Surface Science Division
Fachverband Oberflächenphysik (O)

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Overview of Invited Talks and Sessions

Lecture Rooms: A 053, A 151, HE 101, MA 005, MA 041, MA 042, MA 043, and MA 141
Poster Rooms: MA 141/144 (called Poster F area)

Invited Talks

PV I	Mon	8:30– 9:15	H 0105	**The Interior of Single Molecules** — •Wilson Ho
O 2.1	Mon	9:30–10:15	HE 101	**The Perfect Lens: Resolution Beyond the Limits of Wavelength** — •John Pendry
O 3.1	Mon	10:15–11:00	HE 101	**Graphene Single Electron Transistors** — Christoph Stampfer, Francoise Molitor, Johannes Güttinger, Thomas Ihn, •Klaus Ensslin
O 16.1	Mon	17:00–17:45	HE 101	**The Surfaces of Bulk Semiconducting Metal Oxides** — •Ulrike Diebold
O 17.1	Mon	17:45–18:30	HE 101	**Charge-Density Waves and Superconductivity in Two Dimensions: The ARPES View** — •Sergey Borisenko
PV III	Mon	20:00–21:00	Urania	**Reaktionen an Festkörper-Oberflächen: Vom Atomaren zum Komplexen** — •Gerhard Ertl
O 21.1	Tue	9:30–10:15	HE 101	**Electrons at Surfaces Taking an Unexpected Turn** — •Stefan Blügel
O 22.1	Tue	10:15–11:00	HE 101	**Adsorption Processes on SiC Surfaces: First-Principles Theory** — •Johannes Pollmann
O 41.1	Tue	17:00–17:45	HE 101	**Nonadiabatic Processes in Surface Femtochemistry at Metals** — •Christian Frischkorn
O 42.1	Tue	17:45–18:30	HE 101	**Lateral Interactions on Surfaces: An Empirical Perspective** — •Gil Alexandrowicz, Pepijn R. Kole, Everett Y. M. Lee, Holly Hedgeland, Riccardo Ferrando, Andrew P. Jardine, William Allison, John Ellis
PV VI	Wed	8:30– 9:15	H 0105	**Graphene: Exploring Carbon Flatland** — •Andre Geim
O 47.1	Wed	14:15–15:00	HE 101	**Ab Initio Treatment of Strongly Correlated Electron Materials** — •Emily Carter
PV VIII	Wed	20:00–21:00	Urania	**Vom Riesenmagnetowiderstand zur Computerfestplatte** — •Peter Grünberg
O 79.1	Thu	17:45–18:30	HE 101	**Bonding, Structure and Function of Highly Ordered Molecular Adsorbate Layers on Metal Surfaces** — •Stefan Tautz
O 80.1	Thu	18:30–19:15	HE 101	**Imaging Quantum Phase Information Using Isospectral Electronic Nanostructures** — •Hari Manoharan
O 96.1	Fri	14:00–14:45	HE 101	**Electrochemical Surface Science** — •Klaus Wandelt
O 97.1	Fri	14:45–15:30	HE 101	**Energetics of Metal Atom Adsorption on Surfaces of Oxides and Polymers** — •Charles Campbell

Sessions

O 1	Mon	8:30– 9:15	H 0105	**Plenary Talk Wilson Ho**
O 2	Mon	9:30–10:15	HE 101	**Invited Talk John Pendry**
O 3	Mon	10:15–11:00	HE 101	**Invited Talk Klaus Ensslin**

O 4.1–4.5	Mon	11:15–12:30	MA 042	**Nanostructures at Surfaces**
O 5.1–5.6	Mon	11:15–12:45	MA 043	**Magnetic Nanostructures**
O 6.1–6.7	Mon	11:15–13:00	MA 005	**Metal Substrates: Clean Surfaces**
O 7.1–7.7	Mon	11:15–13:45	HE 101	**Symposium: Atomic Wires at Surfaces I (Invited Speakers: Franz Himpsel, Hanno Weitering, Han Woong Yeom)**
O 8.1–8.11	Mon	12:00–14:45	MA 041	**Metal Substrates: Adsorption of Organic/Bio Molecules I**
O 9	Mon	13:00–13:45	H 0105	**Plenary Talk Sankar Das Sarma**
O 10.1–10.14	Mon	13:15–16:45	MA 042	**Semiconductor Substrates: Epitaxy and Growth**
O 11.1–11.6	Mon	13:30–15:00	MA 043	**Time-Resolved Spectroscopy I**
O 12.1–12.9	Mon	13:30–16:45	MA 005	**Symposium: Size-Selected Clusters at Surfaces I (Invited Speakers: Karl-Heinz Meiwes-Broer, Heinz Hövel, Thorsten Bernhardt)**
O 13.1–13.10	Mon	14:00–16:30	HE 101	**Heterogeneous Catalysis**
O 14.1–14.6	Mon	15:15–16:45	MA 043	**Surface or Interface Magnetism**
O 15.1–15.5	Mon	15:30–16:45	MA 041	**Methods: Other Experimental Techniques I**
O 16	Mon	17:00–17:45	HE 101	**Invited Talk Ulrike Diebold**
O 17	Mon	17:45–18:30	HE 101	**Invited Talk Sergey Borisenko**
O 18.1–18.80	Mon	18:30–19:30	Poster F	**Poster Session I - MA 141/144 (Atomic Wires; Size-Selected Clusters; Nanostructures; Metal Substrates: Clean Surfaces+Adsorption of Organic / Bio Molecules+Solid-Liquid Interfaces+Adsorption of O and/or H; Surface or Interface Magnetism; Oxides and Insulators: Clean Surfaces)**
O 19	Mon	20:00–21:00	Urania	**Evening Talk Gerhard Ertl**
O 20	Tue	8:30– 9:15	H 0105	**Plenary Talk James Hudspeth**
O 21	Tue	9:30–10:15	HE 101	**Invited Talk Stefan Blügel**
O 22	Tue	10:15–11:00	HE 101	**Invited Talk Johannes Pollmann**
O 23	Tue	10:30–13:15	A 151	**SYNF: Ferroic Materials and Novel Functionalities I (FV: MA+O+MM+DF+DS+HL+TT)**
O 24	Tue	9:30–10:45	H 0105	**SYSA: Tayloring Organic Interfaces: Molecular Structures and Applications I (Invited Speaker: Fernando Flores; FV: DS+CPP+HL+O)**
O 25	Tue	10:45–13:00	H 0105	**SYSA: Tayloring Organic Interfaces: Molecular Structures and Applications II (Invited Speakers: Norbert Koch, Antoine Kahn; FV: DS+CPP+HL+O)**
O 26.1–26.5	Tue	11:15–12:30	MA 042	**Methods: Electronic Structure Theory**
O 27.1–27.6	Tue	11:15–12:45	MA 043	**Time-Resolved Spectroscopy II**
O 28.1–28.4	Tue	11:15–13:00	MA 005	**Symposium: Size-Selected Clusters at Surfaces II (Invited Speakers: Steven Buratto, Stefan Vajda, Matthias Arenz)**
O 29.1–29.6	Tue	11:15–13:30	HE 101	**Symposium: Surface Spectroscopy on Kondo Systems I (Invited Speakers: Wolf-Dieter Schneider, Fakher Assaad, Serguei Molodtsov)**
O 30.1–30.8	Tue	12:00–14:00	MA 041	**Phenomena at Semiconductor Surfaces**
O 31	Tue	13:00–13:45	H 0105	**Prize Talk Bernard Barbara (Gentner-Kastler Prize)**
O 32.1–32.15	Tue	13:00–16:45	MA 042	**Oxides and Insulators: Clean Surfaces**
O 33.1–33.7	Tue	13:45–16:15	MA 005	**Symposium: Frontiers of Surface Sensitive Electron Microscopy I (Invited Speakers: James Hannon, Raoul van Gastel, Thomas Schmidt)**
O 34.1–34.11	Tue	13:45–16:30	MA 043	**Metal Substrates: Adsorption of Organic/Bio Molecules II**
O 35.1–35.7	Tue	14:00–16:45	HE 101	**Symposium: Atomic Wires at Surfaces II (Invited Speakers: Erio Tosatti, Serge Lemay, Shuji Hasegawa)**
O 36.1–36.10	Tue	14:15–16:45	MA 041	**Surfaces and Films: Forces, Structure and Manipulation**
O 37	Tue	14:30–17:30	A 151	**SYNF: Ferroic Materials and Novel Functionalities II (Invited Speakers: Jochen Mannhart, Warren Pickett, Yoshinori Tokura, Ramamoorthy Ramesh, Agnes Barthelemy, Evgeny Tsymbal; FV: MA+O+MM+DF+DS+HL+TT)**
O 38	Tue	14:30–16:30	H 2013	**SYSA: Tayloring Organic Interfaces: Molecular Structures and Applications III (Invited Speaker: Alberto Salleo; FV: DS+CPP+HL+O)**

