An SXPS Study** — •Stephan Breuer[1], Knud Gentz[1], Duc Thanh Pham[1], Thanh Hai Phan[1], Thomas Mayer[2], Peter Broekmann[3], and Klaus Wandelt[1] — [1]Universität Bonn, Institut für Physikalische und Theoretische Chemie, Wegelerstraße 12, D-53115 Bonn — [2]Technische Universität Darmstadt, FB Materialwissenschaft, Petersenstraße 23, D-64284 Darmstadt — [3]Universität Bern, Departement für Chemie und Biochemie, Freiestraße 23, CH-3012 Bern

Several Anions adsorb specifically from aqueous solution on copper electrodes. In case of copper single crystals, the electrode acts as a template for the anion adsorption and well ordered superstructures are observable. These, negatively charged, anion layers are used as secondary templates for the adsorption of cationic organic molecules.

The adsorption of TMPyP (Tetramethylpyridiniumporphyrin) has been extensively studied by in-situ EC-STM [1] which provides structural and electrochemical data, but there are less data about the chemical composition of the adsorbate layer. We have characterized (ex-situ) the chemical composition of the adsorbed TMPyP molecules on halide and sulfide modified Cu(100) and Cu(111) using XPS at the synchrotron radiation facility BESSY II.

[1] N.-T.M. Hai, B. Gasparovic, P. Broekmann, K. Wandelt, Surf. Sci. 601, 2007, 2597-2602.

O 59.70 Wed 17:45 Poster B1

**Electrospray Ion Beam Deposition of Molecules and Nanoparticles** — •Gordon Rinke[1], Nicha Thontasen[1], Zhitao Deng[1], Nikola Malinowski[1], Stephan Rauschenbach[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 vacuum deposition of complex molecules and nanoparticles is an important technological step towards applications, for instance in molecular devices or as surface functionalization. Vacuum based processing assures well defined and clean structures in contrast to deposition under ambient conditions or from solution. A possibility to deposit non-volatile particles is given by electrospray ion beam deposition (ES-IBD) [1]. In-situ sample preparation, beam preparation, and sample analysis by scanning tunneling microscopy (STM) allows full control over all deposition parameter [2]. Here, we present recent results of the deposition of molecules and nanoparticles by ES-IBD. We demonstrate the control of coverage, cleanliness, deposition energy, and beam composition and give examples for the in-situ characterization by STM.

[1] Small 2 (2006), 540-547

[2] ACS Nano 3 (2009), 2901

O 59.71 Wed 17:45 Poster B1

**Electronic properties of metal-organic coordination bonding** — •Christoph Limbach[1], Robert Drost[1], Nils Henningsen[1], Riccardo Rurali[2], Katharina J. Franke[1], and Nacho Pascual[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]Institut de Ciència de Materiales de Barcelona (ICMAB), Barcelona, Spain

Metal organic networks are a promising system for tuning the electronic and magnetic properties of single metal atoms. Using low temperature scanning tunneling microscopy and spectroscopy (STM/STS) we investigate the coadsorption of di-metacyano azobenzene (DMC) molecules and cobalt atoms on a Au(111) surface leading to metal-organic chains. dI/dV spectroscopy and conductance maps plotting the distribution of unoccupied resonances are used to localize and characterize the coordination bonds between Co adatoms and DMC. We find that Co-molecule coordination bonds are formed distinguishably at different intramolecular sites, i.e. at the lone-pair electrons at the cyano termination and the di-azo bridge (-N=N-). Density functional theory simulations find a different degree of charge transfer and hybridization of the atomic and molecular orbitals for the two different sites, thus sustaining the experimental observations.

O 59.72 Wed 17:45 Poster B1

**Ab initio investigation of surface adsorption phenomena: from pyridine gold complexes to larger system** — Doreen Mollenhauer, Johannes Floss, •Elena Voloshina, and Beate Paulus — Institut für Chemie und Biochemie - Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustraße 3, 14195 Berlin, Germany

The investigation of the adsorption of organic molecules on metal substrates plays an important role for the understanding of multivalent interactions. Due to the enhancement of the adsorption new architectures of multivalent molecules can appear on metal surfaces. Taking into account recent molecular electronic experiments involving molecules linked via N-heterocycles to gold electrodes and nanoclusters[1], pyridine derivates are seen to be interesting objects for theoretical studies. The interaction of the parent compound pyridine and some substituted derivates with a single gold atom has been investigated. Different quantum-chemical methods and basis sets have been used to find a reliable description. We plan to extend our studies to gold clusters, gold nanoparticles and para-linked pyridine derivates. The main purpose is to analyze the nature of multivalent bonding in comparison to monovalent interaction.

[1] M. J. Crossley and J. K. Prashar, Tetrahedron Lett. 38, 6751

(1997).

O 59.73 Wed 17:45 Poster B1

**What encodes the diversity and ordering of self-organized monolayers?** — •Carsten Rohr[1], Marta Balbás Gambra[2], Kathrin Gruber[1], Edwin C. Constable[3], Erwin Frey[2], Thomas Franosch[2], and Bianca A. Hermann[1] — [1]Walther-Meissner-Institute (WMI) of Low Temperature Research of the Bavarian Academy of Science and Center for Nano Science (CeNS), Germany Walther-Meissner-Strasse 8, 85748 Garching b. München — [2]Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for Nano Science (CeNS), Department of Physics, LMU München, Theresienstraße 37, 80333 München, — [3]Department of Chemistry, University of Basel, Spitalstrasse 51, 4056 Basel, Switzerland

The a priori prediction of patterns formed by molecular self-organization is of crucial importance for the deliberate application of monolayers in functionalizing surfaces. We used scanning tunneling microscopy (STM) to image self-organized monolayers of Fréchet dendrons, which display a large variety of 2D ordering motifs. The ordering of the different phases was simulated by molecular mechanics (MM) energy optimizations. We conceived a coarse-grained interaction-site model, which condenses the essential molecular properties determined by MM modeling. In a Monte Carlo (MC) approach based on this interaction site model placed on a lattice allowing discrete $\pi/3$ rotations the various ordering motifs were successfully predicted. With this model we could confirm that geometry as well as a few salient interaction sites encode the observed variety of structural motifs.

O 59.74 Wed 17:45 Poster B1

**Hydrocarbon contamination of different ruthenium surface orientations** — •Thanh-Nam Nguyen[1], Sina Gusenleitner[1], Marius Ernst[1], Holger Wetzstein[1], Dirk Ehm[2], and Friedrich Reinert[1] — [1]University of Würzburg, Experimental Physics VII, Am Hubland, 97074 Würzburg — [2]Carl Zeiss SMT AG, Rudolf-Eber-Str. 2, 73447 Oberkochen

Multilayer mirrors for Extreme Ultraviolet (EUV) Lithography applications are threatened by various damaging processes. 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 limit these lifetime risks is to coat the mirror with a dedicated capping material, such as Si, Ti, Mo, Pd, Ru, or their oxides. To study the general interaction mechanisms of adsorbates with the capping materials, organic model molecules are used. In this work, the interaction of 3,4,9,10-perylene tetracarboxylic dianhydride (PTCDA) with single crystalline Ru(0001) and Ru(1-100) surfaces as well as evaporated thin Ru films is presented. PTCDA molecules are deposited on the Ru surfaces by organic molecular beam epitaxy. The structural and electronic properties of the resulting interfaces are investigated by various surface analytical techniques, including low energy electron diffraction (LEED), scanning tunnelling microscopy (STM), X-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS).

O 59.75 Wed 17:45 Poster B1

**A Nanocalorimeter for Adsorption Studies of Organic Molecules** — •H.-J. Drescher, F. Bebensee, O. Lytken, H.-P. Steinrück, and J. M. Gottfried — Lehrstuhl für Physikalische Chemie II, Egerlandstraße 3, 91058 Erlangen

Surface nanocalorimetry (SNC) is an UHV based technique for the measurement of adsorption enthalpies on well defined substrates. It is the only technique that provides access to adsorption enthalpies in cases of non-reversible adsorption, i.e., if decomposition occurs at lower temperature than desorption. Typical examples are large organic molecules on metal substrates. SNC relies on the direct measurement of very small temperature changes induced by the adsorption of molecules on single-crystal surfaces. Its outstanding sensitivity in the nanojoule and picomole regimes is achieved by pyroelectric detectors in combination with pulsed molecular beams and highly accurate flux, sticking probability and reflectivity measurements. The adsorption enthalpy is a direct measure for the strength of the adsorbate-substrate interaction and thus one of the most important parameters for the quantitative characterization of chemical bonds at surface and interfaces. We focus especially on metal/organic interfaces, which occur in organic electronic devices. The character of the interfacial bond determines crucial parameters for the device performance, such as the charge injection rate. A setup of an advanced adsorption calorimeter is presented, which is optimized for the studies of $\pi$-conjugated molecular semiconductors on metal single-crystal surfaces. It features several new technical developments, which lead to improved sensitivity and accuracy.

O 59.76 Wed 17:45 Poster B1

**Electron Spectroscopy of Organic Heterointerfaces: SnPc/PTCDA/Ag(111)** — •Michael Greif[1], Marc Häming[1], Michael Wiessner[1], Achim Schöll[1], and Friedrich Reinert[1,2] — [1]Universität Würzburg, Experimentelle Physik VII, D-97074 Würzburg — [2]FZK Karlsruhe, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe

Heterointerfaces between different organic molecules are an issue of great technologic relevance. However, structurally well-defined ultra-thin interfaces which are suited for the investigation with surface sensitive techniques are difficult to prepare. In order to exploit its potential as a model system in this respect we have investigated hetero-layers consisting of tin-phthalocyanine (SnPc) and perylene-tetracarboxylic acid dianhydride (PTCDA) deposited on clean Ag(111) surfaces with photoelectron spectroscopy (XPS and UPS), x-ray absorption and low energy electron diffraction (LEED). The spectroscopic signatures of the two compounds can be distinguished unambiguously in the core and valence spectra. For ultra-thin SnPc layers deposited on a single layer of PTCDA on Ag(111) structural information can be derived from angle resolved XPS and NEXAFS. The data indicates that a closed monomolecular layer of flat lying SnPc is established. This is corroborated by the UPS spectra which show a characteristic splitting of the SnPc HOMO signal due to dimer formation only for SnPc coverages beyond one layer. Moreover, LEED was applied in order to investigate the lateral ordering.

O 59.77 Wed 17:45 Poster B1

**Self-assembled metal-organic networks of tripyridyl-triazine on Au(111) and Cu(111) surfaces** — •Hendrik Mohrmann, Christian Lotze, Katharina J. Franke, and Jose I. Pascual — Institut für Experimentalphysik, Freie Universität Berlin

Self-assembled metal-organic networks have lately attracted a lot of interests since they possibly provide arrays of spins which have promising properties for applications in molecular electronics. We investigate the coadsorption of tripyridyl-triazine (t4pt) and Cobalt on noble metal surfaces by low and variable temperature scanning tunnelling microscopy and spectroscopy (STM/STS) in ultrahigh vacuum.

On Au(111), several highly ordered structures with a wide range of Co-N bond lengths and packing densities, depending on the Co/t4pt deposition rates and annealing temperatures, are observed. We also observe double layer islands in which Co atoms are coordinated in a 3-dimensional complex.

When deposited on Cu(111) t4pt forms a long-range ordered honey comb nanomesh. This structure is stabilized by coordination bonds of the lone-pair electrons of the pyridil groups to Cu adatoms as evidenced by conductance maps.

O 59.78 Wed 17:45 Poster B1

**Surface assisted oxidation of flat lying organic molecules - a real-time STM study** — •Thomas Waldmann[1], Daniela Künzel[2], Michael Roos[1], Achim Breitruck[1], Harry E. Hoster[1], Axel Gross[2], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — [2]Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

Using time resolved scanning tunneling microscopy (STM), we tested the interaction of $O_2$ from gas-phase with ordered adlayers of the Bis(terpyridine) derivative 2,4'-BTP [1,2] on Au(111) [3], Ag(111) [3,4] and graphite (HOPG) [1-3,5] surfaces at T = 300 K. At an $O_2$ pressure of $10^{-5}$ mbar, the adlayers on Ag(111) undergo chemical and structural changes. These include modifications of the 2-pyridyl rings of individual 2,4'-BTP adsorbates and rearrangements of the hydrogen bonded adlayer. Since we do not observe similar changes on HOPG and Au(111), we assume that Ag(111) acts as catalyst for the underlying processes. Based on our STM data in combination with DFT calculations, we conclude that the observed reaction is pyridyl-N-oxide formation. Furthermore, we derive reaction yields, enantiomeric excess, reaction rates and reaction orders from the time-resolved STM data.

[1] U. Ziener et al., *Chem.Eur.J.* 8, **2002**, 951.
[2] C. Meier et al., *J.Phys.Chem.B* 109, **2005**, 21015.
[3] H.E. Hoster et al., *Langmuir* 23, **2007**, 11570.

[4] M. Roos et al., *Phys.Chem.Chem.Phys.* 9, **2007**, 5672.
[5] M. Roos et al., *Phys.Chem.Chem.Phys.*, DOI:10.1039/b920481d

O 59.79 Wed 17:45 Poster B1

**Multi-molecular networks on Ag(111) displaying a novel bonding scheme** — •Wolfgang Krenner[1], Dirk Kühne[1], Florian Klappenberger[1], Svetlana Klyatskaya[2], Mario Ruben[2], and Johannes V Barth[1] — [1]Physikdepartment E20, TU München, München, Germany — [2]Institute of Nanotechnology, Forschungszentrum Karlsruhe, Karlsruhe, Germany

The combination of different types of molecular building blocks provides a wide range of possibilities for the hierarchic construction of molecular networks on metallic surfaces via self-assembly. We present a UHV, low-temperature scanning tunneling microscopy study of the formation of multi-molecular networks constructed with two different bonding schemes.

After deposition of the two building blocks, namely dicarbonitrile polyphenyl (A) and diphenyl oxalic amide (B), at room temperature onto Ag(111), hydrogen-bonded networks formed by molecular self-assembly can be observed. The shape of the molecular networks depends on coverage and stoichiometry.

By tuning the growth conditions highly regular molecular networks can be achieved providing rhombic cavities of an approximate size of 8 $\text{nm}^2$. The elementary binding motif features a hydrogen bond from a carbonitrile group of molecule A to the amine group of molecule B. This type of hydrogen bond has not been observed so far for surface confined self-assembly.

O 59.80 Wed 17:45 Poster B1

**A photoelectron diffraction investigation of vanadyl phthalocyanine on Au(111)** — David Duncan[2], •Werner Unterberger[1], Tsenolo J. Lerotholi[2], Kirsty Hogan[3], Christine Lamont[3], and Phillip Woodruff[1,2] — [1]Fritz-Haber-Institute — [2]Physics Department, University of Warwick — [3]Deptartment of Chemical and Biological Sciences, University of Huddersfield

Scanned-energy mode photoelectron diffraction (PhD) is a well-established method to determine quantitatively the local structure of adsorbates at surfaces. Here we describe its application to adsorption of vanadyl phthalocyanine (VOPc) on Au(111) which was used as a model system for vanadyl species (V=O) on the clean $V_2O_3$ surface.

VOPc was dosed at 130°C on the clean Au(111) surface and a coverage of approximately 0,015ML was reached which is half of that found by STM experiments (Hipps et. al.). O 1s and V 2p scanned-energy mode photoelectron diffraction has been used to investigate the adsorption structure of VOPc. The V=O vanadyl bond is found to point out of the surface with a bondlength of 1.60+-0.04 A. Relative to bulk VOPc, the V atom is pulled down into the approximately planar region defined by the N and C atoms by 0.52 (+0.14/-0.10) A.

O 59.81 Wed 17:45 Poster B1

**Thin vacuum deposited films of charge transfer compounds on the Au(111) surface investigated by SPA-LEED** — •Benjamin Fiedler, Oliver Bauer, and Moritz Sokolowski — Institut für Physikalische und Theoretische Chemie der Universität Bonn

Thin films of different charge transfer compounds were prepared on the Au (111) surface and studied by spot profile analysis LEED (SPA-LEED). For tetrathiafulvalene / tetracyanoquinone (TTF/TCNQ) the films were obtained via two different routes. In the first, we prepared the films by vacuum sublimation from a single crucible containing the charge transfer compound. In the second, the single components (TTF and TCNQ) were evaporated from two different crucibles. Findings of both preparation methods are compared with each other. From the LEED patterns a unit cell of the monolayer was derived and is compared with those unit cells concluded from earlier STM investigations [1,2]. We also studied the larger molecule tetrathiatetracene (TTT) as donor component in combination with dimethyl-dicyanoquinondiimine (DCNQI) and TCNQ as acceptors. First results are presented.

[1] M. D. Ward, J. Am. Chem. Soc. 1994, 116, 6806
[2] J. I. Pasqual, Phys. Rev. Lett. 100, 156805 (2008)

O 59.82 Wed 17:45 Poster B1

**Investigation of self-sustained molecular wires** — •Kerrin Dössel[1], Maya Lukas[1], Alexandrina Stuparu[1], Christophe Stroh[1], Karin Fink[1], Marcel Mayor[1,2], and Hilbert von Löhneysen[3,4] — [1]Institut für Nanotechnologie, KIT, D-76021 Karlsruhe — [2]Department of Chemistry, University of Basel, CH-4056 Basel — [3]Physikalisches Institut, KIT, 76128 Karlsruhe — [4]Institut für Festkörperphysik, KIT, 76021 Karlsruhe

In recent years the conductance of organic molecules has been investigated in a growing number of scanning tunneling microscopy (STM) experiments since STM is capable of characterising the investigated system with (sub)molecular resolution. However, conductance measurements with the current along the long axis of a wire-like molecule are difficult to achieve by STM because the molecules have the tendency to "lie" with their long axis parallel to the surface. We investigate the electronic properties of taylor-made organic molecules: While one wire-like part of the molecule is lying with the long axis parallel to the surface another identical wire is sticking out freely from the surface, accessible by the tip of our STM. We used scanning tunneling microscopy and scanning tunneling spectroscopy to investigate the molecules' position and surrounding on the surface and the electronic properties at low temperature (30K). Due to the special geometry of our molecules we are able to investigate and compare the transport across the wire as well as along the wire in the same experiment without altering further parameters which might otherwise influence the conductance behaviour.

O 59.83 Wed 17:45 Poster B1

**Cobalt porphyrin and phthalocyanine complexes on Ag(111) and Au(111): Interfacial coordination interactions** — •Yun Bai, Martin Schmid, Michael Sekita, Thomas Bischof, Hans-Peter Steinrück, and Michael Gottfried — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II

Metalloporphyrins and metallophthalocyanines are of increasing technological interest due to their potential applications in heterogeneous catalysis, sensor systems, photovoltaics and organic electronics. In most of these applications the interfacial electronic interactions and the chemical bonds between the metal complexes and a solid substrate (metal or oxide) plays an important role. To obtain fundamental insight especially into the contributions of the coordinated metal centers to the surface chemical bond, we studied monolayers of cobalt(II)-phthalocyanine (CoPc), cobalt(II)-octaethylporphyrine (CoOEP), and cobalt(II)-tetraphenylporphyrine (CoTPP), adsorbed on Ag(111) and Au(111), using XPS and UPS. On Ag(111), uniform core level shifts and the appearance of a new valence state indicate that the Co ions interact strongly with the substrate and that the interactions are laterally homogenous, i.e., virtually all Co ions interact in a same way with the Ag substrate. On Au(111), however, a split Co $2p_{3/2}$ signal suggests the presence of two different cobalt species in the monolayer. This observation is discussed in the context of the herringbone reconstruction of the Au(111) surface, which leads to lateral variations of geometric and electronic structure and thus potentially different adsorption sites. Supported by the DFG through SFB 583.

O 59.84 Wed 17:45 Poster B1

**Substrate- and temperature-dependent adsorption studies of azobenzene molecules.** — •Alex Krüger[1], Marten Piantek[1], Matthias Bernien[1], Felix Hermanns[1], Jorge Miguel[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 dimetacyano-azobenzene (DMC) evaporated onto Cu(100) and Au(111), as well as on CoO/Ag(100), was studied at different substrate temperatures in order to ascertain the influence of substrate and coverage. Angle-dependent NEXAFS spectroscopy was used to resolve the adsorption geometry of the molecules. By XPS the formation of additional bonds between the molecules and surface was investigated. For the adsorption on Au(111) at room temperature (RT), and on Cu(100) at 150 K, we find the molecules physisorbed in a planar conformation parallel to the surface. In the case of molecules adsorbed at 100 K on CoO/Ag(100), we observe a change in the angle dependence of the $\pi^*$ resonances of the N-K edge NEXAFS. After annealing the Cu(100) substrate to RT, the angle dependence and intensity of the $\pi^*$ resonances change significantly. From the peak assignment derived from DFT-based simulation of the NEXAFS spectra, we conclude that chemisorption takes place at the azo-nitrogen on Cu(100) at RT, whereas a mixed phase of physisorbed and chemisorbed molecules is found on CoO/Ag(100) at 100 K, and on Cu(100) at 150 K. In contrast, only the physisorbed phase was found for DMC on Au(111) at RT. This work has been supported by Sfb 658.

O 59.85 Wed 17:45 Poster B1

**Binding chemistry and interface dipole formation of dithiol-**

**based monolayers on gold** — •Philip Schulz[1,2], Christopher D Zangmeister[2], Dominik Meyer[1], Matthias Wuttig[1], and Roger D Van Zee[2] — [1]Institute of physics (IA), RWTH Aachen University of Technology, 52062, Aachen, Germany — [2]Chemical Science and Technology Laboratory, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA

The conditioning of metal surfaces via self-assembled monolayers (SAM) of molecules anchored by a sulfur endgroup is a widely studied issue in the field of organic electronics. In particular the electronic properties of the interface between electrode and subsequent functional organic layer in organic light emitting diodes (OLED), thin film transistors (OTFT) and photovoltaic devices (OPV) can be altered in order to promote charge transfer and improve the overall device efficiency. In our study we investigated the growth and electronic structure of dithiol-based monolayers on a Au(111) surface. We focus on the influence of this linker chemistry on the energy level alignment of the SAM and the workfunction change of the gold substrate. FTIR measurements were employed to verify the film formation while the electronic structure was further investigated by photoelectron spectroscopy. Not only did we derive the coverage and film perfection from XPS measurements but could also show a distinct charge rearrangement in the molecular layer while UPS measurements revealed a considerable lowering of the workfunction. DFT calculations have been employed in order to describe these phenomena.

O 59.86 Wed 17:45 Poster B1

**L-tyrosine on Ag(111): universality of the amino acid 2D zwitterionic bonding scheme?** — •Joachim Reichert[1,3], Agustin Schiffrin[2], Willi Auwärter[1], Alexander Weber-Bargioni[3], Matthias Marschall[1], Martina Dell'Angela[4], Dean Cvetko[4], Gregor Bavdek[4], Albano Cossaro[4], Alberto Morgante[4], and Johannes V. Barth[1,3] — [1]Physik Department E20, TU München, Germany — [2]Max-Planck-Institut für Quantenoptik, Garching, Germany — [3]Department of Physics & Astronomy, University of British Columbia, Vancouver, Canada — [4]C.N.R.-INFM, Laboratorio Nazionale TASK, Trieste, Italy

We present a combined study of the adsorption and ordering of the L-tyrosine amino acid on close-packed noble-metal surfaces in ultra-high vacuum by means of low-temperature STM, XPS and NEXAFS spectroscopy. Our high resolution topographical STM data reveal noncovalent molecular dimerization within the highly ordered one-dimensional nanostructures, which recalls the geometrical pattern already seen in the L-methionine/Ag(111) system and supports a universal bonding scheme for amino acids on the Ag(111) surface. XPS measurements reveal a zwitterionic adsorption, whereas NEXAFS experiments show a tilted adsorption configuration of the phenol moiety. This enables the interdigitation between aromatic side-chains of adjacent molecules via parallel-displaced Pi-Pi interactions which, along with the hydrogen-bonding capability of the hydroxyl functionality, could provide an explanation for the emergence of the self-assembled supramolecular nanoribbons.

O 59.87 Wed 17:45 Poster B1

**Coordination networks of the charge transfer compounds TTF and TCNQ on Pb(111)** — •Mario Konschake, Isabel Fernandez-Torrente, Katharina Franke, and Jose Ignacio Pascual — Freie Universität Berlin, Berlin, Germany

The charge transfer complex TTF-TCNQ has recently attracted considerable interest due to its electronic and magnetic properties when adsorbed on a Au(111) surface [1]. Here, we use low-temperature scanning tunnelling microscopy and spectroscopy to investigate the influence of a different substrate, i.e. Pb(111), on the adsorption properties.

As individual components, TTF and TCNQ exhibit very distinct bonding properties with the substrate. TTF adsorbs with its molecular skeleton perpendicular to the surface, giving rise to domains of $\pi$-stacked molecular islands. TCNQ, on the other hand, remains in a flat adsorption configuration and leads to an intriguing network, which is stabilized by Pb adatoms and their coordination bonding to the lone-pair electrons of the cyano terminations.

The coadsorption of TTF-TCNQ gives rise to a variety of phases with or without lead adatoms. Indications of a negative charging of the TCNQ molecules can be found in those forming metal-organic coordination networks.

[1] I. Fernández-Torrente et al. PRL 101(21):217203, 2008

O 59.88 Wed 17:45 Poster B1

**Porphyrin based molecular switches and quantum corrals** — Felix Bischoff, •Willi Auwärter, Knud Seufert, Daniel Heim, and Johannes V. Barth — Physik Department, E20, Technische Universität München, James-Franck Str. 1, D-85748 Garching, Germany

Porphyrin molecules exhibit an intriguing variety of functional properties, which are exploited in both biological and artificial systems. Hereby, particular interest lies on the porphyrin macrocycle, which can act as a chemical pocket and host either two hydrogen atoms or a metal ion. Here, we present first results on the tautomerization of free-base tetraphenylporphyrin molecules (H2-TPP) anchored on a Ag(111) surface. STM experiments proof that the switching of the two H's in the porphyrin pocket can be induced by voltage pulses. This process is directly monitored by current versus time (I-t) spectra, which exhibit two characteristic current levels. In addition, a tip induced process can be applied to remove one H atom from the porphyrin pocket. As a result, the remaining H atom can be switched between four possible positions (the four nitrogen atoms of the macrocycle).

In a different set of experiments, we show that the TPP's chemical pocket plays a non-neglibible role for the interaction of the porphyrin with the electronic structure of the supporting surface. By STM manipulation, individual TPP molecules are removed one-by-one from highly ordered TPP arrays on Ag(111), to construct artifical structures confining the Ag(111) surface state electrons. Hereby, the chemical nature of the corral walls, i.e. the use of either H2-TPP or Co-TPP arrays, affects the electron confinement and the coupling of resonators.

O 59.89 Wed 17:45 Poster B1

**Diffusion of 1,4-butanedithiol radicals on Au(111) and Au(100): A DFT-based comparison** — Andreas Franke and •Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel, 24098 Kiel, Germany

Organic molecules chemisorbed on surfaces hold the perspective of surface functionalization. The 1,4-butanedithiol radical chemisorbed at the Au(111) or Au(100) surface serves as a model system for the S-Au molecule-substrate bond. Density functional total-energy calculations have been carried out for the chemisorption of the radical on the unreconstructed Au surfaces, which are both known to be stabilized under electrochemical conditions [1]. Local minima with close-by energies indicate multi-valley potential-energy surfaces, which originate from the interplay between the two S-Au adsorbate-substrate bonds and the internal degrees of freedom of the butanedithiol radical. Diffusion paths of the radical on both Au surfaces have been calculated within DFT using VASP [2]. The diffusion barriers for translation and rotation of the radical differ. They can be fine-tuned by varying the applied potential in the electrochemical cell. This is considered theoretically by inspecting the variation of the dipole moment along the reaction paths. Consequences for the dynamics of succeeding diffusion hops are discussed.

[1] M. Schneeweiss *et al.*, Appl. Phys. A **69**, 537 (1999). H. Striegler *et al.*, J. Electroanal. Chem. **471**, 9 (1999).

[2] http://cms.mpi.univie.ac.at/vasp

O 59.90 Wed 17:45 Poster B1

**STM study of the structual formation of $C_{60}$ on a thiol tethered Au(111) surface** — •Patrick Mehring, Axel Beimborn, and Carsten Westphal — Fakultät Physik - Technische Universität Dortmund, Otto-Hahn-Str. 4, D 44221 Dortmund, Germany

Since the discovery of fullerenes and their unique properties a large variety of potential applications was predicted. Different structures of fullerenes including ring, ball, and tube variations attracted attention especially in the fields of molecular electronics and nanotechnology. The understanding of the structural formation on different substrates is important for future applications of these carbon molecules. The influence of a methylthiol tethered Au(111) surface on the self assembly of $C_{60}$ buckyballs was investigated by means of scanning tunneling microscopy. Methylthiol arranges in several structures on Au(111) depending on the monolayer coverage. $C_{60}$ was prepared by evaporator deposition on two different striped phases of $CH_3S$. Both exhibit domains with 3 distinct orientations but different line spacing between single molecule rows. Instead of the typical hexagonal orientation of $C_{60}$ on noble metals, domains of a striped phase can be found. Single domains show 6 possible orientations on the $CH_3S$ monolayer. The spacing between $C_{60}$ molecules varied depending on the orientation of the methylthiol layer. They are clearly located on top of the $CH_3S$ rows.

O 59.91 Wed 17:45 Poster B1

**Scanning Tunneling Microscopy and Spectroscopy of Phthalocyanine Molecules on Insulating Films** — •Christof Uhlmann, Ingmar Swart, Tobias Sonnleitner, and Jascha Repp — Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Ultrathin insulating films on metal substrates can be used to electronically decouple individual molecules from the metallic substrate. As electrons can still tunnel through the films, scanning tunneling microscopy can be used to characterize these molecules. This geometry represents a double-barrier tunneling junction, in which at the resonances in conductance spectra, an electron is temporarily added to or removed from the molecule. Here we present a study of Cu-phthalocyanine molecules on different substrate systems. For a neutral Cu-phthalocyanine molecule the lowest unoccupied molecular orbital (LUMO) and the LUMO+1 are degenerate. By varying the substrate system, and thereby also varying the work-function, it is possible to permanently charge the molecules. Consequently, either the former LUMO or the former LUMO+1 is occupied with one electron. Due to the Jahn-Teller effect, the degeneracy of these orbitals is lifted. This manifests itself in a lowering of the symmetry as deduced from STM images.

O 59.92 Wed 17:45 Poster B1

**Morphology, geometric and electronic structure of ultra thin films of perylene bisimide dyes on Ag(111)** — •Markus Scholz[1], Rüdiger Schmidt[2], Achim Schöll[1,3], Frank Würthner[2], and Friedrich Reinert[1,3] — [1]Universität Würzburg, Experimentelle Physik VII, 97074 Würzburg — [2]Universität Würzburg, Institut für Organische Chemie, 97074 Würzburg — [3]Gemeinschaftslabor für Nanoanalytik, Forschungszentrum Karlsruhe, 76021 Karlsruhe

Perylene tetracarboxylic acid bisimides dyes (PBI) are among the best n-conducting organic materials. The molecular structure and electronic properties of these molecules can be tailored by halogen substituents attached to the perylene core which induces a twist angle in the planar perylene backbone. We studied the morphology, geometric and electronic structure of ultra thin epitaxial films of the planar $PBI-H_4$, the slightly twisted $PBI-F_2$ and the strongly twisted $PBI-Cl_4$ on Ag(111) substrates. At coverages below one molecular layer a long range order was observed at room temperature. From the characteristic LEED patterns we deduced real space models for each sample. Incommensurate superstructures were found were the size of the unit cell increases from $PBI-H_4$ to $PBI-Cl_4$. Moreover, the bonding at the interface and consequently the electronic structure is significantly influenced by the molecular conformation thus providing a possible route for tailor the properties of metal-organic interfaces.

O 59.93 Wed 17:45 Poster B1

**Impact of central metal atoms and F-substituents on the adsorption geometry of phthalocyanine molecules on Cu(111)** — •Christoph Bürker[1], Takuya Hosokai[1], Alexander Gerlach[1], Steffen Duhm[2], Norbert Koch[3], Hiroyuki Yamane[4], and Frank Schreiber[1] — [1]Universität Tübingen — [2]Chiba University — [3]HU Berlin — [4]Institut for Molecular Science

The adsorption geometry of large organic molecules on metal surfaces is essential for understanding and controlling the interface electronic structure, thin film structure and growth mechamism. The X-ray standing wave (XSW) technique is one of the most precise methods to determine the vertical positions of specific atoms relative to the substrate and can therefore establish the adsorption geometry of organic molecules.

Metal Phthalocyanines (MPc) as typical organic semiconductors are one of the most suitable systems for XSW experiments due to their chemical stability, high structural symmetry and variability of both the central metal atom and substituents. Using the XSW technique we show how fluorination and a central metal atom affect the adsorption geometry of Pc molecules. We compare the structural differences of metal-free Pc ($H_2$Pc), zinc-Pc (ZnPc) and perfluorinated ZnPc ($F_{16}$ZnPc) on Cu(111). The XSW data reveal significant deviations for both the bonding distance and molecular distortion. These results indicate an interaction strength of each atom with the surface depending on its chemical vicinity.

O 59.94 Wed 17:45 Poster B1

**"Unbinding" an adsorbed organic molecule: K plus PTCDA on Ag(110)** — •Oliver Bauer[1], Giuseppe Mercurio[2], Sergey Subach[2], Christoph H. Schmitz[1], Benjamin Fiedler[1], Frank Stefan Tautz[2], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Bonn — [2]Institut für Bio- und Nanosysteme 3, Forschungszentrum Jülich

We have doped the well-known brick-wall structure of pristine PTCDA which is present in the monolayer on the Ag(110) surface with potassium (K) and investigated the induced structural and electronic changes at the interface. SPA-LEED measurements reveal that the structural order of the PTCDA molecules is strongly altered upon K dosing: A variety of co-existing binary phases is observed within the monolayer. In addition we have conducted XPS and NIXSW measurements on K + PTCDA / Ag(110). The photoemission experiments indicate that the K atoms preferentially interact with the carboxylic groups of the co-adsorbed PTCDA molecules. This interpretation is further supported by the NIXSW results: The adsorption geometries of the carboxylic and the anhydride oxygen (O) atoms are highly influenced by the presence of K on the surface, the bonding distances are extended. The adsorption height of the perylene core is also increased by K doping. Hence we conclude that the local Ag-O bonds at the interface are partially lifted by the co-adsorbed K and that K and Ag atoms compete for the interaction with the carboxylic groups of PTCDA while the bonding across the interface is weakened. Supported by the DFG and the ESRF.

O 59.95 Wed 17:45 Poster B1

**Kondo effect on a mixed Na-TCNQ layer** — •Tobias R. Umbach, Isabel Fernández-Torrente, Robert Drost, Jose I. Pascual, and Katharina J. Franke — Institut für Experimentalphysik, Freie Universität Berlin, Animallee 14, 14195 Berlin, Germany

Mixing organic molecules with dopant atoms is a key issue in the field of organic electronics, as charge transfer processes may be used to tune the electronic properties of the compound. Here we report, by means of low-temperature scanning tunneling microscopy and spectroscopy measurements (LT-STM, STS), the doping of TCNQ by Na on a Au(111) surface. The addition of NaCl to previously formed TCNQ domains breaks the hydrogen network structure of the pure molecular island, leading to the formation of a new ordered Na-TCNQ phase with a bidimensional *wind-mill*-like structure. This self-assembling provokes a lateral electron transfer from the alkali metal to the organic molecule, inducing the localization of an unpaired spin on TCNQ. This free radical state can be demonstrated by the observation of a Kondo resonance arising in the Na-TCNQ unit cell. By STS we can plot the Kondo intensity of this unpaired spin: the Kondo resonance exhibits a different height along the Na-TCNQ layer, being largest at the center of the *wind-mill*structure and smaller at the center of the molecule.

O 59.96 Wed 17:45 Poster B1

**DFT Studies on the Interaction of Sulfur with Transition Metal Surfaces** — •Porntip Seema, Jörg Behler, and Dominik Marx — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

The interaction of sulfur atoms with transition metal surfaces plays an important role for example in the poisoning of heterogeneous catalysts and the formation of self-assembled monolayers of thiolates. In the present work, the sulfur adsorption on Cu(111), Ag(111) and Au(111) surfaces has been studied within the framework of density-functional theory (DFT). Calculations have been carried out for a variety of adsorbate phases, and the sulfur binding sites and binding energies have been investigated systematically as a function of coverage at ideal surfaces as well as at defects. We find that the order of the adsorption energies of the sulfur atoms on the different defect-free metal slabs is Cu(111) > Ag(111) > Au(111). This result is independent of the coverage of the surface.

O 59.97 Wed 17:45 Poster B1

**Vibrational Spectroscopy of Adsorbate Molecules on Roughened Cu(111)** — Heiner Maslosz, •Jan Pischel, Olaf Skibbe, and Annemarie Pucci — Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, D-69120 Heideberg

In order to close the so-called material gap between pristine low-index single crystal surfaces and rough surfaces we study slightly roughened copper surfaces. The roughness is introduced by evaporation of small amounts of copper to the cooled Cu(111) surface. Vibrational spectroscopy (HREELS and IRRAS) has shown in the past several interesting findings regarding the interaction of the roughened surface with adsorbed molecules (e.g. [1,2]). In this study, we present high-resolution electron energy loss spectroscopy (HREELS) measurements of the system $O_2$/Cu/Cu(111). We found already at oxygen exposures of 0.01 Langmuir spectral features that we attribute to atomically adsorbed oxygen. Since the sticking probability for oxygen on the smooth Cu(111) surface is quite low, this system provides a sensitive tool to quantify the introduced roughness.

[1] O. Skibbe, M. Binder, A. Otto, and A. Pucci. J. Chem. Phys., 128:194703, 2008.

[2] O. Skibbe, D. Vogel, M. Binder, A. Pucci, T. Kravchuk, L. Vattuone, V. Venugopal, A. Kokalj, and M. Rocca. J. Chem. Phys., 131:024701, 2009.

O 59.98 Wed 17:45 Poster B1

**Interaction of Fe and $Fe_2O_3$ with $H_2O$ and CO** — •Kai Volgmann[1], Anselm Hahn[1], Florian Voigts[1], and Wolfgang Maus-Friedrichs[1,2] — [1]Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — [2]Clausthaler Zentrum für Materialtechnik, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld

Basic investigations have been done on the interaction of Fe and $Fe_2O_3$ with molecular oxygen[1]. MIES/UPS and XPS measurements revealed that a passivating oxide layer has been formed and inhibits a further oxidation. The scope of this work is to examine the interaction of Fe and $Fe_2O_3$ with water and CO. This is a further step towards a basic data set for further research on the photocatalytical processes on hematite surfaces found under Martian conditions.

Iron and Iron(III) oxide films are investigated by means of their interaction with $H_2O$ and CO. These reactions have been studied with photoelectron spectroscopy. X-ray photoelectron spectroscopy is used to determine stoichiometry of the samples, while Ultraviolet photoelectron spectroscopy and Metastable Induced Electron Spectrocopy are used to analyse the valence band region and to gain information about changes in workfunction due to reactions on the surfaces.

[1] K.Volgmann, F. Voigts, W. Maus-Friedrichs, *The interaction of oxygen molecules with iron films studied with MIES, UPS and XPS*, Surface Science, submitted

O 59.99 Wed 17:45 Poster B1

**Adsorption of CO on clean and oxidized Pt3Ti(111)** — •Marco Moors[1], Séverine Le Moal[2,3], Jan Markus Essen[1], Conrad Becker[2], and Klaus Wandelt[1] — [1]Institut für phys. und theoret. Chemie, Universität Bonn — [2]Centre Interdisciplinaire de Nanoscience de Marseille — [3]Technische Universität München

The adsorption of CO on Pt3Ti(111) before and after its oxidation has been investigated by AES, TDS, LEED and HREELS. The adsorption of CO has clearly been evidenced on clean Pt3Ti(111). The LEED patterns exhibit either a diffuse or a sharp c(4x2) structure (stable up to 300 K) attributed to CO depending on the adsorption temperature. Remarkably, the adsorption / desorption behavior of CO on clean Pt3Ti(111) exhibits similarities to that previously reported for CO on Pt(111). Our results clearly evidence a partial CO decomposition on Ti sites and molecular adsorption of CO on on-top Pt sites. Therefore, the clean surface can not be terminated by a pure Pt plane as previously discussed in the literature. Lowly oxidized Pt3Ti(111) surfaces ($<$ 135 L O2 exposure at 1000 K) exhibit a CO adsorption / desorption behavior similar to that of the clean surface with again a c(4x2) structure (stable up to 250 K) attributed to CO adsorption. These results indicate that some areas of the substrate remain non-oxidized upon low oxygen exposures. Highly oxidized and therefore completely oxide covered Pt3Ti(111) surfaces ($>$ 220 L O2 exposure at 1000 K) allow no CO adsorption at sample temperatures over 100 K.

O 59.100 Wed 17:45 Poster B1

**Electron beam induced effects in ice on Pt(111)** — •Daniel Schwarz, Herbert Wormeester, and Bene Poelsema — Solid State Physics, IMPACT, University of Twente, The Netherlands

The interactions at the water-solid interface determine a wide range of physical and chemical properties, relevant in nature and technology. The growth of a thin water layer on Pt(111) is considered a model system for studying this interaction. A series of complex crystalline structures were found as a function of the thickness of a thin ice film on this metal surface when grown at temperatures above 135K [1]. Below this temperature strongly amorphous ice growth is found. The thin ice layers (1-50ML) form a delicate structure. A fast restructuring of the film under the influence of an electron beam was found [2]. These energetic electron induced changes prohibit a detailed structural analysis with LEED. Although some lateral lattice structure determination is reported, an IV analysis is beyond the capabilities of a standard LEED system.

Electron induced phenomena can be reduced by using MCP-LEED which allows to use much lower electron current densities compared to conventional LEED. This does not only allow to measure in detail the development of the lattice parameter parallel to the interface with ice thickness, but also opens the possibility for a more detailed analysis via IV-LEED. A quadrupole is used to identify kinetics and composition of the desorbed species after prolonged electron bombardment.

[1] A. Glebov et al., J. Chem. Phys. 106 (1997) 9382

[2] J. Harnett et al., Surface Science. 528 (2003) 15

O 59.101 Wed 17:45 Poster B1

**Particle Size Dependent Heat of Adsorption for CO on supported Pd Nanoparticles** — •Jan-Henrik Fischer-Wolfarth[1], Jose Manuel Flores-Camacho[1], Jason Farmer[2], Charles Campbell[2], Jens Hartmann[1], Swetlana Schauermann[1], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, 14195 Berlin, Germany — [2]Department of Chemistry, University of Washington, Seattle, USA

The particle size dependence of the heat of adsorption for carbon monoxide on supported Pd nanoparticles has been investigated at 300 K with a new single crystal microcalorimeter and compared to the heat of adsorption on Pd(111). The average Pd particle size was varied systematically in the range of 100 to 4900 Pd atoms, i.e. 2 to 8 nm diameter. All nanoparticles were supported on $Fe_3O_4$(111)/Pt(111). The initial heat of adsorption was found to decrease monotonically with decreasing particle size below 4 nm. The correlation of the heat of adsorption with a particle size dependent reduction of the particle lattice constant [1] will be discussed.

Further, the microcalorimetry technique used to determine the adsorption energies and its performance will be presented.

[1] Nepijko *et al.* Langmuir 15 **1999** 5309

O 59.102 Wed 17:45 Poster B1

**Manipulation of the wetting layer of $H_2O$ on Pt(111)** — •Sebastian Standop[1], Alex Redinger[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

Previous LEED experiments unveiled strong effects of electron exposure on the structure of the adsorbed water layer on Pt(111) [1]. A transition from the $\sqrt{39} \times \sqrt{39}$ R16.1° structure to the simple commensurate $\sqrt{3} \times \sqrt{3}$ R30° arrangement was observed. Upon electron beam induced restructuring also exposure of bare Pt was found.

Using scanning tunneling microscopy we investigated the influence of electron dose, energy and scanning parameters on the $\sqrt{39} \times \sqrt{39}$ R16.1° overlayer. Our results show that above a threshold electron energy of about 4 eV the high order commensurate phase transforms into the $\sqrt{3} \times \sqrt{3}$ R30° overlayer through partial dissociation of water molecules. This superstructure has a higher molecular density than the initial domains with a $\sqrt{39}$ arrangement which explains the occurrence of uncovered substrate areas after electron beam manipulation. We could rule out that the tip electrical field is of relevance for the structural transition.

[1] J. Harnett, S. Haq and A. Hodgson, Surface Science 528 (2003) 15

O 59.103 Wed 17:45 Poster B1

**Formation of copper oxide surface structures via pulse injection of air onto Cu(111) surfaces** — •Carmen Pérez León[1], Michael Marz[1], Christoph Sürgers[1], and Hilbert v. Löhneysen[1,2] — [1]Karlsruher Institut für Technologie (KIT), Physikalisches Institut and DFG-Center for Functional Nanostructures (CFN), D-76131 Karlsruhe — [2]Karlsruher Institut für Technologie (KIT), Institut für Festkörperphysik, D-76131 Karlsruhe

The pulse-injection method is widely used for deposition of molecules in solution onto clean surfaces. A potential source of contamination of the solution in the valve can be the ambient air. Therefore we have investigated the clean Cu(111) surface after injection of air by Auger electron spectroscopy and scanning tunneling microscopy (STM). The results show that mainly oxygen is adsorbed on the copper surface. The initial stages of oxidation of Cu(111) are governed by the restructuring of the surface, since Cu atoms from the step edges and terraces are incorporated into the growing surface oxide. The nucleation and growth of the oxide is strongly influenced by the substrate temperature during deposition as well as by the oxygen coverage. At submonolayer coverage three different kind of oxide islands are observed, whereas at monolayer coverage these are reduced to two. High resolution STM images reveal that oxidation at room temperature produces poorly ordered oxide structures. In contrast, surface oxides produced at higher temperature (∼ 200 °C) exhibit additional highly ordered structures corresponding to the strained $Cu_2O(111)$ lattice that coincides with the Cu(111) substrate.

O 59.104 Wed 17:45 Poster B1

**Electronic structure of oxygen/W(110): photoemission study** — Martin Weser[1], Alexander Generalov[1,2], Karsten Horn[1], and •Yuriy Dedkov[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]St. Petersburg State University, Russia

The study of oxygen interaction with W(110) has been a focus of many surface-science studies. Thermodynamics of the oxygen adlayer, including the phase diagram and critical behavior [1], have been investigated in series of LEED studies [2] and in later STM study [3]. Because of the relative simplicity in adsorption behavior, the W(110) surface provides an ideal surface to study the electronic structure of the initial stages of the interaction of oxygen with tungsten metal, and this system can be considered as a model for the consideration of catalysis effects on the heavy *d*-metal surfaces. Here we present the results of angle-resolved photoemission studies of the clean and oxidized W(110) surface. The both systems are examined via analysis of the electron dispersions at the particular regions of the Brillouin zone and the effect of the oxygen chemisorption on the electronic structure of W(110) is discussed.

[1] G. C. Wang et al., J. Chem. Phys. 69, 479 (1978).
[2] M. C. Tringides, Phys. Rev. Lett. 65, 1372 (1990).
[3] K. E. Johnson et al., Phys. Rev. Lett. 71, 1055 (1993).

O 59.105 Wed 17:45 Poster B1

**DFT studies on the hydrogen adsorption on Pt(111) and Pt(111)-hydride surfaces** — •Fedir Strygunov and Timo Jacob — Universität Ulm, Albert-Einstein-Allee 47, D-89069 Ulm, Germany

The catalytic reaction of hydrogen on Pt electrodes is one of the simplest, most fundamental and important reactions in electrochemistry. However, despite the apparent simplicity of the hydrogen oxidation and evolution reactions (HOR/HER) and a large numbers of studies, there is still no consensus about adsorption states of hydrogen on Pt electrodes.

Using periodic density functional theory in combination with the extended *ab initio* atomistic thermodynamics approach [1, 2] the structure and stability of clean Pt(111) and Pt(111)-hydride electrodes have been investigated. We find that at low coverages hydrogen prefers surface positions, but above 2 ML hydrogen also occupies subsurface tetrahedral positions, leading to the formation of a surface hydride. The electrochemical surface phase diagram showed that such a surface hydride might be stabilized with negative electrode potentials. On the basis of the most relevant surface hydride structures, further studies will aim on the electrocatalytic hydrogen reactions.

[1] M. Scheffler, J. Dabrowski, *Phil. Mag.*, **A 58**, 107 (1988).
[2] T. Jacob, *J. Electroanal. Chem.*, **607**, 158, (2007).

O 59.106 Wed 17:45 Poster B1

**DFT Studies on the Oxygen Adsorption at Copper Surfaces** — •Björn Hiller, Nongnuch Artrith, and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Oxide-supported copper clusters are important catalysts used for example in methanol synthesis. The surface structures and the morphologies of the copper clusters strongly depend on the composition of the surrounding gas phase [1], which therefore must have a significant influence on the catalytic activity and the reaction mechanisms. Using density-functional theory, we determine the stability of a variety of possible oxygen adsorbate phases and discuss the consequences for the equilibrium shape of the clusters under different catalytic conditions.
[1] P.L. Hansen et al., Science, 295 (2002), 2053.

O 59.107 Wed 17:45 Poster B1

**Surface oxidation of planar and stepped Pt(111) surfaces studied by DFT** — •Jochen Bandlow and Timo Jacob — Universität Ulm, Albert-Einstein-Allee 44, 89069 Ulm, Germany

The surface oxidation of Pt(111) seems to be a rather basic and quite simple reaction but nevertheless 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 stepedges, 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. By comparing the $(p,T)$ phase diagram for the system in contact with a gaseous $O_2$ atmosphere with the corresponding electrochemical $(p,T,\phi)$ 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.

O 59.108 Wed 17:45 Poster B1

**Quantum kinetics of electrons at plasma boundaries** — •Franz Xaver Bronold, Holger Fehske, Rafael Leslie Heinisch, and Johannes Marbach — Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, 17489 Greifswald, Germany

Macroscopic objects in contact with an ionized gas are usually negatively charged. They accumulate electrons more efficiently than ions leading to the build-up of a quasi-stationary electron film at the plasma boundary. The plasma is strongly affected by surface charges, via sheath formation, electron-ion recombination, and secondary electron emission. A kinetic description of surface charges on par with the kinetic modeling of the bulk plasma is however still missing. As a first step in this direction, we propose a physisorption-inspired model for the formation of surface charges at plasma boundaries and their interaction with the bulk plasma [1]. Besides identifying key issues of the electronic microphysics at plasma boundaries we also discuss results of exploratory calculations for clean metallic boundaries focusing in particular on the electron sticking coefficient $s_e$, the thermal electron desorption rate $1/\tau_e$, and the secondary electron emission coefficient due to de-excitation of metastable molecules in front of the boundary $\gamma_e^m$.

[1] F. X. Bronold et al., Eur. Phys. J. D 54, 519-544 (2009).

O 59.109 Wed 17:45 Poster B1

**Electron-induced emission of correlated electron pairs from Fe(001)** — •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

As an essential prerequisite we have calculated the electronic structure of the ground state of a thick Fe(001) film by means of an ab initio Full-Potential Linear Augmented-Plane-Wave method. On the basis of the ground state spin densities we constructed effective quasi-particle potentials, which in particular incorporate a spin-dependent mean free path for the primary electron and the two outgoing electrons. Using these potentials and a screened Coulomb interaction model, we calculated (e,2e) equal-energy angular distributions from Fe(001) by means of a Green function formalism involving Coulomb-correlated two-electron states. For primary spin up and down these distributions are resolved according to parallel and antiparallel alignment of the spins of the primary electron and the relevant valence electron. For parallel spins the outgoing two electrons are thus correlated by exchange and Coulomb interaction, whereas for antiparallel spins there is only the Coulomb correlation. The central depletion zones, which we find in the angular distributions, may therefore – with the proviso of some modification by matrix element effects – be viewed as manifestations of an exchange-correlation hole or a correlation hole in momentum space. Like in the well-known real-space case, the former is significantly larger than the latter.

O 59.110 Wed 17:45 Poster B1

**Theoretical investigation of the InN/In2O3 interface** — •Giancarlo Cicero[1,2], Antonio Aliano[1], and Alessandra Catellani[2] — [1]Chemical Engineering and Materials Science Department, Politecnico of Torino, Torino, Italy. — [2]CNR-IMEM, Parma, Italy

Contribution has been withdrawn by the author.

O 59.111 Wed 17:45 Poster B1

**A quantum-mechanical study of ZnO and TiO2 based Dye Sensitized Solar Cells** — •Giancarlo Cicero[1], Giuseppe

Mallia[2], Leandro Liborio[2], and Nicholas M Harrison[2,3] — [1]Chemical Engineering and Materials Science Department, Politecnico of Torino, Torino, Italy. — [2]Imperial College London - Thomas Young Centre - Chemistry Department, London UK — [3]STFC, Dares- bury Laboratory, Daresbury, Warrington WA4 4AD, UK

Since the pioneering work of Regan and Graetzel [1], a great attention has been paid to dye sensitized solar cell (DSC) as cheap, effective and environmentally benign candidates for a new generation solar power devices. Optimization of the DSC is still a challenging task as it is a highly complex interacting molecular system. Surface properties of the oxide and in particular proper sensitization with dye molecules may highly affect the efficiency of these cells. Aim of this study is to address the binding of cathecol and isonicotinic acid to oxide surfaces usually employed in DSC, namely ZnO and TiO2, in terms of geometry, stability, electronic structure and band alignment. To this end, we employ quantum mechanical simulations based on hybrid density functional theory. Our analysis helps understanding whether the difference between ZnO and TiO2 in photoeletricity generation efficiency is due to the changes in the bonding geometry of the dye anchoring groups or to electronic effects.

[1] B. O. Regan and M. Graetzel Nature, 353, 737 (1991).

O 59.112 Wed 17:45 Poster B1

**Calculation of GW electronic structure for large systems : application to amorphous silica** — •David Waroquiers[1,2], Matteo Giantomassi[1,2], Gian-Marco Rignanese[1,2], and Xavier Gonze[1,2] — [1]Unité de Physico-Chimie et de Physique des Matériaux (PCPM), Université Catholique de Louvain, B-1348 Louvain-la-Neuve, Belgium. — [2]European Theoretical Spectroscopy Facility (ETSF)

For accurate ab initio electronic structure calculations, many-body perturbation theories such as GW approximation or Bethe-Salpeter equation are essential. Up to recently, these methods could only be applied to small systems because of the large computational cost of these techniques. New theoretical and algorithmic developments (extrapolar method to reduce the number of empty states needed in *GW* calculations [1], band parallelism [2], and PAW formalism [3]) now enable us to perform GW calculations in supercells with more than 50 atoms within a reasonable amount of CPU time.

We applied these methods [4] to study the electronic structure of amorphous silica. More than twenty different configurations have been considered, each of them being obtained by relaxing 72-atom supercells at fixed volume. Then, different charged states of atomic hydrogen have been incorporated and relaxed in the larger voids of the systems. Defect energy levels have been calculated within the GW approximation.

[1] F. Bruneval and X. Gonze, Phys. Rev. B **78** (2008) 085125.
[2] X. Gonze *et al.*, Comput. Phys. Comm. **180** (2009) 2582.
[3] M. Torrent *et al.*, Comput. Mater. Sc. **42** (2008) 337.
[4] As implemented in the version 6 of ABINIT (http://www.abinit.org).

O 59.113 Wed 17:45 Poster B1

**Optical switching of sodium nitroprussides** — •Mirco Pötter, Mirco Imlau, and Michael Rohlfing — Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49069 Osnabrück

The optical switching of the NO ligand groups in sodium nitroprussides (e.g. $Na_2[Fe(CN)_5NO]\cdot 2H_2O$) constitutes a prototypical photoactivation process in solid-state optics. The key issue is the existence of several (local) minima in the electronic ground-state total-energy landscape, separated by barriers that do not occur in the photoexcited states, thus allowing switching via the excited state. Here we present theoretical investigations aiming at a detailed understanding of the total-energy landscapes and the transitions between them. Based on density-functional (DFT) calculations, the excitations are described by constraint-DFT, as well as by a simplified version of many-body perturbation theory. Our results show that in the excited state the energy landscape is rather flat, thus facilitating the configurational changes leading to the switching of the NO groups.

O 59.114 Wed 17:45 Poster B1

**Influence of the XC Functional on Band Parameters of AlN, GaN and InN** — •Luiz Claudio de Carvalho, Andre Schleife, Frank Fuchs, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany

The group III-nitrides have a great potential for optoelectronic devices operating in the visible spectrum and deep ultraviolet. Therefore, a detailed knowledge of their structural, electronic and optical parameters is necessary for the interpretation of experimental data and theoretical results. The most successful theoretical method is the DFT, but its accuracy depends on the choice of the functional of the exchange-correlation (XC) energy. Different choices yield slightly varying results for the structural properties. However, this effect is usually believed to be small, when comparing the results of ab-initio calculations using different XC functionals. In this work we investigate the influence of the structural deviations, introduced by different XC functionals, on the quasiparticle-band structure. We present our results for AlN, GaN, and InN, comparing the XC functionals LDA, PBE, and AM05. DFT as implemented in the VASP code is used to calculate the lattice constants, bulk moduli, band-gap energies, volume deformation potentials and hydrostatic pressure coefficients. The quasiparticle band structures are obtained by GW calculations, using the hybrid XC functional HSE03 as a starting point. We compare our results with experimental data reported in the literature, and discuss the influence of the XC induced structural changes on the band parameters.

O 59.115 Wed 17:45 Poster B1

**Non adiabatic effects in photo excited electronic states from ab initio Green's function method** — •Marcin Kaczmarski, Yuchen Ma, and MIchael Rohlfing — University of Osnabrueck, Department of Physics, Barbarastrasse 7, 49076 Osnabrueck, Germany

In this work we apply a universal diabatization method by Baer [Chem. Phys. Lett. 35, 112 (1975)] for the description of electronic excited states. A diabatization denotes a unitary transformation which allows for incorporating non adiabatic effects into the quantum Hamiltonian expressed in the adiabatic representation. A typical example is the occurrence of avoided crossings in the potential energy surface as a result of the Born-Oppenheimer approximation, for instance in the case of the retinal chromophore. We present analytical and numerical calculations for the diabatic states in the context of Green's function based ab initio many body perturbation theory (density functional theory plus GW method plus Bethe-Salpeter equation, DFT-GW-BSE). We present the calculation of the adiabatic and diabatic lowest excited electronic states of $HeH^+$ and the retinal chromophore molecule.

O 59.116 Wed 17:45 Poster B1

**Optical spectra of AlN and CaO from first principles** — •Arthur Riefer, Frank Fuchs, André Schleife, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany

Modern ab-initio calculations can nowadays reliably predict the optical and electronic properties of semiconductors and insulators, also for non-equilibrium crystal structures. Recently, AlN has been grown and characterized by optical ellipsometry also in the unfavored zincblende structure. Therefore, we compute the electronic and optical properties for the zincblende and wurtzite polytype from first principles. Further we investigate the experimentally well studied CaO employing the same approach. More precisely we compute the band structure and its key quantities by applying quasiparticle corrections to the results of a self-consistent calculation using the nonlocal hybrid HSE03 functional as approximation to exchange and correlation. Based on the so obtained electronic structure the optical properties including electron-hole attraction and local field effects are calculated. The so computed optical spectra and exciton-binding energies are analyzed and compared to available experimental data.

O 59.117 Wed 17:45 Poster B1

**Ab initio study of structural stability of InAs nanowires** — •Leila Salimi[1], Nahid Ghaderi[2], Seyed Javad Hashemifar[1], and Hadi Akbarzadeh[1] — [1]Department of Physics, Isfahan University of Technology, 84156-83111 Isfahan, Iran — [2]Theory@Elettra Group, INFM-CNR DEMOCRITOS, c/o Sincrotrone, I-34012 Trieste, Italy

We have studied the structural stability of InAs nanowires with different diameters by using density functional theory - pseudopotential computations. The stable structure of bulk InAs is Zinc Blende (ZB) although under special experimental conditions Wurtzite (WZ) InAs has also been observed. Due to the high symmetry and low ratio of dangling bonds, we have considered hexagonal and triangular WZ nanowires in [0001] direction and hexagonal ZB nanowires in [111] direction. In order to select facets of the nanowires, we calculated formation energy of nonpolar surfaces of both structures and found that ZB(110) and WZ($10\bar{1}0$) surfaces are more stable than others. All nanowires were calculated in the optimized and relaxed supercells. Calculating the cohesive energy of nanowires with small diameters, we found WZ structure more stable than ZB, in good agreement with experimental results. The obtained cohesive energy of the small diameter nanowires were fitted by a phenomenological model to obtain dangling bond energies and then extrapolate the cohesive energy of large diameter nanowires. The extrapolated results indicate that for diameters up to 50 Angstrom, the WZ nanowires are more stable than ZB nanowires while for larger diameters, the contribution of dangling bonds reduces and the results converge to that of bulk InAs.

**The poster O 59.118 has been withdrawn.**

# O 60: Poster Session III (Methods: Atomic and electronic structure; Methods: electronic structure theory; Methods: Molecular simulations and statistical mechanics; Methods: Sanning probe techniques; Methods: other (experimental); Methods: other (theory) )

Time: Wednesday 17:45–20:30 Location: Poster B2

O 60.1 Wed 17:45 Poster B2

**Two-Photon Photoelectron Spectroscopy using a Display Analyzer** — •Daniel Niesner, Tobias Bierlein, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Two-Photon Photoelectron Spectroscopy is a pump and probe technique which allows observation of excited electronic states in solids. After excitation by a first laser pulse a second one removes electrons into vacuum where they are detected by an analyzer. In the display analyzer the sample is placed in one of the focal points of an ellipsoidal mirror which serves as a low pass filter. Subsequently the photoelectrons pass through a retarding high pass filter and are detected by microchannel plates. While most common analyzers are able to detect only electrons emitted in one angular direction, in this setup the two-dimensional angular distribution of electrons emitted into a cone of 90° is measured. We present data from image-potential states on the (001) surfaces of copper and iridium. An energy resolution of 90 meV and an angular resolution of 5° is found.

O 60.2 Wed 17:45 Poster B2

**Tight-Binding Parameterizations Derived from Density-Functional Calculations** — •Alexander Urban[1], Konstantin Weber[1], Martin Reese[2,3], Matous Mrovec[2,3], Christian Elsässer[2], and Bernd Meyer[1] — [1]Interdisziplinäres Zentrum für Molekulare Materialien ICMM, Universität Erlangen-Nürnberg — [2]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg — [3]Institut für Zuverlässigkeit von Bauteilen und Systemen IZBS, Universität Karlsruhe

With the semiempirical Tight-Binding (TB) method it is possible to compute the electronic structure and total energy of systems with thousands of atoms. We present a straightforward method for the systematic derivation of TB parameters from first-principles DFT calculations of arbitrary model systems. Our method is conceptionally different from previous approaches [1] as it is based on a projection [2] of the fully converged wavefunction from a mixed-basis DFT computation onto an optimized minimal basis of atomic orbitals. The Slater-Koster tables are then calculated within that minimal basis using the fully converged DFT Hamiltonian. The electronic structures, total energies and forces resulting from derived TB models are compared to the DFT reference for different benchmark simulations.

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

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

O 60.3 Wed 17:45 Poster B2

**Optical properties of LiF, NaF and KF based on self-interaction corrected pseudopotentials** — •Christoph Sommer, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster, D-48149 Münster, Germany

Many-body perturbation theory yields optical properties of semiconductors and insulators in good agreement with experiment. In this approach, the Bethe-Salpeter equation is solved for an effective two-particle problem. Very good one-particle excitation energies – as given, e. g., by the GW approximation – are a necessary prerequisite for obtaining reliable results. The GWA is very demanding, however. In turn, self-interaction corrected (SIC) pseudopotential calculations can also provide very accurate electronic energies for ionic wide-band-gap materials. At the same time, they are only about as costly as regular DFT-LDA calculations.

We investigate the applicability of SIC energies and wavefunctions in the Bethe-Salpeter equation using the alkali metal fluorides LiF, NaF and KF as examples. This is done on the basis of SIC pseudopotentials [1] that have been shown to yield bandstructures in good agreement with experiment. We arrive at optical spectra that are in accord with the results available in the literature for these systems.

[1] B. Baumeier, P. Krüger, J. Pollmann, and G. Vajenine, Phys. B **78**, 12511 (2008)

O 60.4 Wed 17:45 Poster B2

**Excess electron at the ice surface: an approach via mixed quantum/molecular mechanics simulations** — •Volker Mosert and Michel Bockstedte — Theor. Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

Electron solvation shows a rich varity of phenomena, like surface vs. interior bound states in water clusters. *Ab initio* theory greatly helped to understand these phenomena. However, regarding ice-surfaces, it is desirable to go beyond present *ab initio* models of $I_h$ (0001) and to address, for first insight, the complex morphology of ice films as well as the solvation on the long time scale with a less costly approach.[1] Such an alternative is the mixed QM/MM approach.[2] It treats the water-water interaction via classical potentials and the electron-water interaction via a pseudopotential quantum-mechanically. Although its relevance has been demonstrated for water clusters,[2] applications to the electron solvation at the ice surface are scarce [3] and address the temperature regime where pre-melting occurs. For an evaluation of the method, we address the traping of excess electrons at the $I_h$ surface. For prototypical surface defects, the formation energy as well as the electron binding energy are evaluated using different models of the water-interaction. In comparision to recent DFT-calculations, we obtain a good description with TIP4P potentials.

[1] M. Mehlhorn and K. Morgenstern, Phys. Rev.Lett. **99**, 246101 (2007); Bovensiepen *et al* J. Chem. Phys. C **113**, 979 (2009).

[2] L. Turi, W.-S. Sheu, and P. J. Rossky, Science **309**, 914.

[3] A. Madarász *et al*, J. Chem. Phys. **126**, 234707 (2007).

O 60.5 Wed 17:45 Poster B2

**Analysis of Neural Network Potential-Energy Surfaces for Atomistic Simulations** — •Tobias Morawietz, Nongnuch Artrith, and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

In recent years, artificial Neural Networks (NN) have become a promising new method to represent accurate potential energy surfaces (PES) for molecular and condensed systems. NN potentials are constructed using a set of reference points obtained in electronic structure calculations, which are then interpolated to a continuous PES by the very flexible functional form of the NNs. The NN potentials can then be evaluated several orders of magnitude faster than the underlying electronic structure data. Therefore NN potentials are ideal tools to perform long molecular dynamics simulations of large systems. However, because of the a priori non-physical functional form, NN potentials have to be constructed with care. Using various molecules, clusters and solids we analyze how the physical functional form is approximated by NNs and discuss the scope and limitations of the method.

O 60.6 Wed 17:45 Poster B2

**Atomic-resolution AFM imaging of single molecules** — •Fabian Mohn, Leo Gross, Nikolaj Moll, Peter Liljeroth, and Gerhard Meyer — IBM Research - Zurich, 8803 Rüschlikon, Switzerland

We have recently developed a technique, which enables imaging of individual admolecules with atomic resolution using noncontact atomic force microscopy [L. Gross et al., *Science* **325**, 1110 (2009)]. The key to achieving intramolecular contrast is a controlled functionalization of the microscope's tip apex. We compare the imaging capabilities of different tip terminations and present measurements of the distance-dependence of the imaging contrast. These investigations – along with first-principle density functional theory calculations – indicate, that AFM operation in the regime of maximal attractive forces is crucial for achieving atomic contrast on molecules. Such close-distance operation is facilitated by using oscillation amplitudes in the sub-angstrom range.

O 60.7 Wed 17:45 Poster B2

**Atomic charge state determination by AFM** — •Leo Gross[1], Fabian Mohn[1], Peter Liljeroth[1], Jascha Repp[2], Franz J. Giessibl[2], and Gerhard Meyer[1] — [1]IBM Research - Zurich, 8803 Rüschlikon, Switzerland — [2]Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

We investigated the charge state switching of individual gold and silver adatoms on ultrathin NaCl films on Cu(111) using a qPlus tuning fork atomic force microscope (AFM) operated at 5 Kelvin with oscillation amplitudes in the sub-Ångstrom regime. Charging of a gold adatom by one electron charge increased the force on the AFM tip by a few piconewtons. Employing Kelvin probe force microscopy (KPFM) we also measured the local contact potential difference (LCPD) as a function of the tip height above differently charged adatoms. We observed that the LCPD is shifted depending on the sign of the charge and allows the discrimination of positively charged, neutral, and negatively charged atoms. [L. Gross, et al., Science 324, 1428 (2009)]

O 60.8 Wed 17:45 Poster B2

**Magnetokraftmikroskopie in starken externen Magnetfeldern** — •Lars Ungewitter, Ivo Knittel und Uwe Hartmann — Fachbereich Experimentalphysik, Campus C6.3, 66123 Saarbrücken

In einen Kryostaten mit Raumtemperaturbohrung und supraleitender Magnetfeldspule wird ein modifiziertes kommerzielles Raumtemperatur-Rasterkraftmikroskop eingeführt und als Magnetokraftmikroskop (MFM) bei Feldern bis 1.5 Tesla betrieben. Die Vorteile in der Handhabung sind im Vergleich zum Betrieb eines MFM im variable temperature insert (VTI) ein leichter Zugang zu Probe und Spitze, größere Scanbereiche, und die Abbildung auch ungünstiger Topografien. MFM-Studien über vollständige Hysteresekurven von epitaktischen Magnetitfilmen, SmCo-Filmen und patterned media - Speichermedien werden vorgestellt und diskutiert.

O 60.9 Wed 17:45 Poster B2

**The open source scanning probe control software package Gxsm** — Percy Zahl[1], •Thorsten Wagner[2], Rolf Möller[3], and Andreas Klust[4] — [1]Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, USA — [2]Institute of Experimental Physics, Johannes Kepler University Linz, Austria — [3]Department of Physics, University Duisburg-Essen, Germany — [4]Lewven, Belgium

Gxsm is a full featured and modern scanning probe microscopy (SPM) software. It can be used for powerful multidimensional image/data processing, analysis and visualization. Connected to an instrument, it is operating many different flavors of SPM, e.g. scanning tunneling microscopy (STM) and atomic force microscopy (AFM) or, in general, two-dimensional multi channel data acquisition systems. The Gxsm core can handle different data types, e.g. integer and floating point numbers. An easily extendable plug-in architecture provides many image analysis and manipulation functions. A digital signal processor (DSP) subsystem runs the feedback loop, generates the scan signals and acquires the data. The programmable Gxsm vector probe engine can perform any thinkable spectroscopy and manipulation task, such as scanning tunneling spectroscopy (STS) and tip formation. Due to the support for a new DSP hardware (SoftdB SR-MK2&A810) new developments like multi channel feedback mixing and adaptive infinite response for the tunneling current had been implemented. The Gxsm software is released under the GNU general public license (GPL) and can be obtained free of charge via internet from http://gxsm.sf.net.

O 60.10 Wed 17:45 Poster B2

**Forces in Molecular Electronics** — •Mathias Neu, Andreas Pöllmann, and Jascha Repp — Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

In recent years low-temperature scanning tunneling microscopy (STM) and spectroscopy have been very successfully used to study electron transport through individual molecules. However, STM investigations are limited to conducting substrates and the experimental data is determined by both the geometry and the electronic structure of the sample in a complex and often ambiguous manner. To overcome these two limitations we plan to experimentally implement force detection as an additional measure in molecular electronics. To this end a combined STM and scanning force microscope is being build up. The force detection scheme is based on using tuning forks as force sensors [1]. Unlike in the case of cantilever-based AFM, in this setup the scanning tip is not an integral part of the force sensor and can be a metal tip as is usually used in STM, thus making it an ideal force-detection technique to be combined with STM. On our poster we present our progress on the experimental setup.

[1] Giessibl, Appl. Phys. Lett. 73, 3956 (1998)

O 60.11 Wed 17:45 Poster B2

**Atomic Force Microscopy meets Field Ion Microscopy** — •Jens Falter[1], Daniel-Alexander Braun[1], Udo D. Schwarz[3], Hendrik Hölscher[2], André Schirmeisen[1], and Harald Fuchs[1] — [1]Physikalisches Institut, University of Münster and CeNTech, Center for Nanotechnology, Münster, Germany — [2]IMT, Forschungszentrum Karlsruhe, Germany — [3]Department of Mechanical Engineering, Yale University, New Haven, USA

In atomic force microscopy (AFM), the contrast stems from the interaction between the probing tip and the sample. Although the AFM is even able to measure interaction forces with the force spectroscopy method, the underlying contrast mechanism is still not completely understood. In some extend this is due to the unknown tip shape in an AFM, which is able to resolve atomic resolution of sample surfaces - but not of the tip apex. The Field Ion Microscope (FIM) is a technique which resolves the apex of metal tips with atomic precision. The images of the tip gained with this method allow an atom by atom reconstruction of the foremost atom layers of the tip. We present our home-build system which combines these two microscope techniques: an AFM-head which has been proven to operate at low temperatures in ultra high vacuum [1] and a FIM, which can image the apex of the tungsten tip. The force sensor is based on a tuning fork in the q-plus concept [2] with an electrochemical etched tungsten tip at the end of the free prong. This setup enables us to perform force spectroscopy experiments with well characterized tips from the FIM images. [1] B.Albers et. al., Rev. Sci Instrum. 79 033704 (2008) [2] F.J.Giessibl, APL. 76 1470 (2000)

O 60.12 Wed 17:45 Poster B2

**Quantitative Kelvin probe force microscopy imaging on locally doped Si** — •Christine Baumgart[1], Anne-Dorothea Müller[2], Falk Müller[2], Manfred Helm[1], and Heidemarie Schmidt[1] — [1]Forschungszentrum Dresden-Rossendorf, Institut für Ionenstrahlphysik und Materialforschung, P.O. Box 510119, 01314 Dresden — [2]Anfatec Instruments AG, Melanchthonstr. 28, 08606 Oelsnitz

Failure analysis and optimization of nanoelectronic devices require knowledge of their electrical properties. Kelvin probe force microscopy (KPFM) is a standard technique for the investigation of the surface potential. Since KPFM was developed in 1991 the measured KPFM signal was attributed to the contact potential difference (CPD) between conductive probe and sample. We show that the CPD is not suitable to describe the measured Kelvin bias in semiconductors quantitatively and introduce a unique KPFM model [1] which successfully correlates the measured Kelvin bias with the difference between Fermi energy and respective band edge. Quantitative dopant profiling is demonstrated on cross-sectionally prepared Si epilayer structures and on a Si dynamic random access memory cell.

[1] C. Baumgart, M. Helm, H. Schmidt, Phys. Rev. B 80 (2009) 085305.

O 60.13 Wed 17:45 Poster B2

**Growth of Co-Salen on NiO(001): An atomic force microscopy study in ultrahigh vacuum** — •Johannes Hattendorff, Alexander Schwarz, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, 20355 Hamburg, Germany

Co-Salen is a paramagnetic metal-organic Schiff-base-complex with a central cobalt atom that carries spin. In previous studies the adsorption and growth of Co-Salen was investigated with atomic force microscopy (AFM) on bulk NaCl(001) [1]. The latter investigation revealed that at room temperature the physisorbed molecules are very mobile on NaCl(001) and exhibit a three-dimensional Vollmer-Weber type of growth. Step decoration and two different well ordered crystalline morphologies with bulk-like structures could be identified.

Here we deposit Co-Salen on NiO(001) which is an insulator like NaCl but with a smaller band gap (3.8 eV instead of 9 eV). First results obtained with AFM for sub-monolayer coverage show a step-flow growth and the formation of islands on terraces. At higher coverage the growth appears to be layer-wise. These observations indicate that the molecule-surface interaction on the transition-metal oxide NiO is very different compared to the alkali-halide NaCl. Note that although both surfaces are ionic with rock salt structure bonds in NiO exhibit a significant covalent character and the lattice constant is much smaller (417 pm instead of 564 pm). Both properties might alter the adsorption geometry and interaction strength drastically.

[1] S. Fremy et al., Nanotechnology 20, 405608 (2009).

O 60.14 Wed 17:45 Poster B2

**Observation of Spin Excitation by Inelastic Tunneling Spectroscopy of Fe atoms on a Semiconductor Surface** — •Alexander A. Khajetoorians, Bruno Chilian, Sergei Schuwalow, Frank Lechermann, Jens Wiebe, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Hamburg, Germany

We present a combined experimental and theoretical study of single Fe atoms on a III-V (110) semiconductor surface. Using tunneling spectroscopy at very low temperature (300mK), we observe a zero-field gap in the differential conductivity measured on the Fe atom which can be attributed to magnetic anisotropy. The total spin of the Fe atom as well as its anisotropy is also calculated by first principles calculations within density functional theory and related to the experimental data utilizing a simple quantum magnetic Hamiltonian. In the context of this model, we discuss the predicted magnetic field dependent magnetization and relate it to experimental data in high magnetic fields (12T).

O 60.15 Wed 17:45 Poster B2

**Study on automated atom manipulation** — •Boris Wolter[1], André Kubetzka[1], Roland Wiesendanger[1], Bernd Schütz[2], and Jianwei Zhang[2] — [1]Institut für Angewandte Physik, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg — [2]Technical Aspects of Multimodal Systems (TAMS), Universität Hamburg, Vogt-Kölln-Str. 30, 22527 Hamburg

Recent years have shown an increasing number of investigations concerning automation of atom manipulation via STM [1, 2]. In our study, we employed a Monte-Carlo simulation to model the interactions between tip, sample and adsorbates [3]. Based on this simulation, we explored the prospects of automated lateral manipulation of single atoms. Required techniques like adsorbate detection, learning of manipulation parameters, path planning with uncertainty [4] and manipulation tracing were developed and tested within the simulated STM environment.

In more recent work, we focus on a local scan method for exact positioning of the tip above specified adsorbates [1]. The primary goals of this method are to prevent time consuming scans of large areas, to counter drift in long-term experiments and to increase experimental accuracy. Once finished, it will be combined with automation techniques for tunneling spectroscopy and atom manipulation.

[1] H. Chen *et al.*, Proc. of ICRA, 169-174 (2005)
[2] T. Knepper *et al.*, Proc. of ROBIO, 95 (2005)
[3] A. Kühnle *et al.*, Surf. Sci. 449, 15 (2001)
[4] J.P. Gonzalez *et al.*, Proc. of IROS, 2435-2442 (2005)

O 60.16 Wed 17:45 Poster B2

**Mechanical Behaviour of Graphenes on a Solid Surface** — •Stefan Eilers and Jürgen P. Rabe — Department of Physics, Humboldt-Universität zu Berlin, Germany

Graphene is a promising candidate for future generation electronic devices. Structuring and, more general, manipulation of graphenes are needed for the development of possible applications. Scanning force microscope (SFM) techniques are promising for the investigation of single or multilayer graphenes, because of their thinness, flexibility and flatness. Here we demonstrate the manipulation of graphene on a SiO2 surface. Contrary to the cutting of single polymers with an SFM tip, which always results in only one cut, cutting graphenes results in two cuts. Therefore nanogaps and nanoribbons can be readily produced. This effect is attributed to the one- and two-dimensionality of polymers and graphene, respectively. Simple explanations are provided to understand the behaviour. It is demonstrated inhowfar basic models for describing bending and breaking of macroscopic objects are applicable also for these nanoscopic systems.

O 60.17 Wed 17:45 Poster B2

**A Dynamic Force and Scanning Tunneling Microscopy Study of Line Defects and Step Edges in the Alumina Film on NiAl(110)** — •Lars Heinke, Leonid Lichtenstein, Georg Hermann Simon, Thomas König, Markus Heyde, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14196 Berlin, Germany

The aluminum oxide thin film on NiAl(110) is an often used model system in catalysis. Line defects in the film like step edges and antiphase domain boundaries are prominent structure elements and they are referred to as active sites [1]. In this study, frequency modulation dynamic force microscopy (FM-DFM) and scanning tunneling microscopy (STM) are applied to determine the atomic structure of the thin film and its line defects in ultra high vacuum at 5 K [2]. By means of bias spectroscopy and contact potential measurement different density of electronic states as well as the electrostatic potential were determined. We would like to link the electronic structure of the line defects to catalytic processes.

[1] S. Schauermann et al., Chem. Phys. Lett. 381 (2003) 298-305
[2] G. H. Simon et al., New J. Phys. 11 (2009), 093009

O 60.18 Wed 17:45 Poster B2

**SPM tip cleaning by electron-bombardment for investigation of samples prepared by applying nanospherelithography (NSL)** — •David Hellmann, Uli F. Wischnath, and Achim Kittel — EHF, Fak. V, Physik, Carl von Ossietzky Universität Oldenburg

The heat transfer between a sample and a probe can be measured using a Near-field Scanning Thermal Microscope (NSThM) [1,2]. The NSThM combines a STM tip with a thermocouple sensor. Thus data concerning the heat transfer a few nm above the scanned surface can be collected by measuring the thermovoltage. Cleanliness of the tip and the sample is an issue of great importance as the NSThM seems to be more sensitive to adsorbates than traditional STM techniques. By applying nanospherelithography (NSL), structured surfaces have been prepared and subsequently scanned using a NSThM tip. Residues of unknown origin seem to persist on either the tip or the sample though intensive cleaning procedures have been applied to the latter. X-Ray-Photoelectron-Spectroscopy (XPS) conducted on the sample did not reveal the presence of residues. Therefore electron-bombardment has been applied to the tip, as this has been reported in [3] to be an established method to heat a tip to several hundred degrees Celsius. As the tip used here gives a thermovoltage when its temperature is changed, it should be possible to measure the heating effect of the bombardment directly. Interestingly, no clear evidence could be gathered that the tip can be heated up significantly. Literature: [1] A. Kittel et al., PRL 95, 224301 (2005) [2] U. Wischnath, RSI 79, 073708 2008 [3] S. Ernst et al., Science and Technology of Advanced Materials 8 (2007)

O 60.19 Wed 17:45 Poster B2

**Investigating structured surfaces with a near-field scanning thermal microscope using a new scanning method** — •Lars Hoelzel, Uli F. Wischnath, and Achim Kittel — University of Oldenburg - Energy an Semiconductor Research Laboratory - C. v. Ossietzkystr. - D 26111

The near-field scanning thermal microscope (NSThM) [1] is able to measure the thermal flux between a modified tip of a STM and a heated or cooled sample surface under ultra-high vacuum conditions. Hence, the main contribution is mediated by evanescent electro-magnetic fields. Up to now the heat flux was investigated in constant current mode of the STM on which the NSThM is based [2]. While the tunnelling current decays on a short length scale the heat flux decays on a roughly ten times larger length scale. The new scan mode employs a control loop which keeps the heat current constant. Therefore, it is possible to investigate the influence of the surface morphology on the heat flux at larger distances. The results gained by the constant thermovoltage mode suggest that the evanescent field reaches farther out in trenches compared to a convexly curved surface or even a flat surface.

[1] Uli F. Wischnath et al., Rev. Sci. Instrum. 79, 073708 (2008)
[2] Achim Kittel et al., Appl. Phys. Lett. 93, 193109 (2008)

O 60.20 Wed 17:45 Poster B2

**Appearence of Adsorbates in Near-field Scanning Thermal Microscopy** — •Ludwig Worbes, Uli F. Wischnath, and Achim

Kittel — Universität Oldenburg - EHF - EPKOS

The Near-field Scanning Thermal Microscope (NSThM) is an STM using a probe featuring a miniaturized thermocouple temperature sensor. Therefore it is possible to measure the heat flux between the probe and a heated or cooled sample, in this case Au(111), at distances of a few nanometres [1,2]. By operating in UHV the heat transfer should be restricted to radiation dominated by evanescent electromagnetic fields at this distances.

In reality heat transport measurements turn out to be highly sensitive to adsorbates on the surfaces. Electrically nonconducting adsorbates possibly form a bridge between sample and probe, resulting in phononic heat transfer, without any influence to the electric conductivity of the tunnel gap. Indications can be seen in heat flux versus distance measurements. These measurements are performed with different distance sweep procedures and velocities to survey occurrence and dynamic behaviour of adsorbate bridges.

Even NSThM measurements performed on in situ cleaned samples display this indications, even though STM images show a clean reconstructed surface. Apparent-barrier-height measurements by STM and XPS measurements display inconsistent results.

[1] Uli F. Wischnath et al., Rev. Sci. Instrum. 79, 073708 (2008)

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

### O 60.21 Wed 17:45 Poster B2

**Infrared near-field nanospectroscopy of SiO2 structures embedded at Si[100] surfaces** — Marc Tobias Wenzel[1], •Hans-Georg von Ribbeck[1], Anja Krysztofinski[1], Phillip Olk[1], Andreas Hille[1], Oliver Mieth[1], Peter Milde[1], Lukas M. Eng[1], Rainer Jacob[2], and Manfred Helm[2] — [1]Institut für Angewandte Photophysik, TU Dresden, George-Bähr-Straße 1, 01069 Dresden — [2]Institut für Ionenstrahlphysik und Materialforschung, Forschungszentrum Dresden-Rossendorf, 01214 Dresden

Scattering scanning near-field optical microscopy (s-SNOM, or s-NSOM) allows for optical inspection of nanostructures and materials with a resolution far better than the diffraction-limited resolution of far-field microscopy methods. This is of particular interest in case of mid-infrared investigations. The combination of such an s-SNOM with the wavelength-tunable free-electron laser (FEL) located at the Forschungszentrum Dresden-Rossendorf provides a versatile tool for the nondestructive sample investigation in the IR fingerprint region at nanoscopic resolution.

Here, we present the IR-s-SNOM nanospectroscopy investigations of 400-nm-deep $SiO_2$ trenches, embedded in intrinsic silicon [100]. Measurements were performed in the wavelength range from 9 to 11 $\mu$m (1100 $cm^{-1}$to 910 $cm^{-1}$). We experimentally demonstrate the expected contrast reversal of the near-field amplitude signals of Si and $SiO_2$. This contrast reversal is due to the material-specific near-field enhancement at the reststrahlen band of $SiO_2$. We also present comparative measurements using a $CO_2$ laser at 10.6 $\mu$m (943 $cm^{-1}$).

### O 60.22 Wed 17:45 Poster B2

**Development of a modular multiple temperature UHV Scanning Tunneling Microscope** — •Carsten Tröppner, Lutz Hammer, and Menko Alexander Schneider — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

We present our newly constructed low temperature scanning tunneling microscope (STM) designed for high resolution scanning tunneling spectroscopy (STS) measurements under ultra high vacuum (UHV) conditions. A standard non-UHV helium bath magnet cryostat is used for cooling the STM down to 4.2K and below (Eigler-Design). With the aim to carry out STM measurements at room temperature as well as low temperature we implemented the STM as a mobile unit, which can be transferred within the UHV chamber between regions of different temperature. The mobility of the STM furthermore provides an easy sample transfer and the possibility to transfer it out of the UHV chamber through a load-lock system. Hence the full instrument or the tip only can be exchanged.