O 39	Tue	14:30–20:00	Poster A	**SYSA: Tayloring Organic Interfaces: Molecular Structures and Applications IV (Poster; FV: DS+CPP+HL+O)**
O 40	Tue	16:30–18:30	H 2013	**SYSA: Tayloring Organic Interfaces: Molecular Structures and Applications V (Invited speaker: Henning Sirringhaus; FV: DS+CPP+HL+O)**
O 41	Tue	17:00–17:45	HE 101	**Invited Talk Christian Frischkorn**
O 42	Tue	17:45–18:30	HE 101	**Invited Talk Gil Alexandrowicz**
O 43.1–43.46	Tue	18:30–19:30	Poster F	**Poster Session II - MA 141/144 (Surface Spectroscopy on Kondo Systems; Frontiers of Surface Sensitive Electron Microscopy; Methods: Scanning Probe Techniques+Electronic Structure Theory+Other; Time-Resolved Spectroscopy of Surface Dynamics with EUV and XUV Radiation; joined by SYNF posters)**
O 44	Wed	8:30– 9:15	H 0105	**Plenary Talk André Geim**
O 45	Wed	9:15–10:00	H 0105	**Plenary Talk Knut Urban**
O 46	Wed	13:30–14:15	HE 101	**Invited Talk Stefan Mayr (Gaede Prize)**
O 47	Wed	14:15–15:00	HE 101	**Invited Talk Emily Carter**
O 48	Wed	14:30–17:30	H 2013	**SYSA: Tayloring Organic Interfaces: Molecular Structures and Applications VI (Invited Speaker: Ivan Stich; FV: DS+CPP+HL+O)**
O 49.1–49.10	Wed	15:15–17:45	MA 005	**Particles and Clusters**
O 50.1–50.8	Wed	15:15–18:00	HE 101	**Symposium: Surface Spectroscopy on Kondo Systems II (Invited Speakers: Jonathan Denlinger, Johann Kroha, Alexander Schneider)**
O 51.1–51.13	Wed	15:15–18:30	MA 041	**Metal Substrates: Adsorption of Organic/Bio Molecules III**
O 52.1–52.13	Wed	15:15–18:30	MA 042	**Time-Resolved Spectroscopy III**
O 53.1–53.13	Wed	15:15–18:30	MA 043	**Surface Nanopatterns**
O 54	Wed	17:45–19:30	H 2013	**SYSA: Tayloring Organic Interfaces: Molecular Structures and Applications VII (Invited Speaker: Stephan Roth; FV: DS+CPP+HL+O)**
O 55.1–55.77	Wed	18:30–19:30	Poster F	**Poster Session III - MA 141/144 (Methods: Atomic and Electronic Structure; Particles and Clusters; Heterogeneous Catalysis; Semiconductor Substrates: Epitaxy and Growth+Adsorption+Clean Surfaces+Solid-Liquid Interfaces; Oxides and Insulators: Solid-Liquid Interfaces+Epitaxy and Growth; Phase Transitions; Metal Substrates: Adsorption of Inorganic Molecules+Epitaxy and Growth; Surface Chemical Reactions; Bimetallic Nanosystems: Tuning Physical and Chemical Properties; Oxides and insulators: Adsorption; Organic, polymeric, biomolecular films; etc.)**
O 56	Wed	20:00–21:00	Urania	**Evening Talk Peter Grünberg**
O 57	Thu	8:30– 9:15	H 0105	**Plenary Talk Helmut Grubmüller**
O 58.1–58.4	Thu	9:30–11:00	HE 101	**Symposium: Beyond Optical Wavelengths: Time-Resolved Spectroscopy of Surface Dynamics with EUV and XUV Radiation I (Invited Speakers: Reinhard Kienberger, Martin Aeschlimann)**
O 59.1–59.10	Thu	9:30–12:00	MA 041	**Molecular Nanostructures**
O 60.1–60.8	Thu	9:30–12:15	MA 005	**Symposium: Bimetallic Nanosystems: Tuning Physical and Chemical Properties I (Invited Speakers: Harald Brune, Michael Hilgendorff, Konstantin Neyman)**
O 61	Thu	9:30–12:30	A 151	**SYEC: Exact-Exchange and Hybrid Functionals Meet Quasiparticle Energy Calculations I (Invited Speakers: Gustavo Scuseria, Andreas Görling, Georg Kresse, Angel Rubio, Mark van Schilfgaarde, Michael Rohlfing; FV: O+HL+DF+TT)**
O 62.1–62.12	Thu	9:30–12:30	MA 042	**Metal Substrates: Adsorption of Inorganic Molecules**
O 63.1–63.8	Thu	9:30–12:30	MA 043	**Symposium: Frontiers of Surface Sensitive Electron Microscopy II (Invited Speakers: Jürgen Kirschner, Liviu Chelaru, Michael Bauer, Claus Schneider)**
O 64.1–64.6	Thu	11:15–12:45	HE 101	**Metal Substrates: Adsorption of Organic/Bio Molecules IV**
O 65.1–65.11	Thu	12:00–14:45	MA 141	**Methods: Theory and Experiment**
O 66.1–66.10	Thu	12:45–15:15	MA 041	**Metallic Nanostructures I (on Metals)**