### O 60.23 Wed 17:45 Poster B2

**Electronic characterisation of thin metallic films using Kelvin Probe Force Microscopy and 4-Point-Probe** — •Oliver Ochedowski, Benedict Kleine Bussmann, Florian Meinerzhagen, and Marika Schleberger — Universität Duisburg-Essen, Lotharstrasse 1, 47057 Duisburg

We are investigating the electronic structure of thin metallic films, especially graphene on insulating substrates like siliconoxide. To achieve this, we are combining atomic force microscopy with Kelvin probe technology under UHV conditions and ex situ to map the surface contact potential of these films. This method, first utilized by M. Nonnenbacher, uses the measured force between between the tip and the sample as the control variable [1]: An ac voltage $U_{mod}$ between the tip and sample is modulated on a dc part $U_{Bias}$ until the frequency shift due to electrostatic forces is minimized. As a result the difference in contact potentials can be mapped. We also measure the electrical surface resistance directly by using a four-point-probe mounted on a small micromanipulator. We present first test measurements under ambient conditions.

[1]M.Nonnenmacher, M.P. O Boyle, and H.K.Wickramasinghe Appl. Phys.Lett. 58 (25),2921-2923 (1991)

### O 60.24 Wed 17:45 Poster B2

**Electronic characterisation of thin metallic films using Kelvin Probe Force Microscopy and 4-Point-Probe** — •Oliver Ochedowski, Benedict Kleine Bussmann, Florian Meinerzhagen, and Marika Schleberger — Universität Duisburg-Essen, Lotharstrasse 1, 47057 Duisburg

We are investigating the electronic structure of thin metallic films, especially graphene on insulating substrates like siliconoxide. To achieve this, we are combining atomic force microscopy with Kelvin probe technology under UHV conditions and ex situ to map the surface contact potential of these films. This method, first utilized by M. Nonnenbacher, uses the measured force between between the tip and the sample as the control variable [1]: An ac voltage $U_{mod}$ between the tip and sample is modulated on a dc part $U_{Bias}$ until the frequency shift due to electrostatic forces is minimized. As a result the difference in contact potentials can be mapped. We also measure the electrical surface resistance directly by using a four-point-probe mounted on a small micromanipulator. We present first test measurements under ambient conditions.

[1]M.Nonnenmacher, M.P. O Boyle, and H.K.Wickramasinghe Appl. Phys.Lett. 58 (25),2921-2923 (1991)

### O 60.25 Wed 17:45 Poster B2

**Near-field infrared microscopy with a broadband light source** — •Stefanie Bensmann[1], Christoph Janzen[1], Reinhard Noll[1], Jón Mattis Hoffmann[2], and Thomas Taubner[1,2] — [1]Fraunhofer-Institut für Lasertechnik (ILT), Aachen — [2]I. Physikalisches Institut IA, RWTH Aachen

Scattering-type near-field infrared microscopy offers a wavelength-independent spatial resolution of approximately 30 nm together with chemical sensitivity [1]. Spectra are usually recorded by consecutive measurements that are performed at different wavelengths, which is time-consuming. Additionally, the limited spectral range covered by conventional MIR laser sources does not cover samples like e.g. certain semiconductors (GaAs), polar crystals and different polymers.

Broadband IR light sources allow circumventing these problems by recording a full spectrum with a single measurement in an extended frequency range [2, 3]. However, a laser power of only a few $\mu$W restricts measurements to samples with a strong resonance like SiC. We present work on combining a broadband IR laser (power of several mW at $5 - 12$ $\mu$m) that is currently developed at the ILT with the NeaSNOM (near-field optical microscope from Neaspec, www2.neaspec.com). This new system will extend the spectral range covered and allow to examine samples with weaker resonances.

[1] F. Keilmann, R. Hillenbrand, in: Nano-optics and Near-field Optical Microscopy, p. 235; X. Zhang, K. Wang (eds), Artech House 2009.

[2] M. Brehm et al., Optics Express 15, p. 11222, 2006.

[3] S. Amarie et al., Optics Express 17, p. 21794, 2009.

### O 60.26 Wed 17:45 Poster B2

**STM and STS studies of ferroelectric domain structures on BaTiO$_3$(001) and BaTiO$_3$(111) single crystals** — •Maik Christl, Christian Hagendorf und Wolf Widdra — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Germany

A new method of characterizing ferroelectric domain structures on nanometer scale by using a STM is presented. We demonstrate a domain contrast of various domain arrangements based on dI/dV maps. On $BaTiO_3(001)$ we can differentiate between ferroelectric $c^+$, $c^-$, and a domains based on STM and STS. Additionally domain boundaries between 90° in-plane polarized domains become visible in STS maps. During heating $BaTiO_3(111)$ above the Curie temperature, a modified domain pattern is found. The ferroelectric domain structure can be modified locally by tunneling at higher bias voltages. This STM-induced domain nanostructuring will be discussed in comparison to recent AFM studies [1].

[1] A. Gruverman et al., *Scanning Force Microscopy Studies of Domain Structure in* $BaTiO_3$ *Single Crystals*, Jpn. J. Appl. Phys. Vol. 36 (1997) pp.2207-2211

O 60.27 Wed 17:45 Poster B2

**Chirped Pulse Two Photon Photoemission technique to study adsorbate dynamics** — •Marianne Bader, Indranil Sarkar, Felix Steeb, Andreas Ruffing, and Martin Aeschlimann — Department of Physics, University of Kaiserslautern, 67663 Kaiserslautern, Germany

Time resolved Two Photon Photoemission (TR 2PPE) is a well-known method in surface physics to study adsorbate dynamics. However, it's temporal resolution is limited by the Heisenberg uncertainty principle. Here we propose a novel method to observe dynamics of adsorbate states using Chirped Pulse Two Photon Photoemission (CP 2PPE). This method utilizes a suitable modified spectral phase of the exciting femtosecond laser pulse, modulated by a Fork prism pair [1]. We apply this technique in the case of Cs/Cu(111), where we observe significant energy shifts of the excited adsorbate state (Cs*) as well as a peak broadening. The obeserved asymmetry in peak position is suggestive of possible adsorbate motion [2]. We further propose to apply the method of CP 2PPE to systems with shorter time constants where time resolved methods are restricted.

[1] R. L. Fork et al, Opt. Lett. 9 (1984) 150

[2] F. Steeb, PhD Thesis, TU Kaiserslautern, 2008

O 60.28 Wed 17:45 Poster B2

**Analysis of XPD-patterns by means of Genetic Algorithms** — •Tobias Lühr[1], Daniel Weier[1,2], Frank Schönbohm[1,2], and Carsten Westphal[1,2] — [1] Fakultät Physik - TU Dortmund, Otto-Hahn-Str.4, D 44221 Dortmund, Germany — [2] DELTA - TU Dortmund, Maria-Goeppert-Mayer-Str. 2, D 44227 Dortmund, Germany

Angle-scanned X-Ray Photoelectron Diffraction (XPD) is a powerful technique for the investigation of crystalline interfaces and surfaces. This technique provides the atomic structure of the investigated sample as well as the chemical state of the atoms. In order to determine the accurate structure from the recorded data it is necessary to simulate the XPD-pattern. A genetic algorithm was developed that generates and optimizes different surface structure models. Each structure is defined by a basic model structure and a transformation that depends on a reasonable size of variable parameters (genes). After generating a set of modified structures by variation of the genes the algorithm calculates the multiple scattering pattern for each structure and evaluates the pattern with an R-factor. If no R-factor has reached a specified value, the algorithm creates a new generation of parameter sets by a combination or mutation of the genes of the last generation. In this procedure the genes with a low R-factor are preferred to be chosen. With algorithm we present here it was possible to determine several atomic surface structures like Cyclopentene/Si(100), Pyridine/Si(100), and $ZrSi_2$/Si(100).

O 60.29 Wed 17:45 Poster B2

**Analysis of optical systems, caustic formation and contrast depth in mirror electron microscopy** — •Sergej Nepijko and Gerd Schönhense — Institute of Physics, University of Mainz, 55099 Mainz, Germany

The conditions of realization of positive and negative contrasts in electron mirror microscope are shown. The contrast depth is analyzed as well, that is the sensitivity of electron mirror microscope to disorders of homogeneity on the object (local magnetic and electric fields, surface relief). Because of these, electron trajectories are distorted and electrons acquire additional velocity components in radial and azimuthal directions. This leads to the shift of the observed point on the screen and, as a consequence, to an image contrast. Since the electron energy, when reflected, is close to zero, electrons are influenced by heterogeneities for a long time. It causes high sensitivity to heterogeneities, up to the crossing of electron trajectories (caustics are generated). The conditions of caustic generation due to local electric or magnetic fields are analyzed: (i) the larger the distance $r$ from the centre of the image, the easier the caustic is generated, (ii) after generation, the caustic expands with growth of distance $r$ from the centre of the image, (iii) the value of azimuthal linear shift $S = \gamma r$ ($\gamma$ - azimuthal angular shift) reverses sign when passing through the centre ($r = 0$). A dark wedge will be the continuation of the bright wedge opposite the centre. The caustic disappears in the centre of the screen. The contrast increases with growth of $r$. This differs from the contrast due to electric fields, which does not depend on $r$.

O 60.30 Wed 17:45 Poster B2

**Comparative EELS on carbon-based materials** — •Thomas Haensel, Stefan Krischok, Juergen A. Schaefer, and Syed Imad-Uddin Ahmed — Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany

Carbon-based materials are of great interest, due to the many possible applications in various fields. For example regenerative wood-based biopolymers made of cellulose, lignin and additives are expected to be low-cost ground materials for the use in various typical polymer applications such as fuel cells. Additionally, hard synthetic materials like diamond-like (DLC) and nanocrystalline diamond (NCD) films are relevant as transparent protective coatings, use in bio-sensor systems and electron emitters. In contrast to DLC films, graphite (HOPG) is very soft and has a high electric conductivity. In this contribution various carbon-based materials were analyzed with electron energy loss spectroscopy (EELS), which is a surface sensitive technique and provides information about plasmons in the surface and mean surface region. Additionally, these materials were characterized with XPS to extract further information about the chemical composition and functional groups at the surface. The so called $\pi$-plasmon as well as other energy losses will be discussed and a comparative survey of EELS of surfaces with different surface preparations will be presented.

O 60.31 Wed 17:45 Poster B2

**The High Resolution Diffraction Beamline P08 at PETRA III - First Experiments** — •Carsten Deiter, Florian Bertram, Kathrin Pflaum, and Oliver H. Seeck — Hasylab am DESY, Notkestr. 85, 22607 Hamburg, Germany

Since fall 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 (HV and UHV) 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 close by in the near future. First user experiments have been performed and the results from first in-house experiments will be presented which show the benefits of the PETRA III beam parameters.

O 60.32 Wed 17:45 Poster B2

**Molecular trapping and scattering at ionic liquid surfaces** — •Andre Dorsch, Matthias Schöppke, and Reinhard Denecke — Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnéstr. 2, 04103 Leipzig, Germany

Gas uptake in ionic liquids is an important process for the technological use of such substances [1,2]. Using a supersonic molecular beam setup and a moveable quadrupole mass spectrometer, the interaction of $CO_2$ and $N_2$ with surfaces of imidazolium-based ionic liquids have been studied. Employing angle-resolved measurements, trapping and inelastic scattering events can be determined. Parameters like the kinetic energy of the impinging molecules, which influence the behaviour, are systematically varied. From the results residence times of gases in ionic liquids are derived.

[1] J. F. Brennecke, E. J. Maginn, Purification of Gas with Liquid Ionic Compounds. US Patent 6,579,343 (2003).

[2] A. Yokozeki, M. B. Shiflett, Appl. Energy 84, 351 (2007).

O 60.33 Wed 17:45 Poster B2

**Diffusion of Xe on Multilayer Xe** — •Anuschka Schmitt, Matthias Buschmann, Thomas M. Ernst, and Heinz J. Jänsch — Philipps-Universität Marburg

Diffusion of Xe on Xe-multilayers or inside the multilayers is largely unexplored. This mainly reflects a lack of methods. We employ NMR of $^{129}$Xe to investigate surface phenomena. The sensitivity is greatly enhanced by the use of laser-polarized $^{129}$Xe.

Here we explore different NMR-techniques to study diffusion: surface layer to second layer exchange could be monitored through the strong chemical shift difference ($\Delta\sigma \approx 100$ ppm) of the two; disorder in the solid is spectrally seen by broad lines due to chemical shift fluctuations, so that annealing is detected by line narrowing; direct diffusional motion is measured in pulsed magnetic field gradients.

UHV-compatible gradient coil design was tested and a proof of principle demonstrated by sodium diffusion in a NaCl aqueous solution.

O 60.34 Wed 17:45 Poster B2

**Contrast formation in the SEM at lowest landing energy of the electrons** — •Philipp Tonndorf, Steffen Schulze, and Michael Hietschold — Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany

The primary electrons initially have normal energies of several keV and are slowed down until just before the sample to a few 100 eV by an electric opposing field. This ensures that the chromatic error in the electron optics remains low.

Electron with reduced energy can't penetrate so far into the sample. So they have a smaller interaction volume, which promises to improve the resolution. For example, you can see the walls of the studied carbon nanotubes, which you can't recognize with higher electron energies.

There is also a change in the secondary electron yield and the backscatter coefficient, which causes other contrasts. For gold on carbon the contrasts reversed under 500eV landing energy.

Even charges of the sample can be reduced. You could represent structures from Al on Si3N4 with opposing field better than without opposing field.

This technique is very surface sensitive and can detect details, which are hidden at higher energies and you can investigate samples that would be destroyed by higher landing energies. Poorly or nonconductive samples can be scanned without the need to evaporate a conductive layer.

O 60.35 Wed 17:45 Poster B2

**Real-time simulation of Si(001) 2PPE spectra** — •Henning Husser and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel, 24098 Kiel, Germany

The photo-current induced by a fs laser-pulse is simulated by real-time *ab initio* TDDFT molecular dynamics. The electronic structure of the Si(001) surface is described within density-functional theory using a slab geometry. To account for the finite escape depth of the photo-electrons emitted from a solid surface like Si(001), an optical potential acting on the conduction states only is included in the integration of the time dependent Kohn-Sham equations. The calculation is carried through at frozen-in effective potential. We note, however, that the time-dependent Kohn-Sham equations could be integrated self-consistently in the case of atoms and small clusters, if no optical potential is included. The photo-emission spectrum is derived from the Fourier transform of the single-particle wave-functions. Normal emission 2PPE spectra from Si(001) for s and p-polarized light are presented. We analyze the photon energy and polarization dependence of the theoretical spectra and we compare to experimental 2PPE spectra by Kentsch *et al.*[1].

[1] C. Kentsch, M. Kutschera, M. Weinelt, T. Fauster, M. Rohlfing, Phys. Rev. B **65**, 035323 (2001).

## O 61: Invited talk (Van Bokhoven, Jeroen)

Time: Thursday 9:30–10:15 Location: H36

**Invited Talk** O 61.1 Thu 9:30 H36

**Shining light on catalysis** — •Jeroen A. van Bokhoven — ETH zurich HCI e127 8093 Zh CH

Understanding the functioning of a heterogeneous catalyst is essential to the design and control of the structure of the catalyst of the future. There is close interplay between the reactant and the catalytically active site, which determines the ultimate performance of the latter. I will discuss insights into the roles played by the structure of a catalytically active site and its immediate surroundings on the activity and selectivity of reactions. This, in turn, is the basis for understanding how a heterogeneous catalyst functions.

## O 62: Graphene III

Time: Thursday 10:30–12:30 Location: H31

O 62.1 Thu 10:30 H31

**Structural properties and site specific interactions of Pt with the graphene/Ru(0001) moiré overlayer** — Kerstin Donner, Martin Willenbockel, and •Peter Jakob — Fachbereich Physik, Philipps-Universität Marburg, Germany

The growth, structure, and adsorptive properties of graphene on Ru(0001) has been investigated in detail [1]. Thereby the coherence of graphene layers on Ru(0001) over extended distances has been employed to discriminate between A and B types of Ru(0001) steps and to identify fcc as well as hcp regions of the associated moiré superstructure. We demonstrate that the individual regions of the graphene/Ru(0001) overlayer exhibit pronounced variations in interaction strengths with deposited metal atoms, recommending this substrate to serve as a template for growing periodic arrays of uniform nanoislands. In fact Pt clusters have been grown at 140-180 K and they are found to organize in a well-ordered periodic array defined by the moiré superlattice. Their preferred location within the graphene/Ru(0001) moiré unit cell is identified to be the fcc region. Pt islands are found to be structurally stable at room temperature; they may, however, exhibit some distinct frizzyness which is attributed to some of the islands consisting of stable cores with one or two weakly bound Pt atoms additionally attached to them. Occasionally, pick-up or lateral displacement of Pt islands by the STM tip is observed, which can be avoided by working at tunneling resistances $R_T > 10^9\ \Omega$ and tunneling currents $I_T < 50$ pA.

[1] K. Donner and P. Jakob, J. Chem. Phys. 131 (2009) 164701.

O 62.2 Thu 10:45 H31

**Atomic structure of graphene on Rh(111)** — •Mikhail Fonin[1], Ole Zander[1], Muriel Sicot[1], Samuel Bouvron[1], Ulrich Rüdiger[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

Exceptional transport properties of graphene, a two-dimensional honeycomb lattice of sp$^2$-bonded carbon atoms [1], recently observed on exfoliated quasi-free-standing samples make it a promising material for applications in microelectronics and sensing.

Here, we present a systematic scanning tunneling microscopy (STM) study of the atomic structure of graphene monolayer on the Rh(111) surface. Depending on the preparation conditions a multi-domain or a single domain graphene monolayer can be obtained. Atomically-resolved imaging of the graphene surface shows a moiré structure with pronounced buckling due to a strong interaction with the metal substrate. We show the most abundant moiré pattern in the multi-domain graphene which has the same structure as that in the single domain layer differs distinctly from those previously reported for graphene on Ir(111) or Ru(0001) as well as for *h*-BN nanomesh on Rh(111). Moreover, STM reveals a small rotation between graphene superstructure and metal lattices resulting in the formation of chiral domains.

This work is supported by DFG through SFB 767 (TP C5).

[1] A. K. Geim and K. S. Novoselov, Nature Mater. **6**, 183 (2007).

O 62.3 Thu 11:00 H31

**Bimetallic nanoclusters self-assembled on Ru(0001) supported monolayer graphene** — •Albert K. Engstfeld, Otavio B. Alves, Petra M. Erne, Harry E. Hoster, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

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]. Pt clusters formed this way on graphene/Ru(0001) have heights of 1-5 atomic layers and lateral diameters in the range 1-4 nm. In view of a potential utilization as model systems in electrocatalysis, 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 size distributions of Ru and PtRu clusters in comparison to the properties of Pt clusters. For the bimetallic clusters, we will also elucidate the structural differences depending on whether Pt or Ru is deposited first, and we will discuss possible consequences for their (electro-)chemical properties.

[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 62.4 Thu 11:15 H31

**The electronic structure of graphene on Ru(0001) studied with STS** — Mike Gyamfi, •Marta Waśniowska, Oswald Pietzsch, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, D-20355 Hamburg

The epitaxial monolayer graphene (MLG) on Ru(0001) displays a Moiré pattern with a strong electronic coupling with the substrate[1,2]. The unit cell of the Moiré pattern of MLG contains carbon atoms in high, low and intermediate positions. The periodic structure can produce spatial charge redistribution in the graphene and modify its electronic structure. In order to provide insight into the electronic structure of the different areas of the Moiré pattern, we performed scanning tunneling spectrocopy/microscopy at low temperatures. We observe different features in $dI/dU$ spectra for high and low areas revealing the strong or weak bonding between graphene and the Ru substrate. The experimental results are in good agreement with previous theoretical study of graphene on Ru(0001)[3].

[1] S. Marchini *et al.*, *Phys. Rev. B* **76**, 075429 (2007)
[2] P. Sutter *et al.*, *NanoLett.* **9**, 2654 (2009)
[3] B. Wang *et al.*, *Phys. Chem. Chem. Phys.* **10**, 3530 (2008)

O 62.5 Thu 11:30 H31

**Graphene on Ir(111): A tensile structure** — •Carsten Busse[1], Predrag Lazić[2], Rabia Djemour[1], Johann Coraux[3], Timm Gerber[1], Nicolae Atodiresei[2], Vasile Caciuc[2], Alpha T. N'Diaye[1], Sven Runte[1], Stefan Blügel[3], Jörg Zegenhagen[4], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, Germany — [3]Institut Néel / CNRS-UJF, Grenoble, France — [4]ESRF, Grenoble, France

Epitaxial growth on metal surfaces is an established method to produce highly ordered, extended graphene sheets. Ir(111) stands out from other substrates as the graphene grown on it is of extraordinary structural quality, shows an electronic structure almost equivalent to the one of free graphene, and can serve as a template for the growth of ordered superlattices of metal clusters.

Here we report measurements of the structure of graphene / Ir(111) based on X-ray standing waves (XSW), density functional theory (DFT) and scanning tunneling microscopy (STM). XSW reveals a bonding distance of (3.42 ± 0.02) Å between graphene and the substrate. This height can be accurately confirmed in DFT if Van-der-Waals-interaction is taken into account. STM experiments show that due to the mismatch of graphene and Ir(111) an incommensurate moiré pattern is formed. The chemical interaction between C and Ir as determined by DFT is attractive only in some regions of the superstructure, whereas it is even repulsive for other parts. This is the reason for the significant corrugation of the graphene.

O 62.6 Thu 11:45 H31

**Nucleation and growth of nickel and cobalt nanoclusters on graphene Moiré on Rh(111)** — •Muriel Sicot[1], Samuel Bouvron[1], Ole Zander[1], Mikhail Fonin[1], Ulrich Rüdiger[1], and Yuriy. S. Dedkov[2] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Fritz-Haber-Institut der Max-Planck Gesellschaft, 14195 Berlin, Germany

The development of advanced routes to fabricate highly-ordered monodispersed metallic nanostructures is one of the key challenges in nanotechnology. One of the promising ways to produce arrays of monodispersed nanoclusters (NCs) is to use a bottom-up approach where self-organization growth phenomena on template substrates are used. In this work, we use a graphene Moiré grown on Rh(111) as a template. The possibility to create arrays of magnetic clusters on this graphene Moiré is investigated by means of scanning tunneling microscopy. Regularly sized Ni and Co NCs have been grown. We determine that the initial growth of Co and Ni at 150 K leads to preferential nucleation of monodispersed NCs at specific sites of the Moiré superstructure. The NCs exhibit a typical diameter of about 3 nm and are 4 monolayers high. However, a defined long-range ordering of NCs with increasing coverage is not observed. These results suggest that the graphene nanomesh on Rh(111) is suitable for the growth of low density superlattices only. Room temperature growth of Co shows the same behaviour than at 150 K whereas Ni forms large triangular-shaped nanoislands which are well-matched to the Moiré registry. This work was supported by DFG through SFB 767 (TP C5).

O 62.7 Thu 12:00 H31

**graphene monolayer on Ru(0001) as a good template for metal deposition** — •bin wang and marie-laure bocquet — Université de Lyon, Laboratoire de Chimie, Ecole Normale Supérieure de Lyon, CNRS, F69007 Lyon, France

Perfectly ordered graphene overlayers can be easily obtained on Ru(0001) surface and display a moiré pattern with large periodicities resulting from the mismatch between graphene and Ru lattices [1-2]. In previous works using DFT calculations, we have unveiled that the graphene overlayer displayed periodic ripples of 1.5 Å amplitude, alternating chemical and physical distances with Ru [3-6].

Here we show by an extensive screening over different substrates (Ir and Rh) and a related organic network (h-BN) the uniqueness of the C/Ru interface in terms of local graphitic morphology and reactivity. Next we explore the adsorption properties of several adatoms like Transition Metal atoms (Ru, Pt, Au) and find an enhanced reactivity of the graphene area chemically interacting with the Ru substrate [7]. Consequently, it makes epitaxial graphene a promising template for material science and catalysis.

[1] S. Marchini et al, Phys. Rev. B. 76, 075429 (2007)
[2] J. Wintterlin et al, Surface Science, 603, 1841 (2009)
[3] B. Wang et al, Phys. Chem. Chem. Phys. 10, 3530 (2008)
[4] B. Wang et al, Phys. Rev. Lett. 101, 099703 (2008)
[5] W. Moritz et al, submitted (2009)
[6] T. Brugger et al, Phys. Rev. B 79, 045407 (2009)
[7] B. Wang et al, submitted (2009).

O 62.8 Thu 12:15 H31

**In situ monitoring of graphene growth on Ru(0001) by STM: new growth mode leading to extremely well ordered graphene** — •Sebastian Dänhardt[1], Sebastian Günther[1], Joost Wintterlin[1], and Stefan Schmitt[2] — [1]Department Chemie, Universität München, Butenandtstr. 11, 81377 München, Germany — [2]SPECS GmbH, Voltastr. 5, 13355 Berlin, Germany

We present the results of an in situ study of graphene growth using a novel high temperature STM (SPECS STM 150 Aarhus HT). Graphene was grown by chemical vapor deposition of ethylene on Ru(0001) at temperatures between 380 and 780 °C while STM images were recorded. Three different growth modes were observed. At relatively low temperatures fractal structures form consisting of triangular units. At temperatures between 500 and 680 °C and at ethylene pressures of ~ 1*10-8 mbar graphene grows in a "downhill" fashion as found before by LEEM [E. Loginova, N. C. Bartelt, P.J. Feibelman, K.F. McCarty, New Journal of Physics 11 (2009) 063046]. At temperatures above 750 °C a new growth mode was observed. This mode is connected with massive etching of ruthenium step edges, while coherent, defect free graphene islands of micrometer size grow. Because the graphene islands are restricted to single terraces of the Ru substrate, the step structure of the Ru completely rearranges, and step bunches of up to 10 monoatomic step heights are formed. In this way, by applying the correct growth conditions, flat, defect-free graphene films can be grown on single terraces. The findings may lead to a massive improvement of graphene preparation via the "metal route".

# O 63: Plasmonics and Nanooptics V

Time: Thursday 10:30–13:00 Location: H32

O 63.1 Thu 10:30 H32

**Enhancing higher harmonics generation using plasmonic nanostructures** — •Thomas Paul, Christoph Menzel, Carsten Rockstuhl, Shakeeb Bin Hasan, and Falk Lederer — Institute of Solid State Physics and Optics, Friedrich Schiller Universität Jena, Germany

Exploiting the properties of plasmon polaritons sustained by metallic nanostructures opens up great opportunities in engineering linear and nonlinear optical properties of conventional optical matter. Whereas the linear properties are usually at the focus of interest, also the nonlinear properties may benefit. If the metallic nanostructures are operated in resonance, the enhanced electrical field concentration facilitates the nonlinear interaction of light with matter. In our work we aim to detail such processes from a theoretical point of view. Particularly, we investigate the potential to enhance the higher harmonics generation by periodically arranged metallic nanostructures incorporated into a (nonlinear) dielectric host material. The geometries we are interested in are pairs of gold nanowires and split cylinder resonator structures. Emphasis is put on $\chi(2)$-nonlinearities for which it is reasonably assumed that the intrinsic nonlinearities of the dielectric host material prevails against those of the metallic nanostructures. Independent of the structure, we reveal the peculiarities of how the various types of resonances (dipolar or quadrupolar) may boost the conversion efficiency of the fundamental light into its higher harmonics (i.e. second harmonic). Possible implications to use the process of parametrical amplification for compensating absorption losses will be discussed.

O 63.2 Thu 10:45 H32

**Theoretical Investigation of the Electron Emission from Metal Nanotips** — •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 metallic nanotips illuminated by low-power 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 of an initial value problem [3] via an exponential split-operator method and a real space product formula algorithm [4] in one and two spatial dimensions. The time-dependent electric potential used for the study of the electron emission is derived from the charge distribution on the tip apex. The electric field and the photoelectron current are compared with 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 63.3 Thu 11:00 H32

**Electromagnetic field enhancement at nanostructured surfaces** — •Natalia Garcia Rey and Heike Arnolds — Surface Science Research Centre, University of Liverpool, Oxford Street, Liverpool L69 3BX, UK

Metal surfaces with nanometer scale roughness have been found to be photochemically more active than flat surfaces. This is believed to be caused by the excitation of surface plasmons, which create enhanced electromagnetic fields at the surface.

In this contribution, we explore the field enhancement obtainable from sub-wavelength periodic ripple structures created by argon ion sputtering in UHV, where we model the ripple surface structure as quasi-sinusoidal and solve Maxwell's equations in 2D with the help of finite-element modelling. We calculate the average surface field enhancement for various substrates (noble and transition metals) and vary incident wavelength and ripple periodicity and height.

Based on these results we discuss to which degree it is possible to maximize the electric field strengths and in turn the photochemical cross section using simple large-scale surface patterning techniques like sputtering.

O 63.4 Thu 11:15 H32

**Optical response of metallic nanostructures: simulation vs. measurement** — •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

Today various different tools for calculating the optical response of metallic nanostructures are available. All of them are based on a geometric description of the nanostructures, which makes it difficult to take into account production-based variations in the shape of the structure under investigation. In the context of plasmon resonances in the optical wavelength range and related effects, such as field enhancement, this discrepancy can generate significant deviations between simulation and measurement. To address this problem, we performed a series of FEM-based simulations on Au-nanoparticles, aiming to approach as closely as possible the structures available using today's state-of-the art production techniques. The simulations were carried out using JCMsuite (axis-symmetric model) and Comsol (full 3D), and special attention was paid to corners, triple-points and particle deformation. The calculated results were then compared with nanoparticles produced and analyzed in-house.

O 63.5 Thu 11:30 H32

**Modeling Metallic Nanostructures using a Discontinuous Galerkin Approach** — •Jens Niegemann[1,2], Michael König[1,2], Richard Diehl[1], Christopher Prohm[1], and Kurt Busch[1,2] — [1]Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie — [2]DFG Forschungszentrum Center for Functional Nanostructures (CFN), Karlsruher Institut für Technologie

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.

Here, we present our recent advances in using the DGTD method for the simulation of metallic nanostructures. In particular, we present the advantages of using higher-order curved elements. Furthermore, we will discuss some of our recent developments with respect to the improvement of the time integration.

O 63.6 Thu 11:45 H32

**Mode Tuning in Microresonators Using Uniaxial Anisotropy and Resonator Shaping** — •Stefan Declair, Cedrik Meier, Torsten Meier, and Jens Förstner — University of Paderborn, Department of Physics and CeOPP, Warburger Str. 100, D-33098 Paderborn, Germany

We numerically investigate resonant modes in microdisks and photonic crystal cavities. Mode tuning of the resonant modes, which is desirable for many applications, e.g. for achieving strong coupling, in a broad frequency range is shown using (a) uniaxial anisotropy of either the surrounding environment or the photonic structure and (b) in non-cylindrical microdisks. In both cases anticrossing behavior is observed when modes of different mode order approach each other. Additionally, we compare our simulations with experimental results from a 3 $\mu$m microdisk embedded in a liquid crystal environment.

O 63.7 Thu 12:00 H32

**Microcavity Plasmonics** — •Ralf Ameling and Harald Giessen — 4th Physics Institute, University of Stuttgart, Germany

We couple hybridized plasmon modes in cut-wire metamaterials with resonator modes of a microcavity. Depending on the position of the cut-wire pair in the resonator, the symmetric (electric) or antisymmetric (magnetic) plasmon mode is coupled, manifested by an anticrossing of the resonances. We explain this behavior by taking the symmetry and spatial distribution of the electric fields in the resonator into account. Experimental results verify the predicted mode-splitting due to the strong resonant coupling and agree well with theory. Our work can serve as a model system for far-field plasmon-plasmon coupling and paves the way towards enhanced plasmon-plasmon interaction in photonically coupled three-dimensional Bragg structures.

O 63.8 Thu 12:15 H32

**Functional elements on subwavelength plasmonic waveguides** — •Andreas Reiserer[1], Philip Tuchscherer[1], Christian Rewitz[1], Dmitri V. Voronine[1], Jer-Shing Huang[2], Bert Hecht[2], and Tobias Brixner[1] — [1]Institut für Physikalische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Nano-Optics and Biophotonics Group, Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Plasmonic functional elements are promising to combine the advantages of photonics and electronics – high speed and small spatial extent. We employ numerical simulations and an analytic approach based on transmission line theory to demonstrate several functional elements that consist of so called stub structures – terminated ends on metal–insulator–metal waveguides.

Splitters are presented that allow arbitrary adjustment of the transmission ratio from an input to two different output arms; frequency filters are designed that provide steep transmission resonances; and, finally, nanoscale all-plasmonic switching is proposed with an operating frequency of more than 20 THz.

The suggested device components are promising for future applications in ultrafast nanoscale information processing.

O 63.9 Thu 12:30 H32

**Optimally Shaped Laser Pulses for Hybrid Metal-Semiconductor Nanostructures** — •Matthias Reichelt[1], Torsten Meier[1], Andrea Walther[2], and Michael Dellnitz[2] — [1]Department Physik, Universität Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany — [2]Institut für Mathematik, Universität Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany

A hybrid nanostructure which consists of a metal aperture and a semiconductor quantum wire is studied theoretically. [1] It is shown that one can concentrate the optically excited electron density at an arbitray position for a given time using sophistically shaped laser pulses. To obtain the optimized laser field a genetic algorithm [2] and a more rigorous mathematical approach [3] are applied. Full three-dimensional finite-difference time-domain calculations [4] confirm the predicted spatiotemporal control.

[1] M. Reichelt and T. Meier, Opt. Lett. **34**, 2900 (2009).
[2] A.E. Eiben and J.E. Smith, *Introduction to Evolutionary Computing*, Springer (2003)
[3] S. Sertl and M. Dellnitz, Journal of Global Optimization **34**, 569-587, (2006).
[4] A. Taflove, *Advances in Computational Electrodynamics*, Artech House, (1998).

O 63.10 Thu 12:45 H32

**Analytic Theory of Linear Plasmonic Antennas** — Jens Dorfmüller[1], Ralf Vogelgesang[1], •Moritz Esslinger[1], Worawut Khunsin[1], Christian Ettrich[2], Carsten Rockstuhl[2], and Klaus Kern[1] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Institute of Condensed Matter Theory and Solid State Optics, Friedrich-Schiller Universität Jena

At radio-frequencies, antenna theory is a well understood topic. At optical frequencies, however, antenna sizes are in the order of skin depths so that electromagnetic fields penetrate substantially into the volume of metallic nanostructures, rendering classic radio antenna theory not applicable. We develop a fully analytical model for the electromagnetic behavior of plasmonic wires. Therefore, we model thin, linear plasmonic antennas based on the assumption of homogeneous volume currents. Our model requires only a handful, physically motivated, adjustable parameters. It successfully predicts measured and simulated data in full detail: emission patterns, nearfield optical amplitudes and phases, as well geometric resonances.

## O 64: Solid/liquid interfaces I (focussed session)

Time: Thursday 10:30–13:00 Location: H33

**Invited Talk** O 64.1 Thu 10:30 H33

**Metal/Electrolyte interfaces under atmospheric corrosion conditions** — •Michael Rohwerder — Max-Planck-Institut für Eisenforschung, Max-Planck-Str.1, D-40237 Düsseldorf, Germany

Atmospheric corrosion conditions are characterized by ultra-thin electrolyte layers covering the metal surface. As will be shown, although in not too diluted electrolytes the electrochemical double layer extends only about a nanometre from the metal surface, the corrosion behaviour of metals covered by an electrolyte layer of a few hundred nanometres is different from the one of an immersed metal. This can not easily be studied with standard electrochemical set-ups. An indispensable method for electrochemical investigations in ultra-thin electrolyte layers is the Kelvin probe. Indeed, the Kelvin probe technique can be considered as a natural reference electrode that is applicable to immersed electrodes, metals covered by ultra-thin electrolyte layers and even "dry" surfaces alike. It will also be shown that the potentials measured on "dry" surfaces are of real physical importance as they have a direct impact on corrosion mechanisms.

**Invited Talk** O 64.2 Thu 11:00 H33

**Copper Damascene Process: From the wafer to the atomic scale** — •Alexander Flügel[1], Dieter Mayer[1], Werner Reckien[3], Thomas Bredow[3], N.T.M. Hai[2], and Peter Broekmann[2] — [1]BASF SE, Ludwigshafen — [2]University of Bern — [3]University of Bonn

Copper plating is one of the key processing steps in the state-of-the-art fabrication of high-end microprocessors. The internal wiring of highly integrated circuits is achieved by an electrochemical copper deposition route also known as Copper (Dual) Damascene Process. Trenches and vias in the dielectric are filled defect-free with the copper material due to an enhanced deposition rate at the feature bottom with respect to a suppressed deposition rate at the wafer surface. This non-uniform deposition rate is triggered by the time-dependent interplay of various inorganic and organic additives at the copper surface or the near-surface regime upon electrodeposition. This presentation comprises a surface science approach providing an atomistic understanding of the additive action at the interface under reactive conditions with an electrochemical engineering approach providing a phenomenological characterization of the synergistic and antagonistic additive action at the interface. Our results are discussed in the light of successful fill experiments of sub-50nm Damascene structures relevant for the forthcoming 32-nm technology node.

**Invited Talk** O 64.3 Thu 11:30 H33

**Atomic-scale dynamics and interactions at solid-liquid interfaces** — •Olaf Magnussen — Institut für experimentelle und angewandte Physik, Universität Kiel, Kiel, Germany

A wide variety of interface reactions, such as dissolution and growth, self-assembly, or catalytic reactions, are crucially affected by the surface transport and the interactions of species at solid-liquid interfaces. Understanding how the presence of the liquid phase and the precise interface structure influence these atomic-scale dynamic processes is hence of great interest. Using well-controlled electrochemical model systems and scanning tunnelling microscopy at video-frequency image acquisition rates, direct in-situ observations of such dynamic events are possible, providing quantitative data on surface diffusion barriers and interaction energies in these complex systems. As examples, the diffusion and interaction of different types of adsorbates as well as the collective dynamics of nanostructures are discussed for the case of Cu(100) electrode surfaces in aqueous solution.

O 64.4 Thu 12:00 H33

**Computation of the interfacial excess free energies of solid-liquid interfaces by molecular dynamics simulation and thermodynamic integration** — •Frédéric Leroy and Florian Müller-Plathe — Eduard-Zintl-Institut für Physikalische und Anorganische Chemie, Technische Universität Darmstadt, Darmstadt, Germany

Solid-liquid interfacial tension is a key quantity in the thermodynamics of systems where a liquid is in the vicinity of a solid substrate. While fluid-fluid surface tensions have received a lot of attention, calculation of the solid-liquid interfacial tension is still an on-going task. We present an algorithm[1] that allows the computation of that quantity.

Rather than trying to compute an absolute interfacial free energy, we intend to obtain the free energy difference between the system where the liquid is interacting with the structured solid surface of interest and a reference system where the liquid is in contact with a flat surface, by performing thermodynamic integration from one system to the other. For example, the algorithm is useful in determining the change in free energy with respect to a modification of the chemical composition of the solid or a change in its topography.

We discuss the applications of the method in the frame of wetting in nano-scale systems and present its advantages through results dealing with Lennard-Jones model systems and water in interaction with graphite-based surfaces.

[1] F. Leroy, D.J.V.A. dos Santos and F. Müller-Plathe, Macromolecular Rapid Communications 2009, vol. 30, pp 864-870.

O 64.5 Thu 12:15 H33

**Temperature-dependence of molecular self-organization at solid-liquid interfaces** — •Sissi de Beer, Peter Wennink, and Frieder Mugele — University of Twente, PCF, Enschede, the Netherlands

When a liquid is confined it behaves different from the bulk. A specifically interesting confinement-effect is called layering; close to the solid wall the liquid molecules structure and form layers. When the two surfaces are approached, this layering effect gives rise to an oscillatory disjoining pressure, which can be measured as the oscillatory forces. We present measurements of the effect of temperature on layering of an organic long-chained hydrocarbon (hexadecane) and a quasi-spherical liquid (octamethylcyclotetrasiloxane; OMCTS) confined upon approach of an atomic force microscope tip towards a solid Highly Ordered Pyrolytic Graphite (HOPG) surface. When the distance between the tip and the surface is reduced, both liquids rupture in discrete steps corresponding to the squeeze-out of individual liquid-layers. We measured the force required to squeeze-out the last liquid layers for various temperatures close to the melting-temperature. For OMCTS we found no change in the squeeze-out force. However, for hexadecane we found that the structuring at the wall strongly increases when the melting temperature is approached and surprisingly, the squeeze-out force is not maximum closest to the melting temperature, but around 3-5 degrees above. We argue that this is due to epitaxial effects between the alkanes and the HOPG surface; the hydrogen-atoms of hexadecane exactly occupy the centers of the graphite hexagons.

O 64.6 Thu 12:30 H33

**Adsorption and Phase Transition of Heptylviologen on HOPG observed by EC-STM** — •Knud Gentz and Klaus Wandelt — Institut für Physikalische und Theoretische Chemie der Uni Bonn, Wegelerstraße 12, 53115 Bonn

Heptyl Viologen (1,1'-diheptyl-4,4'-bipyridin, HV) has been the focus of several publications which derived possible structures of the adsorbate films and it's behavior during phase transitions by means of cyclic voltammetry and chronoreflectometry. The purpose of this contribution is to verify these proposed structures as well as the behavior upon adsorption and phase changes by scanning tunneling microscopy. We adsorbed Heptylviologen on an HOPG electrode surface from a supporting electrolyte of sulfuric acid and potassiumchloride (-bromide). In the CV the characteristic voltammetric spikes of the surface phase transition were observed both in the presence of chloride as well as bromide. The STM images clearly show a stripe structure on the surface in the regime negative of the spike voltammetric peaks indicating the presence of the radical cationic phase ($HV^{\bullet +}$) stabilized by $\pi$–$\pi$-interaction of the individual molecules. A single row and a double row structure were found showing a herringbone-like arrangement of the molecules. Above the spike peak no ordered layer was observed. The proposed dimers of the radical cation were not found on the surface at any given potential, instead we observed long-chained oligomers. In the presence of bromide an insoluble viologen bromide is formed on the surface hampering the stabilization of the surface phase which causes the spike peak to fade with progressing voltammetric cycles.

O 64.7 Thu 12:45 H33

**Preparation, characterization and reactivity of submonolayers of platinum on carbon based model surfaces** — •Tine Brülle[1] and Ulrich Stimming[1,2] — [1]Technische Universität München, Department of Physics E19, James-Franck-Str. 1, D-85748 Garching, Germany — [2]Bavarian Center for Applied Energy Research (ZAE Bayern) Division 1 Walther-Meißner-Strasse 6, D-85748, Germany

In connection with fuel cell related research, catalyst nanoparticles on porous carbon supports got into the focus of attention. However, the complex morphology of these technical catalysts makes a thorough understanding of the influence of parameters such as noble metal particle size and morphology as well as particle distance on reactivity rather difficult. Therefore, we aim at a better understanding of these effects by using nanostructured flat surfaces as model systems in our investigations. Platinum nanoparticles supported on HOPG (highly oriented pyrolytic graphite) were prepared. This crystalline form of carbon provides a well-defined support regarding geometric and electronic structure. The platinum nanostructured surfaces were used to investigate catalytic properties for hydrogen related reactions.

Another form of crystalline carbon is diamond. High doping rates cause a sufficient electronic conductivity that make electrochemical measurements possible, while the very flat surfaces diamond monocrystals make imaging of metal nanoparticles via SPM-methods possible. Preliminary results on platinum nanostructured diamond surfaces will be shown.

## O 65: Density functional theory and beyond for real materials III

Time: Thursday 10:30–13:15 Location: H34

O 65.1 Thu 10:30 H34

**Mott transition and Mahan exciton in MgO and ZnO from first principles** — •André Schleife, Claudia Rödl, Frank Fuchs, Karsten Hannewald, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Jena, Germany

Under the name “Transparent Electronics” a field is emerging, which already attracted interest, mainly due to the demand for transparent conducting materials for solar cells. Driven by the next generation of optoelectronic devices it is expected to grow even further.
Especially important in this context are the transparent conducting oxides. To combine transparence and conductivity, free carriers have to be present in the conduction bands of these semiconducting materials, which in turn affects the optical properties.

We approach this topic from the theoretical point of view: the solution of the Bethe-Salpeter equation is perfectly suited to describe the optical properties of a system. With this method we gain insight into the optical properties of a system from first-principles and obtain a quantitative understanding of the interplay of additional free carriers and many-body effects.

After introducing our approach along with necessary approximations and technical tweaks, we present results for MgO and ZnO taking into account the influence of an additional free electron gas by including Thomas-Fermi screening and Pauli-Blocking. We relate the resulting effects in the absorption spectrum to the Fermi-edge singularity or Mahan excitons. The comparison with experimental spectra is excellent, but the Mott transition of the excitons is difficult to observe.

O 65.2 Thu 10:45 H34

**Unravelling the enigma of the F center in MgO with many-body perturbation theory** — •Patrick Rinke[1,2], Anderson Janotti[2], Andre Schleife[3], Emmanouil Kioupakis[2], Claudia Roedl[3], Friedhelm Bechstedt[3], Chris G. Van de Walle[2], and Matthias Scheffler[1,2] — [1]Fritz-Haber-Institut der MPG, 14195 Berlin, Germany — [2]Materials Dep., University of California Santa Barbara, CA, USA — [3]Friedrich-Schiller-Universität Jena, 07743 Jena, Germany

The anion vacancy in bulk MgO (also called F- or color center) can probably be regarded as *the* classic intrinsic point defect in compound insulators. Its characterization has been impeded for decades by the fact that the neutral and the positively charged F-center (denoted F and F$^+$, respectively) absorb at nearly identical energies [1]. To unravel this problem we apply a recently developed formalism that combines density functional theory (DFT) with many-body perturbation theory (MBPT) in the $G_0W_0$ approximation [2,3]. We find that this approach corrects the DFT formation energies in the local-density approximation (LDA) significantly. To describe the optical spectrum, however, it proves to be necessary to go one step further in the hierarchy of MBPT, i.e. solving the Bethe-Salpeter equation. After inclusion of the electron-hole and electron-phonon interaction we observe unprecedented agreement between the calculated and the experimental optical absorption spectra for the F and F$^+$ center [1]. [1] L. A. Kappers, *et al.*, Phys. Rev. B **1**, 4151 (1970). [2] Hedström *et al.* Phys. Rev. Lett. **97**, 226401 (2006). [3] P. Rinke, *et al.*, Phys. Rev. Lett. **102**, 026402 (2009).

O 65.3 Thu 11:00 H34

**Atomic-level elucidation of the initial stages of self-assembled monolayer metallization** — •John Keith and Timo Jacob — Universität Ulm, Albert-Einstein-Allee 47, D-89069 Ulm, Germany

Developing high performance nanotech applications and molecular electronics requires deep understanding of atomic level structural, electronic, and magnetic properties of electrode/molecular interfaces. To clarify the initial stages of interface formation during self-assembled monolayer (SAM) metallization, we used first principles density functional theory (DFT) calculations to study Pd diffusion on top of 4-mercaptopyridine (4MP)-SAMs on Au(111). After distinguishing potential energy surfaces (PESs) for different spin configurations for Pd on the SAM, we find adatom diffusion and expected Ostwald ripening is not possible over the clean 4MP-SAM surface. Pre-adsorption of Pd, however, facilitates Pd diffusion that appears to explain multiple reports on experimentally observed island and monolayer formation on top of SAMs. Furthermore, these diffusions most likely occur by moving across low-lying and intersecting PESs of different spin states. Vertical diffusion processes were also investigated, and the electrolyte was found to play a key role in preventing Pd permeation through the SAM to the substrate. Initial stages of nanoparticle formation on top of SAMs are presented, as well as their electronic structures.

O 65.4 Thu 11:15 H34

**Benzene on Cu(111): Adsorption and Assembly by Lateral van der Waals and Surface-State-Mediated Interactions** — Kristian Berland[1], •Theodore L. Einstein[2], and Per Hyldgaard[1] — [1]Chalmers U. Tech., Sweden — [2]U. Maryland, USA

Combining a van der Waals density functional (vdW-DF) [PRL 92 (2004) 246401] and estimation of lateral vdW and indirect electronic interactions, we study the adsorption, surface diffusion, and lateral assembly of benzene on Cu(111) [KB,TLE,PH, PRB 80 (2009) 155431]. The vdW-DF inclusion of nonlocal correlations changes the relative stability of 8 high-symmetry binding positions and increases the adsorption energy over tenfold. We find that benzene can move almost freely along a honeycomb web of "corridors" linking fcc and hcp sites via bridge sites, consistent with the low diffusion barrier in experiment.

We further present an extended vdW-DF scheme which accounts well for the structural phases of benzene on Cu(111). Experiments show that benzene condenses into two different structural phases: a compact and a sparse phase, both of approximately hexagonal symmetry. The vdW-DF calculations demonstrate that the denser benzene-overlayer phase, with lattice constant 6.74 Å, is due to direct benzene-benzene vdW attraction. The structure of the second, sparser phase, with lattice spacing 10.24 Å, is attributed to the indirect electronic interactions mediated by the well-known metallic surface state on Cu(111). To support this claim, we use a formal Harris-functional approach to evaluate nonperturbatively the asymptotic form of this indirect interaction.

Supported by [1]Vetenskapsrådet 621-2008-4346 & [2]NSF CHE07-50334

O 65.5 Thu 11:30 H34

**Kohn-Sham potential for spherical fullerenes** — •Yaroslav Pavlyukh and Jamal Berakdar — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Heinrich-Damerow-Strasse 4, 06120 Halle, Germany

Majority of the known cage molecules has low symmetry elongated shapes. Fortunately for the theoretical analysis the most stable fullerenes are spherical and highly symmetric. This makes them accessible for electron correlation methods used up to now only for the closed shell atoms. Starting from valence densities from the first principles quantum chemistry calculations we determine accurate Kohn-Sham potentials for icosahedral C$_{20}^{2+}$ and $C_{60}$ molecules. Assuming that the density is $N$-representable the Hohenberg-Kohn theorem guarantees the uniqueness of such potential. The potential is iteratively constructed following the method suggested by van Leeuwen and Baerends (Phys. Rev. A **49**, 2421 (1994)). High symmetry of the molecules allows to parametrize angular dependence of the densities and potentials with a small number of symmetry-adapted spherical harmonics. Radially, these quantities are represented on the grid and the density is constructed from the approximate potential by numerically solving the coupled-channel Kohn-Sham equation. This is followed by an update of the potential and the procedure is continued until convergence is achieved.

O 65.6 Thu 11:45 H34

**Reliable Kohn-Sham eigenvalues and self-interaction: a study on organic semiconductors** — •Thomas Körzdörfer and Stephan Kümmel — Physikalisches Institut, Universität Bayreuth, D-95440 Bayreuth, Germany

Photoelectron spectroscopy is an important tool for investigating organic semiconductor materials such as PTCDA and NTCDA. Kohn-Sham (KS) eigenvalues obtained from density functional theory are frequently used as a tool to facilitate the interpretation of the measured spectra. So far, however, it was difficult to predict when the spectrum of occupied KS eigenvalues obtained from commonly used (semi-)local functionals bears physical relevance and when not. Clearly, this considerably limits the practical usefulness of the approach and triggers the need for an easy criterion which can serve as a warning against possible misinterpretation of the eigenvalue spectrum. In this work, we demonstrate that such a criterion can be based on evaluating each orbital's self-interaction error [1]. With PTCDA and NTCDA serving as examples it is shown that the spatial structure of the highest lying KS orbitals is decisive for the physical reliability of the eigenvalue spectrum obtained from (semi-)local functionals. We further demonstrate that a recently introduced generalized optimized effective potential scheme [2] that is based on the self-interaction correction of Perdew and Zunger leads to reliable eigenvalues also in difficult cases such as PTCDA where (semi-)local functionals fail.

[1] T. Körzdörfer, et al., Phys. Rev. B 79, 201205(R) (2009).

[2] T. Körzdörfer, et al., J. Chem. Phys. 129, 014110 (2008).

O 65.7 Thu 12:00 H34

**A DFT study on electronic structure and vibronic properties of $d^8$ (Ni-, Pd-, and Pt-) phthalocyanines** — •Davoud Pouladsaz[1], Thiruvancheril G. Gopakumar[2], and Michael Schreiber[1] — [1]Institut für Physik, Technische Universität Chemnitz — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel

We studied the HOMO-LUMO gap shrinking in order to investigate the tip-induced polarization in scanning tunneling spectroscopy of $d^8$ (Ni, Pd, and Pt) phthalocyanines [1]. By means of density functional theory (DFT), the molecular orbital energies have been calculated for Ni-, Pd-, and PtPc single neutral molecules and singly and doubly ionized cations and anions of all molecules. Interestingly, the position of the HOMO decreases systematically with increasing the atomic number of the central metal atom. The first ionization energies of neutral molecules increase by changing the central metal atom, while the electron affinities remain constant. This causes an increase in the HOMO-LUMO gap. These results show a clear correlation to experimental observations. Furthermore, we performed a DFT study on photoelectron spectra of the first and the second ionizations of these molecules, computing the vibronic couplings and the reorganization energies. The partitioning of the reorganization energy into normal mode contributions shows that the major contributions are due to several vibrational modes with $a_{1g}$ symmetry lower than 1600 $cm^{-1}$.

[1] Th. G. Gopakumar, J. Meiss, D. Pouladsaz, and M. Hietschold, J. Phys. Chem. C, **112**, 2529 (2008)

O 65.8 Thu 12:15 H34

**Modeling the electronic properties of Pi-conjugated self-assembled monolayers** — •Egbert Zojer[1], Ferdinand Rissner[1], and Georg Heimel[2] — [1]Institut für Festkörperphysik, Technische Universität Graz, Petersgasse 16, A-8010 Graz, Österreich — [2]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstrasse 15, 12389 Berlin

The modification of electrode surfaces by depositing self-assembled monolayers (SAMs) provides control over various key parameters in organic and molecular electronic devices. These include the work-function of the electrode and the relative alignment of its Fermi level with the conducting states in the SAM and with those in a subsequently deposited organic semiconductor. This contribution summarizes [1] recent progress in developing a proper understanding of the relation between the chemical structure of a molecule, its molecular electronic characteristics, and the properties of a SAM formed by such molecules. This is achieved by linking the insight that can be gained from fundamental electrostatic considerations with a quantum-mechanical description. The roles played by substituents, molecular backbones, chemical anchoring groups, and the packing density of molecules on the metallic surface are elucidated. Also the properties of multilayer structures are addressed. [1] reviewed in: G. Heimel, F. Rissner, and E. Zojer, Progress Report, Adv. Mater., (in print).

O 65.9 Thu 12:30 H34

**Charge transport through O-deficient Au-MgO-Au junctions** — •Mohamed Fadlallah[1,2], Cosima Schuster[1], Udo Schwingenschlögl[3], Ivan Rungger[4], and Ulrich Eckern[1] — [1]Universität Augsburg, 86135 Augsburg, Germany — [2]Benha University, Benha, Egypt — [3]KAUST, Thuwal 23955-6900, Kingdom of Saudi Arabia — [4]Trinity college, Dublin 2, Ireland

Metal-oxide heterostructures have been attracting considerable attention due to various technological applications as photovoltaic and spintronic devices. We present results of electronic structure and transport calculations for Au/MgO/Au tunnel junctions based on density functional theory and scattering theory on the level of non-equilibrium Green's functions. In particular, we study the dependence of the conductance of the heterostructure on the thickness of the MgO interlayer, the interface termination, and the interface spacing. In addition, we address the effect of O vacancies. The exponential decay with interlayer thickness is modified when Au-O bonds are formed at the interface. Electronic states tracing back to O vacancies change the conductance depending on the position of the vacancy. By increasing the interface spacing, the vacancy induced gap states are shifted towards the Fermi energy, leading to an enhancement of the conductance. Thus, we have identified two mechanisms which determine the conductance of the Au/Mgo/Au-junction: O vacancies are able to increase the transparency of the MgO interlayer; the interface coupling then can be used to fine tune these states.

O 65.10 Thu 12:45 H34

**Functionalized Tips Leading towards Ultimate Resolution of Atomic Force Microscopy** — •Nikolaj Moll, Leo Gross, Fabian Mohn, Alessandro Curioni, and Gerhard Meyer — IBM Research, Säumerstrasse 4, 8803 Rüschlikon, Switzerland

Ultimate resolution can be achieved by functionalizing the tip with a molecule like carbon monoxide with the tip molecule significantly contributing to the measured force. The force and therefore the resolution crucially depends on the chemical nature of the terminating tip molecule. In this work molecules such as pentacene are imaged with unprecedented resolution by employing such functionalized tips. The interactions of the tip molecule with imaged molecule are studied with ab initio density functional theory (DFT) calculations. The calculations show that Pauli repulsion is the source of the high resolution, whereas van-der-Waals and electrostatic forces only add a diffuse attractive background. This enhancement of the resolution is also observed experimentally and compares very well with the theoretical findings.

O 65.11 Thu 13:00 H34

**Yttria stabilized Zirconia: A first principles study** — •Christian Carbogno[1], Hepeng Ding[2], Feng Liu[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin, Germany — [2]Department of Materials Science and Engineering, University of Utah, Salt Lake City, USA

Yttria-stabilized Zirconia is widely used in a variety of different technological fields, for instance as a thermal barrier coating in turbine engines due to its extremely low thermal conductivity. Although it is still a topic of scientific debate, it is generally presumed that its macroscopic properties are strongly related to the dynamics of the occurring oxygen vacancies that are induced due to charge compensation by the aliovalent substitutional doping with Yttrium. Previous ab initio studies (e.g. [1]) were able to shed some light on the complex interactions of these vacancies, but the exact mechanism determining the dynamic processes and thus the thermodynamic properties of this ceramic could not be identified by first principles. By exploiting the availability of massively parallel linear-scaling DFT codes [2] we overcome the numerical limitations affecting these previous studies and thus lay the basis for further multi-scale ab initio studies: We investigate how various fundamental properties of Yttria-stabilized Zirconia depend upon the employed exchange-correlation functional and additionally discuss the implications of these results on the simulation of the thermodynamics of the crystal by inspecting the phonon free energies.

[1] F. Pietrucci et al., Phys. Rev. B 78, 094301 (2008).

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

## O 66: Nanotribology I

Time: Thursday 10:30–12:15 Location: H36

O 66.1 Thu 10:30 H36

**Tuning mechanical properties of single silica capsules** — •Doris Vollmer[1], Lijuan Zhang[1], Alfons van Blaaderen[2], Robert Graf[1], and Michael Kappl[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Debye Institute for Nanomaterials Science, Utrecht University, Utrecht, The Netherlands

The shell's mechanical properties determine their stability and flow behavior. We investigated the mechanical properties of single silica shells by force-distance spectroscopy. The spherical capsules of different diameters (800 nm and 1.9 $\mu$m) and shell thickness (15 nm thickness 70 nm) were immobilized on a silicon substrate.

We probed the elastic response of the hollow particles by applying a point load, successively increasing the load until the shell broke. In agreement with the predictions of shell theory the deformation increases linearly with applied force for small deformations. For thicknesses larger than 20 nm the Young modulus is independent of shell thickness. However, it depends on the thermal history of the sample. It increases from 10 GPa for unheated shells to close to that of fused silica (80 GPa) after heating the hollow particles to 1100 °C. Heating transforms the large number of silanol groups into Si-Si bonds. This transformation leads to a compaction of the shells, which is reflected in a reduction of the diameter of the hollow particle as well as its shell thickness. Amazingly, tempering at 1100 °C induces smoothing of shells although the particles still remain spherical as shown by atomic-force-microscopy and scanning-electron-microscopy.

O 66.2 Thu 10:45 H36

**Crystallographic Orientation Maps by Transverse Shear Microscopy (TSM)** — •Quan Shen[1], Gregor Hlawacek[1], Markus Kratzer[1], Heinz-Georg Flesch[2], Thomas Potocar[2], Roland Resel[2], Adolf Winkler[2], and Christian Teichert[1] — [1]Institute of Physics, University of Leoben, 8700 Austria — [2]Institute of Solid State Physics, Graz University of Technology, 8010 Graz, Austria

For organic semiconductor devices (OTFTs, OLEDs and organic solar cells, etc.), the grain boundary and domain size of organic thin films have a strong effect on the final device performance [1]. In this work, we use transverse shear microscopy (TSM) to characterize crystallographic domains in a para-sexiphenyl (6P) polycrystalline thin layer [1] and a thiophene based self assembled monolayer (SAM). TSM is a special mode of conventional lateral force microscopy (LFM). The elastic anisotropy [2] in different crystallographic arrangements can be recognized by TSM sensitively. The generated TSM image can be considered as a Crystallographic Orientation Map to reveal information on shape, size, boundary and crystallographic orientation of domains in the molecular films.

This work is funded by Austrian Science Fund NFN "Organic Thin Films" Projects S9707, S9708 + P19197, and the SAMs are provided by Dago de Leeuw, Philips Research, Einhoven.

[1] G. Hlawacek, et al., Science, 2008, 321, 108-111.

[2] K. Puntambekar, et al., Adv. Funct. Mater. 2006, 16, 879-884.

O 66.3 Thu 11:00 H36

**A miniature high vacuum microtribometer: from conception to calibration** — Mikhail Kosinskiy[1], Yonghe Liu[2], Juergen A. Schaefer[1], and •Syed Imad-Uddin Ahmed[1] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany — [2]European Patent Office, Bayerstr. 115, München 80335, Germany

A newly developed microtribometer for evaluating the tribological performance of materials and coatings in vacuum and controllable atmospheres on the micro- and milli-Newton scale is presented. The microtribometer consists of a piezo driving table, an elastic force sensor and two laser interferometers to precisely detect normal and lateral deflections of the force sensor. The driving unit and the force sensor are located in the vacuum chamber, while the laser interferometers are installed outside. Force sensor deflections are measured with accuracy down to nanometers by focusing laser beams on small mirrors attached to the sensor. Various types of counterbodies can be attached to the sensor allowing examination of a wide variety of tribopairs. Results of friction tests of Si-Si tribopairs in ambient and vacuum conditions were performed using the UHV microtribometer and compared with measurements performed on a commercial microtribometer as well as with values published in literature using other types of tribometers.

O 66.4 Thu 11:15 H36

**Wear-less floating contact imgaging of polymer surfaces** — Armin Knoll, Hugo Rothuizen, Bernd Gotsmann, and •Urs Duerig — IBM Research GmbH - Zurich, Saeumerstrasse 4, 8803 Rueschlikon, Switzerland

An atomic force microscopy (AFM) technique is described combining two operating modes that previously were mutually exclusive: Gentle imaging of delicate surfaces requiring slow dynamic AFM techniques, and passive feedback contact mode AFM enabling ultra-fast imaging. A high frequency force modulation is used to excite resonant modes in the MHz range of a highly compliant cantilever force sensor with a spring constant of 0.1 N/m. The high order mode acts as a stiff system for modulating the tip-sample distance and a vibration amplitude of 1 nm is sufficient to overcome the adhesion interaction. The soft cantilever provides a force-controlled support for the vibrating tip enabling high-speed intermittent contact force microscopy without feedback control of the cantilever bending. Using this technique, we were able to image delicate polymer surfaces and to completely suppress the formation of ripple wear patterns that are commonly observed in contact AFM.

O 66.5 Thu 11:30 H36

**Large-scale MD simulations of the contact and sliding of nanoscale metallic asperities** — •Joël Peguiron[1] and Michael Moseler[1,2] — [1]Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstraße 11, 79108 Freiburg — [2]Physikalisches Institut, Albert-Ludwigs Universität Freiburg, Hermann-Herder-Straße 3, 79104 Freiburg

Molecular dynamics simulations of the tribology of nanoscale gold contacts are reported. Contact formation, sliding, and fracture between two asperities are investigated, bearing special interest on the mechanisms of material flow underlying these processes. In particular, the formation of long atomic chains, a known property of gold, is observed. The influence of the presence of a liquid lubricant is also explored. Large-scale simulations (hundreds of thousands atoms) are set up in order to make one step further, with respect to earlier works, towards connection with experiments from the literature.

O 66.6 Thu 11:45 H36

**Friction on Graphene/SiC(0001)** — •Christian Held and Roland Bennewitz — INM-Leibniz Institute for New Materials, 66123 Saarbrücken, Germany

Layers of graphene are grown on SiC(0001) samples by means of thermal decomposition in ultra-high vacuum [1]. The resulting structure consists of atomically flat terraces of SiC with a width of tens on nanometer, covered with single and bilayer patches of graphene. Single and bilayer coverage can be identified by Kelvin force microscopy. Strong friction contrast is observed across the surface structure when measured in situ by means of friction force microscopy. Friction on the SiC substrate is greatly reduced even by a single layer of graphene.

[1] K. V. Emtsev et al. , Nat. Mater. 2009, 8, 203.v

O 66.7 Thu 12:00 H36

**Atomic stick-slip friction on a metal vs. a monolayer lubricant surface.** — •Nitya Nand Gosvami, Philip Egberts, and Roland Bennewitz — INM-Leibniz Institut für Neue Materialien, Saarbrücken, Germany

We study friction at the atomic scale on a Au(111) surface with and without an alkanethiol self-assembled monolayer (SAM) coverage. The experiments were performed using an atomic force microscope (AFM), operated in ultra-high vacuum (UHV) conditions. On atomically flat terraces of Au(111), very low friction with clear atomic stick-slip instabilities was observed which did not vary with load in the low load regime. However, as the normal load was increased beyond a threshold, friction showed sharp rise with significant variation in magnitude and accompanied with irregular stick-slip events, indicating wear of the surface. The striking observation of atomic stick-slip without dissipation can not be explained using existing classical models for single asperity friction. Our results also did not show agreement with a recently developed two-mass-two-spring model, which incorporates thermal effects. Alternate mechanisms for the observed friction behaviour are discussed.

We extended atomic scale friction studies to a SAM covered Au(111)surface. We found that the self-assembled molecules support atomic stick-slip friction where friction maps revealed the molecular superstructure of the SAM film. In several cases, frictional contrast down to single molecular level was achieved near the pull-off force.

## O 67: Gerhard Ertl Young Investigator Award (talks of the selected canditates)

Time: Thursday 10:30–13:00 Location: H37

O 67.1 Thu 10:30 H37

**Restructuring of Catalyst Surfaces under Reaction Conditions** — •Feng Tao[1,2], Miquel Salmeron[2], and Gabor Somorjai[1,2] — [1]Department of Chemistry, University of California, Berkeley, California, USA, 94720 — [2]Materials Science Division, Lawrence Berkeley National Lab, Berkeley, California, USA, 94720

The surface structure of catalysts and their evolution under reaction conditions is one of the crucial issues in understanding catalytic mechanisms at molecular and atomic levels. Here bimetallic nanoparticles (Rh0.5Pd0.5 and Rh0.5Pt0.5) were used as model catalysts for the in-situ study of surface structure under reaction conditions. The as-synthesized Rh0.5Pd0.5 nanoparticles are core-shell structured. However, there is no significant depth-dependence of atomic fractions of Rh and Pt in Rh0.5Pt0.5 nanoparticles. Surface structures of two Rh-based bimetallic nanoparticle catalysts during catalysis, oxidation, and reducing reactions have been systematically studied in-situ using XPS in Torr pressure ranges. The Rh0.5Pd0.5 and Rh0.5Pt0.5 nanoparticles undergo reversible changes in both atomic fractions and chemical states corresponding to the switch of reaction environments between oxidizing and catalysis (or reducing) conditions. Rh atoms in Rh0.5Pd0.5 and Rh0.5Pt0.5 segregate to surface region and are largely oxidized under oxidizing conditions, while in reducing atmospheres the Pd atoms in Rh0.5Pd0.5 and Pt atoms in Rh0.5Pt0.5 segregate to the surface regions and Rh oxides are largely reduced. The capability of restructuring nanoparticles through chemical reactions suggests a new method for the development of new catalysts.

O 67.2 Thu 11:00 H37

**Charge Measurement of Atoms and Atomic Resolution of Molecules with Noncontact AFM** — •Leo Gross[1], Fabian Mohn[1], Nikolaj Moll[1], Peter Liljeroth[1], Jascha Repp[2], Franz J. Giessibl[2], and Gerhard Meyer[1] — [1]IBM Research - Zurich, 8803 Rüschlikon, Switzerland — [2]Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Individual gold and silver adatoms and pentacene molecules on ultrathin NaCl films on Cu(111) were investigated using an atomic force microscope (AFM), equipped with a qPlus sensor, operated at 5K.

Charging a gold atom by one electron charge increased the force on the AFM tip by a few piconewtons. Employing Kelvin probe force microscopy (KPFM) we also measured the local contact potential difference (LCPD) which is shifted depending on the sign of the charge. This effect allows the discrimination of positively charged, neutral, and negatively charged atoms.

To image pentacene molecules we modified AFM tips by means of vertical manipulation techniques, i.e. deliberately picking up known atoms and molecules. Using a CO terminated tip we resolved all individual atoms and bonds within a pentacene molecule. By comparison with density functional theory (DFT) calculations we found that atomic resolution is obtained due to the contributions from the Pauli repulsion.

O 67.3 Thu 11:30 H37

**Probing the surface state and reactivity of an active catalytic site: from single-site catalysts to nanoparticles** — •Elena Groppo — Department of Inorganic, Physical and Material Chemistry, NIS Centre of Excellence and INSTM Unità di Torino, University of Torino

The utility of applying advanced spectroscopic techniques in determining the properties of the active catalytic sites, the difficulties encountered and the possible strategies to overcome the problems, will be discussed in this contribution by considering two case studies, which are among the simplest examples of single-site and multiple-site catalysts, respectively:

(i) the CrII/SiO2 system, which catalyses the ethylene polymerization. Interaction with CO was studied since decades by in situ FT-IR spectroscopy and more recently by Raman spectroscopy, both giving a clear, although indirect, proof that an important rearrangement of the local environment of the CrII site at the silica surface occurs upon CO adsorption. Very recently, XAS experiments offer the first direct experimental evidence of adsorption induced mobility of CrII sites, which is the key for understanding the catalytic activity of CrII sites in presence of adsorbates.

(ii) supported Pd nanoparticles, which catalyse hydrogenation reactions. EXAFS, UV-Vis and FT-IR spectroscopies, coupled with TEM microscopy, are used to investigate the structural, optical and vibrational properties of two Pd/polymer systems in all the synthetic steps, starting from the hosted Pd(OAc)2 precursors up to Pd nanoparticles.

O 67.4 Thu 12:00 H37

**Assembly of core-shell superparamagnetic iron oxide nanoparticles and their application to smart materials** — •Erik Reimhult — ETH Zürich, Zürich, Switzerland

Application of superparamagnetic iron oxide nanoparticles (SPIONs) as biomedical imaging contrast agents and as smart materials require them to retain high stability even in extremely dilute suspensions, high salt and elevated temperatures. Furthermore, many applications require close control over their hydrodynamic diameter and interfacial chemistry. These requirements can only be met by irreversible steric stabilization. We describe how such stabilization can be obtained using dispersants anchored by biomimetically inspired, electronegatively substituted catechols, which provide irreversible binding of a high density polymer shell to the particle core by grafting to assembly, in contrast to previously described approaches using e.g. DOPA or dopamine. The novel dispersant stabilization allowed creation of multifunctional SPIONs for targeted biomedical imaging with controlled number of ligands and individually optimized core and shell thicknesses. Furthermore, we present how assembly of core-shell nanoparticles at fluid hydrophobic-hydrophilic interfaces provides a route to create hierarchical smart materials, by allowing control of the geometry of monolayer films of inorganic cores serving as nanoantennas for external stimuli within a responsive matrix. We show how irreversible binding affinity of the hydrophobic or hydrophilic dispersant shell greatly increases NP loading into lipid, polymer and NP only membranes and allows the emergence of well characterized responsive properties.

O 67.5 Thu 12:30 H37

**The structure of surfactants at the nanoscopic oil-in-water droplet interface and the consequence for the interfacial tension** — •Sylvie Roke — Max-Planck Institute for Metals Research Heisenbergstrasse 3, 70569 Stuttgart, Germany

Surfactants such as sodium dodecylsulphate (SDS) can reduce the interfacial tension between bulk water and bulk n-hexadecane by 42 mM/m. Although it is commonly expected that interfacial tension lowering should also take place on the interface of nanoscopic oil droplets in water vibrational sum frequency scattering experiments indicate otherwise. Vibrational sum frequency scattering is a method that can be used to obtain local structural information from the chemical species present at the interface on nanoscopic oil droplets in water. In these measurements we have directly measured the adsorption of SDS onto hexadecane oil droplets with an average radius of 83 nm. We find that the interfacial density of adsorbed SDS is at least one order of magnitude lower than that at a corresponding planar interface. The derived maximum decrease in interfacial tension is only 5 mN/m.

## O 68: Semiconductor substrates: Epitaxy and growth

Time: Thursday 10:30–13:00 Location: H42

O 68.1 Thu 10:30 H42

**Dimer Flipping at the MOVPE-prepared P-rich GaP(100) Surface** — •Peter Kleinschmidt, Henning Döscher, Sebastian Brückner, Anja Dobrich, Oliver Supplie, Christian Höhn, and Thomas Hannappel — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

The structure of the P-rich GaP(100) surface has been known for some time, showing a p(2x2)/c(4x2) reconstruction. The surface is terminated by alternating buckled phosphorus dimers stabilized by one hydrogen atom per dimer. The STM image of this surface consists of zigzag dimer chains where neighbouring chains can be aligned in phase as well as out of phase to each other. The in-phase configuration results in a p(2x2) surface unit cell, while the out-of-phase configuration corresponds to a c(4x2) unit cell.

We prepared the P-rich GaP(100) surface in a commercial MOVPE system and employed a dedicated transfer system, which enables contamination-free transfer from the MOVPE environment to UHV and, using a mobile transfer chamber, to various surface analysis systems including STM. The quality of our STM images enabled us to compare successive images, revealing in some locations flipping of the P-dimers and therefore of the surface reconstruction. This process requires shifting of the H-termination between the P-atoms in the respective dimer. It could be thermally activated, not dissimilar to the dimer flipping on the clean Si(100) surface, where the flipping cannot be resolved at room temperature by STM, or tip-induced, similar to systems where manipulation of surface atoms can be achieved.

O 68.2 Thu 10:45 H42

**Real Time Measurements of Surface Diffusion in a Multi-Reconstruction System: Ag/Si(111)** — •Dirk Wall[1], Ingo Lohmar[2], Kelly Ryan Roos[3], Joachim Krug[2], Michael Horn-von Hoegen[1], and Frank-Joachim Meyer zu Heringdorf[1] — [1]Fakultät Physik und Center for Nanointegration Duisburg-Essen (CeNIDE), Universität Duisburg-Essen, 47057 Duisburg, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, 50937 Köln, Germany — [3]Department of Physics, Bradley University, Peoria, Il 61625, USA

Photoemission Electron Microscopy (PEEM) is used to study the thermal decay (750-850°C) of Ag islands grown on Si(111) surfaces. During decay, Ag atoms are expelled from the island edges and migrate over the surface. Due to continuous desorption, a coverage gradient forms around each island. Depending on local Ag coverage, two different concentric reconstructions form. These reconstructed "isocoverage zones" are imaged with PEEM. A simple continuum model is presented explaining the dynamic decay of the islands for multi-reconstruction systems. Using this model, we extract diffusion parameters for the specific areas in one simple desorption experiment. We demonstrate that the imaging of these reconstructed "isocoverage zones" constitutes a unique experimental method for directly imaging diffusion fields in epitaxial systems. The general applicability of this imaging technique is demonstrated by the decay of other metal islands on Silicon surfaces of various orientations.

O 68.3 Thu 11:00 H42

**Microscopic picture of hydrogen on the (MO)VPE-preparation of Si(100)** — •Anja Dobrich, Henning Döscher, Sebastian Brückner, Peter Kleinschmidt, Oliver Supplie, Christian Höhn, and Thomas Hannappel — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner Platz 1, 14109 Berlin, Germany

The preparation of Si(100) in the (MO)VPE environment usually involves hydrogen as carrier gas and as by-product from precursors. Hydrogen is suggested to have a crucial impact on the step structure of the silicon surface. To study the complete microscopic picture of the Si(100) surface we observed the (MO)VPE-preparation in situ with reflection anisotropy spectroscopy (RAS) and with a variety of surface-sensitive UHV-based techniques using a contamination-free (MO)VPE to UHV transfer system. Correlation between these results led to the conclusion that the surface is covered with hydrogen, in form of monohydrides and the surface is completely terminated with monohydrides. FTIR-spectroscopy in an attenuated total reflection (ATR) configuration served to perform surface-sensitive measurements of silicon-hydrogen bonds. This is in agreement with results from LEED and STM, which indicated that the surface unit cell consists of dimers. While our results were in agreement with the existence of H-Si-Si-H dimers, ATR spectroscopy did not reveal to what extent dangling bonds of the surface silicon atoms were saturated with hydrogen. Therefore we carried out tip-induced H-desorption by STM, which evidenced complete H-termination of the surface.

O 68.4 Thu 11:15 H42

**Structural and electronic properties of MnGa monolayers on wurzite GaN(0001) surface** — •Kangkang Wang, Abhijit Chinchore, Meng Shi, and Arthur Smith — Ohio University, Athens, OHIO, U.S.A.

Ferromagnetic (FM) metal/semiconductor bilayers are of great interest due to their importance in novel spintronics applications, such as spin injection and spin light-emitting diodes[1]. It has been reported[2] that delta-MnGa, a FM alloy with curie temperature higher than room temperature (RT), can be grown epitaxial on top of w-GaN(0001) with sharp interface and controllable magnetism. Using molecular beam epitaxy, we deposit up to 3 monolayers (ML's) of Mn onto w-GaN(0001) "1x1" surface, which forms Mn(x)Ga(1-x) with x varying from 0 to ~0.6. Mn-induced surface reconstructions and formation of Mn(x)Ga(1-x) crystalline phases are observed by reflection high-energy electron diffraction (RHEED), Auger electron spectroscopy as well as in-situ RT-STM. The data suggests large-period reconstructions upon deposition of <0.25ML Mn and quick formation of delta-MnGa at ~1 ML of Mn. Structural and electronic properties at representative stages will be presented, as well as possible magnetic properties of MnGa ML's. This work has been supported by DOE (Grant No.DE-FG02-06ER46317) and NSF (Grant No.0730257). Equipment support from ONR is also acknowledged.

[1] S.A.Wolf et al, Science 294, 1488 (2001)

[2] E.Lu et al, Phys.Rev.Lett. 97, 146101 (2006) K.K.Wang et al, Mater.Res.Soc.Symp.Proc.1118-K06-06 (2009)

O 68.5 Thu 11:30 H42

**Characterization of copper-metallized ZnO and brass surfaces with STM, SEM and XPS** — •Vadim Schott[1], Zhinong Wang[1], David Silber[1], Franziska Traeger[1], Alexander Birkner[1], Martin Kroll[2], Ulrich Köhler[2], and Christof Wöll[1,3] — [1]Chair of physical chemistry I, Ruhr-Universität Bochum, Germany — [2]Experimental Physics IV, Surface Science Group, Ruhr-Universität Bochum, Germany — [3]Institute of functional interfaces, Karlsruhe Institute of Technology, Germany

The metal-substrate interaction is of particular importance for a better understanding of the methanol synthesis process using Cu/ZnO containing catalysts. Scanning tunneling microscopy (STM) and scanning electron microscopy (SEM) was used to investigate the topography of the copper-metallized ZnO and brass surfaces. Addionally x-ray photoelectron spectroscopy (XPS) reveals information about the chemical composition and the oxidation states of surface atoms. Our ultrahigh vacuum (UHV) apparatus allows STM-, SEM-Imaging and XPS measurements at the same sample position. The initial preparation of the ZnO single crystals is done by cycles of Ar-sputtering (E=800eV) and annealing up to 700°C. Then Cu is deposited by molecular beam epitaxy (MBE). In this work we focus on the growth of Cu on the different ZnO surfaces, diffusion of Cu into ZnO and the feasibility of brass formation. The next step of our research is the characterization of brass single crystals. After initial preparation of the crystals and additional oxidation ZnO layers are growing on the surface. The orientation of this ZnO layer was determined using pyridine as a probe molecule.

O 68.6 Thu 11:45 H42

**Analysis of Anti-Phase-Domains for GaP Heteroepitaxie on Si(100) by LEEM** — •Benjamin Borkenhagen[1], Henning Döscher[2], Gerhard Lilienkamp[1], Peter Kleinschmidt[2], Anja Dobrich[2], Sebstian Brückner[2], Ulrike Bloeck[2], Thomas Hannappel[2], and Winfried Daum[1] — [1]Institute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin

Anti-phase disorder in polar epilayers on non-polar substrates is one of the major obstacles to overcome during the growth of III-V/Si heterojunctions, e.g., for multi-stack solar cells. As a model system, thin heteroepitaxial GaP films were grown on Si(100) substrates with metal-organic vapour phase epitaxy (MOVPE). Despite the use of stepped single-domain Si(001)(2x1) substrates, the complete prevention of anti-phase domains (APD) in the GaP layer is still an unsolved problem. We have applied low energy electron microscopy (LEEM) to retrieve APDs in the main phase matrix. APDs and main phase can be distinguished by dark-field LEEM using specific diffraction spots for imaging. The results are in good agreement with TEM images of identically prepared samples. In contrast to TEM, LEEM needs no further sample preparation and allows for non-destructive investigations. A further advantage is the possibility to analyze large sample areas and find scattered defects. LEEM can also be applied to study the initial growth of such films and to inspect defect formation from the beginning.

O 68.7 Thu 12:00 H42

**Symmetry and Shape of Reconstructed Two-dimensional Nanostructures** — •Bert Voigtländer, Konstantin Romanyuk, and Vasily Cherepanov — Institute of Bio and Nanosystems (IBN-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology

We show that the symmetry of the shape of reconstructed 2D islands (nanostructures) on reconstructed surfaces can deviate from both the symmetry of the underlying substrate and the symmetry of the reconstruction. Only an analysis of the symmetry of the *combined system* of reconstructions on substrate and island and of the substrate lattice can deduce predictions for the island shapes (equilibrium shape or steady state growth shape). In explicit case studies we analyze the symmetry of islands on simple cubic (100), fcc(100), fcc(110) and diamond lattice (111) surfaces and present predictions for the expected island shapes. We introduce a general method for the symmetry analysis of the combined system. Our symmetry analysis includes as a special case also the symmetry of any kind of epitaxial reconstruction domain surrounded by a reconstruction at a surface.

O 68.8 Thu 12:15 H42

**Surface electronic structure and morphology of epitaxial $CuInSe_2$** — •Andreas Hofmann — Helmholtz-Zentrum Berlin für Materialien und Energie, Institut für Ladungsträgerdynamik (E-I4)

Solar cells based on chalcopyrite absorbers reach the highest efficiencies of all thin-film devices. However, the best laboratory cells still lag dramatically behind the theoretical energy conversion limit. So far, calculations for the surface reconstructions and electronic properties exist [1,2], but experimental data on crystalline material is sparse. Therefore, our approach is to study epitaxial $CuInSe_2$ films as a model system with surface analytic techniques.

Samples of different orientation and stoichiometry were prepared by molecular beam epitaxy, the analysis was performed in-situ in a dedicated UHV system. LEED measurements confirmed the c(4x2) surface for near-stoichiometric $CuInSe_2$(112) which was also predicted by calculation [1]. For the copper-depleted surface, however, a (1x1) structure is found. Angle-resolved photoemission data obtained for the (001) surface showed a good agreement with the band structure from DFT [2]. The morphology of surface with different orientation was investigated with scanning tunnelling microscopy.

[1] S.B. Zhang et al., Phys. Rev. B **57**, 9642 (1998)

[2] S.B. Zhang and S.-H. Wei, Phys. Rev. B **65**, 081402 (2002)

O 68.9 Thu 12:30 H42

**Evolution of the surface reconstructions during the growth**

**of an InAs wetting layer on GaAs(001)-c(4×4)** — •Holger Eisele, Jan Grabowski, Christopher Prohl, Britta Hoepfner, and Mario Daehne — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin

We studied the growth of the first monolayer of InAs on the GaAs(001)-c(4×4) surface using a combined UHV-MBE-(RHEED)-STM setup, which provides atomically resolved images of the growth surfaces. For a coverage below about 2/3 of an monolayer of deposited InAs we observe single signatures of the deposited material at the GaAs(001)-c(4×4) surface. The number of these signatures is proportional to the amount of deposited InAs. They occur first at the domain boundaries and further at the hollow sites of the GaAs(001)-c(4×4) reconstruction. At a coverage of about 2/3 of a monolayer an abrupt phase transition occurs in the RHEED. Also the STM images changes completely from the c(4×4) reconstruction to a flat topmost layer, showing an (n×3) periodicity along [110] direction. The detailed analysis of this layer exhibits an in-line (4×3) reconstruction alternating with a brick-lined c(4×6) reconstruction, shifted to each other along the [-110] direction by the insertion of an (6×3) surface unit cell. The stoichiometry of the (4×3) could be determined to $In_{2/3}Ga_{1/3}As$ for the topmost layer and the complete structural model for this surface reconstruction can be given, due to comparison of the STM images with DFT-calculations. On top of this layer, the InAs grows in pure stoichiometry and forms chains and 2D islands with $\alpha2(2\times4)$ and $\beta2(2\times4)$ reconstructions.

O 68.10 Thu 12:45 H42

**In situ RAS Analysis of MOVPE prepared GaP/Si(100) heterointerfaces** — •Oliver Supplie, Henning Döscher, Sebastian Brückner, Anja Dobrich, Peter Kleinschmidt, Christian Höhn, and Thomas Hannappel — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

For high-quality optoelectronic devices built on III-V/Si(100) heterostructures, it is crucial to reduce the defect concentration induced by the heterointerface. As an extremely surface sensitive optical probe, reflectance anisotropy spectroscopy (RAS) can be applied *in situ* in the MOVPE environment. Utilizing RAS, we monitor and characterize the growth of thin GaP layers on a silicon substrate as a model system for III-V/Si(100) heterostructures.

Since RA spectra of the homoepitaxial GaP(100) and heteroepitaxial GaP/Si(100) show characteristic deviations, it is necessary to distinguish the different origins of the RAS signal contributions. Homoepitaxial spectra change with measurement conditions and surface reconstructions. Buried heterointerfaces lead to additional reflections and interference affecting both the reflectance and anisotropy signal. We correct this interference with an empirical method. At III-V/Si(100) heterointerfaces, anti-phase disorder and strain may affect the RAS signal as well. Potentially the interface itself is anisotropic. Applying multiple thin film optical models and reflection simulations, we separate the surface and interface dielectric anisotropy from our measured RAS data.

## O 69: Symposium Polarization Field Control in Group-III-Nitrides

Time: Thursday 9:30–12:15 Location: H1

**Invited Talk** O 69.1 Thu 9:30 H1

**Growth and applications of N-polar (Al,Ga,In)N** — •Stacia Keller and Umesh K Mishra — Electrical and Computer Engineering Department, Univerisity of California, Santa Barbara, CA 93106, USA

While the properties of Ga-polar (Al,In,Ga)N/GaN structures have been widely studied in the past, N-polar nitride films were much less investigated, largely related to difficulties in the growth of smooth N-polar films, in particular by metal organic chemical vapor deposition. Due to the hexagonal symmetry of the GaN crystal, the properties of (Al,Ga,In)N heterostructures grown in both directions are strongly influenced by polarization effects, resulting in strong electric fields in the crystal. The opposite direction of the electric fields in N-polar in comparison to Ga-polar heterostructures is interesting in particular for applications such as enhancement mode transistors, and highly scaled transistors, photodetectors, and solar cells. After a discussion of growth and materials properties of N-polar (Al,Ga,In)N, special emphasis will be given to the fabrication and properties of N-polar GaN/AlGaN and GaN/AlInN transistors. Differences in the properties of N- and Ga-polar two dimensional electron gasses will be addressed as well.