O 67	Thu	13:00–13:45	H 0105	**Prize Talk Fedor Jelezko (Walter Schottky Prize)**
O 68.1–68.6	Thu	13:15–14:45	MA 043	**Metal Substrates: Solid-Liquid Interfaces**
O 69.1–69.4	Thu	14:00–15:00	MA 042	**Symposium: Size-Selected Clusters at Surfaces III**
O 70	Thu	14:00–17:00	A 151	**SYMS: Modern Developments in Multiphysics Materials Simulations I (Invited Speakers: David Pettifor, Alessandro De Vita, Chris Wolverton, Ingo Steinbach, Walter Thiel, Karsten Reuter; FV: O+HL+MM)**
O 71	Thu	14:00–17:00	A 053	**SYEC: Exact-Exchange and Hybrid Functionals Meet Quasiparticle Energy Calculations II (FV: O+HL+DF+TT)**
O 72.1–72.8	Thu	14:00–17:00	HE 101	**Symposium: Beyond Optical Wavelengths: Time-Resolved Spectroscopy of Surface Dynamics with EUV and XUV Radiation II (Invited Speakers: Wilfried Wurth, Hermann Dürr, Shik Shin)**
O 73.1–73.10	Thu	14:00–17:30	MA 005	**Symposium: Bimetallic Nanosystems: Tuning Physical and Chemical Properties II (Invited Speakers: André Fielicke, Thomas Risse, Jürgen Behm)**
O 74.1–74.9	Thu	15:00–17:15	MA 141	**Metal Substrates: Adsorption of O and/or H**
O 75.1–75.8	Thu	15:15–17:15	MA 042	**Oxides and Insulators: Epitaxy and Growth**
O 76.1–76.9	Thu	15:15–17:30	MA 043	**Organic, Polymeric, Biomolecular Films - also with Adsorbates**
O 77.1–77.8	Thu	15:30–17:30	MA 041	**Methods: Scanning Probe Techniques I**
O 78	Thu	17:00–18:30	H 2032	**SYSA: Tayloring Organic Interfaces: Molecular Structures and Applications VIII (Invited Speaker: Tomasz Kowalewski; FV: DS+CPP+HL+O)**
O 79	Thu	17:45–18:30	HE 101	**Invited Talk Stefan Tautz**
O 80	Thu	18:30–19:15	HE 101	**Invited Talk Hari Manoharan**
O 81	Thu	18:30–19:30	Poster F	**Poster Session IV - MA 141/144: SYMS II and SYEC III (Modern Developments in Multiphysics Materials Simulations; Exact-Exchange and Hybrid Functionals Meet Quasiparticle Energy Calculations)**
O 82	Thu	19:30–20:00	HE 101	**General Meeting of the Surface Science Division**
O 83	Thu	20:00–21:00	HE 101	**Post Deadline Session (followed by Surface Science Symposion)**
O 84	Fri	8:30– 9:15	H 0105	**Plenary Talk Wolfgang Kleemann**
O 85	Fri	9:15–10:00	H 0105	**Prize Talk Hagen Kleinert (Max Born Prize)**
O 86.1–86.7	Fri	9:30–11:15	MA 141	**Oxides and Insulators: Adsorption**
O 87.1–87.7	Fri	9:30–12:00	HE 101	**Symposium: Beyond Optical Wavelengths: Time-Resolved Spectroscopy of Surface Dynamics with EUV and XUV Radiation III (Invited Speakers: Christian Spielmann, Matias Bargheer, Philippe Wernet)**
O 88.1–88.12	Fri	9:30–12:30	MA 005	**Metallic Nanostructures II (on Semiconductors)**
O 89.1–89.12	Fri	9:30–12:30	MA 041	**Metal Substrates: Epitaxy and Growth**
O 90.1–90.7	Fri	10:15–12:00	MA 042	**Methods: Scanning Probe Techniques II**
O 91	Fri	10:15–12:30	A 151	**SYEC: Exact-Exchange and Hybrid Functionals Meet Quasiparticle Energy Calculations IV (FV: O+HL+DF+TT)**
O 92	Fri	10:15–13:00	A 053	**SYMS: Modern Developments in Multiphysics Materials Simulations III (FV: O+HL+MM)**
O 93.1–93.11	Fri	10:15–13:00	MA 043	**Surface Chemical Reactions**
O 94.1–94.5	Fri	12:00–13:15	MA 141	**Methods: Other Experimental Techniques II**
O 95	Fri	13:15–14:00	H 0105	**Special Talk Theodore Postol**
O 96	Fri	14:00–14:45	HE 101	**Invited Talk Klaus Wandelt**
O 97	Fri	14:45–15:30	HE 101	**Invited Talk Charles Campbell**

Evening Talks by Nobel Laureates 2007

Monday, 8:00 p.m., Urania	Gerhard Ertl
Wednesday, 8:00 p.m., Urania	Peter Grünberg

Urania is best reached by subway U1 from Ernst-Reuter-Platz to Wittenbergplatz (just a 4 min. train ride + 8 min. walk). Both lectures will also be presented in a live broadcast in H 0105.

Annual General Meeting of the Surface Science Division

Thursday, 7:30 p.m., HE 101

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

NOTES

Poster Sessions O18 (Monday), O43 (Tuesday), O55 (Wednesday), and O81 (Thursday) at 6:30-7:30 p.m. in MA 141/144 (Poster F area) - Posters should be put up between 10:00 and 11:00 a.m. and must be removed before 10:00 a.m. on the following day. The poster presenter should be present at the poster between 6:30 and 7:30 p.m.

Post Deadline Session O83 on Thursday, 8:00-9:00 p.m., in HE 101, followed by the Surface Science Symposion at the TU Mensa (first floor), Hardenbergstraße 34.

Deadline for submission of abstracts is January 11, 2008; Notification on acceptance will be on February 4, 2008. Support from Elsevier (Surface Science), SPECS together with Bestec, Createc Fischer, and Surface Concept, and from IBM is gratefully acknowledged.

O 1: Plenary Talk Wilson Ho

Time: Monday 8:30–9:15 Location: H 0105

The Interior of Single Molecules

O 2: Invited Talk John Pendry

Time: Monday 9:30–10:15 Location: HE 101

Invited Talk O 2.1 Mon 9:30 HE 101
The Perfect Lens: Resolution Beyond the Limits of Wavelength — •John Pendry — Imperial College London

The lens is one of the most basic tools of optics but the resolution achieved is limited, as if the wavelength of light defined the width of a pencil used to draw the images. This limit intrudes in all kinds of ways. For example it defines the storage capacity of DVDs where the laser can only *see* details of the order of the wavelength.

Two types of light are associated with a luminous object: the near field and the far field. True to its name the far field escapes from the object and is easily captured and manipulated by a lens, but high resolution details are hidden in the near field and remain localised near the source and cannot be captured by a conventional lens. The near field is familiar to surface scientists in the form of surface plasmons, for example. To control the near field we have developed a new class of materials with properties not found in nature. These new materials derive their properties not from the atomic and molecular constituents of the solid, but from microstructure which can be designed to give a wide range of novel electromagnetic properties.

The lecture will describe the new materials and the principles behind them and show how they may be used to control and manipulate the near field. Finally a prescription will be given for a lens whose resolution is unlimited by wavelength provided that the ideal prescription for the constituent materials is met.

O 3: Invited Talk Klaus Ensslin

Time: Monday 10:15–11:00 Location: HE 101

Invited Talk O 3.1 Mon 10:15 HE 101
Graphene Single Electron Transistors — Christoph Stampfer, Francoise Molitor, Johannes Güttinger, Thomas Ihn, and •Klaus Ensslin — Solid State Physics Lab, ETH Zurich, Switzerland

Graphene flakes are patterned into nanostructures using electron beam lithography and dry etching. A mesoscopic Hall bar is investigated by low-temperature magnetotransport experiments. The potential inside the Hall bar is tuned by graphene side gates. We demonstrate that the carrier density can be tuned over typical lateral distances of 90 nm. This way a tunable graphene single electron transistor is realized. Clear conductance resonances and Coulomb diamonds are resolved at a temperature of T=2 K. We present data for several graphene single electron transistors and discuss the tunability of the tunnel barriers as well as the overall electronic configuration of the device.

O 4: Nanostructures at Surfaces

Time: Monday 11:15–12:30 Location: MA 042

O 4.1 Mon 11:15 MA 042
Dynamic processes in metalorganic networks based on oligopyridines and copper — •Achim Breitruck[1], Harry E. Hoster[1], Christoph Meier[2], Ulrich Ziener[2], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm — [2]Institute of Organic Chemistry III, Ulm University, D-89069 Ulm

We report on the dynamics of chiral metalorganic networks on the basis of Bis-terpyridines (BTP) and copper which were studied by time-resolved scanning tunneling microscopy (STM). Using highly oriented pyrolytic graphite (HOPG) as substrate, the samples were prepared by vapor deposition of oligopyridines to form a quadratic 2D molecular network[1] and post-deposition of copper under ultra high vacuum (UHV) conditions. At Cu coverages below phase saturation, we observed the formation of an Cu-organic network, consisting of copper-free and copper-containing BTP trimers. At room temperature, this allows the migration of Cu atoms within the network via a hopping mechanism from Cu-containing to Cu-free trimers on a timescale of seconds. The mechanism is accompanied by a local rearrangement of the BTP molecules. Despite the high adlayer dynamics, we find very large enantiopure domains with sizes $> 10^4$ nm^2.