**Invited Talk** O 69.2 Thu 10:00 H1

**Green light-emitting diodes and laser heterostructures on semi-polar GaN(11-22)/sapphire substrates** — •Andre Strittmatter — Palo Alto Research Center, Palo Alto, CA, USA

The performance of nitride-based light emitting diodes (LED) and laser diodes (LD) is subject to polarization charges at the interfaces between the quantum well active region and surrounding barrier material. Reduction or even elimination of such interface charges will enable improved light emitters with power-independent emission wavelength and increased internal quantum efficiency. Different strategies exist to reduce or even eliminate the strength of polarization fields in nitride semiconductor light emitting heterostructures. However, for their potential application within device structures further issues such as strain relaxation, In incorporation and material quality due to the growth itself need to be considered. Semi-polar (11-22) oriented heterostructures offer high In incorporation, low polarization fields in InGaN/GaN quantum wells plus reduced cracking vulnerability of thick AlGaN layers which makes them attractive for long wavelength LEDs and LDs. Experimental results are presented demonstrating reduced blue-shift of long-wavelength emitters and lasing at 500 nm.

**Invited Talk** O 69.3 Thu 10:30 H1

**Pros and cons of green InGaN lasers on polar GaN substrates** — •Uwe Strauss, Adrian Avramescu, Teresa Lermer, Jens Müller, Christoph Eichler, and Stephan Lutgen — Osram Opto Semiconductors, Leibnizstr. 4, 93055 Regensburg, Germany

One of the big challenges of InGaN lasers is the development of a device for the green spectrum. In 2009, first direct green InGaN lasers are demonstrated. The next step forward to a product will be cw operation at long wavelength > 515nm combined with wall plug efficiencies of several percent and power levels up to 50mW. However, the question about polar or non-polar orientation is still open and researchers investigate different substrates: (1) c-plane GaN: Nichia reported 515nm at 8mW cw operation on this GaN substrate, OSRAM presented R&D samples operating already at 50mW cw and 515nm. (2) Rohm published 499nm lasing on non-polar m-plane GaN. (3) Recently, Sumitomo used semi-polar substrates [20-21] to achieve 520nm lasing with 2mW of cw output power. The longest wavelengths of pulsed lasing were 526nm on c-plane (OSRAM) and 531nm on [20-21] (Sumitomo), respectively. The big advantage of c-plane is that 2 inch c-plane substrates are commercially available in high volume. The wafer size, availability and costs of semi-polar / non-polar substrates are still not clear. We will present recent results on c-plane GaN and we will discuss the advantages and disadvantages related to lasers grown on this orientation. The lasers already reached more than 2% wall plug efficiencies in cw operation at 515nm and power levels of 50mW.

**15 Min. Coffee Break**

**Invited Talk** O 69.4 Thu 11:15 H1

**Molecular beam epitaxy as a method for the growth of free-standing zinc-blende GaN layers and substrates.** — •Sergei Novikov, Thomas Foxon, and Anthony Kent — School of Physics and Astronomy, University of Nottingham, Nottingham, NG7 2RD, UK

The group III-nitrides normally crystallise in the hexagonal (wurtzite) structure. The unique feature of wurtzite group III-nitrides, in comparison with conventional III-V semiconductors, is the existence of very strong electric fields inside the crystal structure. The electric fields can be eliminated in wurtzite material by growing in non-polar directions. However, a direct way to eliminate electric fields would be to use non-polar (001) oriented zinc-blende (cubic) III-nitride layers. The thermodynamically metastable cubic GaN layers have, so far, received less attention than the more familiar hexagonal films.

We have developed a process for growth by molecular beam epitaxy (MBE) of free-standing cubic GaN layers with potential application as substrates. Undoped thick cubic GaN films were grown on semi-insulating GaAs (001) substrates by a modified plasma-assisted molecular beam epitaxy (PA-MBE) method and were removed from the GaAs substrate after the growth. The resulting free-standing GaN wafers with thickness in the 30-100$\mu$m range may be used as substrates for further epitaxy of cubic GaN-based structures and devices. We will discuss the fabrication and properties of cubic GaN substrates. The first GaN/InGaN LEDs on our zinc-blende GaN substrates have been demonstrated by our collaborators.

**Invited Talk** O 69.5 Thu 11:45 H1

**Three-dimensional GaN for semipolar light emitters** — •Thomas Wunderer[1], Frank Lipski[1], Stephan Schwaiger[1], Ferdinand Scholz[1], Martin Feneberg[1], Klaus Thonke[1], Andrey Chuvilin[1], Ute Kaiser[1], Sebastian Metzner[2], Frank Bertram[2], Jürgen Christen[2], Clemens Vierheilig[3], and Ulrich Schwarz[3] — [1]Ulm University — [2]Otto-von-Guericke-University — [3]University of Regensburg

Semipolar group III-nitrides are thought to be possible candidates for improving the problems of the so-called green gap and the efficiency droop during high current operation. The reduced piezoelectric fields lead to an improved radiative recombination probability even within thick InGaN quantum wells (QWs).

In this paper, a detailed description of the fabrication technology of 3D GaN structures providing semipolar facets will be presented. The high material quality is confirmed by structural and optical investigation methods showing that effective defect reduction can be realized. Extremely low threading dislocation density and stacking fault-free surfaces can be achieved. InGaN QWs deposited on the 3D structures show interesting phenomena as semipolar emitters. Structural properties will be explained by growth models of selective area epitaxy. Besides, the effectiveness of the method will be discussed by evaluating the internal quantum efficiency for different Indium compositions. Therefore, locally resolved measurement methods contributed from several groups are analyzed and combined. Additionally, a complete LED device is demonstrated.

## O 70: Invited talk (Loth, Sebastian)

Time: Thursday 14:00–14:45 Location: H36

**Invited Talk** O 70.1 Thu 14:00 H36

**Sensing and controlling the spin of an atom by electric current** — •Sebastian Loth — IBM Research Almaden, San Jose CA, USA

Electrons interact with the magnetic moment of the material they flow through [1]. This effect is harnessed in the spin transfer torque (STT) to manipulate the relative alignment of the magnetization directions of ferromagnetic thin films in magnetic multilayer devices. We show that similar electrical control is possible for quantum magnetic systems where magnetic excitations are energetically discrete. Individual transition metal atoms adsorbed to a copper nitride layer on a copper substrate serve as model system. We use a low temperature scanning tunneling microscope (STM) to address individual adatoms and probe their energetically discrete excitations by inelastic tunneling [2]. By attaching one magnetic atom to the probe tip and positioning it above another magnetic atom on the surface electric current flows between them and efficiently transfers spin-angular momentum. Similar to the macroscopic STT, the direction of current flow determines whether the magnetic moments of the atoms are driven towards alignment or anti-alignment and a magnetoresistive elastic tunnel current enables sensing it. This technique gives access to the dynamic behavior of the surface-bound spin. We study the mechanism for spin relaxation out of the highly excited spin states and quantify the spin lifetimes in these quantum magnetic systems.

[1] Chappert, et al., Nature Materials 6, 813 (2007). [2] Hirjibehedin, et al., Science 317, 1199 (2007).

## O 71: Metal substrates: Epitaxy and growth

Time: Thursday 15:00–18:00 Location: H31

O 71.1 Thu 15:00 H31

**Interaction of gold with clean and oxygen-covered Re$(10\bar{1}0)$ surfaces** — Sebastian Schwede, •Susanne Schubert, Christian Pauls, and Klaus Christmann — Freie Universität Berlin, Takustr. 3, 14195 Berlin

The structure, growth and morphology of thin Au films deposited on both clean and oxygen-covered rhenium $(10\bar{1}0)$ surfaces has been studied as a function of coverage $\Theta$ and temperature T using LEED, STM and thermal desorption spectroscopy (TDS). In the absence of oxygen, Au forms a variety of ordered $(1 \times n)$ phases (n = 3, 4, 5, 6 and 1) with the Au adsorption energy increasing from $\sim$ 320 kJ/mol at low $\Theta$ to $\sim$ 380 kJ/mol near the bilayer $(1 \times 1)$ structure ($\Theta = 2$), where the heat of sublimation of bulk Au, $\Delta H_{sub}$, is reached. Au wets the Re surface completely, for $\Theta > 2$, a simultaneous multilayer growth is observed. On the oxygen covered Re surface with its well-known (reconstructed) $(1 \times 3)$-2O phase ($\Theta = 2/3$), however, Au deposition at 300 K causes immediate 3D clustering with rough and heterogeneous films pointing to a clear non-wetting behavior. Annealing of these films at 850 K gives the Au atoms sufficient mobility to coalesce to cylindrically shaped aggregates of ca. 50 Å diameter and 100 Å average length which are aligned parallel to the troughs of the Re surface. At elevated temperatures, Au desorbs first from the bulk phase ($E_{des} = \Delta H_{sub}$), only as oxygen desorption becomes competitive, Au atoms can diffuse to and interact with the bare Re sites and desorb with the characteristic energy.

O 71.2 Thu 15:15 H31

**Study of the growth of bismuth thin film on graphite with STM and UPS at low temperature** — Fei Song, Justin Wells, Magne Saxegaard, Anne Borg, and •Erik Wahlstrøm — Department of Physics, Norwegian University of Science and Technology(NTNU),Trondheim 7491, Norway

Bismuth, a novel semimetal material, which has been widely studied recently as topological insulator in the form of alloy with some other metals. In this talk, we will foucs on the growth behaviour of Bi film from very thin coverage to thick layer at low temperature, in the light of scanning tunnelling microscopy (STM) and photoemission spectrocopy (PES), to have a close look at the interface morphology and electronic structure. Similar to other reports about Bi on Si substrate at critical coverage, interesting phenomenon, such as quantum well states will show up together with surface states which can be easily resolved from bulk states from the valce band.

O 71.3 Thu 15:30 H31

**Structural analysis of Ag growth on Ni(111)** — •Axel Meyer[1], Jan Ingo Flege[1], Sanjaya Senanayake[2], Faisal Alamgir[3], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, 28359 Bremen, Germany — [2]Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973-5000, USA — [3]Georgia Institute of Technology, Atlanta, GA 30332-0245, USA

The growth structure and morphology of ultra-thin metal films on metallic substrates strongly influence the physical and chemical properties of the resulting bimetallic system. Therefore, a particular knowledge of these properties is crucial for creating functional materials with novel characteristics. In this contribution, a detailed study of the growth of ultra-thin silver films on the Ni(111) surface employing in-situ low-energy electron microscopy and diffraction (LEEM/LEED) is presented.

In the entire temperature range from 470 K to 850 K, silver is observed to grow in a Stranski-Krastanov mode with a wetting layer exhibiting a critical thickness of two atomic layers. For lower temperatures, the Ag films take on a collinear $(7 \times 7)$ structure or a 1° tilted $(\sqrt{57} \times \sqrt{57})R6.59^\circ$ structure, respectively, the latter as predicted by Chambon et al. (Phys. Rev. B **79** 125412 (2009)). Elevated temperatures over 675 K lead to a $(\sqrt{52} \times \sqrt{52})R13.9^\circ$ reconstruction with extended rotational domains on the Ni(111) surface, while Ag/Ni intermixing is not observed throughout the whole temperature range. Furthermore, by quantitative intensity-voltage analysis of the specular beam, layer-dependent surface relaxations were determined.

O 71.4 Thu 15:45 H31

**Rare earth metals - Au surface compounds** — •Martina Corso[1,2], Matthieu Verstraete[3], Frederik Schiller[4], Laura Fernández[1], Maider Ormaza[5], Thomas Greber[6], Angel Rubio[3], and J. Enrique Ortega[1,3,5] — [1]Donostia International Physics Center, San Sebastián, Spain — [2]Institut für Experimentalphysik, FU Berlin, Germany — [3]ETSF, Centro Joxe Mari Korta, San Sebastián, Spain — [4]Centro de Física de Materiales, San Sebastián, Spain — [5]Departamento de Física Aplicada I, San Sebastián, Spain — [6]Physik Institut, Universität Zürich, Switzerland

The high temperature reactive deposition of rare earths on Au(111) leads to the formation of surface compounds with extraordinary crystallinity. Gd on Au(111) is the most promising system we studied so far. Under specific growth parameters, we are able to obtain alloyed single- and double-layers whose optimum surface atomic structure corresponds to the $GdAu_2$ stoichiometry. Moreover, the lattice mismatch between the $GdAu_2$ layers and the Au substrate gives rise to a long-range periodic Moiré pattern, with a lattice parameter of 3.8 nm as detected by STM. We measured in detail with ARPES the electronic structure of the surface compound and based on theoretical calculations we identified the origin of the bands. This robust and highly ordered nanostructure is a perfect template to grow magnetic clusters. Co deposited at RT forms a regular network of homogeneously-sized dots that faithfully follow the underlying Moiré periodicity. By changing the Co coverage, we can obtain cluster arrays with areal densities up to 54 Teradots/inch$^2$ and remanent magnetization at 300 K.

O 71.5 Thu 16:00 H31

**Small Pt adatom clusters on Pt(111): When fewer bonds are better than more** — •Michael Schmid[1], Andreas Garhofer[1,2], Josef Redinger[1,2], Florian Wimmer[1], Philipp Scheiber[1], and Peter Varga[1] — [1]Institut f. Angewandte Physik, TU Wien — [2]Center for Computational Materials Science, Wien, Österreich

Bonding of face-centered-cubic metals is usually characterized by a preference for high a coordination number of each atom. In sharp contrast to this picture, we find that small clusters of Pt adatoms on Pt(111) behave differently. Creating a high number of small Pt adatom clusters by pulsed laser deposition at low temperature, we find that up to 1/3 of all clusters are linear chains of Pt atoms with lengths of up to 9 atoms. This finding cannot be explained by a simple diffusion-limited-aggregation model. We have therefore analyzed the binding energies of Pt adatom clusters by density functional theory and found that bonding of such clusters does not follow the rule of “higher coordination is stronger bonding”. Instead, short linear chains are bound more strongly than some more compact configurations, explaining the preference for such structures observed experimentally. We ascribe the unusually low energies of short chains to strong bonding towards atoms at opposite sides, induced by $d_{z^2}$-like orbitals. We have also obtained time-lapse STM movies of diffusing Pt adatoms and their coalescence. The data show no strong long-range interaction between adatoms, which would otherwise provide a different route towards an explanation of the phenomena observed.

O 71.6 Thu 16:15 H31

**Submonolayer growth of Cu on Cu(110)** — •Georg Ciobotea, Andreas Dobler, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

The submonolayer growth of Cu on Cu(110) was investigated by scanning tunneling microscopy. Due to the geometry of the Cu(110) surface, diffusion in $(1\bar{1}0)$ direction is expected to be dominant.

Island densities and shapes are measured after varying particle flux, coverage and temperature. Below 180 K, long and narrow islands of nearly constant width are found indicating a one-dimensional growth mode. At higher temperature island widths are strongly increasing. A comparison to nucleation theory is presented.

Thermal deposition and pulsed-laser deposition were compared at variable temperatures below 260 K. For pulsed-laser deposition, higher island densities are expected because of the high instantaneous particle flux. This behavior is found at low temperatures, where small adatom mobility is given.

O 71.7 Thu 16:30 H31

**Pulsed-laser deposition of Cu on Cu(001) - the crucial role of particle mobility and flux** — •Andreas Dobler and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Pulsed-laser deposition (PLD) provides for some $\mu s$ up to $10^5$ times higher particle flux than thermal deposition (TD). For homoepitaxial submonolayer growth, nucleation theory predicts island densities on the substrate scaling with a power law of flux $F$ over the temperature-dependent diffusion coefficient $D$. Thus, significantly higher island densities are expected for PLD than for TD.

At 300 K, we found identical island densities for PLD and TD which were measured by scanning tunneling microscopy. Systematic variation of $D$ (temperatures from 150 to 300 K) and $F$ shows that this unexpected behavior is limited to low $F/D$ values. At high $F/D$, the island density created by PLD is significantly higher than by TD. Nucleation is modeled by numerical integration of rate equations to explain this behavior.

O 71.8 Thu 16:45 H31

**Anomalous Size-Dependent Reconstruction Behavior of Cu-Islands on Ag(100)** — •Michael Rieger[1], Christopher Zaum[2], Karina Morgenstern[2], and Karsten Reuter[1,3] — [1]Fritz-Haber-Institut, Berlin (Germany) — [2]ATMOS Leibniz Universität Hannover, (Germany) — [3]Technische Universität München, (Germany)

Fast-STM reveals an unusual structure and mobility of smaller Cu-islands on clean Ag(100) at room temperature. Small islands show a complex structure with Cu atoms also adsorbed in bridge sites, and a diffusivity and decay time that is significantly higher than any previously measured value. These observations are supported by our DFT calculations, which indicate a complex reconstructed structure of islands in this size range. Driven by the large lattice mismatch between Ag and Cu, this reconstruction enables shorter Cu-Cu bonds and thereby a stabilization through intra-island strain release. With the concomitantly weakened Cu-Ag bonds, the computed lower binding energy of reconstructed islands to the Ag(100) substrate is consistent with the measured higher diffusivity. In order to better explore the configuration space of island structures we validate an EAM potential for the Ag/Cu system against our DFT data set and employ it for an extensive structure search. The semi-empirical potential enables us to predict a critical island size for the reconstruction that is in perfect agreement with the experimental estimate for the shape turnover.

O 71.9 Thu 17:00 H31

**Temporal evolution of Pb-islands on Ni(111)** — •Tjeerd R.J. Bollmann, Raoul van Gastel, and Bene Poelsema — MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

Low Energy Electron Microscopy (LEEM) allows real-time imaging of epitaxial growth of metals on metal substrates. We have used LEEM in combination with micro Low Energy Electron Diffraction to study the structure, size and height evolution of Pb islands on top of a Pb wetting layer on a Ni(111) surface, as well as the diffusion of islands across steps during epitaxial growth at elevated temperatures. Pb islands diffusing across nickel steps show remarkable self-organization in that they can half their surface area by doubling their layer in height. Concerted rapid coarsening of (larger) Pb islands within seconds is also observed. In both cases mass transport of Pb leads to new island equilibrium shapes with increased uniform (integer) heights. We present a systematic LEEM investigation of the effects that play a role in the area versus height evolution of Pb islands at elevated temperatures. The results are discussed in view of quantum size effect driven growth where specific heights are particularly stable.

O 71.10 Thu 17:15 H31

**Adsorbate-induced segregation of $C/Pt_{25}Rh_{75}(100)$: ab-initio predictions** — •Tobias Kerscher, Wolfgang Landgraf, and Stefan Müller — Universität Erlangen-Nürnberg, Lehrstuhl für Theoretische Physik 2, Staudtstr. 7, 91058 Erlangen, Germany

The segregation profile of alloy surfaces can strongly depend on the presence of adsorbates, a fact that is especially interesting for catalysts. The (100) surface of the alloy $Pt_{25}Rh_{75}$ provides an example:

For the clean surface, the experiment [1] shows a strong Pt enrichment in the top atomic layer and a depletion underneath. Yet, even a small amount of carbon impurity (8% of a monolayer) leads to a considerable decrease in the Pt top layer concentration [1]. We use an ab-initio-based cluster-expansion in the framework of the UNCLE code [3] to efficiently model this adsorbate-induced change in segregation. The properties of the system are found to be controlled by two competing effects: the different segregation energies of Pt and Rh, and their individual binding energies to C. We discuss the substitutional ordering of the system as a function of C-coverage.
Supported by Deutsche Forschungsgemeinschaft

[1] E. Platzgummer et al., Surf. Sci. **419** (1999), 236
[2] S. Müller, M. Stöhr, O. Wieckhorst, Appl. Phys. A. **82** (2006), 415 [3] D. Lerch *et al*, Modelling Simul. Mater. Sci. Eng. **17** (2009), 055003

O 71.11 Thu 17:30 H31

**Oblique incidence ion impact pattern formation on Cu(001) along the [100] and [110] azimuthal directions** — •Frank Everts, Herbert Wormeester, and Bene Poelsema — Solid State physics, MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

Oblique incidence sputtering is a versatile tool for nanopattern creation on different types of surfaces. Often ripple patterns are observed as a result of an erosion instability. The orientation of the ripples is governed by the polar angle of incidence of the ion beam. High resolution low energy electron diffraction reveal an unanticipated azimuth dependence for Cu(001) at 200 K. Near normal incidence sputtering along [110] gives rise to a diffraction pattern showing a fourfold symmetry of the etch structures. Surprisingly, a further increase of the polar angle shows that this surface imposed fourfold symmetry is preserved up to grazing incidence. In marked contrast are the results for sputtering along the [010] azimuth. Already for near normal incidence the fourfold symmetry in the diffraction pattern is broken, reflecting ripple formation. The orientation of these ripples changes with more oblique incidence sputtering. The explanation for this strong azimuth sensitivity is found by varying the ion energy, showing a strong dependence on the details of the ion substrate interaction.

O 71.12 Thu 17:45 H31

**Surface structures of thin silver films on the Re**$(10\bar{1}0)$ **surface** — •Viktor Scherf, Lyria Messahel, Christian Pauls, and Klaus Christmann — Freie Universität Berlin, Takustr. 3, 14195 Berlin

We have studied the growth of silver on the Re$(10\bar{1}0)$ surface in UHV between 300 and 700 K by means of MEED and LEED as well as with TPD. The phenomena depend strongly on coverage and temperature: At 300 K a $(1 \times 4)$ LEED phase exists in the large coverage range $0.1 < \Theta < 2$. For $T > 400$ K Ag forms a $c(2 \times 2)$ structure which reversibly transforms to the $(1 \times 4)$ phase upon cooling. *In-situ* MEED was performed during Ag deposition at various temperatures; grazing incidence ($\sim 2°$) and off-Bragg scattering conditions provided high sensitivity with respect to surface electron reflectivity. At 700 K, we find a pronounced correlation between the (0,0) MEED beam intensity and the growth of the Ag phases which helps to calibrate the (local) Ag coverages. *Nominal* Ag coverages are obtained from Ag TPD peak areas. Systematic LEED intensity-temperature meassurements at fixed $\Theta_{Ag}$ reveal optimum values of $\Theta = 1.3$ for the $c(2\times2)$ and $\Theta = 1.5$ for the $(1 \times 4)$ structure, respectively. Near the monolayer saturation a pseudomorphic $(1\times1)$ structure forms. According to dynamical LEED calculations, it contains two Ag atoms/unit cell and manifests $\Theta = 2$ for this bilayer, in which both troughs and ridges of the Re surface are covered by Ag atoms. The data are discussed and compared with the previously studied Au-on-Re$(10\bar{1}0)$ system.

## O 72: Plasmonics and Nanooptics VI

Time: Thursday 15:00–18:00 Location: H32

O 72.1 Thu 15:00 H32

**Surface plasmon polaritons on arrays of nanostructures with three-fold symmetry** — •David Leipold, Stephan Schwieger, and Erich Runge — Institut für Physik und Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau

Surface plasmon polaritons (SPPs) are optical excitations that are confined to a metal-dielectric interface. They interact with propagating light if the metal is structured on the scale of the wavelength of the incident light. Here, we consider the coupling properties of quadratic arrays of nano-holes cut into a silver film. In particular, we investigate the influence of nano-holes with three-fold symmetry, which is incompatible with the four-fold symmetry of the array. Our numerical results reproduce aspects of earlier experimental findings [1]. Namely, there are shifts in the SPP-related minima and maxima in the reflectivity of specific reflection orders as function of the polarization of the incident light.

[1] B. Ashall, M. Berndt, and D. Zerulla, *App. Phys. Lett.* **91**, 203109 (2007)

O 72.2 Thu 15:15 H32

**Determination of surface plasmon polariton velocity measured by scattering scanning nearfield optical microscopy** — •Brian Ashall and Dominic Zerulla — School of Physics, University College Dublin, Dublin 4, Ireland.

Surface Plasmon Polaritons (SPPs) are electromagnetic waves, propagating at the interface of a metal and a dielectric material, that are coupled to a charge density oscillation of the free electrons of the metal. In order to examine the optical nearfields of SPPs as they interact with nanoscale topography features, the technique of scattering Scanning Nearfield Optical Microscopy (sSNOM) is used. Presented here is an example of direct imaging of standing SPP interference patterns following interaction with a sharp topographic reflector. Analysis of this SPP interference pattern demonstrates a SPP propagation velocity of 0.93 times the speed of light. In addition to this, interaction of SPPs with specifically designed surface patterns will be demonstrated to yield a focussing of the plasmon nearfield.

O 72.3 Thu 15:30 H32

**Surface Plasmon Mapping using Photoelectron Emission Microscopy combined with Huygens principle** — •Christian Schneider, Alexander Fischer, Martin Rohmer, Daniela Bayer, Pascal Melchior, and Martin Aeschlimann — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern

Photoelectron emission microscopy (PEEM) is a very powerful tool to investigate electron dynamics simultaneously in time and space with femtosecond temporal and nanometer spatial resolution. This microscopy technique is also suitable to study plasmonic behaviour in metal nanostructures, which combines the advantages of photonics and electronics. In this talk, we will show PEEM measurements of structures exhibiting surface plasmon polariton (SPP) resonances and present a novel simulation method based on Huygens' principle. As only the beating between the exciting light wave and the SPP wave can be observed by PEEM, a direct access to the surface plasmon wave isn't possible. Applying the simple wave model of Huygens in combination with a fast and reliable fitting algorithm to the complex PEEM data allows us to recalculate the propagating SPP wave for different shaped nanostructures. Examples like gold-squares as well as L-shaped structures are presented.

O 72.4 Thu 15:45 H32

**Photoemission Microscopy with Surface Plasmon Polaritons** — Niemma Buckanie[1], Nicolai Rass[1,2], Pierre Kirschbaum[1], Michael Horn-von Hoegen[1], and •Frank-J. Meyer zu Heringdorf[1] — [1]Universität Duisburg-Essen, Fakultät für Physik and Center for Nanointegration (CeNIDE), Lotharstrasse 1, 47057 Duisburg, Germany — [2]present address: E.ON Gastransport GmbH, 45141 Essen, Germany

The interaction of frequency doubled femtosecond laser pulses with Silver provides a fantastic opportunity to study surface plasmon polariton (SPP) phenomena in Ag nanostructures. In two photon photoemission microscopy (2PPE PEEM) using femtosecond laser pulses, SPPs are imaged as a superposition of the electric field of the travelling SPP wave with the electric field of the laser pulse that hits the surface under grazing incidence. As the SPP and the fs laser pulse travel at different speeds, a moiré pattern is formed across the island that can be directly imaged in 2PPE PEEM. The period and orientation of the moiré pattern are influenced by the angle between the propagation direction of the SPP wave and the projection of the direction of incidence of the laser pulse into the surface plane. In a pump-probe experiment, where two coherent fs laser pulses are mutually time-delayed, it is possible to shift the moiré pattern across the island, to visualize the propagation of the SPP, and to control the location of maximum intensity behind the particle.

O 72.5 Thu 16:00 H32

**Free-Space Excitation of Propagating Surface Plasmon Polaritons** — •Jan Renger[1], Romain Quidant[1], Niek van Hulst[1], Stefano Palomba[2], and Lukas Novotny[2] — [1]ICFO-Institut de Ciencies Fotoniques, 08860 Castelldefels (Barcelona), Spain — [2]Institute of Optics, University of Rochester, Rochester, NY 14627, USA

A unique feature of surface plasmon polaritons (SPPs) is that their in-plane momentum is larger than the momentum of free-propagating photons of the same energy. Therefore, it is believed that they can be excited only by evanescent fields created by total internal refection or by local scattering. Here, we provide the first demonstration of free-space excitation of surface plasmons by means of nonlinear four-wave mixing [1]. The process involves the vectorial addition of the momenta of three incident photons, making it possible to penetrate the light cone and directly couple to the SPP dispersion curve. Using this technique, surface plasmons can be launched on any metal surface by simply overlapping two beams of laser pulses incident from resonant directions. The excitation scheme is also applicable to other bound modes, such as waveguide modes, surface phonon-polaritons, and excitations of two-dimensional electron gases. [1] J. Renger et al. Phys. Rev. Lett. accepted (2009)

O 72.6 Thu 16:15 H32

**Femtosecond Surface Plasmon Characterisation on Metallic Dielectric Interfaces** — Jose Francisco Lopez-Barbera, Brian Ashall, and •Dominic Zerulla — University College Dublin, School of Physics, Dublin 4, Ireland

As result of the latest advances in ultrashort pulse measurements, it is now possible to investigate ultrashort processes such as surface plasmon polariton (SPP) dynamics on a sub 20 fs time scale. SPPs are one of the fastest events in nature with time scales varying from 100s of attoseconds to 100s of nanoseconds. Using advanced autocorrelation techniques based on optical gating (FROG and GRENOUILLE) in combination with a 12 fs broadband Ti:Sa laser system, we have characterised the resonant photon-SPP coupling processes on metallic thin films. In particular we focus on the excitation, propagation and life-time of the SPPs at high temporal and frequency resolution. We will present surprising insights into the behaviour of SPPs on this short timescales, including data on the interference of the SPP emission with the directly reflected/diffracted channel.

O 72.7 Thu 16:30 H32

**Light guiding in para-hexaphenylene based nanofibers in interaction with a gold substrate studied by photoemission electron microcopy** — •Till Leissner[1], Michael Bauer[1], Kasper Thilsing-Hansen[2], Roana Melina de Oliveira Hansen[2], Jakob Kjelstrup-Hansen[2], and Horst-Günther Rubahn[2] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel — [2]NanoSYD, Mads Clausen Institute, University of Southern Denmark

Para-hexaphenylene (p-6P) based nanofibers have been proven to support almost loss-free and broadband optical wave guiding up to wavelengths as short as 400 nm [1]. As a dielectric distortion on top of a metallic substrate, they can, additionally, support the localized propagating of interface plasmon modes. P-6P nanofibers may therefore be useful as light-channeling sub-units and highly localized emitters in future ultrafast nanophotonic devices. To address the interaction between optical waveguiding and surface plasmon excitations we deposited well aligned p-6P nanofibers onto microstructured gold films. Photoemission Electron Microscopy was used to image the local light modes excited by a femtosecond laser pulse. Within the nanofibers, periodic beating patterns are observed which exhibit a strong dependence on the polarization the excitation laser field. The pattern periodicity can quantitatively be modeled and assigned to the interference between a propagating interface plasmon and the excitation light field, thus given evidence for plasmon guiding by the nanofibers.

[1] H.-G. Rubahn et al., Appl. Phys. Lett. 82, 10 (2003)

O 72.8 Thu 16:45 H32

**Surface Plasmon Excitation on Magnetoactive Hybrid Materials** — •Dominic Zerulla and Brian Ashall — UCD Dublin, School of Physics, Dublin 4, Ireland

The interaction of surface plasmons polaritons (SPPs) - fluctuations in the electron density at the interface between media with dielectric constants of opposite sign - with magnetically ordered systems has attracted a significant interest in recent years, as a result of the possibility of enhancing magneto-optical properties, like the Faraday and Kerr effect. More recently, research has been focused on the merging of the areas of spintronics and plasmonics, thus developing a new field called spin-plasmonics. Here, we will present a systematic study of the excitation of SPPs on ferromagnetic materials in multilayered structures composed of thin films of nickel, iron, cobalt, capped by a silver layer [1]. The electromagnetic properties of the systems are theoretically and experimentally investigated as a function of the metal layers' thickness and the critical parameters in this study of the interaction between surface plasmon waves and the magneto-active material are discussed. Finally, an optimized structure for the investigations of spin-plasmonic effects in thin films is proposed.

[1] L. Sapienza, D. Zerulla, "Surface Plasmon Excitation on Magnetoactive Materials", Phys. Rev. B 79, 033407 (2009)

O 72.9 Thu 17:00 H32

**Loss compensation of surface plasmon polaritons in multilayer structures with optically pumped gain media** — Patrick Scholz[1,2], •Stephan Schwieger[1], and Erich Runge[1] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Climate Science Division, Alfred Wegener Institut für Polar- und Meeresforschung, 27570 Bremerhaven, Germany

Surface plasmon polaritons (SPPs) that are excited at metal gratings have large losses due to metallic absorption and re-radiation into propagating far-field modes. These losses can be possibly compensated by energy transfer from thin layers of optically excited media, such as semiconductor quantum wells in close vicinity to the metal surface [1,2]. In this contribution, the loss compensation is investigated theoretically as a function of the geometry of the sample. Parameters, such as the grating period, the slit width, the thickness of the metal film, and the spatial separation between the quantum well and the metal are varied. Furthermore, the formation of coupled SPP-exciton modes and some of their properties, as, e.g., their life times, propagation lengths, and group velocities, are discussed.

[1] P. Vasa, R. Pomraenke, S. Schwieger, Yu. I. Mazur, Vas. Kunets, P. Srinivasan, E. Johnson, J. E. Kihm, D. S. Kim, E. Runge, G. Salamo, and C. Lienau, *Phys. Rev. Lett.* **101**, 116801 (2008).

[2] S. Schwieger, P. Vasa, and E. Runge, *Phys. Stat. Sol. (b)* **245**, 1071(2008).

O 72.10 Thu 17:15 H32

**Electrically influencing the surface plasmon dispersion relation** — •Brian Ashall[1], Michael Berndt[2], and Dominic Zerulla[1] — [1]School of Physics, University College Dublin, Dublin 4, Ireland. — [2]Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden, Germany.

Surface Plasmon Polaritons (SPPs) are a resonant coupling of electromagnetic radiation to charge density oscillations of the conduction electrons at the surface of a metal. As this SPP charge density oscillation is based on electron movement, it is intuitive to consider the possibility of influencing SPPs with an applied electric current, which also moves the charges to which the SPPs are coupled. This possibility to directly influence SPPs is examined experimentally, along with indirect electrical influences, such as electric Joule heating. Additionally, the inverse process is examined; i.e. the potential for the creation of a direct net movement of electrons by propagating SPPs. The possibility for this to occur is supported by the fact that the electromagnetic waves describing SPPs possess electrical field components along the propagation direction of the plasmons, and so they should have some potential to move the charge carriers to which they are coupled.

O 72.11 Thu 17:30 H32

**Efficient Coupling of Single NV Centres to Surface Plasmon Polaritons** — •Bernhard Grotz[1], Merle Becker[1], Sebastian Macke[2], Julia Tisler[1], Gopalakrishnan Balasubramanian[1], Fedor Jelezko[1], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, Universität Stuttgart, Germany — [2]Max-Planck-Institut für Metallforschung, Stuttgart, Germany

When light interacts with metal surfaces it excites electrons which can form propagating charge-density waves called surface plasmon polaritons. These collective electronic excitations have many applications due to their ability to produce strong electric fields localized to subwavelength distance scales. It was shown that nanodiamonds containing single nitrogen-vacancy (NV)centres can be attached efficiently to silver nanowires where they are used to excite single surface plasmon polaritons [1]. We discuss recent approaches to address this problem and in particular how to increase the coupling strength between NV and nanowires.

[1] R. Kolesov, B. Grotz, G. Balasubramanian, R. J. Stöhr, A. A. L. Nicolet, P. R. Hemmer, F. Jelezko & J. Wrachtrup, Wave-particle duality of single surface plasmon polaritons, Nature Physics 5, 470-474 (2009)

O 72.12 Thu 17:45 H32

**Plasmonic Collimation for near-IR Laser Diodes** — •Xinghui Yin[1,2], Justin White[3], Mark Brongersma[3], and Thomas Taubner[1,2] — [1]RWTH Aachen — [2]Fraunhofer-Institut für Lasertechnik — [3]Stanford University

It is known that one can use gratings to couple freely-propagating light to plasmon modes. Ebbesen [1] examined the reverse process at a metallic slit-grating structure and discovered a beaming effect. Subsequently, Capasso [2] successfully combined such a structure with a Quantum Cascade Laser at a mid-infrared wavelength of $\lambda = 9.8\ \mu$m to reduce the beam divergence in one direction.

In our work, we investigate plasmonic collimators for laser diodes at near-infrared wavelengths. We focus on optimizing the structure parameters for $\lambda = 960$ nm. In this region, it is important to take the higher surface plasmon propagation losses into consideration. Also, we examine the efficiency of plasmonic collimation compared to conventional laser diode collimation by cylindric lenses.

The simulations are carried out using a 2D Finite Difference Frequency Domain code developed by J. White. Using the obtained parameters, we fabricate the plasmonic collimator and characterize it.

[1] Ebbesen et al., 2002, Vol 297, Science

[2] Capasso et al., Nature Photonics, 2008

## O 73: Solid/liquid interfaces II (focussed session)

Time: Thursday 15:00–17:45 Location: H33

**Invited Talk** O 73.1 Thu 15:00 H33

**Theoretical studies on the electrocatalytic Oxygen reduction reaction on Pt** — •Timo Jacob — Universität Ulm, Albert-Einstein-Allee 47, D-89069 Ulm

The oxygen reduction reaction (ORR) is one of the most important reactions in basic electrochemistry and for various applications such as fuel cells. However, due to the high complexity of this reaction the exact mechanisms is still unknown.

Using density functional theory, we investigated different mechanisms of the ORR on Pt electrodes [1]. Among the three main mechanisms (i.e., $O_2^{ad}$-Dissociation, $OOH^{ad}$-Formation, and $HOOH^{ad}$-Formation) we found that $HOOH^{ad}$-Formation is the preferred process in gas phase. When including water solvation as an environmental effect, the reaction paths were modified, leading to drastic changes in the energetics and a nearly identical preference for the $O_2^{ad}$-Dissociation and the $OOH^{ad}$-Formation mechanisms. Interestingly, inclusion of solvent as well as electrode potential effects resulted in a picture showing that both Langmuir–Hinshelwood and Eley–Rideal mechanisms could be at play, making the ORR a rather complex reaction, where rigorous evaluation of the kinetics of all paths coupled together under certain environmental parameters was required to further elucidate the complicated nature of the overall reaction process.

[1] S. Venkatachalam, T. Jacob, *Handbook of Fuel Cells Vol. 5&6*, W. Vielstich, H. A. Gasteiger, H. Yokokawa (Eds.), John Wiley & Sons Ltd., Chichester, UK (2009)

**Invited Talk** O 73.2 Thu 15:30 H33

**Investigations on Pt based catalysts for PEM fuel cells: from model systems to high surface area catalysts** — •Matthias Arenz — Technische Universität München, Physikalische Chemie, Lichtenbergstr. 4, D-85748 München

The long term stability as well as the slow rate of the oxygen reduction reaction (ORR) are the main fundamental problems in the catalysis concerning polymer electrolyte membrane fuel cells. On Pt based model electrodes (single crystals and polycrystalline samples), it has recently been demonstrated how by fine-tuning the electronic structure of the surface, the specific activity for the oxygen reduction can be drastically enhanced. However, there is still a great challenge to create catalyst particles with the electronic and structural properties of the most active bulk crystal surfaces. For this task, the testing of high surface area catalysts, especially establishing the true specific activity of nanoparticle catalysts, is of highest importance. In the presentation the testing of high surface area catalysts by the so-called thin film rotating disc electrode method is critically discussed. It will be shown how reproducible activity measurements can be performed. In this respect it is demonstrated how the treatment of catalysts affects their surface composition and structure. Furthermore, a new TEM methodology for testing the stability of catalysts in accelerated ageing tests is introduced as well as new results on size selected Pt particles are shown.

**Invited Talk** O 73.3 Thu 16:00 H33

**Computer Simulation of Electrolyte / Solid Interfaces** — •Eckhard Spohr — Lehrstuhl fuer Theoretische Chemie, Universitaet Duisburg-Essen, D-45141 Essen, Germany

This talk will review the state of the art and recent advances of atomistic computer simulations of interfaces between electrolytes and electrolyte solutions and solid interfaces. I will focus on the simulation of charged interfaces and systems of electrochemical importance. Simulation methodology and several examples from various research groups including our own will be discussed in some detail. The examples will cover structural aspects, interfacial dynamics, and prototypical electrochemical reactions such as proton discharge on metal electrodes.

O 73.4 Thu 16:30 H33

**Multilayer passivated AlGaN/GaN-sensors for stable pH-measurements** — •Stefanie Linkohr, Volker Cimalla, Christoph Nebel, and Oliver Ambacher — Fraunhofer Institute for Applied Solid State Physics Tullastraße 72, 79108 Freiburg, Germany

Due to its high chemical stability in physiological fluid and the large spontaneous polarization AlGaN/GaN-sensors are of particular importance for pharmaceutical and medical sensors. They are advantageous for the fabrication of very sensitive and robust biosensors to detect ions, bio-molecules and the bioactivity of cells in solutions, gases and polar liquids. The ion-sensitive field effect transistor (ISFET) is realized by an open gate surface placed in a measuring solution and controlled by a reference electrode. Based on the sensing principle of an AlGaN/GaN-heterostructure ions cause a change of the two-dimensional electron gas (2DEG) near the surface. Negative charge depletes and positive charge accumulates the 2DEG. With an achievable sensitivity of 57 mV/pH these sensors are able to measure the pH-value close to Nernst limit. The sensors have to be appropriately protected. The passivation has to protect the inactive areas and the contacts but should be biocompatible and chemical stable in acidic and alkaline liquids. In this work, we investigate various passivations such as SiNx, DLC (diamond like carbon), SiO2-SiNx-doublelayer (up to 500 nm) and various SiO2-SiNx-SiO2-SiNx-multilayers (up to 700nm). The multilayer passivations show the best chemical stability, no memory effects, no ionic diffusion and a minimal drift less than 0.01 pH/h.

O 73.5 Thu 16:45 H33

**Electrochemical experiments in sulphuric acid with electronic devices** — •Andreas Barmscheid, Damian Bürstel, Eckart Hasselbrink, and Detlef Diesing — Institut für Physikalische Chemie, Universität Duisburg Essen

With chemical experiments on the surfaces of thin film devices one can monitor for example adsorbate induced changes in the film resistivity or the existence of excited charge charriers in the course of a reaction. We show that thin platinum films on Si-SiOx-substrates show a well defined surface chemistry in 0.1 M sulphuric acid. Parts of the eletrochemical charge transfer at the Pt-acid interface can be monitored as a device current flowing from the Pt to the silicon. This transfer ratio depends on the inner potential difference of the device across the SiOx layer as well as on the outer electrode potential across the platinum-sulphuric acid interface. The transfer of charge carriers generated at the platinum-acid interface within the adsorption and desorption reaction of hydrogen is found to have a dependence on the inner device potential which is very similar to that one of photo excited carriers. On the other hand, charge carriers generated during the sulphate adsorption or platinum oxidation reaction do not exhibit similiarities in the transfer through the internal interfaces of the device with photo excited carriers.

O 73.6 Thu 17:00 H33

**Investigations on Pt based catalysts for PEM fuel cells: The stability of Pt-Co alloys** — •Katrin Hartl and Matthias Arenz — Technische Universität München, Physikalische Chemie, Lichtenbergstr. 4, D-85748 München

The long term stability as well as the slow rate of the oxygen reduction reaction (ORR) are the main fundamental problems in the catalysis concerning polymer electrolyte membrane fuel cells. On Pt based model electrodes (single crystals and polycrystalline samples), it has recently been demonstrated how by fine-tuning the electronic structure of the surface, the specific activity for the oxygen reduction can be drastically enhanced. However, there is still a great challenge to create catalyst particles with the electronic and structural properties of the most active bulk crystal surfaces. For this task, the testing of high surface area catalysts, especially establishing the true specific activity of nanoparticle catalysts, is of highest importance. In the presentation the testing of high surface area catalysts by the so-called thin film rotating disc electrode method is critically discussed. It will be shown how reproducible activity measurements can be performed. In this respect it is demonstrated how the treatment of catalysts affects their surface composition and structure. Furthermore, a new TEM methodology for testing the stability of catalysts in accelerated ageing tests is introduced as well as new results on size selected Pt particles are shown.

O 73.7 Thu 17:15 H33

**Electrokinetics and Charge Inversion as studied by Single Colloid Electrophoresis** — Ilya Semenov, •Gunther Stober, Periklis Papadopoulos, and Friedrich Kremer — Institute for Experimental Physics I (MOP), University of Leipzig, Linnestrasse 5, 04103 Leipzig, Germany

Single Colloid Electrophoresis (SCE) is employed to measure in a specifically designed microfluidic cell the electrophoretic and electroosmotic mobility for the identical colloid. Charge inversion in dependence on concentration, valency and acidity is observed and is proved to be fully reversible. The results are discussed with in terms of overcharging as caused by ion-ion correlations.

The determination and prediction of the surface charge density of the particle's surface are thus of prime importance. This requires an accurate model for the electric double layer at the solid/liquid interface. The standard electrokinetic model is not accurate in strongly coupled systems. That is, for systems containing multivalent ions, high ionic concentration and/or strong surface charge.

A phenomenon known as charge inversion may be seen in electrokinetic measurements such as electrophoresis in presence of multivalent ions, where the sign of the electrokinetic potential appears to be opposite to the expected one. The interpretation of such a result is still controversial. Often it is explained by specific chemical adsorption of multivalent counter-ions. However, the pure electrostatic interactions, i.e. the ion-ion correlations, can cause overcharging by the strong accumulation of counter-ions in contact with a charged surface.

O 73.8 Thu 17:30 H33

**Step bunching instability of Au(11n) vicinal surfaces in electrolyte** — •Mohammad Al-Shakran[1], Guillermo Beltramo[1], Harald Ibach[2], and Margret Giesen[1] — [1]Institute of Bio-and Nanosystems ,IBN4, Jülich Forschungszentrum GmbH — [2]Institute of Bio-and Nanosystems ,IBN3, Jülich Forschungszentrum GmbH

Flame annealed vicinal Au(11n) electrodes, n=5, 7, 9 11, 17, were studied by means of electrochemical scanning tunneling microscopy (STM), cyclic voltametry (CV) and capacitance curves in sulfuric and perchloric acid solution. STM results show that Au(11n) is unstable against step bunching. The surfaces arrange into alternating stripes of reconstructed surface (almost free of steps) and steep, unreconstructed step bunches. Though very stable, the step bunches still show a high mobility of individual steps within the bunch, indicating that the step bunches formed after flame annealing represent an equilibrium structure even at higher electrode potentials. Analyzing the step-step distance distribution shows that the relative amount of reconstructed area shifts with potential. As a consequence, the CVs of Au(11n) show a distinct change in the peak structure as well as in the minimum of the capacitance curves representing the potential of zero charge (pzc) which surprisingly is still well defined. We could show that a well-defined minimum in the capacitance curves exists below a maximum structure size of reconstructed and unreconstructed areas. Our results offers for the first time a comprehensive interpretation of the complex structure of CVs and capacitance curves on vicinal Au(11n) surfaces.

## O 74: Nanostructures at surfaces: Other

Time: Thursday 15:00–18:00 Location: H34

O 74.1 Thu 15:00 H34

**UTAM based Surface Nano-Structuring for Functional Surfaces** — •Stefan Ostendorp, Yong Lei, Christian Heckel, and Gerhard Wilde — WWU Münster, Institut für Materialphysik, Wilhel-Klemm-Straße 10, 48149 Münster, Germany

Versatile surface nano-structuring techniques with high throughput and low costs are highly desirable. The UTAM (Ultra-Thin Alumina Membrane) technique is such a method to create highly regular surface structures: nano-pores, nanodots and free-standing one-dimensional nanostructures (wires and tubes). Based on a wet-chemical anodization process of Aluminum, there is in principle no limitation to the patterning-area of the nano-structured surface. We want to present our latest results concerning this UTAM surface nano-structuring technique. Besides porous layer structures and metallic or semiconducting nano-particles and wires, we are able to create surface arrays or 3D-structures of functional molecules. All these structures have in common, that we can adjust their size and spacing within certain limitations by changing the preparation conditions for the UTAM.

Especially some functional molecules were sublimated through and along the pores of UTAMs on different substrates to obtain tubular structures. To determine the properties of these molecules, which have a wide range of possible applications e.g. in the field of opto-electronics, we use different techniques like AFM, SEM, IV-characterization or PL-spectrometry.

O 74.2 Thu 15:15 H34

**Generation of Clean Iron Structures by Electron Beam Induced Deposition and Catalytic Decomposition of Iron Pentacarbonyl on Rh(110)** — •Michael Schirmer, Thomas Lukasczyk, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstraße 3, D-91058 Erlangen

The fabrication of nanostructures with arbitrary shape and well defined chemical composition still is a major challenge. Our approach is the electron beam induced deposition (EBID) in which a focused electron beam induces the local decomposition of precursor molecules, resulting in the deposition of non-volatile fragments. Here, we present an EBID study with $Fe(CO)_5$, on clean and modified Rh(110) surfaces. By utilizing an ultra high vacuum (UHV) system, we achieved a very high iron purity of more than 88 %, similar to previous findings on Si(100) [1]. For Rh(110) the process strongly depends on the surface properties: On a perfect, clean Rh(110) surface iron is found on irradiated and non-irradiated surface regions, due to catalytic decomposition of the $Fe(CO)_5$. However, on a structurally non-perfect Rh(110) surface and on a Ti-precovered Rh(110) surface a high selectivity is found, i.e. Fe deposits are formed in irradiated regions only. The role of catalytic and autocatalytic growth of iron is discussed [2]. This work was supported by the DFG under grant MA 4246/1-1. [1] T. Lukasczyk, et al., Small 4(6) (2008) 841. [2] T. Lukasczyk, et al., Langmuir 25(19) (2009) 11930.

O 74.3 Thu 15:30 H34

**Local Surface Activation of SiO$_x$ by a Focused Electron Beam as a Means for Nanoscale Lithography** — •Florian Vollnhals, Marie-Madeleine Walz, Michael Schirmer, Thomas Lukasczyk, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Friedrich-Alexander- University Erlangen-Nuremberg, Egerlandstr. 3, 91058 Erlangen

The fabrication of arbitrarily shaped nanostructures is of key interest for industrial applications as well as for scientific research. Suitable fabrication techniques include resist-based and resist-free techniques, e.g. electron beam induced deposition (EBID).

In EBID, a precursor gas adsorbs on a substrate and is decomposed locally by a focused electron beam. Non-volatile fragments then form a deposit on the surface. It was shown that this process can yield almost pure Fe deposits (95%) from Fe(CO)$_5$ under UHV conditions [1].

Our recent results expand the EBID concept. If the focused electron beam is used to locally irradiate a thin (300nm, commercial) or an ultra thin (few nm) SiO$_x$ layer on Si(100) without offering any precursor gas, the exposed areas can later be "developed" by dosing Fe(CO)$_5$. The resulting formation of Fe deposits is attributed to electron induced activation of the surface and enhanced by autocatalytic growth of iron in the presence of Fe(CO)$_5$.

This work was supported by the DFG through grant MA 4246/1-1. [1] T. Lukasczyk et al., Small, 4 (6) (2008) 841

O 74.4 Thu 15:45 H34

**Surface Nano-Patterning in Realizing Diverse Functional Surface Nanostructures with High Structural Regularity** — •Yong Lei, Stefan Ostendorp, Nina Winkler, Peter Hess, Christian Heckel, and Gerhard Wilde — Institute of Materials Physics and Center for Nanotechnology, University of Muenster, Wilhelm-Klemm-Str. 10, D-48149 Muenster, Germany

Here we want to show you the results in our group concerning the surface nano-structuring using UTAM (ultra-thin alumina mask) surface nano-patterning technique. UTAM technique is an emerging approach in fabricating ordered arrays of different surface nanostructures. Besides nanodots and nanoholes, three-dimensional surface nano-patterns (mainly free-standing one-dimensional nanostructures of metals and semiconductors) can be prepared using electrochemical processes and CVD processes. Moreover, functional molecular surface patterns are realized based on the UTAM-prepared pre-patterns on substrates. The structural parameters (size, spacing, and shape) of all these UTAM-fabricated surface nanostructures can be adjusted by controlling the structural parameters of the UTAMs, which consequently results in the tenable properties of the UTAM-synthesized surface patterns. Different applications in optical, sensing, and electronic devices will be presented based on the advantageous features of the UTAM surface patterning technique, including the tuneable structural parameters and properties, large pattern area and high throughput of surface nanostructures, and low equipment costs.

O 74.5 Thu 16:00 H34

**Magnetotransport in anisotropic Pb-films and monolayers** — •Daniel Lükermann, Christoph Tegenkamp, and Herbert Pfnür — Uni Hannover, Inst. für Festkörperphysik, Abt. ATMOS

Pb chain structures with strong anisotropic conductance are formed by adsorption of Pb monolayers (ML) on Si(557). In the case of 1.3 ML, even 1D transport is found along the wire's direction. The perpendicular direction shows localization due to perfect Fermi nesting for the (223) facet orientation. Above 78 K thermal activation annihilates this phase and a refactting transition switches the system back into an anisotropic transport regime.

In order to learn more about the scattering mechanisms magnetotransport measurements have been performed and analysed using the fromalism by Hikami, which allows to deduce inelastic($\tau_i$), elastic ($\tau_0$) and spin–orbit ($\tau_{so}$) scattering times . While for multilayers weak localization, i.e. increase of the resistance by contructive interference of elastically backscattered electrons, has been found, the ML phases show weak anti localization. Contrary to the Pb multilayers, spin-orbit coupling is essential for the ML phases. The anisotropy seen by conductivity measurements is nicely reflected by elastic and spin–orbit scattering rates. Interestingly, for 1.3 ML, a strong increase by three orders of magnitude in $\tau_{so}$ is seen in the parallel direction. As judged from ARPES one of the two split-off bands is nested by the modulation of the wires, while the other crosses the Fermi energy, responsible for the high conductance. This would suggest that spin-flip processes are strongly suppressed, in agreement with the magnetotransport data.

O 74.6 Thu 16:15 H34

**Studies of Growth of Epicuticular Wax (nonacosan-10-ol) on Model Surfaces by Atomic Force Microscopy (MAC mode)** — •Sujit Kumar Dora[1], Adrian Niemietz[2], Kerstin Koch[2], Wilhelm Barthlott[2], and Klaus Wandelt[1] — [1]Institute for Physical and Theoretical Chemistry, University of Bonn, Germany. — [2]Nees Institute for Biodiversity of Plants , University of Bonn, Germany.

Plant surfaces are often covered by crystalline self-assembled waxes forming hydrophobic microstructured surfaces. Out of the vast variety of wax morphologies found on plant surfaces, nonacosan-10-ol wax tubules are considered as one of the most important type, found on the leaf surface of lotus (Nelumbo nucifera) and are responsible for the famous self-cleaning phenomena known as "Lotus-effect". The formation of a hydrophobic nanostructure of nonacosanol tubules on lotus leaves is responsible for its superhydrophobicity. In this contribution we describe and discuss the results of the effect of various factors e.g., concentration, presence of water, salt etc. on the growth of wax tubules on various model substrates like HOPG, Mica, Glassy Carbon and Glass as obtained by atomic force microscopy (MAC mode). The rate of tubule formation is faster on nonpolar substrates e.g., HOPG, Glassy Carbon in comparison to polar substrates e.g., Mica, Glass. Only on HOPG tubules were standing perpendicular to the substrate surface. Whereas water considerably increases the growth rate, salts and different concentrations have no effect on growth. In our investigation we developed a systematic approach to understand the different factors affecting the growth of nonacosanol tubules on model substrates.

O 74.7 Thu 16:30 H34

**Spatially modulated differential conductance in nm narrow Cu channels between and on Co islands** — •Safia Ouazi, Yasmine Nahas, Marco Corbetta, Hirofumi Oka, Dirk Sander, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle (Saale), Germany

Electron scattering off step edges and due to confinement in nanostructures leads to interference effects which induce a spatially modulated local density of states [1]. We measure maps of the differential conductance dI/dV on Cu(111) in a 7 nm narrow channel between Co islands by scanning tunneling microscopy and spectroscopy at 8 K. We observe a spatially modulated dI/dV signal in the channel, and also on the adjacent Co islands. We extract the energy and position dependence of the modulation pattern. The electron energy dispersion is discrete in the wave vector k. Our results are well described by a quantization rule for k, which identifies the channel width and the island height as the decisive length scales. The role of structural relaxation and electronic rim states for electron confinement in channels and islands is discussed.

O 74.8 Thu 16:45 H34

**Contrast inversion of the h-BN nanomesh on Rh(111) investigated by nc-AFM and KPFM** — •Markus Langer[1], Sascha Koch[1], Shigeki Kawai[1], Bartosz Such[1], Jorge Lobo-Checa[3], Thomas Brugger[2], Thomas Greber[2], Juerg Osterwalder[2], Ernst Meyer[1], and Thilo Glatzel[1] — [1]Department of Physics, University of Basel, Klingelbergstr. 82, 4056 Basel, Switzerland — [2]Physik-Institut, Universität Zürich, Winterthurerstrasse 190, 8057 Zürich, Switzerland — [3]Centre d'Investigaci'o en Nanoci'encia i Nanotecnologia, CIN2 (CSIC-ICN), Esfera UAB, Campus de Bellaterra, 08193-Barcelona, Spain

Boron-Nitride forms a highly regular, hexagonal, corrugated monolayer (h-BN nanomesh) on a Rhodium(111) substrate [1,2]. High resolution measurements by non contact atomic force microscopy (nc-AFM) as well as the analysis of the electronic structure by Kelvin probe force microscopy (KPFM) will be shown. A contrast inversion of the topography and the local contact potential difference was observed frequently and will be discussed. Two possible scenarios based on a local deformation of the tip apex or of the nanomesh will be presented and are compared to existing theoretical and experimental work.

[1] S. Berner et al., Angewandte Chemie, Int. Edition 46, 5115 (2007).
[2] R. Laskowski et al., Phys. Rev. Lett. 98, 106802 (2007).

O 74.9 Thu 17:00 H34

**Transport properties of single atom and single molecule junctions** — •Guillaume Schull — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — Institut de Physique et de Chimie de Strasbourg, Université Louis Pasteur, CNRS UMR 7504, 67034 Strasbourg, France.

The study of the current passing through single atoms or molecules has revealed fascinating phenomena such as the observation of a quantization of the conductance or a reduction of the shot noise at single atom contacts... A next step is to determine how transport properties of atoms and molecules are influenced by the contacts geometry. We used a scanning tunneling microscope (STM) which provides a way to precisely localize and characterize the structures of interest before probing their transport properties. First, I will focus on the transport properties of single C60 molecules and show how atomic scale variations of the molecule-metal interfaces influence the junction conductance. Using a STM tip with a C60 attached at the apex, the transport properties of a suspended chain made of two C60 have been probed. Here, the molecule-molecule interface is revealed to be the limiting factor to the contact conductance. Finally, I will show that specific inelastic contributions to the current (under tunnelling and contact conditions) can be probed by studying the light emitted at the STM junction.

These works were performed in collaboration with Thomas Frederiksen, Michael Becker, Nicolas Néel, Peter Johansson, Mads Brandbyge and Richard Berndt.

O 74.10 Thu 17:15 H34

**Excitonic luminescence of pentacene nanocrystals induced by STM** — •Klaus Kuhnke[1], Alexander Kabakchiev[1], Theresa Lutz[1], and Klaus Kern[1,2] — [1]Max-Planck Institut für Festkörperforschung, D-70569 Stuttgart — [2]Institut de physique de la matiere condensee, EPFL, CH-1015 Lausanne

The local injection of charge carriers by scanning tunneling microscopy (STM) can be employed to excite luminescence from nanostructures. We study the luminescene of pentacene nanocrystals grown on a thin insulating KCl layer on different metals. The observed electroluminescence spectrum at liquid He temperature exhibits up to 3 features and is dominated by the emission of the self-trapped singlet exciton at 1.60 eV. It compares well to low temperature spectra reported for photoluminescence on macroscopic single crystals. We find the onset bias of light emission at 1.8 eV - close to the energy of the free exciton and still below the transport gap in bulk pentacene. The charge injection conditions for luminescence involve a high electric field between STM tip and metallic substrate. The field results in a Stark shift of the dominating emission line of about 20meV. This strong shift may indicate a charge-transfer (CT) contribution to the Frenkel exciton.

O 74.11 Thu 17:30 H34

**Theoretical investigation of the switching mechanism in a single-molecule memory unit** — •Felix Hanke and Mats Persson — University of Liverpool, Liverpool, United Kingdom

The storage and retrieval of information at the sub-nanometer scale is one of the outstanding challenges in nanoelectronics. It was recently proposed that the molecular switch naphthalocyanine can be controlled using scanning-tunneling microscopy (STM) [1] when it is adsorbed on a thin layer of NaCl. The on/off state of naphthalocyanine is determined by the orientation of two central hydrogen atoms, which changes with the application of a high STM voltage, while a low voltage allows to read out the molecular state. Despite the wealth of available experimental information, the electronic processes responsible for the STM-induced configurational changes in naphthalocyanine are poorly understood theoretically. This project aims to explain the switching property based on density functional theory. From the adsorption geometry on the NaCl surface, the reaction path for the switching pathway is computed. This result leads to a detailed investigation of the molecular orbitals responsible for the tunneling-induced motion of the central hydrogen atoms. In particular, the evolution of the lowest two unoccupied and nearly degenerate molecular orbitals is shown to be an important piece in the puzzle. Finally, a model is developed to take into account the electron-induced motion of naphthalocyanine along its switching pathway. - [1] P. Liljeroth *et al.*, Science **317**, 1203 (2007)

O 74.12 Thu 17:45 H34

**Nanocones and Nanowires Analysed with Scanning Auger Microscopy.** — •Andrey Lyapin[1], Stefan Reichlmaier[1], Denis Paul[2], John Hammond[2], and Sakar Raman[2] — [1]Physical Electronics GmbH, Ismaning, Germany — [2]Physical Electronics, Chanhassen, USA

The increased interest in nanotechnological material, such as nanocone, nanorods and nanowires, has pushed the development of analytical techniques to determine the growth mechanisms of these nanostructures. Scanning electron beam techniques, including Scanning Auger Microscopy, have provided valuable imaging and elemental characterization tools for these structures with a spatial resolution better than 10 nm. Using the combination of high energy resolution chemical state spectroscopy and imaging of the Scanning Auger Microscopy allows to obtain quantitative elemental results on the different parts of the nanocone and nanowire as well as the imaging of different chemical states and depth profiling. In this talk we present results of the Auger analysis of the nanocones and nanowires which provide further insights into the growth mechanisms of these nanostructures.

## O 75: Nanotribology II

Time: Thursday 15:00–17:00 Location: H36

O 75.1 Thu 15:00 H36

**Atomic Friction on Electrode Surfaces** — •Nikolay Podgaynyy and Helmut Baltruschat — University of Bonn, D-53117 Bonn, Germany

Friction under ambient conditions often involves wet surfaces, and thus electrochemical interfaces. Yet, measurements of friction at an atomic scale under electrochemical conditions are scarce. For HOPG, a change of friction forces at steps edges was observed with a change of potential. We recently started to measure friction by AFM and the influence of potential, Cu UPD on Au(111) and other parameters thereupon. We will present friction measurements performed on Au(111) single crystal electrodes and the effect of potential thereupon. Friction increases upon adsorption of anions (sulphate). An increase of friction is also observed at step edges. Here, a careful analysis is necessary to separate geometric effects from true changes of friction. The range of a normal force necessary to observe stick-slip resolution depends on the type of ionic adsorbates and tip radius. Atomic resolution is easily observed if sulfate anions are adsorbed on the gold or copper submonolayer surface. However, with the type of cantilever we used, it was not possible to observe stick-slip resolution on a monolayer of Cu on Au(111) and on Cu bulk deposits. In contrast to Couloumb*s friction law the tip scan rate has an influence on the friction force, however, only when sulfate is adsorbed on the clean Au surface. Such effects were found and explained with conditions when atomic stick-slip occurs.

O 75.2 Thu 15:15 H36

**Frictional changes upon modification of single crystal electrodes with anions** — •Florian Hausen and Roland Bennewitz — INM - Leibniz Institute for New Materials, Campus D2 2, 66123 Saarbrücken

Considering that most tribological processes occur at a solid - liquid interface, friction measurements under electrochemical conditions are scarce. Compared to similar experiments in ultra high vacuum the surfaces are as clean and well defined. A unique tool offered by electrochemical methods is the possibility to alter the surface structure and to deposit various adsorbates by changing the applied potential at the working electrode.

We present friction force measurements on Au(111) and Au(100) single crystal electrodes performed by means of atomic force microscopy (AFM). The influence of a surface modification with anions is explored by using electrolytes containing sulphate. With adsorbing sulphate to the surface a strong increase of the friction force compared to the bare gold substrate is found. Furthermore we observe a strong correlation between friction forces and the anion structure. Complementary studies were done by using perchlorate, which is isoeletronical to sulphate but shows a different electrochemical behaviour. Additionally the effect of chloride on friction and wear due to the enhanced mobility of the surface atoms in the presence of chloride will be discussed.

O 75.3 Thu 15:30 H36

**Friction Induced Deformation of Microstructured Rubber Surfaces** — •Katrin Brörmann and Roland Bennewitz — INM - Leibniz-Institut für Neue Materialien, Saarbrücken

In an attempt to bridge the gap between macroscopic and microscopic friction measurements, R. Bennewitz et al. [1] introduced a method to analyse friction by means of optical diffraction. In the experiment, a microstructured sample is dragged over a glass surface, resulting in a deformation of the sample due to friction. While sliding, a diffraction pattern of the surface structure is recorded and the strain across the contact, i.e. the average distance between the asperities, is extracted. Simultaneously, the force in normal and lateral direction is measured. PDMS samples with different periodically structured surfaces were used, representing a simple model of multi-asperity contacts.

In a second experiment, the deformation of the sample was observed in real space using an optical microscope. The movement and deformation of the surface structure was tracked and the local trajectories of specific sites on the patterned surface were recorded.

Results of both experiments indicate three phases in the deformation process: first shearing, then the transition from static to kinetic friction and last stick-slip motion. Furthermore, a 2D Poisson's ratio of the structure can be determined. Details on the phases will be presented and briefly compared to a recent theoretical model.

[1] R. Bennewitz et al., *J. Phys.: Condens. Matter* **20** (2008) 015004

O 75.4 Thu 15:45 H36

**Friction Force Microscopy on a Layer Compound with Organic Surfaces** — •Gregor Fessler[1], Iwan Zimmermann[2], Thilo Glatzel[1], Sascha Koch[1], Pascal Steiner[1], Enrico Gnecco[1], Tony Keene[2], Shi-Xia Liu[2], Silvio Decurtins[2], and Ernst Meyer[1] — [1]Dept. of Physics, University of Basel — [2]Dept. of Chemistry and Biochemistry, University of Bern

We investigated the surface structure of a layer compound crystal formed by a stack of copper oxalate layers sandwiched between stereoregular organic cations. Friction force microscopy in ultra-high vacuum on the (001) surface revealed a friction contrast between different molecular rows along the [100] direction. High resolution measurements were possible without any preparation of the sample in ultrahigh vacuum. Excellent agreement with the experimental results is obtained with numeric simulations reproducing the scan process based on the phenomenological Prandtl-Tomlinson model in 2D.

O 75.5 Thu 16:00 H36

**Frictional properties of a mesoscopic contact with engineered surface roughness** — •Johannes Sondhauss[1,2], Harald Fuchs[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

Friction force microscopy (FFM) is a standard tool to perform friction experiments on the nanoscale. However, with a conventional tip used in FFM, only contact areas of a few $\mathrm{nm}^2$ are realizable. To get access to friction experiments with larger contact geometries typical for, e.g., MEMS, new concepts to prepare mesoscale tip-sample contacts are necessary. In this work, we used a focused ion beam (FIB) to engineer both sliding partners, i.e. tip and sample. Cantilever with spherical apexes with diameters of 5 and 16 $\mu$m were fabricated by attaching a titanium microparticle to the modified tips. To investigate the influence of interface roughness of the contact, a silicon surface was patterned with arrays of grooves with a lattice periodicity ranging from 1 to 9 $\mu$m and a depth of 26 nm. The average friction coefficient was determined systematically for the two tips as a function of the lattice periodicity of the sample grooves. For both tips the maximum friction force was found where the geometry of the spherical tip and the lattice are commensurate. These findings highlight the importance of surface structure on tribological properties of mesoscale contacts.

O 75.6 Thu 16:15 H36

**Oxygen-induced degradation of carbynoid structures on carbon surfaces: a DFT study** — •Gianpietro Moras[1,2], Lars Pastewka[1], Peter Gumbsch[1,2], and Michael Moseler[1,3] — [1]Fraunhofer Institut für Werkstoffmechanik, Freiburg (Germany) — [2]Universität Karlsruhe, Institut für Zuverlässigkeit von Bauteilen und Systemen, Karlsruhe (Germany) — [3]Albert-Ludwigs Universität Freiburg, Physikalisches Institut, Freiburg (Germany)

Carbynoid structures - sp-bonded carbon chains - have recently gained in importance in materials science as they have been reported to form during the growth of diamond-like carbon and nanostructured carbon films, as well as during diamond polishing. The interaction of these structures with air is crucial to the final structure of the deposited or polished surfaces. In particular, oxygen was found to cause the degradation of carbynoid strutures. This may play an important role in the wear mechanism of the diamond polishing.

Here we present a DFT study of the oxidation mechanisms of carbynoid structures. Due to the lack of reference experimental studies specifically devoted to the oxidation mechanisms of supported carbon chains, the accuracy of our simulations is assessed by studying the oxidation of small cationic carbon cluster in the gas phase, for which detailed experimental data exist. This allows us to gain insight into unclear oxidation mechanisms of cyclic cationic carbon clusters. Moreover, the extension of our simulation approach to supported linear carbon clusters yields possible mechanisms for the oxygen-induced degradation of such structures.

O 75.7 Thu 16:30 H36

**Scaling laws in superlubric sliding of metallic nanoparticles** — •Dirk Dietzel[1], Tristan Mönninghoff[1], Michael Feldmann[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, CT, USA

If an interface between two incommensurate surfaces is atomically clean, a state of virtually frictionless sliding is anticipated, often referred to as 'superlubricity'. Theory predicts that the lattice mismatch at the interface causes a decrease of shear stress with increasing contact area, ultimately leading to vanishing friction. Analyzing the contact area dependence of superlubric friction should therefore confirm the concept of superlubricity. To measure the interfacial friction we have manipulated metallic nanoparticles of different size on atomically flat surfaces by contact mode atomic force microscopy techniques. An optimized experimental setup allowed us to quantify friction of nanoparticles which previously appeared to be sliding frictionless[1]. As theoretically expected, interfacial friction showed a nonlinear contact area dependence with a shear stress decreasing with contact area. This confirms the superlubric sliding of the nanoparticles under investigation. [1]Dietzel et al., Phys. Rev. Lett. 101, 125505 (2008).

O 75.8 Thu 16:45 H36

**Ultra-thin films as wear resistive coatings** — •Tassilo Kaule[1], Sascha Pihan[1], Sebastian G. J. Emmerling[1], Yi Zhang[1], Renate Förch[1], Jochen Gutmann[1], Hans-Jürgen Butt[1], Rüdiger Berger[1], David Pires[2], Armin Knoll[2], Bernd Gotsmann[2], and Urs T. Dürig[2] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz — [2]Zurich Research Laboratory, IBM Research, 8803 Rüschlikon, Switzerland

Here we report on developing and characterizing ultra-thin polymer films with certain mechanical and chemical properties. The films were deposited via plasma-polymerisation from the monomers hexamethyldisiloxane or norbornene. The variation of the reaction conditions, e.g. plasma power, reaction time, pulse modes and additional gases allow adjusting mechanical and interface properties like hardness or hydrophility. We discuss the feasibility of such ultra-thin films as mechanical protection layers for softer polymers such as polystyrene. In particular, we optimized the ultra-thin films for the use as a protection layer for storage media as used for thermomechancial probe based storage. The mechanical stability of the layered medium was tested with scanning force microscopy tribology tests [1], the thickness of the films were measured by profilometry and X-ray reflectivity measurements. Furthermore contact angle studies were performed to characterize the film surface. We found that film thicknesses $< 10$ nm can be used as suitable wear resistant protection layers for polystyrene but still allow thermomechancial read and write operations.

[1] R. Berger et al., Langmuir, 23, 3150 - 3156 (2007)

# O 76: Nanostructures at surfaces: Wires, tubes

Time: Thursday 15:00–17:15 Location: H38

O 76.1 Thu 15:00 H38

**Tuning Ag nanowire growth on Cu(110) based templates** — •Thorsten Wagner, Thomas Brandstetter, and Peter Zeppenfeld — Johannes Kepler University Linz, Institute of Experimental Physics, Austria

The Cu(110) surface can be readily structured by adsorbing oxygen: If the coverage of oxygen is less than required to form a complete (2×1) overlayer, CuO stripes are formed which are separated by bare copper areas. These stripes are regularly arranged and parallel to the [001] direction. On such an oxygen pre-covered surface silver was adsorbed at 660 K. As revealed by scanning tunneling microscopy, submonolayer silver coverages lead to a phase separation between CuO and a Ag/Cu alloy [1]. The original Cu-CuO stripe phase is destroyed and larger CuO areas (‘ponds’) are formed. The ponds are separated by Ag rich stripes which are again parallel to the [001] direction. These template surfaces can be used to manipulate the further growth of Ag nanowires at 300 K. Since on our template, the nanowires grow only on the Ag rich stripes, their extension along the [$1\bar{1}0$] direction is limited by the width of these stripes. By carefully choosing the parameters for the preparation of the template, one can even produce Ag nanowires which are aligned along [001] direction, which is perpendicular to the natural extension of Ag nanowires on pure Cu(110).

[1] Brandstetter *et al.*, Surf. Sci. **603**, 3410-3413 (2009)

O 76.2 Thu 15:15 H38

**Morphology and electronic properties of Co nanorods on Cu(110)-p(2x3)N** — •Sebastian Wedekind[1], Fabio Donati[1,2], Hirofumi Oka[1], Guillemin Rodary[1], Dirk Sander[1], and Jürgen Kirschner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]NEMAS, Politecnico di Milano, Milano, Italy

Copper nitride systems are of high current interest in nanoscience as they offer a venue towards decoupling the electronic properties of nanostructures or adatoms from those of the substrate. We have prepared a Cu(110)-p(2x3) ($Cu_3N$) substrate by N-ion bombardment (600 eV, 30 min, 550 K) of clean Cu(110) [1]. Deposition of Co leads to the formation of several ten nm long Co wires, extending along [1-10]. Our scanning tunneling microscopy and spectroscopy studies at 8 K reveal the positions of all atoms within the rectangular surface unit cell, where we measure unit vectors of 1.094 and 0.502 nm for the $Cu_3N$ structure. Surprisingly, spectroscopy on clean $Cu_3N$ and on Co nanowires on $Cu_3N$ shows very similar results. No special spectroscopic features are identified near the Fermi energy, but peaks at +1.8 and +3.5 eV of presently unknown electronic character of the unoccupied sample states are observed for both $Cu_3N$ and Co/$Cu_3N$. This suggests a rather strong electronic coupling between substrate and nanowire, questioning the electronic decoupling between this copper nitride system and nanostructures deposited on top. [1] X. Ma, D. Bazhanov, O. Fruchart, F. Yildiz, T. Yokoyama, M. Przybylski, V. Stepanyuk, J. Kirschner, Phys. Rev. Lett. **102** (2009) 205503.

O 76.3 Thu 15:30 H38

**Potentiometry measurements of Pb wires on vicinal Si(557) produced by electron-beam stimulated thermal desorption of oxygen** — •Jan Rönspies and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, 30167 Hannover, Germany

We explored the structural limits of unconventional electron beam lithography by directly writing with an electron beam into ultra-thin $SiO_2$ films. These bare silicon window structures are suitable for growing contiguous metallic nanowires with a thickness of a few monolayers. The Auger excitation process necessary for electron-beam stimulated thermal desorption of oxygen (EBSTD) allows generation of single wire structures between two macroscopic metallic contact pads. The prepared line was filled with Pb and by subsequent processing steps a wetting layer remains inside the wire structure. Applying this combination of processes to a regularly stepped $Si(557)$ sample which consists of a periodic array of small (111) and (112) oriented mini-facets with an average periodicity of $5.7nm$ normal to the steps, line widths close to the resolution of the electron microscope of $5nm$ were obtained. Using a STM tip and the macroscopic pads in a potentiometric geometry we were able to identify the quantized nature of ultrasmall structures and their conductance behavior over a range of a few micrometers. These uncovered structures with lateral dimensions down to $10nm$ were analyzed further by potentiometry using scanning tunneling microscopy. We found a significant potential drop in the order of $200\mu V/nm$ at step sites which are probably related to contact resistance.

O 76.4 Thu 15:45 H38

**STM induced electroluminescence from individual CdSe nanowires** — •Theresa Lutz[1], Alexander Kabakchiev[1], Thomas Dufaux[1], Christian Wolpert[1], Marko Burghard[1], Klaus Kuhnke[1], and Klaus Kern[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Scanning tunneling microscopy (STM) not only provides the ultimate tool to obtain atomic scale information in both topographic and spectroscopic measurements at surfaces, but can also be employed to stimulate local photon emission. Here we show STM induced luminescence on individual semiconducting CdSe nanowires in combination with topographic and tunneling spectroscopic measurements at liquid He temperature. We investigate individual CdSe nanowires[1] with average diameters of 8 nm to 22 nm deposited onto a gold surface. The generated luminescence is ascribed to electron-hole recombination in the wire and requires hole injection from the STM-tip in excess of several hundred meV above the luminescence energy. The luminescence spectra are similar to the ones obtained in photoluminescence. Interestingly, the STM-induced luminescence is found even in the absence of tip-induced plasmonic emission, which stands in contrast to studies on similar systems in which light emission and plasmon observation seem to be coupled. We find that the energy of the emission line depends on the diameter of the wire as expected for quantum confinement of the charge carriers to one dimension.

[1] Z. Li et al., Small 4, 1698-1702 (2008)

O 76.5 Thu 16:00 H38

**Ab-initio studies of Au-induced atomic wires on Ge(001)** — •Simeon Sauer[1,2], Frank Fuchs[1], Friedhelm Bechstedt[1], Christian Blumenstein[3], and Jörg Schäfer[3] — [1]Institut für Festkörpertheorie und -optik, Universität Jena, D-07743 Jena — [2]Physikalisches Institut, Universität Freiburg, D-79104 Freiburg — [3]Physikalisches Institut, Universität Würzburg, D-97074 Würzburg

Au-induced atomic wires on Ge(001) are a promising model system to study the physics of one-dimensional electron liquids [1]. However, the results of scanning tunneling microscopy (STM) experiments do not permit to unambiguously determine the arrangement of surface atoms. Several questions remain unresolved: Are the observed protrusions formed by Au atoms only or do they incorporate Ge as well? What is their absolute height?

Therefore, we theoretically investigate possible atomic geometries of the surface in the framework of density functional theory. For each model, features like surface energy, STM images, and band structure are calculated. The computed properties are compared to experimental data and used to evaluate the different models. Due to the large variety of possible geometries no final statement about the atomic structure of the surface can be made. However, the calculations give good indications towards the correct geometry, e.g. ruling out models proposed in literature or identifying stabilizing building blocks [2].

[1] J. Schäfer et al., Phys. Rev. Lett. 101, 236802 (2008).

[2] S. Sauer, F. Fuchs, F. Bechstedt, C. Blumenstein, and J. Schäfer, submitted for publication.

O 76.6 Thu 16:15 H38

**Is Au/Ge(001) a model system for a 1D Electron Liquid?** — Arie van Houselt, Daan Kockmann, Tijs Mocking, Bene Poelsema, and •Harold Zandvliet — MESA+ instute for Nanotechnology and University of Twente, Enschede, The Netherlands

Recently it has been claimed that the Au induced nanowires on Ge(001) represent an outstanding case for a one-dimensional electron liquid [1]. Here we show, based on the data of the authors of ref. [1], that the differential conductivity of the Au induced nanowires and the troughs between the nanowires are comparable in magnitude [2]. Therefore, this system cannot be considered as a model system for a one-dimensional electron liquid [2-4].

[1]. J. Schäfer et al. Phys. Rev. Lett. 101, 236802 (2008). [2].

A. van Houselt et al. Phys. Rev. Lett. 103, 209701 (2009). [3]. D. Kockmann, A. van Houselt, T.F. Mocking, B. Poelsema and H.J.W. Zandvliet, Journal of Physical Chemistry C 113, 17156 (2009). [4]. K. Nakatsuij, R. Niikura, Y. Shibata, M. Yamada, T. Iimori and F. Komori, Phys. Rev. B 80, 0814069R (2009).

O 76.7 Thu 16:30 H38

**Temperature-dependent Study on the Superstructure of Atomic Gold Nanowires on Ge(001)** — •Christian Blumenstein[1], Jörg Schäfer[1], Sebastain Meyer[1], Ralph Claessen[1], Sbeastian Mietke[2], and Rene Matzdorf[2] — [1]Experimentelle Physik 4, Universität Würzburg, 97074 Würzburg, Germany — [2]Fachbereich Naturwissenschaften, Universität Kassel, 34132 Kassel, Germany

Self-organized atomic nanowires on semiconductor surfaces form ideal model systems for the study of physics in low dimensions. A lot of research has been conducted on the Au induced reconstructions on Si(111) and its vicinal surfaces. These wires have been discussed in terms of a Peierls-distorted state at low temperature. A relatively high transition temperature for this charge density wave (CDW) points at a significant coupling between the chains. The recently discovered Au/Ge(001) nanowires can serve as an alternative system to question the origin of the low-temperature structure. They grow in a regular c(8x2) reconstruction and cover the whole sample surface. Their lateral confinement reaches the atomic limit, while the separation between the wires is several Ge lattice constants. Therefore these exceptionally narrow chains represent a new playground for 1D physics. The talk will address the structural elements of the Au/Ge(001) chains, which have been investigated by Low Energy Electron Diffraction and Scanning Tunneling Microscopy over a wide temperature range. Special attention will be paid to superstructure periodicities and their relation to a possible CDW.

O 76.8 Thu 16:45 H38

**Structural and electronic properties of the Bi:Si(001) Haiku reconstruction.** — •Sigrun A. Köster[1], James H. G. Owen[1], François Bianco[1], Daniel Mazur[1], David R. Bowler[2], and Christoph Renner[1] — [1]Université de Genève, Section Physique/DPMC, Quai Ernest-Ansermet 24, 1211 Genève 4, CH — [2]London Centre for Nanotechnology (LCN), University College London, UCL 17-19 Gordon Street, WC1H 0AH, London, UK

There is substantial interest in probing the physical properties of low dimensional systems motivated by the interest in fundamental physics of these systems but also for the development of increasingly small technological devices. Self-assembled bismuth nanolines appear when Bi is deposited onto the Si(001) surface and subsequently annealed [1]. They can reach one micrometer in length and their width is fixed at 1.54 nm owing to the complex underlying Si reconstruction known as the Haiku structure [2]. Exposing the Bi-nanolines to atomic H, we were able to strip off the Bi from the nanoline and expose for the first time the Haiku structure. We present a detailed spectroscopic and structural characterization of the Bi-nanoline and the Haiku using scanning tunneling microscopy and spectroscopy. These results are in excellent agreement with theoretical modelling of the nanowire.

[1] J. H. G. Owen, K. Miki, and D. R. Bowler, J. Mater. Sci. 41, 4568 (2006) [2] J.H.G.Owen, K.Miki, H.Koh, H.W.Yeom and D.R.Bowler, Phys. Rev. Lett. 88, 226104 (2002)

O 76.9 Thu 17:00 H38

**Production and electrical properties of nanostructures on graphite surfaces** — •Lukas Patryarcha[1], Stefan Balk[1], Karl Bauer[1], Axel Rudzinski[2], Lars Bruchhaus[2], and Heinz Hövel[1] — [1]TU Dortmund, Experimentelle Physik I — [2]Raith GmbH, Dortmund

A Focused Ion Beam (FIB) of $Ga^+$ ions with 25 keV kinetic energy was used to produce defects in a graphite (HOPG) crystal up to a depth of about 50 nm. Subsequently carbon atoms at the defect positions were oxidized in an $Ar/O_2$ atmosphere and released from the bulk. Using the ionLiNE FIB instrument (Raith GmbH) bars with different width, length and artificial breaks at different positions were isolated from the surrounding crystal and investigated with STM and AFM. The current distribution in the conductive bars was simulated by an array of discrete resistors. The results of the simulations are planned to be compared to a four tip nanoprobe experiment. Nanostructures with specific electrical properties can be designed on HOPG surfaces if the current distribution is localized sufficiently to the bars.

## O 77: Oxides and insulators: Epitaxy and growth

Time: Thursday 15:00–18:00 Location: H42

O 77.1 Thu 15:00 H42

**Formation of a laterally nanostructured cobalt oxide** — •Matthias Gubo, Christina Ebensperger, Wolfgang Meyer, Lutz Hammer, and Klaus Heinz — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

In this study the growth of ultrathin cobalt oxide on a monolayer cobalt and on a monolayer of a $Co_4Ir$ surface alloy - both prepared on a Ir(100) surface - is investigated by means of low energy electron diffraction (LEED) and scanning tunnelling microscopy (STM). The oxide on a monolayer cobalt reveals a c(4x2) periodic LEED pattern. Its structure consists of a compressively strained CoO(100) layer with cobalt vacancies arranged in a c(4x2) periodicity equivalent to a $Co_3O_4$ stoichiometry of the film. This structure is very different from the oxide on the bare iridium surface [*1*]indicating that the internal structure of this cobalt oxide is strongly coupled to the underlying species of atoms (cobalt or iridium, resp.). Accordingly, by growing the oxide on a well ordered $Co_4Ir$ lateral superlattice - produced via decoration of the reconstructed Ir(5x1)-H phase [*2*] - the cobalt oxide monolayer becomes laterally nanostructured.

So, the oxide's growth appears to be strongly influenced by the local binding conditions to the substrate. In case of a laterally nanostructured substrate the oxide is nanostructured, too.

[*1*] *M. Gubo et al.,* ***J. Phys.: Condens. Matter 21*** *(2009) 474211*

[*2*] *L. Hammer et al.,* ***PRL 91*** *(2003) 156101*

O 77.2 Thu 15:15 H42

**Interface Oxides of Eu on Ni(100)** — •Jürgen Klinkhammer, Daniel F. Förster, Carsten Busse, and Thomas Michely — II. Physikalisches Institut, 50937 Köln

Eu-oxides of submonolayer to few layer thickness were grown on Ni(100) at 350°C through reactive molecular beam epitaxy with Eu fluxes of $2{,}04 \cdot 10^{14}$ atoms $m^{-1}s^{-1}$. The resulting interface oxides are investigated through low energy electron diffraction (LEED) and scanning tunneling microscopy (STM). As a function of the oxygen chemical potential at fixed Eu flux a sequence of interface oxide structures is observed. For the highest oxygen chemical potential polar EuO(111) starts to grow on Ni(100) with the densepacked $[1\bar{1}0]$ EuO direction aligned to the Ni$[(01\bar{1})]$. For medium oxygen chemical potential a phase of small magic clusters coexists with a complex stripe phase. The magic clusters are immobile and decay upon heating. Finally for the lowest oxygen chemical potential applied a 5x5 superstructure forms, which uses as building blocks small, stable square clusters. It turned out that the 5x5 superstructure is well suited as interface oxide for subsequent growth of rather perfect and stoichometric EuO films. The polar EuO(111) interface oxide decays during subsequent growth through the formation triangular pyramids bounded by {100} facets and the film transforms to the nonpolar (100) orientation.