[1] H.E. Hoster et al., Langmuir 23, 11570-11579, (2007)

[2] A. Breitruck et al., Surf. Sci. 601, 4200-4205, (2007)

O 4.2 Mon 11:30 MA 042
Mid infrared microspectroscopy: Characterization od diamond-like (DL) and polymer-like (PL) single nanoparticle — •Jean-Sébastien Samson[1], Raphaella Weiss[2], Erik Bründermann[1], Jörg Winter[2], and Martina Havenith[1] — [1]Physical Chemistry 2, Ruhr-University Bochum, Bochum, Germany — [2]Experimental Physics 1, Ruhr-University Bochum, Bochum, Germany

We report on the infrared spectroscopic characterization of plasma nanoparticles formed in a dusty plasma by scanning near-field infrared microscopy (SNIM). We use high power OPO-lasers with up to 2,7 W output power as radiation source [1] which emit in the so-called fingerprint region (2,5-4 um). We were able to use the characteristic N-H absorption band around 3300 cm-1 to spectrally resolve a shift of the band between the diamond-like and the polymer-like phase. The measurement were carried out on a sample containing 100 nm diamond-like and 400 nm polymer-like plasma nanoparticles. Our results demonstrate the high sensitivity of SNIM for characterization of nanoparticles found in plasma. [1]J.-S. Samson et al. PCCP, (2006), 8, 753-758

O 4.3 Mon 11:45 MA 042
Nanostructuring of the HOPG surface — •Artur Böttcher[1], Markus Cudaj[1], Daniel Löffler[1], Sharali Malik[2], Manfred Kappes[1,2], Patrice Brenner[3], and Dagmar Gerthsen[3] — [1]Institut für Physikalische Chemie, Universität Karlsruhe, Karlsruhe, Germany — [2]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, Germany — [3]Laboratorium für Elektronenmikroskopie, Universität Karlsruhe, Germany

By combining the focused ion beam technique, 30keV-Ga$^+$-FIB, with high-temperature oxidation well defined periodic structures were fabricated on HOPG surfaces [1]. The method exploits the high reactivity of the amorphous surface areas towards the oxidation-induced gasification of undercoordinated carbon sites, C→CO, CO$_2$. Large surface areas covered by periodically arranged nanocavities, gratings and arrays of nm-sized squares have been fabricated routinely. The minimum width of the grooves written is limited by the interaction of the ion beam with the substrate and levels presently off at 80 nm. The mean depth of the grooves can be easily varied in the range up to 55 nm by applying different ionic doses. These parameters enable to fabricate large arrays of nanographene plates with desired size and shape. Two stages are clearly distinguishable in the kinetics of the etching process: within the early stage the amorphous carbon is removed and in the later stage the prism surfaces of the regular graphite are gradually gasified with lower efficiency. The integral removal probability depends on the surface temperature and ranges from 10 $^{-11}$ to 10 $^{-8}$ C/O_2. [1] A. Böttcher et al. Nanotechnology, 17(2006)

O 4.4 Mon 12:00 MA 042

Effect of HF concentration on physical and electronic properties of electrochemical formed nano-porous silicon — •Pushpendra Kumar[1], Manash Ghosh[1], Hongdan Yan[1], Frank Ludwig[2], Meinhard Schilling[2], and Peter Lemmens[1] — [1]IPKM, TU-Braunschweig — [2]EMG, TU-Braunschweig

We report on the preparation and functionalization of porous silicon (PS) using electrochemical etching in hydrofluoric (HF) acid based solutions. The properties of PS such as thickness of the porous layer, porosity and average pore diameter are precisely controlled and characterized using optical absorption, nitrogen sorption isotherms, field emission SEM, Raman and PL spectroscopy. Functionalization was performed by oxidizing and subsequent doping with different dyes and magnetic molecules.

O 4.5 Mon 12:15 MA 042

Preparation and functionalization of porous anodic aluminum oxide templates — •Hongdan Yan[1], Seth White[1], Pushpendra Kumar[1], Peter Lemmens[1], and Pengxiang Zhang[2] — [1]IPKM,TU-Braunschweig — [2]IAMPE, Kunming University of Science and Technology, Yunnan, China

We report on the preparation of porous anodic aluminum oxide templates (AAO) and their functionalization/modification. AAO with nanoporous morphology is a well controlled template material due to the high density and uniformity of nano pores. Free standing, transparent membranes have been prepared and doped with dyes, magnetic molecules. Ni and Fe nano-wires have been grown within the pores by electrodeposition.

O 5: Magnetic Nanostructures

Time: Monday 11:15–12:45 Location: MA 043

O 5.1 Mon 11:15 MA 043

Probing the surface states of single atoms on cobalt nanoislands — •Laurent Limot[1], Benjamin Heinrich[1], Mircea-Vasile Rastei[1], Cristian Iacovita[1], Pavel A. Ignatiev[2], Valeri S. Stepanyuk[2], Patrick Bruno[2], and Jean-Pierre Bucher[1] — [1]Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, Université Louis Pasteur, F-67034 Strasbourg, France — [2]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle/Saale, Germany

With the remarkable downscaling of data-storage bits, both writing and reading processes become extremely challenging, since read sensors need to be comparable to the bit size, and at the same time, their sensitivity must be improved due to the loss in signal-to-noise ratio. Future progress strongly relies on our fundamental understanding of magnetic phenomena in reduced dimensions.

Atoms on magnetic nanoislands represent a model playground for investigating such phenomena. In this study, we focus on the electronic properties of single Ni, Cu and Co atoms adsorbed on cobalt nanoislands grown on the Cu(111) surface. By combining low-temperature scanning tunneling spectroscopy with *ab initio* calculations we reveal the existence of a common electronic resonance, resulting from the localization of the nanoisland surface states at the adsorption site of the atoms.

O 5.2 Mon 11:30 MA 043

Tailoring exchange interactions between magnetic adatoms in engeneered nanostructures: ab initio study — •Pavel A. Ignatiev, Valeri S. Stepanyuk, and Patrick Bruno — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

The controllable modification of quantum states in 1D nanostructures could permit one to manipulate their electronic and magnetic properties. An advanced experimental methods, such as the scanning tunneling microscope (STM), allows one to construct chains on surfaces in atom-by-atom fashion [1,2]. Our ab initio calculations unambiguously demonstrate that both sign and magnitude of the exchange interaction between magnetic impurities incorporated in nonmagnetic chains on metal surfaces can be tailored by an appropriate design of the chain length and composition [3]. Such engineered 1D systems are experimentally feasible [4], and the above effects should be detectable with modern technology, for instance, by probing the Kondo resonance [5].

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[2] N. Nilius T. M. Wallis, and W. Ho, Science 297, 1853 (2002).

[3] P. A. Ignatiev, V. S. Stepanyuk and P. Bruno, submitted to PRL

[4] J. Lagoute, C. Nacci, and S. Folsch Phys. Rev. Lett. 98, 146804 (2007).

[5] P. Wahl, P. Simon, L. Diekhoner, V. S. Stepanyuk, P. Bruno, M. A. Schneider, and K. Kern, Phys. Rev. Lett. 98, 056601 (2007).

O 5.3 Mon 11:45 MA 043

***Ab initio* Study of Spin-polarized Bound States in Magnetic Dimers on Metal Surfaces** — •Oleg O. Brovko, Valeri S. Stepanyuk, and Patrick Bruno — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Interaction of single adatoms with surface state electrons has been shown to produce a bound state below the surface state band bottom [1,2]. Similar states have been revealed at nonmagnetic Cu chains [2]. Using *ab initio* KKR Green's function method we study the spin-polarized bound state arising at magnetic dimers on noble metal surfaces. We demonstrate that the spin-splitting of the bound state can be utilized to determine the exchange coupling of a magnetic dimer.