O 77.3 Thu 15:30 H42

**Epitaxial growth of ultra-thin ceria films on Si(111)** — •Björn Menkens[1], Jan Ingo Flege[1], Sebastian Gevers[2], Daniel Bruns[2], Joachim Wollschläger[2], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, 28359 Bremen, Germany — [2]Physics Department, University of Osnabrück, 49069 Osnabrück, Germany

Rare-earth oxides are of major interest in fundamental research due to their intriguing electronic properties, which provide strong potential for multiple applications. Ceria, e.g., is a prominent compound in catalytic converters because of its high oxygen storage capacity, which results from multiple crystallographic phases and their associated oxidation states. In this contribution, we present a growth study of epitaxial ceria films on Si(111) by chemically sensitive x-ray standing waves (XSW) and grazing-incidence x-ray diffraction (GIXRD).

Under ultrahigh-vacuum conditions only $Ce_2O_3$ can be observed as shown by XPS. Our results show different phases depending on the ceria film thickness. The distinction between a hexagonal phase and the bixbyite (cubic) structure for ultra-thin $Ce_2O_3(111)$ films on Si(111) was achieved by XSW using $Ce3d_{5/2}$ and O1s photoelectrons as secondary signals and subsequent comparison with calculated Fourier components. For film thicknesses exceeding a few nanometers, their crystallinity and surface roughness were investigated by GIXRD and complemented by x-ray relectivity (XRR) measurements. Furthermore, we will discuss the influence of chlorine on ceria growth on Si(111), which acts as a passivating agent for the Si(111) surface.

O 77.4 Thu 15:45 H42

**MOS diodes with BaO, SrO and $Ba_{0.7}Sr_{0.3}O$ thin films on Si(001) as a high-k dielectric** — •Dirk Müller-Sajak[1], Alexandr Cosceev[2], Herbert Pfnür[1], and Karl R. Hofmann[2] — [1]Leibniz-Universität Hannover, Inst. f. Festkörperphysik — [2]Leibniz-Universität Hannover, Bauelemente der Mikro- und Nanoelektronik

We have grown BaO, SrO and $Ba_{0.7}Sr_{0.3}O$ films on clean Si(001) in order to find a new high-k gate oxide. These films are highly hygroscopic and have to be sealed completely by the metal gate electrode in order to perform ex-situ electrical measurements. We show that complete wetting of a Au layer can be obtained by introducing a thin layer (0.5-1ML) of Al after the oxide growth.

All three oxides have remarkable electrical properties: Dielectric constants near the values for volume material were obtained. Low leakage current densities ($<10^{-6}$A/cm$^2$ for $Ba_{0.7}Sr_{0.3}O$) have been measured. These results are supported by band offsets measured on the unstructured oxides by XPS and EELS (all above 1eV). Changing the growth conditions at the interface cause a shift in the band offsets induced by states at the interface. Growth of crystalline and lattice matched $Ba_{0.7}Sr_{0.3}O$ turns out to be superior to the amorphous layers of BaO and SrO in terms of defect densities at the interface and of leakage currents. We observed the lowest density of states at the interface of $6.3 \cdot 10^{10}$eV$^{-1}$cm$^{-2}$ by the Terman method and typically two orders of magnitude lower leakage currents for the crystalline oxide. Structural and chemical reasons will we discussed.

O 77.5 Thu 16:00 H42

**Substrate-induced structural modulation of a CoO(111) bilayer on Ir(100)** — •Lutz Hammer, Christina Ebensperger, Wolfgang Meyer, Matthias Gubo, and Klaus Heinz — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Oxidation of a monolayer of cobalt deposited on the unreconstructed Ir(100) surface leads to the formation of a CoO(111) bilayer [1]. Quantitative LEED and STM reveal a cobalt layer next to the substrate covered by an oxygen layer. Both layers' hexagonal atomic arrangements are, however, strongly distorted by the quadratic substrate and form a c(10x2) superstructure. The Co layer's buckling characteristics and atomic bond lengths to Ir atoms are consistent with the hard sphere radius of metallic Co. The binding of the oxide to the substrate appears to be characterized by two types of oxygen ions. One type is close to the expected rocksalt-type stacking with respect to the cobalt layer whilst the other type oxygen ions reside nearly on top of Ir atoms with a very short bond length. They are practically coplanar with the Co layer and so almost form a boron-nitride-type oxide. The bond to Ir can be interpreted as a local pinning of the oxide to the substrate, so modulating the entire oxide bilayer.

[1] C. Giovanardi et al., Phys. Rev. B 74 (2006) 125429

O 77.6 Thu 16:15 H42

**Comparing the Structure of Line Defects and Step Edges in the Alumina Film on NiAl(110) – A Dynamic Force and Scanning Tunneling Microscopy Study** — •Lars Heinke, Leonid Lichtenstein, Georg Hermann Simon, Thomas König, Markus Heyde, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14196 Berlin, Germany

Thin metal oxide films, like aluminum oxide on NiAl(110), are often used as model systems in catalysis. It was found that line defects like step edges and anti phase domain boundaries (APDB) are particularly active sites for catalysis and, therefore, require detailed investigations. In this context, frequency modulated dynamic force microscopy (FM-DFM) and scanning tunneling microscopy (STM) are used to determine the atomic structure of the thin film and its defects in ultra high vacuum at 5 K [1]. The APDBs are orientated along two different directions, i.e. there exist two possible orientations of the film (domain A and B). A detailed analysis reveals that the step edges, which are uniformly distributed on the substrate before the film growth, prefer orientations along these angles. This suggests that the substrate is influenced by the growth of the thin film.

[1] G. H. Simon et al., New J. Phys. 11 (2009), 093009

O 77.7 Thu 16:30 H42

**Synchrotron radiation spectroscopy studies of the initial interaction between cobalt and titanium dioxide** — •Sebastian Müller and Dieter Schmeisser — BTU Cottbus, Konrad-Wachsmann-Allee 1, 03046 Cottbus

Small metallic particles deposited on oxide surfaces can serve as heterogeneous catalysts, as for example $TiO_2$ supported cobalt is a known Fischer-Tropsch-Catalyst.

The goal of the presented studies is to investigate the interaction between cobalt and $TiO_2$ in the initial step of growth by synchrotron radiation based spectroscopy.

PES studies of $TiO_2$ supported cobalt show a reduction of the oxide support, accompanied by an oxidation of the deposited material. The oxidation is not complete, but metallic cobalt is found already in the very first step of growth. Uniform decrease of both substrate PES lines indicate very weak interaction between overlayer and $TiO_2$.

An atomic multiplet calculation including charge transfer and crystal field effects is applied to simulate the experimental Co 2p XAS and XPS spectra of the oxidized component. The results allow the identification of the local coordination as well as the identification of the oxidation state of cobalt.

O 77.8 Thu 16:45 H42

**From chemisorbed oxygen to ultrathin cobalt-oxides on Ir(100)-(1x1)** — •Christina Ebensperger, Matthias Gubo, Wolfgang Meyer, Lutz Hammer, and Klaus Heinz — Institut für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudstr. 7, 91058 Erlangen

A single monolayer (ML) of cobalt was deposited on Ir(100)-(1x1) and exposed to oxygen at elevated temperatures. As function of oxygen dosage several ordered phases develop, which were studied by means of STM and quantitative LEED.

At low oxygen coverage of 0.25 ML a (2x2) phase develops with hollow site adsorption of chemisorbed oxygen as observed also for other fcc(100) surfaces (R-factor: R = 0.12). With further exposure to oxygen this phase transforms into two different (3x3) phases, $(3x3)_I$ and $(3x3)_{II}$, which can be instantaneously monitored by the LEED intensities. The $(3x3)_I$ structure is a periodic arrangement of isolated suboxide rings with $Co_8O_4$ stoichiometry (R-factor: R = 0.14), while in the second phase these rings are interconnected by additional oxygen ions (R-factor: R = 0.16). The latter attract the surrounding cobalt ions and reduce their bonding to the substrate. The stoichiometry thereby changes towards $Co_8O_5$. With even further exposure to oxygen a c(10x2) phase develops which can be regarded as a heavily distorted bilayer of bulk CoO.

O 77.9 Thu 17:00 H42

**Mixed interface and charge neutrality in the oxide heterostructure $DyScO_3/SrTiO_3$** — •kourosh rahmanizadeh, gustav bihlmayer, and sbtefan blügel — Institut für Festkörperforschung & Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich

Oxide interfaces have attracted considerable attention in recent years due to the emerging novel behavior, which does not exist in the corresponding parent bulk compounds, e.g. joining two simple band insulators $LaAlO_3$ and $SrTiO_3$ with different polarity can induce new properties ranging from conductivity to magnetism, even to superconductivity. The electrostatic potential diverges due to the polar discontinuity at the interface. But intermixing at the interface, defects, or formation of a polarization in the substrate can help to avoid the divergence of the electrostatic potential.

We carried out density functional theory calculations based on the full-potential linearized augmented planewave (FLAPW) method as implemented in the `FLEUR` code (www.flapw.de) for studying sharp and intermixed $DyScO_3/SrTiO_3$ interfaces. $DyScO_3$ layers induce the same polarity as the lanthanum aluminate. Experimental evidence for intermixing was reported for this system in Ref.[1]. We investigated both scenarios avoiding the polar catastrophe, either by forming a mixed layer at the interface or by formation of a polarization in the

$SrTiO_3$ substrate.

[1] M. Luysberg et al., Acta Materialia **57**, 3192 (2009)

O 77.10 Thu 17:15 H42

**The surface termination of $Mn_3O_4(001)$ films on Ag(001)** — Michael Huth, •Klaus Meinel, Roman Shantyr, Sebastian Polzin, Konrad Gillmeister, Henning Neddermeyer, and Wolf Widdra — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Germany

Spinel-like $Mn_3O_4(001)$ films can be imagined as an alternating stacking of (2x1)-like $Mn_2O_4$ and (2x2)-like Mn spinel sublayers (SL). According theory [1], the $Mn_2O_4$ layer is favored for termination. In our investigations, $Mn_3O_4$ films have been grown on Ag(001) and analyzed by means of STM and SPA-LEED. The films grow with the lattice vectors of the $Mn_3O_4(001)$ structure aligned along the [110]-like directions of the Ag(001) substrate. This specific film orientation implies an almost vanishing misfit which explains the brilliancy of the LEED spots. In the submonolayer stage, $Mn_3O_4$ islands are formed displaying either (2x1) or (2x2) surface termination depending on local thickness. For ultrathin continuous films, a (2x1) termination is resolved. However, for film thickness $>$ 12 spinel SL, SPA-LEED yields a (2x2) pattern. STM shows that the films are nevertheless terminated by a $Mn_2O_4$ layer. But it is now composed not only by (2x1) domains but also by domains where the Mn ions form a c(2x2) pattern. The combination of both structures explains the observed (2x2) LEED pattern. The spreading of this more symmetric structure implies a decrease of density of (2x1) domain boundaries and a corresponding decrease of domain boundary energy.

[1] V. Bayer et al., Phys. Rev. B76 (2007) 165428

O 77.11 Thu 17:30 H42

**Epitaxial Europiumoxide on Ni(100) with Single Crystal Quality** — •Daniel F. Förster, Jürgen Klinkhammer, Carsten Busse, Zhiwei Hu, L. Hao Tjeng, and Thomas Michely — II. Physikalisches Institut, Univ. zu Köln, Zülpicher Str. 77, 50937 Köln

EuO is one of the rare ferromagnetic semiconductors. Showing a variety of outstanding electronic properties it is e.g. an ideal candidate for spintronic systems. Growth on metal substrates gives rise to additional effects e.g. due to image charge screening or Schottky barriers. Hence the electronic structure is expected to have a different thickness dependence compared to oxide substrates. The initial growth of EuO films on Ni(100) strongly depends on the flux ratio Eu/O and the growth temperature. We use reactive molecular beam epitaxy (MBE) with a flux ratio Eu/O $\approx 3/2$ to grow stoichiometric EuO(100). For two monolayer thick films grown at 450°C in-situ scanning tunneling microscopy (STM) shows films with large monatomic flat terraces and few defects. The EuO grows quasi-pseudomorphically, hence the EuO is in-plane compressed by 3.1%. Low energy electron diffraction (LEED) measurements show the relaxation of the surface lattice constant close to the bulk value within the first 40 monolayers. 100 nm thick films grown at 320°C and annealed at 600°C have a RMS roughness of only 0.5 nm. The step edges are roundly shaped due to the annealing process and the LEED shows spots as sharp as for a single crystal. Ex-situ X-ray adsorption spectroscopy (XAS) was performed after capping with a 4 nm thick Al film. No signs of $Eu^{3+}$ or oxygen vacancies were found, thus the EuO film is stoichiometric.

O 77.12 Thu 17:45 H42

**Title: Simulation of deposition and growth of Xe-crystals via the low-temperature atom beam deposition method** — •Nicola Toto, Christian Schoen, and Martin Jansen — Max Planck Institute for Solid State Research - Heisenbergstrasse, 1 - 70569 Stuttgart - Germany

We model the deposition of Xe-atoms on a sapphire substrate and the subsequent growth of ordered Xe-phases via the low-temperature atom beam deposition method. This chemical synthesis method (D. Fischer and M. Jansen, J. Am. Chem. Soc. 41, 1755 (2002)) is a successful new way to synthesize metastable solid compounds. The modeling procedure consists of several steps, where we use empirical potentials to model the interactions within the substrate, the Xe-Xe-interactions in the gas phase and the solid, and the interactions between the Xe-atoms and the substrate. In a first step, we established that under the experimental conditions, no Xe-clusters form in the gas phase, and thus the deposition could be described by the adsorption of single Xe-atoms on the substrate at low temperatures. Next, we simulate the Xe deposition process and we study the growth mode depending on various synthesis parameters such as the deposition rate and the temperature of the substrate. Finally, the deposited Xe-layers are annealed, and the structure of the resulting compound is analyzed. We studied the establishment of locally ordered regions as a function of time, both during the deposition and the annealing. We observed that the final configuration is always crystalline, although defects such as stacking faults and dislocations are likely to form.

## O 78: Symposium Density functional theory and beyond for real materials

Time: Thursday 14:45–18:00 Location: H1

**Invited Talk** O 78.1 Thu 14:45 H1

**Downfolded Self-Energy of Many-Electron Systems and the Hubbard U** — •Ferdi Aryasetiawan — Graduate School of Advanced Integration Science, Chiba University, 1-33 Yayoi-cho, Inage-ku, Chiba-shi, Chiba, 263-8522 Japan

Correlated materials are usually characterised by a partially filled narrow 3d or 4f bands crossing the Fermi level. These materials, such as the 3d perovskites, are hosts to many intriguing properties which cannot be satisfactorily explained within the local density approximation (LDA) or its extensions. The usual approach for treating these systems is to adopt a model Hamiltonian that contains input parameters, notably the Hubbard U, which is often treated as an adjustable parameter. It is therefore highly desirable to construct reliable model Hamiltonians, where the input parameters are computed from first-principles, thus avoiding adjustable parameters which may lead to misleading results.

Here we propose a constrained random-phase approximation (cRPA) scheme [1,2] that allows for a systematic downfolding of high energy screening channels resulting in a low-energy model with a screened Coulomb interaction or the Hubbard U [3]. The model Hamiltonian can then be solved by a number of approaches such as the LDA+U method, the dynamical mean-field theory (DMFT) scheme or the recently introduced LDA+Gutzwiller approach.

[1] Phys. Rev. B 70, 195104 (2004) [2] Phys. Rev. B 80, 155134 (2009) [3] Phys. Rev. Lett. 102, 176402 (2009)

**Invited Talk** O 78.2 Thu 15:15 H1

**LDA+Gutzwiller method for correlated electron systems** — •Zhong Fang — Institute of Physics, Chinese Academy of Science

I will introduce our newly developed LDA+Gutzwiller method, in which the Gutzwiller variational approach is incorporated with the density functional theory (DFT) through the generalized Kohn-Sham formalism, such that orbital fluctuations can be treated from ab initio. We will show that its quality for ground state determination is as accurate as dynamic mean field theory (DMFT), and yet its computational cost is as cheap as LDA+U. Then we will concentrate on FeAs-based compounds, which are typical multi-orbital correlated system. Various corrected properties beyond LDA (or GGA), such as Fe-As distance, soft phonon, and Fermi surface shape, will be discussed based on the calculations by LDA+Gutzwiller. The inter-orbital Hund's coupling J rather than U plays crucial roles for the physical properties of FeAs-compounds.

References:

[1] X. Y. Deng, X. Dai, Z. Fang, EPL 83, 37008 (2008). [2] G. T. Wang, X. Dai, Z. Fang, PRL 101, 066403 (2008). [3] X. Y. Deng, L. Wang, X. Dai, Z. Fang, PRB 79, 075114 (2009). [4] G. T. Wang, X. Dai, Z. Fang, Cond-mat:/0903.1385 (2009).

**Invited Talk** O 78.3 Thu 15:45 H1

**Localized and itinerant states in $d/f$-electron systems unified by $GW$@LDA+$U$** — •Hong Jiang — College of Chemistry, Peking University, Beijing 100871, China

Density-functional theory in the local-density or generalized gradient approximation (LDA/GGA) has proven to be inadequate for $d$ and $f$-electron systems that are characterized by the simultaneous presence of itinerant and localized states and interactions between them. The simplest extension that can overcome the major failure of LDA is the introduction of a local Hubbard-like correction (LDA+$U$), however itinerant states are still treated at the LDA level. As a first step towards a unified treatment of localized and itinerant states, we combine many-body perturbation theory in the $GW$ approximation with LDA+$U$ ($GW$@LDA+$U$) to investigate the quasiparticle band structure of prototypical $d/f$-electron systems. We observe good agreement between the $GW$ density of states and experimental photoemission spectra using $U$s determined by constrained DFT. All main features in the experimental band gaps of the lanthanide sesquioxide series ($Ln_2O_3$) are well reproduced by $GW$@LDA+$U$ and can be attributed to the evolution of the occupied and unoccupied $f$-states as the number of $f$-electrons increases. Consistent with other $GW$ approaches, the satellite structure in late transition metal oxides is still absent, and the binding energy of occupied $d/f$-states exhibits a tendency to be underestimated. The implications of our studies for strongly correlated electrons are discussed. *In collaboration with R. I. Gomez-Abal, P. Rinke and M. Scheffler at Fritz-Haber-Institut der MPG.

**15 min. break**

**Invited Talk** O 78.4 Thu 16:30 H1

**Giant polaronic effects in solids and nanstructures** — •Andrea Marini — CNISM and department of Physics, University of Rome *Tor Vergata*

The conjugation of Ab-Initio methods with Many-Body techniques, constitutes a well-established approach to interpret the photoexcited properties of bulk materials, surfaces, nanostructures and organic/biomolecules. In the standard approach, however, atoms are assumed to be frozen in their crystallographic positions, thus neglecting the effect of lattice vibrations. As a consequence quasiparticles and excitons turn out to be insensitive to the temperature T and with an infinite lifetime, in stark contrast with the experimental evidence. In the frozen-atom approaches this temperature dependence is not described at all and, even in the $T \rightarrow 0$ limit, the calculated absorption spectra is commonly convoluted with some artificial, *ad-hoc* numerical broadening function chose to yield the best agreement with the experiment. In this talk I will show how to solve, in a fully Ab-Initio manner, the equation of motion of quasiparticles and excitons including the coupling with the lattice vibrations. The picture obtained within a frozen-atom approximation will turn out to be deeply modified by the electron-phonon coupling, either at zero and finite temperature. I will discuss several important consequences as the bright to dark (and vice versa) transitions of excitons in layered materials, or the beakdown of the quasiparticle picture in conjugated polymers.

**Invited Talk** O 78.5 Thu 17:00 H1

**Excitation energies with time-dependent density *matrix* functional theory** — •Evert Jan Baerends, Klaas J. H. Giesbertz, Oleg Gritsenko, and Katarzyna Pernal — Vrije Universiteit, Amsterdam, The Netherlands

Time-dependent density functional theory in its current adiabatic implementations exhibits three striking failures: a) totally wrong behavior of the excited state surface along a bond-breaking coordinate [1]; b) lack of doubly excited configurations, affecting again excited state surfaces; c) much too low charge transfer excitation energies. We address these problems with time-dependent density matrix theory (TD-DMFT) [2-4].

For two-electron systems the exact exchange-correlation functional is known in DMFT, hence exact response equations can be formulated. This affords a study of the performance of TDDMFT in the TDDFT failure cases mentioned (which are all strikingly exhibited by prototype two-electron systems such as dissociating $H_2$ and $HeH^+$). At the same time, adiabatic approximations, which will eventually be necessary, can be tested without being obscured by approximations in the functional.

[1] K. J. H. Giesbertz, E. J. Baerends, Chem. Phys. Lett. 461 (2008) 338 [2] K. Pernal, O. V. Gritsenko, E. J. Baerends, Phys. Rev. A 75, 012506 (2007) [5] K. J. H. Giesbertz, E. J. Baerends, O. V. Gritsenko, Phys. Rev. Lett. 101 (2008) 033004 [6] K. J. H. Giesbertz, K. Pernal, O. V. Gritsenko, E. J. Baerends, J. Chem. Phys. 130 (2009) 114104

**Invited Talk** O 78.6 Thu 17:30 H1

**Calculations of multipoles in magnetic metals and insulators** — •Lars Nordström — Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

The concept of spherical tensors or multipoles of an open atomic shell is reviewed and discussed. Some of these multipoles play an important rule in e.g. x-ray circular dichroism measurements, where with the use of the famous sum rules by Carra et al. the spin and orbital magnetic moments can be deduced.

Here we will describe how such multipoles can be calculated in general in both the ground state as well as excited states in terms of density functional methods including a local correlation term, as in e.g. the so-called LDA+U or LDA+DMFT methods. It will be demonstrated how these multipoles can contribute significantly to the exchange and correlation energies of transition metal systems. Especially, we will discuss in some depth materials where these multipoles act as the main order parameter, sometimes referred to as an "hidden order". Results for two cases will be presented the magnetic/superconducting iron-pnictide LaOFeAs and the heavy fermion compound $URu_2Si_2$.

## O 79: General Meeting of the Surface Science Division

Time: Thursday 19:30–20:00 Location: H1

**Report of the Chairman of the DPG Surface Science Division**

## O 80: Post Deadline Session

Time: Thursday 20:00–21:00 Location: H1

**4 contributed talks to be determined**

## O 81: Invited talk (Bligaard, Thomas)

Time: Friday 10:15–11:00 Location: H36

**Invited Talk** O 81.1 Fri 10:15 H36

**Towards the computational design of heterogeneous catalysts** — •Thomas Bligaard — Center for Atomic-scale Materials Design, Dept. of Physics, Build. 307, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark

Electronic structure methods based on density functional theory have reached a level of speed and accuracy where they can be used to describe complete catalytic reactions on transition metal surfaces. Simulations now complement experiments to give unprecedented insight into surface processes, allowing one to pinpoint the origin of catalytic activity of a metal in terms of its electronic structure. The use of electronic structure theory as a tool for directly designing or searching for new materials is a computationally rather expensive process, though, and has until now been quite limited. For a limited number of catalytic processes the underlying reactivity trends have been understood well enough that they could subsequently successfully be used to seek out new catalysts. The computational search for such potentially useful catalysts will be discussed. The focus will be on showing the generality of such a trend- and descriptor-based approach by linking a few specific case stories to more fundamental underlying linear-energy relations for the adsorbate-surface bonds [1].

[1] J.K. Nørskov, T. Bligaard, J. Rossmeisl, C.H. Christensen, Nature Chemistry 1, 37 (2009)

## O 82: Graphene IV

Time: Friday 11:15–13:00 Location: H31

O 82.1 Fri 11:15 H31

**Spin-Splitting of Graphene/Au/SiC investigated with Spin- and Angle-Resolved Photoemission Spectroscopy** — •Isabella Gierz[1], Fabian Meier[2], Bartosz Slomski[2], Jan Hugo Dil[2], Jürg Osterwalder[3], Christian R. Ast[1], and Klaus Kern[1,4] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [2]Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [3]Physik-Institut, Universität Zürich, CH-8057 Zürich, Switzerland — [4]Institut de Physique des Nanostructures, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

Due to its high carrier mobility graphene is a promising candidate for electronics applications. For possible applications in the field of spintronics, however, a spin-splitting of the graphene band structure is required. In order to lift the spin degeneracy in graphene we exploit the Rashba-Bychkov effect where the presence of heavy elements with a strong atomic spin-orbit interaction in a symmetry-broken environment leads to a spin-splitting of the two-dimensional band structure on a crystal surface. The intrinsic spin-orbit interaction of carbon is negligible but [1] predicts that defects, i.e. local distortions of the graphene lattice from sp$^2$ to sp$^3$ hybridization, lead to a strong enhancement of the spin-orbit coupling. Furthermore, we have shown recently that it is possible to intercalate epitaxial graphene on SiC with gold atoms, thereby adding heavy atoms to the system. We present spin- and angle-resolved photoemission spectroscopy measurements on pristine epitaxial graphene as well as gold intercalated graphene on SiC.

[1] A. H. Castro Neto et al., *Phys. Rev. Lett.*, **103**, 026804 (2009)

O 82.2 Fri 11:30 H31

**High Resolution Electron Energy Loss Spectroscopy on Graphene/SiC(0001)** — •Roland J. Koch[1], Michael Endlich[1], Thomas Haensel[1], Syed Imad-U. Ahmed[1], Thomas Seyller[2], and Juergen A. Schaefer[1,3] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, TU-Ilmenau, Ilmenau, Germany — [2]Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Erlangen-Nürnberg, Germany — [3]Department of Physics, Montana State University, Bozeman, Montana, USA

The recent experimental realization of single-layer graphene sheets has led to intense efforts to understand its electronic and vibrational properties in the context of solid state materials physics. In this contribution we investigate the interaction of epitaxial graphene with SiC(0001) using high resolution electron energy loss spectroscopy (HREELS). The focus in this contribution is on the coupling of charge carriers in semi-metallic graphene with the optical phonons of SiC(0001). Due to this coupling the surface optical phonons, the so called Fuchs-Kliewer phonons, completely vanish and two new modes $\omega_-$ and $\omega_+$ are observed instead. The energetic position and intensity of these modes depend strongly upon the momentum transferred parallel to the interface ($q_\parallel$), which we investigated in the regime of 0.005 $\mathring{A}^{-1}$ to 0.03 $\mathring{A}^{-1}$. Simulating our HREELS-data using dielectric theory and solving the Poisson- and Schrödinger equations self consistently allows us to determine the carrier density distribution and the conduction band edge normal to the plane of the graphene/SiC heterostructure.

O 82.3 Fri 11:45 H31

**AFM imaging of graphene under ambient conditions** — •Michael Enzelberger[1], Viatcheslav Dremov[1], Florian Speck[2], Catharina Knieke[3], Angela Berger[3], Thomas Seyller[2], Wolfgang Peukert[3], and Paul Müller[1] — [1]Department of Physics and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Germany. — [2]Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Germany. — [3]Lehrstuhl für Feststoff- und Grenzflächenverfahrenstechnik, Universität Erlangen-Nürnberg, Germany.

Routine checks of graphene properties during device production can be facilitated significantly, when these measurements can be carried out under ambient conditions. We report on AFM investigations of epitaxial graphene on SiC(0001) and ball-milled graphite. Tapping-mode AFM and Kelvin-probe force microscopy (KPFM) were applied to reveal morphology and work function distribution. Although the absolute values of the work function differences are not meaningful under ambient conditions, the work function contrast from the KPFM data allows to distinguish between single-, bi- and trilayer graphene. Ball-milled graphite shows small flakes of single or multilayer graphene which are covered with surfactant molecules on either side. Also stacks of several graphene sheets separated by surfactant molecules were observed.

O 82.4 Fri 12:00 H31

**Low Temperature Epitaxial Graphene on SiC by Carbon Deposition** — •Ameer Al-Temimy, Christian Riedl, and Ulrich Starke — Max Planck Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

Epitaxial graphene displays unconventional electronic properties that make it an interesting material for carbon based nanolectronics. The epitaxial growth of graphene on silicon carbide (SiC) is a promising route to achieve large graphene samples. Conventionally, on SiC(0001) in an ultrahigh vacuum (UHV) system, monolayer graphene is prepared by annealing to about 1200 °C. Using low energy electron diffraction (LEED) and angle-resolved ultraviolet photoelectron spectroscopy (ARUPS) we demonstrate that monolayer graphene can also be grown at a lower temperature of about 950 °C under simultaneous carbon deposition. As shown by atomic force microscopy (AFM) the approach of carbon deposition modifies the growth dynamics of graphene so that the initial surface morphology of the SiC crystal is preserved in contrast to the conventional method. On SiC(000$\bar{1}$), LEED demonstrates that the carbon evaporation induced epitaxial graphene grows with a predominant lattice orientation of 0° with respect to the substrate instead of 30° as observed for the conventional UHV preparation. The new approach of carbon evaporation on SiC crystals opens up pathways in the investigation of SiC surface phase diagrams and for low temperature procedures in graphene growth.

O 82.5 Fri 12:15 H31

**Quasi-freestanding Graphene on SiC(0001)** — •Florian Speck[1], Markus Ostler[1], Jonas Röhrl[1], Johannes Jobst[2], Daniel Waldmann[2], Martin Hundhausen[1], Lothar Ley[1], Heiko B. Weber[2], and Thomas Seyller[1] — [1]Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Germany — [2]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Germany

Epitaxial graphene thermally grown on SiC(0001) is a first choice candidate for the development of graphene-based electronics. The graphene layer directly in contact with the substrate is covalently bound and forms the $(6\sqrt{3}\times 6\sqrt{3})R30°$ reconstruction. It lacks the electronic properties of graphene and is thus called buffer layer. Only the next graphene layer, which resides on top of the buffer layer, exhibits the characteristic Dirac cone. Hydrogen can saturate dangling bonds on Si and SiC surfaces and is therefore a promising candidate for a chemical modification of the interface. Riedl et al. demonstrated the conversion of the buffer layer into monolayer graphene by annealing in hydrogen [1]. Here we present a comprehensive spectroscopic study on buffer layer and monolayer graphene samples annealed in hydrogen. Si-H bonds at the interface are detected by infrared absorption spectroscopy, proving the intercalation of hydrogen underneath the buffer layer. The graphene layer formed by this process interacts only weakly with the substrate. Raman spectroscopy indicates the presence of short range defect sites. Hall effect measurements show p-type conduction with hole mobilities up to 1250 cm$^2$V$^{-1}$s$^{-1}$ at room temperature.

[1] C. Riedl et al., arXiv:0911.1953v1

O 82.6 Fri 12:30 H31

**Crystal Symmetry and Stress in Epitaxial Graphene Films** — •Diedrich Schmidt[1] and Taisuke Ohta[2] — [1]Department of Physical Chemistry II, Ruhr-University Bochum, 44780 Germany — [2]Sandia National Laboratories, Albuquerque, NM 87185 USA

We performed combined confocal Raman microspectroscopy and atomic force microscopy (AFM) studies to address discrepancies in the reported electronic properties and characteristic Raman bands of monolayer epitaxial graphene. Monolayer graphene was made by sublimation of Si from a SiC substrate at elevated temperature in an argon environment [1]. Our samples exhibit variation in both the G and 2D peak positions presumably due to strain; similar to previous work [2]. However, our monolayer films show large areas of uniform compressive strain covering ≥40% of the surface with nearly equivalent coverage of smaller, quasi strain-relieved regions which are oriented at multiples of 30° to each other. AFM phase data confirm the quasi strain-relieved areas seen in Raman microspectroscopy are physical effects that exist within the monolayer film, or that are induced in the film by interactions with the interface layer. Due to the high symmetry of the C-rich interface layer [3], we propose that these regions are controlled by the interface layer.

This work is supported in part by the LDRD program at Sandia Labs and by the German BMBF under grant 05KS7PC2.

[1] K. V. Emtsev, *et al.*, *Nature Materials* **8**, 203 (2009).
[2] J. A. Robinson, *et al.*, *Nano Letters* **9**, 964 (2009).
[3] K. V. Emstev, *et al.*, *Phys. Rev. B* **77**, 155303 (2008).

O 82.7 Fri 12:45 H31

**Plasmons in epitaxial graphene: influence of steps and doping concentration** — •Thomas Langer[1,2], Herbert Pfnür[1], Christoph Tegenkamp[1], and Hans Werner Schumacher[2] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, D-30167 Hannover — [2]PTB, D-38116 Braunschweig

Collective excitations of the two dimensional electron gas in epitaxial graphene grown on SiC(0001) have been studied. Structural properties were analyzed by XPS and SPA-LEED. The influence of surface defects on the dispersion and the lifetime of the sheet plasmon has been investigated in detail by angle resolved EELS. The step concentration (10-100nm terrace length) has been varied by using differently ex-situ treated samples and by varying the sublimation rates. The dispersion, which does not depend on the defect concentration, is almost linear and differs strongly from a $\sqrt{k}$ behaviour, which is often found for 2DEG. The strong blueshift in the short wavelength regime can be attributed to nonlocal effects within the highly correlated electron system. For the pristine graphene layer the dispersion shows a pronounced dip at the position of $k_F$, which vanishes after adsorption of 4F-TCNQ. Hence the position can be used to control the filling of the conduction band. The lifetime of the plasmons is inversely proportional to the step density and to the wavelength. As the phase velocities of the plasmons deduced from the linear dispersion coincide with the Fermi velocity of the electrons, steps only have to act as a momentum source to couple effectively plasmons to the electron-hole continuum, thus reducing effectivly the lifetime outside the Landau regime.

## O 83: Plasmonics and Nanooptics VII

Time: Friday 11:15–13:00 Location: H32

O 83.1 Fri 11:15 H32

**Metamaterial sensor for glucose and molecular monolayers using the plasmonic analog of EIT** — •Martin Mesch[1], Na Liu[1], Thomas Weiss[1], Carsten Sönnichsen[2], and Harald Giessen[1] — [1]4th Physics Institute, University of Stuttgart, Germany — [2]Institute of Physical Chemistry, University of Mainz, Germany

We utilize the plasmonic analog[1] of electromagnetically induced transparency (EIT) to construct an optical LSPR (localized surface plasmon resonance) sensor. A combination of stacked gold dipole and quadrupole antennas exhibits a sharp spectral resonance, which shifts for changes in the structures' dielectric environment. To characterize the sensor, aqueous glucose solutions with concentrations between 0% and 25% have been measured in a custom flow cell by Fourier transform infrared spectroscopy. The results reveal a sensitivity of 374 nm per refractive index unit, corresponding to a figure of merit (sensitivity/linewidth) of 4.1. We compare our measurements to S-matrix simulations and give a recipe to determine the most sensitive structure geometry. To our knowledge, this is up to date the most sensitive lithographically manufactured LSPR sensor design. Additional experiments demonstrate the ability to detect a single molecular layer of biotin/streptavidin. [1] N. Liu et al., Nature Materials 8, 758 (2009)

O 83.2 Fri 11:30 H32

**Optical properties of a metallic meander Fabry-Perot cavity** — •Liwei Fu[1], Heinz Schweizer[1], Thomas Weiss[2], Harald Giessen[1], Philipp Schau[3], Karsten Frenner[3], Steffen Maisch[3], and Wolfgang Osten[3] — [1]4th Physics Institute, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [2]LASMEA, Université Blaise Pascal, F-63177 Aubière Cedex, France — [3]Institut für Technische Optik, University of Stuttgart, Pfaffenwaldring 9, 70550 Stuttgart, Germany

A single layer metallic meander structure is favorable to couple photons with surface plasmon polaritons and, as a result, a resonant enhanced transmission can be observed. A combination of two single-meander layers forms a Fabry-Perot cavity with frequency selective mirrors. In this contribution we investigate its optical properties. At the proper distance, the cavity behaves as a single layer meander, in which enhanced transmission and negative mode dispersion are present. In contrast to the single layer, however, the surface waves from the two mirrors are still coupled together, resulting in an amplified longitudinal E-field propagating backwards inside the cavity. The backward wave can be observed at visible frequencies with low loss and high transmittance for structural parameters that are well suited for nanofabrication. Such a compact realization of negative refraction is a promising approach for applications of subwavelength imaging, polarization beam splitting, and delay line approaches.

O 83.3 Fri 11:45 H32

**Dynamical response of split-ring molecules for metamaterials** — •Stephan Bernadotte[1,2,3], Wim Klopper[1,2], and Ferdinand Evers[1,3] — [1]Institut für Nanotechnologie, Karlsruher Institut für Technologie — [2]Lehrstuhl für Theoretische Chemie, Institut für Physikalische Chemie, Karlsruher Institut für Technologie — [3]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie

We investigate the dynamical properties of molecular crystals (matrices) built up from nanometer sized ring shaped, conjugated molecules, which are candidate systems for negative index materials with frequencies in the optical regime. The response properties of such materials near their dynamical resonances can be understood in terms of an LRC circuit. In the conventional modeling of metamaterials, the circuit parameters enter (essentially) as phenomenological quantities. By contrast, in the present work they will be calculated from a microscopic tight binding model of a molecular Hamiltonian employing the Kubo approach.

We find that the LRC resonances of the molecular structures correspond to plasmonic excitations. By comparing to an analytical calculation, we can study in which way the plasmon resonances (and residues) depend on the molecule's electronic structure. On a qualitative level, our study also includes an investigation of the sensitivity of the dynamical response to the damping of the plasmons. Finally, we analyze the impact of cross-talk among the molecules within the matrix and the importance of birefringence terms.

O 83.4 Fri 12:00 H32

**Negative refraction in natural ferromagnetic metals** — •Sebastian Engelbrecht, Alexey Shuvaev, and Andrei Pimenov — Experimentelle Physik 4, Universität Würzburg

It is generally believed that nature does not provide materials which show negative refraction. Up to now, the experiments with negative refraction have been realized with metamaterials or photonic crystals. As has been suggested recently, negative refraction in natural materials can be realized in ferromagnetic metals. Close to the ferromagnetic resonance (FMR) the real part of the magnetic permeability can reach negative values. This may lead to negative refraction as long as the dielectric permittivity is dominated by metallic response. This talk will provide experimental data of ferromagnetic metals (Fe,Co) which indeed show a range of negative refraction close to FMR in millimeter frequency range. In these materials the negative refractive index can be achieved even at room temperature.

O 83.5 Fri 12:15 H32

**Bragg Plasmonics** — •Richard Taubert, Ralf Ameling, Lutz Langguth, Daniel Drégely, and Harald Giessen — University of Stuttgart, Germany

The investigation of plasmon-plasmon coupling has focused on near-field coupling until now. Only little work has been done on far-field interaction in plasmonic structures. We investigate a so-called 3D plasmonic crystal: four layers of nanowires are stacked in Bragg fashion, where the vertical distance matches half the resonance wavelength of the individual nanowire particle plasmon. The resonant far field coupling leads to the formation of a plasmonic band gap spanning almost one octave.

The structure was fabricated using layer-by-layer stacking. We investigate the dependence of the optical spectra on layer number and distance tuning. Scattering matrix calculations agree very well with our experimental findings.

O 83.6 Fri 12:30 H32

**Al nanostructures for metamaterials in visible region and biosensing** — •Shankar K. Jha[1], Yogesh Jeyaram[1], Mario Agio[2], Jörg F. Löffler[1], and Yasin Ekinci[1,3] — [1]Laboratory of Metal Physics and Technology, ETH Zurich, 8093 Zurich, Switzerland — [2]Laboratory of Physical Chemistry, ETH Zurich, 8093 Zurich, Switzerland — [3]Paul Scherrer Institute, 5232 Villigen-PSI, Switzerland

Metamaterials are artificially engineered materials having electromagnetic material properties that are not readily found in nature. Owing to their potential applications like sub-wavelength imaging, negative refractive index, optical cloaking etc., these materials have been extensively studied in the microwave and optical regimes including in red wavelengths. We report development of metamaterials down to blue range. We studied optical properties of two-dimensional arrays of aluminum nanosandwiches. Strong magnetic response and negative permeability are observed down to 400 nm wavelength, paving the way towards metamaterials operating in the visible range. In addition we discuss the superior performance of such structures in biosensing.

O 83.7 Fri 12:45 H32

**Electromagnetic polarisation twisting mediated by plasmon / nanostructure interaction** — •Brian Ashall[1], Brian Vohnsen[1], Stephan Schwieger[2], Erich Runge[2], Michael Berndt[3], and Dominic Zerulla[1] — [1]School of Physics, University College Dublin, Dublin 4, Ireland. — [2]Theoretical Physics I, Technische Universität Ilmenau, 98684 Ilmenau, Germany. — [3]Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden, Germany.

The design and architecture of nanostructures for the purpose of controlling and manipulating Surface Plasmon Polariton (SPP) dynamics is currently a focal point of research. Here, we present the first instance of plasmon mediated polarisation reorientation observed in the farfield with no associated reemission directional change [1]. Specifically, it is demonstrated that, as a result of the interaction between SPPs and tailor designed nanostructures of 3-fold symmetry characteristics [2], a polarisation twisting of the SPP mediated reradiated light is attained. It is shown that the dynamics of such an interaction can be controlled externally, enabling active control of the out-going polarisation orientation. In order to further understand the origin of the processes involved, Green's function based simulations of the interactions are presented and confirm that the origin of the polarisation twisting can be explained via asymmetrical in-plane SPP scattering.

[1] B. Ashall, B. Vohnsen, M. Berndt, D. Zerulla; Phys. Rev. B, 80(20) (2009)

[2] B. Ashall, M. Berndt, D. Zerulla; Appl. Phys. Lett. 91(20), 203109 (2007)

## O 84: Density functional theory and beyond for real materials IV

Time: Friday 11:15–13:15 Location: H34

O 84.1 Fri 11:15 H34

**Evolution of electron traps at ice surface: aggregation of orientational defects** — •Michel Bockstedte[1,2], Anja Michl[1], and Angel Rubio[2] — [1]Theor. Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen — [2]Nano-Bio spectroscopy group and ETSF, Dpto. Física de Materiales, Universidad del País Vasco, Av. Tolosa 72, E-20018 San Sebstián

Water, water clusters and ice possess the fascinating ability to solvate electrons. On crystalline ice long-living solvated electron states were observed that derive from pre-existing surface traps.[1] Theoretical models based on the bi-layer terminated $I_h$-(0001) relate such traps to orientational defects[1] of the otherwise ordered arrangement of water molecules at the surface.[2] At these traps with low formation energy, the electron attaches to the local dipole moment of OH-groups pointing out of the surface. In experiments, however, the solvated electron state was found to evolve in a thermally activated process characterized by an enhancement of its binding energy. The underlying reconstruction of the ice-trap is crucial to understand the long life time. Employing density functional theory we address the mechanism of the evolution of the initial trap. We show that an aggregation of orientational defects results in an enhanced localization of the solvated electron. The solvation-triggered aggregation yields structures with an excess energy $> 500\,\mathrm{meV}$ after the electron detachment. We discuss this mechanism in the light of an alternative evolution via the formation of voids.

[1] Bovensiepen *et al* J. Chem. Phys. C **113**, 979 (2009).

[2] Buch *et al.* PNAS **105**, 5969 (2008).

O 84.2 Fri 11:30 H34

**The role of van der Waals interactions for the cohesive properties of the coinage metals** — •Lorenz Romaner[1], Matthias Scheffler[2], and Claudia Ambrosch-Draxl[1] — [1]Chair of Atomistic Modelling and Design of Materials, University of Leoben, Franz-Josef-Straße 18, A-8700 Leoben, Austria. — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin-Dahlem, Germany.

Density-functional theory has been successfully applied over many years to calculate binding energies and bond lengths for a wide range of systems. More recently, it has been extended to include long-range correlation interactions and hence could be used for purely van der Waals (vdW) bound systems such as noble gas solids or organic crystals. On the other hand, early calculations for noble metals have revealed a vdW contribution to the cohesive energy [Rehr, Zaremba, Kohn, PRB 12, 2062 (1975)]. We investigate this issue by employing the vdW-DF approach [Dion et al., PRL 92, 296401 (2004)], where the exchange interactions are treated within revPBE, and the non-local correlations are based on an approximation to the adiabatic connection formula. We find that the latter give a substantial contribution to the cohesive energies but, overall, vdW-DF underestimates their magnitude while overestimating the lattice parameters. We attribute this shortcoming to the local part of the correlation energy.