[1] L. Limot, E. Pehlke, J. Kröger, and R. Berndt, Phys. Rev. Lett. 94, 036805 (2005). [2] V. S. Stepanyuk, A. N. Klavsyuk, L. Niebergall, and P. Bruno, Phys. Rev. B 72, 153407 (2005)

O 5.4 Mon 12:00 MA 043

Quantum resonators on metal surfaces: theoretical and experimental studies — •L. Niebergall[1], N.N. Negulyaev[2], V.S. Stepanyuk[1], P. Bruno[1], J. Repp[3], G. Meyer[4], and K.-H. Rieder[5] — [1]Max Planck Institute of Microstructure Physics, 06120 Halle, Germany — [2]Physics Department, Martin-Luther-University Halle-Wittenberg, 06099 Halle, Germany — [3]Institute of Experimental and Applied Physics, University Regensburg, 93053 Regensburg, Germany — [4]IBM Research, Zurich Research Laboratory, 8803 Rueschlikon, Switzerland — [5]Institute of Experimental Physics, FU Berlin, 14195 Berlin, Germany

Confinement of surface-state electrons on metal surfaces can lead to many interesting effects [1-3]. Here, we present a combined experimental and theoretical studies on adatom motion in quantum resonators. Using STM technique we construct two parallel monatomic Cu chains on Cu(111). Quantum confinement of surface electrons between chains is revealed. Experimental and theoretical studies demonstrate that adatom motion inside the resonators at low temperature is determined by quantized electronic states in resonators.

1. V.S. Stepanyuk et al., Phys. Rev. Lett. 94, 187201 (2005).
2. L. Niebergall et al., Phys. Rev. Lett. 96, 127204 (2006).
3. V.S. Stepanyuk et al., New J. Phys. 9, 388 (2007).

O 5.5 Mon 12:15 MA 043

Self-organized surface ripples as a source of magnetic anisotropies — •J. Fassbender[1], M. O. Liedke[1], A. Keller[1], S. Facsko[1], D. Marko[1], A. Hanisch[1], J. Grenzer[1], E. Cizmar[2], and S. Zvyagin[2] — [1]Forschungszentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 128, 01328 Dresden, Germany — [2]Forschungszentrum Dresden-Rossendorf, High Magnetic Field Laboratory, Bautzner Landstrasse 128, 01328 Dresden, Germany

In thin film magnetism surface and interface morphologies are important sources of magnetic anisotropy. This can be either due to the reduced coordination of step edge atoms (intrinsic contribution) or due to magnetic stray fields emanating from the film corrugation (extrinsic contribution). Low energy ion erosion is perfectly suited to create a periodic surface modulation (so-called ripples) on the nanoscale. By changing the primary energy of the ions the ripple periodicities can be varied from 20 to 150 nm. Subsequently, thin magnetic films are deposited on these template systems in order to investigate the influence of the surface morphology on the induced magnetic anisotropies. For small ripple periodicities a strong uniaxial magnetic anisotropy is found which rapidly decrease for larger ripple periodicities. In the case of Permalloy ($Ni_{81}Fe_{19}$) the induced anisotropy can be more than a factor of 20 larger compared to the intrinsic anisotropy of flat Permalloy. The microscopic origin of this effect will be discussed.

O 5.6 Mon 12:30 MA 043

Magneto-optical study of hexagonal hole arrays in thin magnetic films — •Georgios Ctistis[1], Evangelos Papaioannou[2], Piotr Patoka[1], Paul Fumagalli[2], and Michael Giersig[1] — [1]Nanoparticle Technology Department, Center of Advanced European Studies and Research, 53175 Bonn, Germany — [2]Institut für Experimentalphysik, Freie Universität Berlin, 14195 Berlin, Germany

Nanostructured surfaces of optically thin films exhibit interesting optical properties as plasmon assisted transmission and are thus interesting for opto-electronic applications. Using magnetic materials such as Fe or Co instead, could result in tailoring the magnetic properties of the materials at desired frequencies.

In this study we present our magneto-optical studies of hexagonal nano-hole arrays of 100 nm thick magnetic films (Fe, Co, Ni). Different meshes were used with hole diameters ranging between 220 nm and 330 nm, while the inter-hole distance was kept constant at 470 nm, respectively. Spectra were taken with a Kerr-spectrometer in the range of 0.8 - 5 eV. A strong change in the response depending on the hole geometry compared to the corresponding closed films is observed. Furthermore, recorded hysteresis loops reveal the magnetization process as a function of the underlying geometry.

O 6: Metal Substrates: Clean Surfaces

Time: Monday 11:15–13:00 Location: MA 005

O 6.1 Mon 11:15 MA 005

Imaging phonon excitation with atomic resolution — •Heiko Gawronski and Karina Morgenstern — Institute of Solid State Physics, Department of Surface Science, Leibniz University Hannover, Appelstr. 2, D-30167 Hannover, Germany

Scanning tunneling microscopy (STM), inelastic tunneling spectroscopy (IETS), and d^2I/dV^2-mapping at low temperature are used to investigate vibrations of Au(111) and Cu(111). The low energy peaks in the IET-spectra at 9 meV on Au(111) and 21 meV on Cu(111) are attributed to phonons at surfaces. This phonon energy on Au(111) is not influenced by the different stacking of the surface atoms, but it is considerably influenced by different atomic distances within the surface layer. In addition, the spatial variation of the phonon excitation is measured in d^2I/dV^2-maps on Au(111). These display a novel type of atomic resolution that is explained in terms of site specific phonon excitation probabilities.

O 6.2 Mon 11:30 MA 005

Diffraction and crystal symmetry in electron pair emission from surfaces — •Frank O. Schumann, Carsten Winkler, and Jürgen Kirschner — Max-Planck-Institut f\"{u}r Mikrostrukturphysik, Weinberg 2 , 06120 Halle, Germany

We have investigated the electron pair emission from a Cu(111) surface excited with a primary electron beam of 30.7 eV kinetic energy via a coincidence time-of-flight experiment. The movement of two interacting particles can be described within the so-called two-body problem, where it is shown that the motion of the center-of-mass can be separated from the relative motion. We adopt this notation in our presentation of the data. If we focus on the motion of the center-of-mass, we compute the sum of the in-plane momentum of the pair. Plotting the coincidence intensity as a function of the sum momentum gives a two-dimensional distribution, which displays intensity peaks, if a reciprocal lattice vector is added to the sum momentum of this electron pair and not to the individual electrons. This highlights the fact that the pair as the whole experiences diffraction at the surface. This in turn means that the electrons must be interacting. The interaction within the pair is described by the relative motion. The intensity distribution of this motion reveals the six-fold symmetry of the surface. Both features are only observed, if the valence band electron comes from the vicinity of the Fermi level, where the Cu(111) surface exhibits a Shockley surface state. For an explanation of our observations this electronic state is important.

O 6.3 Mon 11:45 MA 005

Relaxations at the Ag(001) surface: A LEED study — •Michael Huth, Wolfram Münchgesang, Karl-Michael Schindler, and Wolf Widdra — Martin-Luther Universität Halle-Wittenberg, Institut für Physik, Halle, Deutschland

For low-energy electron diffraction a new approach of data recording and postprocessing has been developed. The improved I(V) curves for Ag(001) show low intensity features and additional fine structure of high intensity peaks. By comparing experimental and calculated I(V) curves significant relaxations of the top two layer distances have been determined. The relaxations found basically confirm recent theoretical predictions [1]. Detailed analysis shows that I(V) curves exhibit a strong dependence on the angle of incidence and show that small deviations from normal incidence can remove essential structures from the I(V) curves.