O 84.3 Fri 11:45 H34

**Ab initio Quantum Monte Carlo: Methods and Applications** — •Norbert Nemec[1,2], Dario Alfè[1], and Richard Needs[2] — [1]University College London, UK — [2]University of Cambridge, UK

Quantum Monte Carlo (QMC) methods allow accurate computations of correlated quantum systems. Using a combination of different variants of QMC, the electronic structure of atomistic systems can be handled in ab initio calculations. We present benchmarks on molecules that demonstrate the accuracy and results on graphitic systems that demonstrate intricate finite size effects arising from van der Waals interactions in anisotropic periodic systems.

O 84.4 Fri 12:00 H34

**Surface Energies of Transition Metals with Density-Functional Theory and beyond** — Aloysius Soon[1], Bo Li[2], Martin Fuchs[1], and •Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]University of California Santa Barbara, California, USA

Determining surface energies of metals is, to date, a great challenge, both theoretically and (even more so) experimentally. Density-functional theory (DFT) calculations of metal surface energies within the local-density approximation have provided understanding of qualitative trends. Yet absolute surface energies, in particular of *d*-metals, exhibit significant uncertainties related to the description of exchange-correlation (XC). A more sophisticated treatment of XC for real metals, beyond present-day gradient-corrected approximations is however still an open challenge. In particular, this requires a careful (re-)analysis of the bonding between metal atoms in the bulk and at the surface in terms of explicitly correlated approaches. Such an analysis is attempted in this paper.

Employing the cluster correction scheme[1], we derive surface energies beyond the (semi-)local DFT, using hybrid-DFT XC functionals as well as higher-level approaches (e.g. exact exchange plus the RPA for correlation – EX+cRPA). We find the surface energies of pristine metals to be poorly described (i.e. largely underestimated by about 30 %) by hybrid-DFT XC functionals, while the EX+cRPA provides a promising approach towards describing surface energetics. [1] Q.-M. Hu *et al.*, Phys. Rev. Lett. **98**, 176103 (2007); **99**, 169903(E).

O 84.5 Fri 12:15 H34

**Assessing the random phase approximation for weakly bonded molecules** — •Xinguo Ren, Patrick Rinke, and Matthias Scheffler — Fritz-Haber-Institut der MPG, 14195 Berlin, Germany

The random phase approximation (RPA) to the electronic correlation energy has generated increasing interest in recent years due to several of its attractive features. One of these is the automatic and seamless inclusion of van der Waals (vdW) interactions, which makes the RPA free of limitations that empirical vdW correction schemes may suffer from. However, RPA is still an approximate theory, and the treatment of vdW will not be perfect. In addition, RPA calculations are presently performed non-self-consistently with input orbitals from a preceding Hartree-Fock (HF) or standard density functional theory (DFT) calculation. For a systematic assessment of the RPA's performance for vdW interactions, we applied our recent implementation of the RPA [1] to the molecular S22 benchmark set [2], which comprises 22 weakly bonded complexes of different nature. Different DFT/HF orbitals have been used to demonstrate the orbital dependence of RPA. We observe a systematic underbinding of the RPA in all cases, whereby the amount of underbinding depends noticeably on the input orbitals. A detailed analysis reveals that both the exchange and the correlation part of the RPA contribute to this dependence, but in a somewhat counteracting manner. [1] V. Blum *et al.*, Comp. Phys. Comm. **180**, 2175 (2009). [2] P. Jurečka *et al.* , Phys. Chem. Chem. Phys. **8**, 1985 (2006).

O 84.6 Fri 12:30 H34

**A simple construction of the GW approximation for molecules** — •Dietrich Foerster[1], Peter Koval[2], and Olivier Coulaud[3] — [1]CPMOH, Bordeaux, France — [2]CNRS, INRIA (Hiepacs), Bordeaux, France — [3]INRIA (Hiepacs), Bordeaux, France

To model the fundamental processes in organic solar cells where light first generates an exciton that is then separated at the donor acceptor interface is a challenging task and requires an extension of existing computational methods to large aperiodic systems. We chose to extend the LCAO approach to excited states in a simple way by defining a space of dominant functions that spans the space of products with exponential accuracy [1]. Using these functions as a basis, we devised an $O(N^2)$ algorithm for computing the Kohn-Sham response function [2] where $N$ is the number of atoms. Our approach simplifies/accelerates the computation of spectra in TDDFT linear response (see the contribution at this symposium of Dr. P. Koval).

In this contribution, we use our construction of the Kohn-Sham response function to give a simple algorithm for the GW approximation. Our results are only "proof of principle" and the complexity of the calculation must still be reduced.

**References** [1] D. Foerster, J. Chem. Phys. **128**, 034108 (2008); P. Koval and D. Foerster, Physica Status Solidi, submitted (2010) arXiv:0910.3796. [2] D. Foerster, P. Koval., J. Chem. Phys. **131** 044103 (2009). [3] F. Aryasetiawan and O. Gunnarsson, Rep. Prog. Phys. **61**, 237 (1998).

O 84.7 Fri 12:45 H34

**An iterative method for TDDFT of large molecules** — •Peter Koval[1], Dietrich Foerster[2], and Olivier Coulaud[3] — [1]CNRS, INRIA (Hiepacs), Bordeaux, France — [2]CPMOH, Bordeaux, France — [3]INRIA (Hiepacs), Bordeaux, France

To model the processes in organic solar cells where light first generates an exciton that is then separated at the donor acceptor interface is a challenging task. The first difficulty is the size of the molecules used in such devices and the absence of any translational symmetry. Recently, a fast method for computing of the Kohn-Sham response function [1] in a localized basis set [2] has been developed. The Kohn-Sham response function serves as a building block for TDDFT in linear response, for Hedin's GW approach and for the Bethe-Salpeter equation. In TDDFT, a drawback of our response function is its large memory requirements. Fortunately, electronic excitation spectra can be computed with an iterative method of moderate computational and memory cost. This method is similar to van Gisbergens iterative method [3] but we use our basis of dominant functions and a more systematic iterative technique (bi-orthogonal Lanczos, GMRES) [4]. In this contribution, we present examples of TDDFT electronic excitation spectra of molecules used in organic photovoltaic.

**References** [1] D. Foerster, P. Koval., J. Chem. Phys. **131** 044103 (2009). [2] D. Foerster, J. Chem. Phys. **128**, 034108 (2008). [3] S. J. A. van Gisbergen, C. Fonseca Guerra, E. J. Baerends, J. Comput. Chem. **21**, 1511 (2000). [4] Y. Saad, *Iterative Methods for Sparse Linear Systems*, (Siam, Philadelphia 2003).

O 84.8 Fri 13:00 H34

**Hybrid Functionals within the All-Electron FLAPW Method: Implementation and Applications** — •Martin Schlipf, Markus Betzinger, Christoph Friedrich, Marjana Lezaic, and Stefan Blügel — Forschungszentrum Jülich, Institut für Festkörperforschung and Institute for Advanced Simulation

Density-functional theory is exceptionally successful in describing the properties of molecules and solids. However, the commonly used approximations for the exchange-correlation functional - the local-density (LDA) and generalized gradient approximation (GGA) - fail to describe the band gaps and structural properties of a number of semiconducting and insulating materials. The self-interaction error in LDA and GGA is mainly responsible for this shortcoming. It is partly corrected in hybrid functionals, which contain a certain fraction of nonlocal Hartree-Fock exchange. So far, most implementations for periodic systems approximate the presence of the core by pseudopotentials and employ a plane-wave basis set. In this contribution, we present an efficient implementation of the PBE0 and HSE06 functionals within the all-electron full-potential linearized augmented planewave method realized in the `FLEUR` (www.flapw.de) code. We demonstrate the improvement over LDA and GGA for oxide materials and focus in particular on systems where the results obtained with the standard functionals disagree with experimental results.

## O 85: Metal substrates: Adsorption of organic / bio molecules VII

Time: Friday 11:15–13:00 Location: H36

O 85.1 Fri 11:15 H36

**Thin films and monolayers of metalloporphyrines and -phthalocyanines: Examination of the reactive sites** — •Martin Schmid, Yun Bai, Michael Sekita, Hans-Peter Steinrück, and J. Michael Gottfried — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen, Germany

Planar metal complexes such as metalloporphyrins and -phthalocyanines show various chemical and structural properties that make them promising candidates for many technological purposes, ranging from gas sensors and catalytic applications to molecular electronic devices. In the absence of axial ligands, those complexes possess coordinatively unsaturated central metal ions which then play a key role as reactive and/or coordinative sites. For a detailed mechanistic understanding of the electronic interactions, especially at the central metal ion, we prepared thin films and monolayers of Co, Fe and Cu porphyrines and -phthalocyanines under ultrahigh vacuum conditions on Ag(111) and Au(111) single crystal surfaces. The systems were analyzed by UV and X-ray photoelectron spectroscopy; these methods are sensitive to the valence electronic structure of the interface and to the oxidation states of the metal centers, respectively. Our investigations revealed that changes in the chemical environment, e.g., by coordination of small reactive molecules such as $O_2$ and CO, as well as subtle differences in the molecular geometry, the nature of the substrate, and even temperature variations can alter the oxidation state of the metal center and the character of its interaction with the substrate.

O 85.2 Fri 11:30 H36

**Complex nanoporous networks from flexible functionalised porphyrin units** — •David Écija[1], Knud Seufert[1], Willi Auwärter[1], Claudia Aurisicchio[2], Davide Bonifazi[2], Daniel Heim[1], and Johannes V. Barth[1] — [1]Physik Department, E20, Technische Universität München, James-Franck Str. 1, D-85748 Garching, Germany — [2]Department of Chemistry, University of Namur, Rue de Bruxelles 61, B-5000 Namur, Belgium

Porous materials are attracting wide interest because of the presence of cavities, which can selectively accomodate guest species. Here we report on a low temperature STM study of the formation of two different bidimensional supramolecular porous networks made of trans- and cis-like porphyrin derivatives on Ag(111) in ultra high vacuum. In either case, there is a high level of homogeneity in the pore size, shape and chemical composition, as required for applications. The trans-like porphyrin self-assembles into a hexagonal porous network, with an inter-pore distance of 5.3 nm and a pore area of 0.9 nm2. Chirality plays a major role, giving as a result two different domains, each of them made of only one kind of enantiomer. The cis-like species self-assembles into a Kagomé porous network, with an interpore distance of 4.8 nm and a pore area of 0.28 nm2.

Due to the donor character of the molecular species involved, on going experiments are focused on the deposition of acceptor molecules on top of the porous templates, with the idea of improving the efficiency of new kind of organic solar cells.

O 85.3 Fri 11:45 H36

**Strategies to fabricate molecular architectures by local anchoring and functionalization of porphyrins** — Florian Buchner, Elisabeth Zillner, Michael Röckert, Stefanie Glässel, Hans-Peter Steinrück, and •Hubertus Marbach — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Friedrich-Alexander-University Erlangen-Nuremberg, Egerlandstr. 3, 91058 Erlangen

For the generation of functional molecular devices the ultimate goal is the control of the position, supramolecular arrangement, intramolecular conformation and electronic coupling of the molecular building blocks to the substrate. Porphyrins appear to be ideal building blocks to generate such devices on surfaces, since they combine an active site, usually a coordinated metal center, with a planar, structure forming element. In this contribution we discuss scanning tunneling microscopy (STM) investigations of the dynamics, supramolecular ordering and intramolecular conformation of different porphyrins on Ag(111), Cu(111) and composite surfaces in ultra-high vacuum, mainly at room temperature. The presented data enables the understanding of the role of molecule-molecule and molecule-substrate interactions. The obtained findings indicate the possibility to locally anchor and/or functionalize (e.g. metalate) the porphyrins on surfaces prestructured with metallic or oxygen islands. Based on these results a technique for large scale patterning with the corresponding molecules will be proposed. This work has been funded by the DFG through Sonderforschungsbereich 583.

O 85.4 Fri 12:00 H36

**Combined STM and theoretical first-principles study of ligated metalloporphyrins adsorbed on noble metal surfaces** — •Knud Seufert[1], Willi Auwärter[1], Marie-Laure Bocquet[2], Nicolas Lorente[3], Alexander Weber-Bargioni[4], Joachim Reichert[1,4], and Johannes V. Barth[1] — [1]Physik Department, E20, Technische Universität München, Garching, Germany — [2]Laboratoire de Chimie, ENS, Lyon, France — [3]CIN2, Barcelona, Spain — [4]Physics Department, University of British Columbia, Vancouver, Canada

Motivated by the importance of metalloporphyrins in many biological processes, such as the transport of respiratory gases, we present a combined experimental and theoretical study of the interaction of gaseous ligands with porphyrins. The metalloporphyrins (M-TPP, M=Fe, Co) were anchored on Ag(111) and Cu(111) surfaces and exposed to small amounts of CO and NO. Based on low-temperature STM experiments, we discuss the M-TPP's appearance and electronic structure dependent on the additional ligand. On both surfaces, bare M-TPPs show an occupied electronic state (HOMO) and an ant-like topographic appearance, which is completely modified through the attachment of NO. The dosage of CO instead yields no drastic changes in the low-energy electronic structure of the porphyrin host.

Our theoretical investigations focus on the well defined Co-TPP/Cu(111) system. The results show that the CO is not exclusively bound to the metal center, but rather to bridge-like positions between the central metal ion and the nitrogen of the porphyrin macrocycle.

O 85.5 Fri 12:15 H36

**Conformational switching of porphyrin derivatives on Au(111) by heating and STM manipulation** — •Johannes Mielke[1,2], Matthew Dyer[3], Mats Persson[3], Stefan Hecht[4], Jesús Martinez-Blanco[2], Karsten Horn[2], and Leonhard Grill[1,2] — [1]Institut für Experimentalphysik, Freie Universität Berlin — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [3]Department of Chemistry, University of Liverpool, United Kingdom — [4]Institut für Chemie, Humboldt-Universität zu Berlin

Molecular switches, which exhibit at least two stable states with characteristic properties, could play an important role in future applications of molecular electronics for the control of the conductance or the implementation of logic functions. Although such molecules have been investigated intensely in solution, the knowledge about their switching properties when being adsorbed on a solid surface is still scarce. We have studied functionalised porphyrin molecules on a Au(111) surface at different temperatures. In STM images, two stable conformations can be distinguished by their characteristic appearance. When applying voltage pulses with the STM tip to single molecules at low temperatures (around 7 K), it is possible to switch the molecules reversibly from one conformation to the other, whereas the voltage thresholds turn out to be characteristic. On the other hand, thermal switching is observed at elevated temperatures of around 300 K. The high number of switching events in the regime of thermal switching can be used to gain detailed insight in the dependence of the switching process on the atomic-scale environment of the molecule.

O 85.6 Fri 12:30 H36

**modification of supramolecular binding motifs induced by substrate registry: formation of self-assembled macrocycles and chain-like patterns** — •Saranyan Vijayaraghavan — Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel,Switzerland

The self-assembly properties of two ZnII porphyrin isomers on Cu(111) are studied at different coverage by means of an STM. Both isomers are substituted in their meso-positions by two voluminous 3,5-di(tert-butyl)phenyl and two 4*-cyanobiphenyl groups, respectively. In the trans-isomer, the two cyanobiphenyl groups are opposite to each other, whereas they are at right angle in the cis-isomer. For coverage up to one monolayer, the cis-substituted porphyrins self-assemble to form oligomeric macrocycles held together by antiparallel CN-CN dipolar interactions and CN-H-C(sp2) hydrogen bonding. Cyclic trimers and tetramers occur frequently but everything from cyclic dimers to hexamers are observed. Upon annealing of the samples at >150 C, dimeric macrocyclic structures are observed, in which the two porphyrins are bridged by Cu atoms, as CN-Cu-NC coordination bonds. LInear chains are seen at low coverages on Cu111 and densely packed structure at high coverages. Both cis- and trans-bis(4*-cyanobiphenyl)-substituted ZnII porphyrins behave very differently on Cu(111) compared to similar porphyrins on less reactive surfaces such as Au(111) and Ag(111). A very strong molecule-substrate interaction is seen on Cu(111) which dominates all observed structures.

O 85.7 Fri 12:45 H36

**Surface-assisted assembly of discrete porphyrin-based cyclic supramolecules** — •Daniel Heim[1], Knud Seufert[1], Willi Auwärter[1], Claudia Aurisicchio[2], Chiara Fabbro[3], Davide Bonifazi[2,3], and Johannes V. Barth[1] — [1]Physik Department, E20, Technische Universität München, James-Franck Str. 1, D-85748 Garching, Germany — [2]Department of Chemistry, University of Namur, Rue de Bruxelles 61, B-5000 Namur, Belgium — [3]Department of Pharmaceutical Sciences, University of Trieste, Piazzale Europa 1, I-34127 Trieste, Italy

We employed de novo synthesized porphyrin modules to construct discrete cyclic supramolecular architectures supported on a copper (111) surface. Hereby, porphyrin derivates exhibiting either one or two functional pyridyl recognition groups, the latter being cis-like and trans-like isomers, were applied. The programmed geometry and functionality of the molecular modules together with their conformational flexibility and substrate interaction yields symmetric discrete assemblies, including dimers and chains as well as three- to six-membered cyclic structures. The area of the molecular cavities is extended by creating bicomponent structures combining building blocks with different symmetry. All these supramolecular architectures are stabilized by Cu surface atom mediated attractive pyridyl-pyridyl interactions. The resulting strength of the intermolecular interactions allows for conformational changes of the entire assemblies by STM manipulation.

## O 86: Organic, electronics and photovoltaics

Time: Friday 11:15–12:45 Location: H40

O 86.1 Fri 11:15 H40

**WO3 under, in and on CuPc - A doping mechanism for organic semiconductors** — •Corinna Hein, Eric Mankel, Thomas Mayer, and Wolfram Jaegermann — TU Darmstadt, FG Oberflächenforschung, Petersenstraße 32, 64287 Darmstadt

Doping of organic semiconductors plays an important role for the development of organic devices like photovoltaic cells or organic light emitting diodes. P-doping of CuPc which is frequently used as hole conductor was performed successfully by coevaporation of the CuPc matrix and the WO3 dopant showing good doping efficiency and limit. The Fermi level determined by synchrotron induced photoemission shifts gradually with the concentration of dopant up to 690meV. To clarify the doping mechanism band alignment of both CuPc/WO3 and WO3/CuPc interfaces was determined. The work function difference of the two materials is overcome by band bending and an interface dipole. The dipole is 2eV for CuPc/WO3 and 1.4eV for WO3/CuPc lowering the amount of transferred charge and therefore limiting the doping efficiency. The sum of band bending at the interface adds up to 0.5eV for the CuPc/WO3 interface and 1.1eV for CuPc deposited on WO3. The Fermi level shift in the composites fits to this range in accord to a doping model assuming cluster growth of WO3 within CuPc. The model could be directly proofed by transmission electron microscopy distinguishing the two phases of CuPc and WO3 with a cluster size of approximately 5nm.

O 86.2 Fri 11:30 H40

**Mixed Self-Assembled Monolayers on Au(111): Understanding the Level Alignment and Work-Function Modification.** — •Ferdinand Rissner[1], David A. Egger[1], Lorenz Romaner[2], Georg Heimel[3], and Egbert Zojer[1] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]Chair of Atomistic Modelling and Design of Materials, University of Leoben, Austria — [3]Institut für Physik, Humboldt-Universität zu Berlin, Germany

In organic electronics, coverage of electrodes with appropriate self-assembled monolayers (SAMs) is a well-known technique for enhancing the performance of devices; by modification of the electrode work function, $\Phi$, charge-carrier injection barriers can be optimized. Mixing molecules which show a work-function increasing effect ($\Delta\Phi > 0$) with molecules decreasing $\Phi$ was experimentally found to allow for tuning of $\Phi$ over a wide range (as a function of the mixing ratio). [1]

For "pure" SAMs of $\pi$-conjugated oligophenylene derivatives, the mechanisms controlling the metal/SAM interface energetics have been extensively investigated over the past years. Here, we present density-functional theory based slab-type band structure calculations on the energetics of mixed monolayers. We find and explain significant differences in the energy-level alignment compared to what is known from the respective pure layers.

[1] K.-Y. Wu, S.-Y. Yu and Y.-T. Tao, Langmuir, **2009**, 25 (11), pp 6232-6238.

O 86.3 Fri 11:45 H40

**Analysis of systematic heat treatment of TiO2 nanocrystalline films for solid-state dye sensitized solar cells using photoelectron spectroscopy** — •Xianjin Feng, René Hock, Eric Mankel, Thomas Mayer, and Wolfram Jaegermann — Institute of Materials Science, Darmstadt UniVersity of Technology, D-64287 Darmstadt, Germany

In this contribution we investigated the effect of heat treatment on the chemical and electronic structures of TiO2 nanocrystalline films for solid-state dye sensitized solar cells (SDSC). The samples were heated in air by an air-gun and a hot plate, respectively, within the temperature range of 300-600°C. The samples were chemically and electronically characterized using synchrotron-induced photoelectron spectroscopy (SXPS) and X-ray photoemission spectroscopy (XPS). The most prominent chemical variation after heating by air-gun was found in the SXPS the intensity increase of the Na2p core level and obvious changes both in the O2s core level and O2p valence band were also observed at 450°C. An increase in the Na1s core level was also observed in the XPS study. For the heat treatment using a hot plate, the intensity of the Na2p core level increased less strongly and no obvious change in the O2s core level and O2p valence band was observed even at 600°C. In both cases of heat treatment, the oxygen vacancies VO-related gap states around 1.3 eV and states just below the Fermi level were observed in the gap region and the intensity of the VO-related gap states decreased obviously after heating and almost vanished at high temperatures.

O 86.4 Fri 12:00 H40

**Vanadyle and perfluoro vanadyle phthalocyanine on gold: unseen metastable modification and interfacial reaction** — •Indro Biswas, Heiko Peisert, and Thomas Chassé — Institut f. Physikalische u. Theoretische Chemie, Universität Tübingen, Auf der Morgenstelle 8, 72076 Tübingen

Vanadyle phthalocyanine (PcVO) and perfluorinated-vanadyle phthalocyanine ($F_{16}$PcVO) are of the same inside-out-umbrella structure as the extensively investigated titanyle phthalocyanine. Just in the recent years, interest on these molecules has grown again. They exhibit some very surprising properties. Thin films of PcVO and $F_{16}$PcVO on polycrystalline gold have been examined using photoemission, X-ray absorption, optical spectroscopy, and Kelvin probe measurements. In addition to surprisingly good self-ordering abilities of both materials, an interface reaction including the fluorine substituents in $F_{16}$PcVO has been observed, and the application of the minimal invasive Kelvin probe method allowed the investigation of the undisturbed metastable Phase I of PcVO with a different interface formation, which will be transformed by conventional spectroscopic methods.

1 C. H. Griffiths, M. S. Walker, P. Goldstein, *Polymorphism in Vanadyle Phthalocyanine*, Mol. Cryst. Liq. Cryst. 33 (1976) 149.

O 86.5 Fri 12:15 H40

**Photoemission spectroscopy investigations of silicon organic dye interfaces for photovoltaic applications** — •Andreas Decker[1], Thomas Mayer[1], Wolfram Jaegermann[1], Sabin Suraru[2], and Frank Würthner[2] — [1]Fachgebiet Oberflächenforschung, Fachbereich Materialwissenschaften, Technische Universität Darmstadt — [2]Institut für Organische Chemie, Universität Würzburg

In a new solar cell concept, organic dyes (small molecules) are embedded in the hydrogenated microcrystalline i-layer of a silicon p-i-n structure to enhance the optical absorption. This approach aims at an increase in efficiency and a decreased silicon absorber layer thickness, thus potentially lowering deposition time and production cost.

The electrical lineup of the dye orbitals versus the silicon band edges plays a vital role for this sensitization process because a driving force is needed for the transfer of photogenerated electrons and holes from the dye molecules to the silicon matrix. For the two dyes $Cl_4$MePTCDI and CuPc the electrical lineup on our model substrate, hydrogen terminated n-type Si(111), was investigated with photoemission interface experiments. Si(111):H was prepared from wafers with a native oxide by two-step wet-chemical etching in $NH_4F$ which leads to clean and flat terraces as shown in AFM measurements. By comparison of calculations with XPS measurements the Si(111):H surface was found to have flat bands, i. e. showing no Fermi level pinning due to dangling bonds or fresh adsorbates originating from the sample transport through air to the UHV system, thus being a suitable substrate for interface experiments.

O 86.6 Fri 12:30 H40

**Band alignment studies of ZnO-ZnS-CIS interfaces** — •Carsten Lehmann, Andreas Hofmann, Alexandra Dombrowa, and Christian Pettenkofer — Helmholz-Zentrum Berlin, Berlin, Deutschland

With respect to thin film solar cells based on $CuInS_2$ and ZnO ZnS is a promising alternative to CdS as buffer layer material [1,2]. A MOMBE process based on diethylzinc and water is investigated on $CuInS_2(112)$ thin films. A ZnS buffer layer grows epitaxially using the surplus of sulfur in the eventually present $CuS_x$ layer. A ZnO film grows on top of the .8 nm thick ZnS layer with its own lattice parameters in (0001) direction. Step-by-step analysis of this ZnO-ZnS-CIS interface yielded a band alignment favorable for photovoltaic applications [2]. We present in-situ preparation and step-by-step investigation on ZnO-ZnS-CIS interfaces with varying CIS substrates. $CuInS_2(001)$ samples were prepared on GaAs(100) by gas source MBE (GSMBE) using TBDS as sulfur precursor. Sulfurization of CuIn films prepared by MBE and sputtering yielded polycrystalline $CuInS_2$ samples of 100nm up to 2.5$\mu$m thickness. The samples were investigated by XPS, UPS and LEED. We will discuss the interfaces with respect to the derived band aligments and their morphology. Furthermore we will compare the results to those of analogous experiments on $CuInSe_2(112)$. [1] M. Bär, et. al., Journal of Applied Physics 99 (2006) [2] S. Andres, et. al., Thin Solid Films 518 (2009)

## O 87: Methods: Other (experimental)

Time: Friday 11:15–12:45 Location: H42

O 87.1 Fri 11:15 H42

**Determining the internal structure and morphology of nanoparticle films using element-specific X-ray techniques** — •Marc Sauerbrey, Ardalan Zargham, Thomas Schmidt, Jan Ingo Flege, and Jens Falta — Institute of Solid State Physics, University of Bremen, 28359 Bremen, Germany

The nanoscopic structure of colloidal nanoparticle films is investigated using X-ray Standing Waves in Total External Reflection (TER-XSW) together with X-ray Reflectometry (XRR). The period of the standing wave field and the distance between the mirror surface and the antinodes are determined by the incidence angle ($\theta$) of the X-ray beam. While varying $\theta$, the interference pattern moves through the adsorbed particles and excites fluorescence. The detection of this angle-dependent fluorescence signal allows to draw conclusions on the vertical position of the nanoparticles with subnanometer resolution. As a model system we investigated an Au-coated Si substrate functionalized with a self-assembled monolayer (SAM) of hexadecanethiol covered by a monolayer of $CoPt_3$ nanoparticles prepared by dip coating. Besides the determination of the vertical position of adsorbed particles, this technique also allows to resolve the internal structure of colloidal particles.

O 87.2 Fri 11:30 H42

**Double Photoemission from Pb(111)** — •Robert Wallauer[1], Stefan Voss[1], Till Jahnke[1], Achim Czasch[1], Lothar Schmidt[1], Nadine Neumann[1], Jasmin Titze[1], Hung-Keun Kim[1], Götz Berner[2], Michael Sing[2], Ralph Cleassen[2], Juan Carlos Campuzano[3], Horst Schmidt-Böcking[1], and Reinhard Dörner[1] — [1]IKF, Universität Frankfurt — [2]EP4, Universität Würzburg — [3]University of Illinois at Chicago

We investigate the angular resolved single photoemission (ARPES) and double photoemission (DPE) from a Pb(111) crystal in the normal and superconducting state using a momentum resolved coincidence detection method(often referred to as COLTRIMS)[1]. The experiment was performed at the synchrotron in Berlin (BESSY-II) in single bunch operation mode at photon energies around 20 to 25eV.

Theory [2] predicts that Cooper-pairs can be observed using coincidence photoemission. We suspect that our energy resolution (around 500 meV) prevents us from observing the pairs, since the calculation predicts differences (between the normal and SC states) only in an energy range of a few meV. For photon energies above 25eV the DPE current is dominated by Auger-processes involving the 5d(5/2) and 5d(3/2) core levels emitting Auger-electrons with a angular dependence on the emission direction of the Photoelectron which is not understood so far.

[1] M.Hattass et. al, Rev. Sci. Instr., 75, 2373 (2004) [2] K. A. Kouzakov and J. Berakdar Phys. Rev. Lett., 91, 257007 (2003)

O 87.3 Fri 11:45 H42

**A fast, full multichannel reflectance difference spectrometer** — •Chunguang Hu[1,2], Lidong Sun[1], Michael Hohage[1], and Peter Zeppenfeld[1] — [1]Institut für Experimentalphysik, Johannes-Kepler-Universität Linz, Austria — [2]State Key Lab of Precision Measuring Technology and Instruments, Tianjin University, China

With its high surface sensitivity, reflectance difference spectroscopy (RDS) has been proven to be a versatile tool for the scientific research in surface science and thin film growth. We report the development of a fast, multiwavelength RD spectrometer using a rotating compensator (RC) for signal modulation. The new spectrometer measures the optical anisotropy in the entire spectral range from 1.5 to >4.5eV simultaneously using a photodiode array with 1024 channels as detector. We will demonstrate that the new RDS is particularly suitable for in-situ monitoring of thin film growth and other surface processes by illustrating its application in the research of organic thin film growth.

O 87.4 Fri 12:00 H42

**SMART-II: the Next Generation of Aberration Corrected Spectro-Microscopy** — Helder Marchetto, Marcel Springer, •Thomas Schmidt, and Hans-Joachim Freund — Fritz Haber Institute of the MPG, Dept. CP, Berlin, Germany

The unique SMART (Spectro-Microscope with Aberration correction for many Relevant Techniques), built up within a collaboration [1] with the University Würzburg, TU Darmstadt, TU Clausthal and Zeiss (LEO) Oberkochen, combines electron spectroscopy with electron microscopy at high lateral and energy resolution to obtain spatially resolved information about the morphology, chemical distribution, work function and structural properties on nanometer scale. The basic instrument is a Low Energy Electron Microscope (LEEM) and Photo-Emission Electron Microscope (PEEM) equipped with an imaging energy analyzer and an aberration corrector, compensating simultaneously for both, the spherical and the chromatic aberrations. This leads to an outstanding lateral resolution of 2.6 nm which is twice as good as for an uncompensated LEEM/PEEM. Basing on the optical design of this prototype instrument, a new microscope is under construction, called SMART-II. It combines a commercial LEEM instrument with the well proven corrector system of SMART-I and a newly designed electrostatic imaging energy filter. We will discuss the advantages of this concept which are threefold: (a) higher electronic stability and therefore improved lateral resolution, (b) an improved reliability and (c) better maintenance for routine operation. [1] R. Fink et al., J. Electr. Spectrosc. Rel. Phen. 84, 231 (1997)

O 87.5 Fri 12:15 H42

**Collinear Generation of ultrashort UV and XUV pulses for pump/probe spectroscopy** — •Elisabeth Bothschafter[1,2], Agustin Schiffrin[1], Vladislav Yakovlev[1,3], Ferenc Krausz[1,3], Ralph Ernstorfer[1,2], and Reinhard Kienberger[1,2] — [1]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Straße 1, D-85748 Garching, Germany — [2]Lehrstuhl für Experimentalphysik I (E11) Technische Universität München, James Franck Strasse, D-85748 Garching, Germany — [3]Department für Physik, Ludwig-Maximilians-Universität, Am Coulombwall 1, D-85748 Garching, Germany

The investigation of the dynamics of excited electronic states in molecular and solid state systems on the few femtosecond time scale is a veritable challenge and requires the availability of ultrashort pulses in different spectral domains.

For application in future UV pump/XUV probe experiments, we demonstrate and characterize the collinear generation of sub-4 fs ultraviolet (UV) pulses and attosecond extreme ultraviolet pulses (XUV) pulses via nonlinear interaction of a sub-1.5 cycle near infrared/visible (NIR) laser pulse with noble gas atoms. The combination of third-order and high harmonic generation in a setup comprising two subsequent gas targets in a single laser focus provides inherently synchronized UV pulses with a photon energy of ∼5 eV and a pulse energy of

∼1 μJ and XUV pulses with a cut-off photon energy of more than 120 eV and up to $\sim 10^7$ photons.

O 87.6 Fri 12:30 H42

**Surfaces of Customary Materials - a LEEM Study on Polycrystalline Iron** — •Benjamin Borkenhagen[1], Thorsten Franz[2], Gerhard Lilienkamp[1], and Winfried Daum[1] — [1]Institute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — [2]ELMITEC GmbH, Albrecht-von-Grodeck-Str. 3, 38678 Clausthal-Zellerfeld

Most contemporary surface science studies are focussed on single crystal surfaces and adsorbates on single crystalline substrates with a limited variety of structural details and surface symmetries. Customary materials, however, are mainly polycrystalline with a large variety of defects and surface orientations which frequently have an important influence on surface processes. The study of such samples needs simultaneously high lateral resolution, information about the local surface symmetry and laterally resolved spectroscopic data. We have applied low energy electron microscopy (LEEM) to polished polycrystalline Fe samples which have been cut from pure bulk material to demonstrate that LEEM/PEEM-related methods meet these requirements. First results exhibit characteristic surface structures depending on the orientation of the grains. Single atomic steps and step bunches are well resolved, and the run of the steps is strongly influenced by grain boundaries and local tension in the microstructure. Small-area LEED with the microscope supplies first information concerning surface lattice and orientation of the grains. Due to the fast image acquisition investigations of thermally activated transformations of the texture and surface reactions appear promising.

## O 88: Symposium Nanotribology

Time: Friday 10:15–13:15 Location: H1

**Invited Talk** O 88.1 Fri 10:15 H1

**Atomic friction under ultrahigh vacuum conditions** — •Ernst Meyer[1], Enrico Gnecco[1], Pascal Steiner[1], Gregor Fessler[1], Sascha Koch[1], Thilo Glatzel[1], Alexis Baratoff[1], Mircin Kisiel[1], Urs Gysin[1], Akshata Rao[1], Shigeki Kawai[1], and Sabine Maier[2] — [1]Department of Physics, University of Basel, Switzerland — [2]Lawrence Berkeley National Labs, USA

It will be shown that atomic-scale stick-slip is relatively well understood, where the dependence on velocity and normal force is experimentally investigated and interpreted in terms of an extended Tomlinson model. It is essential to include thermal actuation to understand the observed phenomena. The transition from atomic-scale stick slip to continuous sliding will be described. The detailed analysis yields the energy corrugation and the lateral contact stiffness as a function of load. Very low lateral contact stiffness values of the order a few N/m are found. Experiments will be shown to determine the normal contact stiffness, simultaneously. Slip distances are related to the atomic lattice, where mostly single but also multiple slips are observed. An important parameter is the damping coefficient of the contact, which can be estimated from histograms of slip distances. Friction can be reduced with rather high accuracy by electrostatic actuation. An essential prerequisite are the high intrinsic resonance frequencies of the nanometer-sized contacts, which gives the opportunity to move in nearly continuous way without instabilities. Therefore, average friction values become negligible and small objects can be moved without extremely small dissipation.

**Invited Talk** O 88.2 Fri 10:45 H1

**Layering and Squeeze-out Damping in Confined Liquid Films** — •Frieder Mugele — University of Twente, Physics of Complex Fluids, Enschede (The Netherlands)

Liquid films confined between solid surfaces play a crucial role as lubricants reducing friction and wear in a wide range of tribological contacts ranging from biological joints to engineering bearings. For separations between the solid surfaces of just a few nanometers, the properties of the fluid deviate substantially from their macroscopic behaviour. Due to the presence of the solid surfaces the liquid arranges itself in well-defined molecular layers, which gives rise to pronounced forces between the solid surfaces, oscillating between attractive and repulsive as a function of the distance between the surfaces. The structural reorganization also affects the dissipation during flow. Compared to the oscillatory conservative forces, however, the effect of confinement on the dissipation has been much more challenging to quantify. Recent experiments using both laterally wide slit pores with atomically smooth surfaces in a surface forces apparatus (SFA) as well as atomic force microscopy (AFM) experiments with nanoscale single asperity contacts indicate that the effect of the structural reorganization is relatively small. Except for the molecular layers in direct contact with the solid surfaces, the effective viscosity of confined liquids remains close to its bulk value within approximately one order of magnitude.

**Invited Talk** O 88.3 Fri 11:15 H1

**Wear on the nanoscale: mechanisms and materials** — •Bernd Gotsmann[1], Mark A. Lantz[1], Harish Bhskaran[1], Abu Sebastian[1], Ute Drechsler[1], Michel Despont[1], Yun Chen[2], Kumar Sridharan[2], Papot Jaroenapibal[3], and Robert Carpick[3] — [1]IBM Research - Zurich, Switzerland — [2]University of Wisconsin-Madison, Madison, WI, USA — [3]University of Pennsylvania, Philadelphia, USA

Endurance requirements in emerging probe technologies, such as probe based data storage and lithography, are extremely demanding. Tip lifetime has been viewed as an unsolved critical issue in this context.

We show, that on the nanoscale the complexity of wear can be simplified to a thermally activated bond breaking process in which the energy barrier is reduced by the frictional shear stress. The resulting atom-by-atom wear deviates strongly from macroscopic wear behavior. Model predictions agree well with wear data obtained using sharp tips sliding in contact with various surfaces at sliding distances up to hundreds of meters.

As an application alternative tip materials are studied: We fabricated a nanoscale silicon-doped Diamond-Like-Carbon tips using a plasma immersion ion implantation and deposition process in conjunction with a molding technique. Silicon carbide (SiC) is another interesting material, in particular for thermo-mechancial applications. Tips were made by a combination of carbon ion implantation and an anneal step.

For both, Si-DLC and SiC tips, we demonstrate an improvement over silicon of several orders of magnitude.

**Invited Talk** O 88.4 Fri 11:45 H1

**Friction at the Nanoscale: Insights from Atomistic Simulations** — •Izabela Szlufarska, Yifei Mo, Yun Liu, and Maneesh Mishra — Department of Materials Science & Engineering, University of Wisconsin, Madison, WI 53706

Controlling tribological properties requires understanding a bewildering array of interrelated mechanisms, including elastic instabilities, plastic deformation, fracture, and chemical reactions. Large scale atomistic simulations have been used to unravel some of these mechanisms. Tribological studies are typically divided into a wearless regime, where deformation is primarily elastic, and a wear regime where permanent deformation occurs. For wearless contacts, I will use the example of H-terminated diamond surface to illustrate the breakdown of continuum mechanics at the nanoscale and to demonstrate that nanoscale contacts can be described using macroscale roughness theories. This discovery lays a foundation for unified friction laws across all length scales. I will also discuss effects of surface chemistry on friction, such as frictional dissipation in the presence of trace moisture. In the wear regime I will focus on the origins of recently observed ductile wear in nominally brittle SiC. Although this ductile wear holds potential for greatly enhancing the ease of machining of high-performance ceramics, its origin is still an open question. I will evaluate potential mechanisms for ductile wear, including the possibility of transformation to more ductile phases, dislocation mediated plasticity, and nanoindentation-induced amorphization.

**Invited Talk** O 88.5 Fri 12:15 H1

**The friction of wrinkles** — •Martin H. Müser[1] and Hamid Mohammadi[2] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]University of Western Ontario, London, Ontario, Canada

When in contact with an adhering particle, elastic sheets possess competing mechanically stable, wrinkled geometries if their thickness is below a critical value. Using molecular dynamics simulations, we show that adhering particles moving laterally over a wrinkled elastic sheet induce instability transitions of the wrinkles. These dynamics produce a frictional force between the particles and the sheet that can be well described with the Coulomb law of friction for solids. Analytical models for buckled rods are presented that allow one to rationalize the frictional response of wrinkles. We will also discuss the implications of our results for tribological experiments of graphite sheets that are only a few layers thick.

**Invited Talk** O 88.6 Fri 12:45 H1

**Influence of humidity on nano- and micromechanical contact adhesion** — •Hans-Jürgen Butt — Planck Institute for Polymer Research, Mainz, Germany

The interaction between hydrophilic surfaces or particles in air is often dominated by capillary forces. In this case capillary forces are caused by liquid menisci forming in the gap between the surfaces by capillary condensation. Significant progress has been made during the last decade in understanding capillary forces. In particular the influence of surface roughness is now better understood. After giving an introduction into the subject recent results are presented. To analyse capillary forces we measured the adhesion forces between atomic force microscope (AFM) tips or particles attached to AFM cantilevers and different solid samples. Humidity was adjusted relatively fast to minimize tip wear during one experiment. It is demonstrated that the results can be interpreted with simple continuum theory of the meniscus force. The capillary force between two fine particles or between the AFM tip and a sample depends on the precise geometry of the contact region on the 1 nm length scale. We demonstrate that vice versa from a measurement of the adhesion force versus humidity one can calculate the shape of the AFM tip. Finally, a simple, approximate formalism is described to calculate capillary forces between solid surfaces analytically.

## O 89: Invited talk (Aebi, Philipp)

Time: Friday 13:30–14:15 Location: H36

**Invited Talk** O 89.1 Fri 13:30 H36

**Evidence for exciton condensation in layered TiSe2: A photoemission study** — •Philipp Aebi — Département de Physique, Université de Fribourg, Switzerland

There is a longstanding open question about the existence of a condensate of electron-hole pairs (excitons) in a way as it is well-known for pairs of electrons, Cooper-pairs, in superconductivity. TiSe2 exhibits an unusual temperature-dependence in transport experiments and a specific band configuration that has been related to the possible formation of excitons.

Here we present a temperature dependent, high-resolution angle-resolved photoemission study of 1T-TiSe2. The material undergoes a phase transition from its room-temperature, normal phase to a low-temperature, charge-density wave phase. At low temperature the photoemission spectra are strongly modified, with large band renormalisations at high-symmetry points of the Brillouin zone and a very large transfer of spectral weight to backfolded bands.

A calculation of the theoretical spectral function for an exciton phase using a BCS-like formalism reproduces the experimental features with very good agreement. This gives strong evidence in favour of the exciton phase in 1T-TiSe.

## O 90: Invited talk (Behm, Jürgen)

Time: Friday 14:15–15:00 Location: H36

**Invited Talk** O 90.1 Fri 14:15 H36

**Surface Science and Electrocatalysis - Where do we stand?** — •R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

The close connection between Surface Science and Heterogeneous Catalysis, both on the experimental and on the theory side, is well established, and bridging the materials and pressure gap initially separating these disciplines has become a highly active field [1]. The existence of similar relations between the fields of Surface Science/Heterogeneous Catalysis and Electrochemistry/Electrocatalysis was much less established, although electrochemical studies on single crystals ('Surface Electrochemistry') have been reported since several decades [2]. Driven also by the recent rise of Electrochemical Energy Technologies (fuel cells, photovoltaics, batteries etc.) in concepts for future sustainable energy supplies, this has changed considerably during recent years [3].

In the present talk I want to illustrate the close correlations between these fields and the validity of similar microscopic concepts for the description of reactions at the solid/gas and the solid/liquid interface, but also point out key differences, using simple reactions such as $O_2$ reduction or $C_1$ oxidation as examples. The potential of combined experimental and theoretical studies is demonstrated.

[1] R. Imbihl, R.J. Behm, R. Schlögl, Phys. Chem. Chem. Phys. 9 (2007) 3459.

[2] D.M. Kolb, Surf. Sci. 500 (2002) 722.

[3] Fuel Cell Catalysis: A Surface Science Approach, M.T.M. Koper, ed. (Wiley and Sons, Chichester, 2009).