[1] J.-M. Zhang, Y. Shu, K.-W. Xu, Sol. Stat. Comm. 137 (2006) 441

O 6.4 Mon 12:00 MA 005

How Au(100) and Pt(100) reorganize themselves: Large-scale surface reconstructions studied by all-electron DFT — •Paula Havu[1], Ville Havu[1], Patrick Rinke[1,2], Volker Blum[1], and Matthias Scheffler[1,2] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]University of California at Santa Barbara, CA 93106, USA

Pt(100) and Au(100) show large-scale quasi-hexagonal, often called (5×20), surface reconstructions that are intimately linked to the external surface conditions (temperature, absorbates, electrochemistry). The reconstruction energy of Pt(100) is known from a careful calorimetric measurement [1], but earlier first principles studies of both surfaces have so far so far restricted to simpler (5×1) models that neglect the long range aspect of the reconstruction. We here use the new numerical atom centered orbital based all-electron code FHI-aims [2] to determine the full (5×20)-reconstructed surface structure, by means of density functional theory (DFT) calcluations. We compare our results to full-potential LAPW results for older (5×1) models. The full surface reconstruction is investigated both in DFT-LDA and -GGA (PBE functional), both to uncover the precise relaxation mechanism, and to compare quantitatively to the experimental reconstruction energy. [1] Y. Y. Yeo, C. E. Wartnaby, D. A. King, Science **268**, 1731-1732 (1995). [2] V. Blum *et al.*, The FHI-aims project, www.fhi-berlin.mpg.de/aims/

O 6.5 Mon 12:15 MA 005

determination of the DOS in Nb(110) from scanning tunneling spectroscopy — •Stefania C. Bobaru, Berndt Koslowski, and Paul Ziemann — Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm, Germany

We investigate the electronic structure of Nb(110)/Al2O3(0001) by means of Scanning Tunneling Spectroscopy (STS) at 6.2 K. To enable a comprehensive analysis of the local electronic structure of niobium, we employ standard I-V as well as I-z and dI/dz-z spectroscopy. The experimental results will be discussed in the framework of a recently developed method for recovering the electronic density of states (DOS) from STS data [1]. Based on the one-dimensional WKB approximation this method should enable recovering the DOS of the sample semi-quantitatively, and it should allow principally a deconvolution of tip and sample DOS. In this contribution we first elucidate the effect of data evaluation on the recovered DOS separating contributions from the bulk and the surface. We then try to deconvolute the DOS of tip and sample at least partially by comparing I-V data and differential barrier measurements taken at different locations of the sample with the same tunneling tip.

References:

[1] B. Koslowski, Ch. Dietrich, A. Tschetschetkin, P. Ziemann, Phys.Rev. B 75, 035421 (2007).

O 6.6 Mon 12:30 MA 005

Surface electronic structure of Y(0001): A consistent picture — •Michael Budke, Juliet Correa, and Markus Donath — Physikalisches Institut, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

The photoemission (UPS) spectra of the (0001) surfaces of rare earth single crystals like Sc, Pr, Y, Gd, Tb, Ho and Er show an intense feature at about 10 eV binding energy. Its sensitivity to the degree of surface order led to the acronym "surface order dependent state" (SODS) in the literature [1]. For more than 20 years it remains an unsolved puzzle why the SODS was not observed in photoemission data obtained from clean rare-earth thin films grown on W(110) or Mo(110). On the one hand, experiments performed on rare earth single crystals are known to suffer from inherent impurities. On the other hand, thin films grown on W(110) or Mo(110) are of higher purity but not as well ordered as single crystals due to the considerable lattice mismatch between substrate and film. In our contribution, we give a consistent picture of the surface electronic structure of Y(0001) that explains the differences between single-crystal and thin-film UPS data. Furthermore, we provide evidence that the SODS is in fact due to carbon contamination, and not, as believed for more than 20 years, an indicator for a well prepared, highly ordered surface.

[1] S.D. Barrett, Surface Science Reports **14**, 271 (1992).

O 6.7 Mon 12:45 MA 005

Efficient ab-initio based modelling of segregation profiles in metal alloys for arbitrary bulk concentrations — •Tobias Kerscher and Stefan Müller — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

As shown recently [1], the combination of density functional theory (DFT) with cluster expansion methods and Monte-Carlo simulations is a powerful tool to model surface segregation in binary metal alloys. However, the predicted surface properties are then restricted to the in-plane lattice parameter defined by the bulk concentration of the alloy. Indeed, a change of the bulk concentration demands the re-calculation of all atomic configurations via DFT being the most time-consuming factor in the used approach. We will present a cluster-expansion Hamiltonian which provides universal and volume-corrected bulk energetics for all bulk concentrations, and simultaneously, minimizes the number of DFT calculation which have to be performed. This is demonstrated for the [100] direction of the bulk systems Pt$_{25}$Rh$_{75}$ and Pt$_{50}$Rh$_{50}$. Our results are in quantitative agreement with experimental measurements.

Supported by Deutsche Forschungs-Gemeinschaft

[1] S. Müller, M. Stöhr, O. Wieckhorst, Appl. Phys. A. **82**, 415 (2006).

O 7: Symposium: Atomic Wires at Surfaces I
(Invited Speakers: Franz Himpsel, Hanno Weitering, Han Woong Yeom)

Time: Monday 11:15–13:45 Location: HE 101

Invited Talk O 7.1 Mon 11:15 HE 101

Low-Dimensional Electrons at Metallic Semiconductor Surfaces — •Franz Himpsel — Dept. Physics, University of Wisconsin, Madison, USA

In recent years, it has become possible to create well-ordered semiconductor surfaces with metallic surface states by using self-assembly of metal atoms. Since these states lie in the band gap of the semiconductor, they completely de-couple from the substrate. The surface structures can be tailored from two-dimensional triangular lattices to nearly one-dimensional atomic chains, which may be considered as the ultimate nanowires. The dimensionality can be varied systematically between 2D and 1D by using vicinal surfaces with variable step spacing. Angle-resolved photoemission and scanning tunneling spectroscopy reveal surprising features, such as a fractional band filling, nanoscale phase separation into doped and undoped chain segments, and a spin-splitting at a non-magnetic surface.

O 7.2 Mon 11:45 HE 101

Properties and origin of one-dimensional Au nanostructures on tungsten surface carbides — •Andrei Varykhalov, Oliver Rader, and Wolfgang Gudat — BESSY Berlin

We introduce a universal template for one-dimensional self-organization. The tungsten surface carbide W(110)/C-R(15×3) displays a large-scale reconstruction with interesting properties [1,2]. We recently showed that this structure which is rotated by 14° relative to W is able to order various atomic species ranging from C$_{60}$ superclusters which show "magic" numbers to Au films which become patterned in a way that they in turn serve as templates for needle-shaped Ni clusters [3]. The Au reconstruction is uniaxial with corresponding one-dimensional $E(\mathbf{k})$ dispersion [3]. We will demonstrate the origin of the self-organization of Au comparing (15×12) and (15×3) templates by STM and LEED. Two principally different mechanisms are identified: At *room temperature*, regular Au clusters develop which are *1 monolayer high* when grown on the (15×12) structure and *2 monolayers high* on (15×3) but always aligned along the *physical potential* of the carbide nanomesh, i. e., off by 14°. *Annealing* rearranges the Au adatoms towards a nanowire-like reconstruction which has rotated back to the [001] of W. The *chemical* driving force for this is revealed in detail by photoemission spectra from the valence band and the W4f core level.

[1] M. Bode et al., Surf. Sci. 344, 185 (1995). [2] A. Varykhalov et al., Phys. Rev. B 72, 115440 (2005). [3] A. Varykhalov et al., Phys. Rev. B 73, 241404(R) (2006); 74, 95420 (2006); 72, 241404(R) (2005).

O 7.3 Mon 12:00 HE 101

Spatial Mapping of the Electronic States of a One-Dimensional System — Arie van Houselt, Bene Poelsema, and •Harold Zandvliet — University of Twente, Enschede, The Netherlands

Using low-temperature scanning tunneling microscopy and spectroscopy we have recorded spatial maps of confined electronic states in the troughs between self-organized Pt nanowires on Ge(001) that are spaced 2.4 nm apart. Two subbands are resolved, which correspond to the lowest energy levels of a quantum mechanical particle in a box. As expected, the spatial dI/dV maps exhibit a maximum and a minimum in the middle of the troughs for the n=1 and n=2 states, respectively.

O 7.4 Mon 12:15 HE 101

Electrons Confined to Atomic Nanowires of Au on Ge(001) — •Jörg Schäfer, Christian Blumenstein, Sebastian Meyer, Marc Wisniewski, and Ralph Claessen — Physikalisches Institut, Universität Würzburg, D-97074 Würzburg

Nanowires reach their lower size limit in metal-induced chains on semiconductors. In such quasi-one-dimensional (1D) systems, the Fermi surface may host a charge density wave (CDW) with concomitant energy gaps. Metallic chain reconstructions on Ge(001) can serve as model systems, such as Au nanowires on Ge(001). In using scanning tunneling microscopy, one finds that the wires are spaced by several Ge lattice constants, with their electron density being laterally strictly confined. In the related system Pt/Ge(001), our data show a conduction path of atomic dimensions [1], yet various dimer elements are detected. In contrast, in Au nanowires the charge density is spread out very evenly in chain direction, as seen for a large range of bias values. This reflects an unusually pronounced delocalization with metallic character at room temperature. Most significantly, at low temperature indication of a periodic superstructure along the chains of twice the unit cell is found. The electronic properties have also been explored with angle-resolved photoemission. These measurements reveal free-electron-like bands close to the Fermi level. Moreover, the observed Fermi level crossings are supportive of a CDW nesting condition. The talk will review the various aspects of this exceptional 1D electron liquid, and present a perspective regarding related systems.

[1] J. Schäfer *et al.*, Phys. Rev. B **74**, 041404(R) (2006).

Invited Talk O 7.5 Mon 12:30 HE 101

Electronic instabilities and fluctuations in quantum chains — •Hanno H. Weitering — Department of Physics and Astronomy, The University of Tennessee, Knoxville, TN 37931, USA — Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

One-dimensional (1D) quantum conductors have always captured the imagination of physicists. While a strictly 1D material remains a theoretical construct, a vast number of materials can be viewed as macroscopic ensembles of weakly-coupled quantum chains, making them interesting test cases for theoretical predictions. I will discuss the electronic and magnetic properties of some quasi 1D systems on Si and Ge surfaces. Highlights include the remarkable self-assembly of rare-earth metal atoms on Si into silicide nanowires. Large strain anisotropy in these wires can lead to extraordinary aspect ratios and uniformity. The thinnest wires exhibit electronic properties reminiscent of a multichannel 1D conductor. These include the stepwise increase of the tunnel current as a function of tip bias in scanning tunneling microscopy, and the appearance of a fluctuating charge density wave or Peierls instability at low temperature. Peierls instabilities are normally attributed to a collective screening response of the 1D electron gas, but in the present case there is no obvious connection to the classical Peierls picture. The remarkable assembly of yttrium atoms into long nanowires with built-in metal/semiconductor junctions is illustrative of how the finite-size- and temperature-scaling behavior of a collective phenomenon may one day be exploited in nano-architectures.

Invited Talk O 7.6 Mon 13:00 HE 101

Phase transitions and fluctuations of metallic atomic wires on silicon — •Han Woong Yeom — CAWL, Yonsei University, Seoul, Korea

Wire-type metals in nano scale are essential for nano/molecular electronics and their fundamental properties are challenging with various exotic ground states and fluctuations. As an unconventional form of such 1D metallic systems, we have investigated the self-organized metallic atomic wires on flat and vicinal Si surfaces such as In/Si(111) [1, 2, 3], Au/Si(111) [4], Au/Si(557) [5], and Au/Si(553) [6], and Pb/Si(557) [7]. For some of these systems, we observed Peierls-type phase transitions due to the 1D bands nested fully with electron fillings of 1/2 or 1/3 [1-3, 5, 6]. In the present talk, I will review the achievements so far and the present debates [8] on these phase transitions. A few issues related to the transitions will be introduced such as (i) the impurity control over the Tc, the band gap [4], and the solitonic dynamic fluctuation [9], and (ii) the atomic-scale characterization of the embryonic charge-density wave order [10]. I also raise the question of why some of these systems like Au/Si(111) and Pb/Si(557) are robust against Peierls instability down to fairly low temperature [7]. [1] H. W. Yeom et al., PRL 82, 4898 (1999); [2] J. R. Ahn et al., PRL 93, 106401 (2004); [3] S. J. Park et al., PRL 93, 106402 (2004); [4] W. H. Choi et al., PRL, submitted; [5] J. R. Ahn et al., PRL 91, 196403 (2003); [6] J. R. Ahn et al., PRL 95, 196402 (2005); [7] K. S. Kim et al., PRL, in press; [8] H. W. Yeom, PRL 97, 189701 (2006); [9] S. J. Park et al., PRL 95, 126102 (2005); [10] P. G. Kang et al., PRL, submitted.

O 7.7 Mon 13:30 HE 101

Peierls instability in platinum chains on Ge(001) — •Arie van Houselt, Daan Kockmann, Bene Poelsema, and Harold Zandvliet — University of Twente, Enschede, The Netherlands

We have studied the structural and electronic properties of atomic Pt chains on a germanium (001) substrate. Using scanning tunneling microscopy we show that these Pt chains undergo a phase transition from a 2x periodicity at room temperature to a 4x periodicity at low temperatures. The coupling between the atomic chains turns out to be of essential importance, since isolated Pt chains and chains located at the edge of an array of chains maintain their 2x periodicity at temperatures as low as 4.7 K. The 2x to 4x transition is accompanied by an opening of an energy gap and can be interpreted as a Peierls instability.

O 8: Metal Substrates: Adsorption of Organic/Bio Molecules I

Time: Monday 12:00–14:45 Location: MA 041

O 8.1 Mon 12:00 MA 041

Surface stress and its consequences: In-situ study of PTCDA induced faceting of vicinal Ag(111) — •Florian Pollinger[1], Pavo Vrdoljak[1], Zhen Tian[2], Dirk Sander[2], Stefan Schmitt[1], Christian Kumpf[1], Achim Schöll[1], Jürgen Kirschner[2], and Eberhard Umbach[1,3] — [1]Universität Würzburg, Experimentelle Physik II, 97074 Würzburg — [2]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle — [3]Forschungszentrum Karlsruhe, 76021 Karlsruhe

Adsorption of organic molecules on vicinal metal surfaces is known to promote faceting and self-organized ordering on mesoscopic scales. The adsorption of PTCDA on vicinal Ag(111) surfaces leads to grating-like structures after annealing [1]. The system PTCDA/Ag(10 8 7) was investigated using two complementary techniques: An optical cantilever bending technique sensitive to changes in surface stress and spot-profile analysis low energy electron diffraction (SPA-LEED) to monitor the development of the interface structure during faceting. The data was compared to the related, non-faceting system PTCDA on Ag(111). Overall, we find a surface stress change of 0.7 N/m due to the PTCDA-induced faceting, whereas the adsorption of PTCDA without faceting induces a change of 0.4 N/m. Moreover, the data allows an explicit and unambiguous correlation of the surface stress change to the structural and morphological evolution of the interface during the adsorption of the PTCDA adlayer. In conclusion, the results provide experimental evidence for significant surface stress induced by an organic adsorbate and for its importance for faceting and long-range ordering at metal-organic interfaces. [1] X. Ma et al., APL 84, 4038 (2004)

O 8.2 Mon 12:15 MA 041

Island formation and diffusion of PTCDA on Ag(100) surface — •Julian Ikonomov, Oliver Bauer, and Moritz Sokolowski — Institut für Physikalische und Theoretische Chemie, Universität Bonn

Perylene-3,4,9,10-tetracarboxylic acid dianhydride (PTCDA) forms a c(8×8) ordered structure with a high symmetry on Ag(100). For submonolayers the attractive interactions between the molecules lead to two-dimensional islands with a quadratic equilibrium shape. The ordered PTCDA islands are in equilibrium with a disordered two-dimensional gas-like phase, consisting of highly mobile molecules. The dynamic behavior of this system was studied by variable temperature scanning tunneling microscopy. At room temperature, the islands were found to grow preferentially at the lower side of substrate steps, while at lower sample temperature, they grow on the terraces. At temperatures of about 680 K, a phase transition to a fully disordered phase was observed. The island decay and the diffusion of the PTCDA molecules were quantitatively investigated in order to obtain surface related energies and the diffusion parameters. Funded by the DFG SFB 624.

O 8.3 Mon 12:30 MA 041

Low temperature phases of NTCDA and PTCDA monolayers on Ag(111) — •Tim Laugks, Johannes Ziroff, and Friedrich Reinert — University of Würzburg, Experimental Physics II, 97074 Würzburg, Germany

The organic semiconductor molecule 1,4,5,8-naphtalene-tetracarboxylic dianhydride (NTCDA) and 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) exhibit phase transitions and variances in the electronic structure for both samples at low temperatures and for low temperatures during the film preparation. These problems are subject of current research because the interface geometry is decisive for the growth mode of organic molecules and the electronic properties of the interface. To improve our understanding of these systems we prepare NTCDA/PTCDA monolayers on Ag(111) at substrate temperatures down to 100 K and monitor their properties in a range from room temperature systematically down to 10 K. We investigate the electronic structure at the various temperature dependant phases, discussing the photoemission parameters of the HOMO and the former LUMO features. These parameters (i.e. binding energy and width) show a significant variation across the phase transitions and therewith we suggest a model for the interactions between molecule and substrate.

O 8.4 Mon 12:45 MA 041

Tuning the interaction at an organo-metallic interface: PTCDA on epitaxial Ag on Au(111) — •Johannes Ziroff, Frank Forster, and Friedrich Reinert — Universität Würzburg, Experimentelle Physik II , 97074 Würzburg

PTCDA (3,4,9,10-perylene-tetracarboxylic acid dianhydrid) monolayers on Au(111) and Ag(111) are widely used model systems in the field of organo-metallic interfaces, featuring the basic adsorbtion types of physisorption and chemisorption respectively. By the growth of epitaxial layers of Ag on Au(111), the electronic states of the substrate can be modified (depending on the thickness of the Ag film) to become more and more "silver-like", up to the point where they resemble the (111) surface of bulk silver. This process includes the formation of quantum well states with well charcterised charge distribution and electronic properties. Therefore, this system enables experiments in which we control the substrates physical properties in small discrete steps, meanwhile tuning the molecular bonding from van der Waals to covalent.

We will show angle-resolved photoemission spectra of PTCDA monolayers on Ag films of various thicknesses on Au(111), focusing on the valence band and its electronic features, namely the Shockley surface state, higher molecular orbitals (HOMO, HOMO-1) and the so-called former LUMO. We will comment on correlations between the substrates distinctive electronic features and the appropriate interface structure, thus fathoming their role in the bonding mechanism and the formation of new valence electronic states.

O 8.5 Mon 13:00 MA 041

Investigation of unoccupied electronic states in PTCDA/Ag(111) — •Sönke Sachs[1], Christian Schwalb[2], Manuel Marks[2], Stefan Krause[1], Achim Schöll[1], Eberhard Umbach[1,3], and Ulrich Höfer[2] — [1]Universität Würzburg, Experimentelle Physik II, Am Hubland, 97074 Würzburg — [2]Universität Marburg, Fachbereich Physik, Renthof 5, 35032 Marburg — [3]Forschungszentrum Karlsruhe, 76021 Karlsruhe

Energetics, momentum and time evolution of electronic states in organic semiconductors and at their interfaces are fundamental properties that strongly determine the performance in electronic applications. All of these properties can be explored with two-photon photoelectron (2PPE) spectroscopy for occupied and in particular for unoccupied electronic states.

In the archetypal system perylene-tetracarboxylic-dianhydride (PTCDA) on single crystal Ag(111) surfaces considerable differences between the electronic states of chemisorbed monolayer films and multilayer films are eminent. These differences, which are due to the altered chemical environment of PTCDA- and as well Ag-derived states in the vicinity of the interface, can be tracked with 2PPE. A new unoccupied interface state at the Ag/PTCDA interface with a free-electron like dispersion and comparatively short lifetime is detected that influences the charge injection characteristics considerably. The results of the 2PPE spectroscopy are compared to the results of complementary spectroscopies like UPS, IPES, and STS.

O 8.6 Mon 13:15 MA 041

Single molecule transport measurements in a well controlled contact geometry — •Ruslan Temirov[1], Adam Lassise[2], Olga Neucheva[1], Frithjof Anders[3], Michael Rohlfing[4], Bo Song[5], Florian Pump[5], Gianaurelio Cuniberti[5], and Stefan Tautz[1] — [1]Forschungszentrum Jülich — [2]Jacobs University — [3]Universität Bremen — [4]Universität Osnabruck — [5]Technische Universität Dresden

Transport properties of single molecules are presently in the focus of intense research. The reliability of experimental transport studies is, however, often hindered by difficulties in controlling contacts to the measured molecule on atomic level. Here we present single molecule transport experiments made on PTCDA/Ag(111) and PTCDA/Au(111) epitaxial interfaces which achieve a very high degree of control over the contacts [1]. Although the presented transport experiments were conducted in the LT STM, the limitation of the two-terminal STM geometry has been overcome by using a mechanical gating effect induced by the retraction of the STM tip [1]. Due to the high degree of control and the rich tunability achieved in the presented experiments, the obtained experimental data are fit for the comparison with the theory on ab-initio level. First results of such theoretical analysis will be discussed.

[1] R. Temirov, A. Lassise, F. Anders, S. Tautz. cond-mat/0612036

O 8.7 Mon 13:30 MA 041

Local control of the conductivity of single atoms and molecule probed by scanning tunneling microscopy and spectroscopy — •Lucia Vitali[1], Robin Ohmann[1], Sebastian Stepanow[2], and Klaus Kern[1] — [1]MPI for Solid State Research, Stuttgart — [2]ICREA, Barcelona

The implementation of molecule-based electronics is a pressing challenge of nanotechnology. The realization of such a circuit is still facing challenges such as the contact of the molecule to the electrodes. In order to clarify this, we studied the conductivity through single atoms and more complex molecular systems. Here, we present an experimental study of the electronic transport through single Co atoms and 4-[trans-2-(pyrid-4-yl-vinyl)] benzoic acid (PVBA) molecules adsorbed on Cu(111) studied by local probe spectroscopy at low temperatures. Morphology and electronic structure of atoms and molecules, obtained by conventional scanning tunneling microscopy/spectroscopy, are combined with transport properties measurements extracted from point contact spectroscopy. For Co single atoms the transport properties are modulated by the Kondo screening. The Kondo temperatures observed in tunneling and in point contact regime are comparable. A general model to explain our experimental evidence is proposed. For the PVBA molecules, the transport properties are strongly affected by the molecule-metal adsorption orientation. This deepens our understanding of the role of the molecular arrangement in the nano-junction and in molecular electronic transport, and addresses the determining role of the molecule-metal contacts.

O 8.8 Mon 13:45 MA 041

Electron transport across single phthalocyanide (Pc) molecules — •Florian Witt[1], Albert Takacs[1,2], Timofey Balashov[1], and Wulf Wulfhekel[1,2] — [1]Physikalisches Institut, Universität Karlsruhe, Wolfgang-Gaede Strasse 1, 76131 Karlsruhe, Germany — [2]CFN-DFG Centrum für Funktionelle Nanostrukturen

Recently molecular electronics is discussed as a future replacement of semiconductor electronics. A detailed knowledge of the electronic properties of the molecules i.e. the HOMO-LUMO gap, the density of states and the conductance is necessary. Scanning Tunneling Microscopy (STM) in combination with Scanning Tunneling Spectroscopy (STS) has become one of the most important methods for studying these molecular properties. We present results on single molecule contact measurements obtained with STM at 4K. A small amount of H_2Pc and CoPc molecules was evaporated on clean Cu(111) and Co/Cu(111). By laterally positioning the STM tip over isolated molecules and approaching the tip towards the molecules we measured the conductance as function of distance. Initially, an exponential increase was observed reflecting electron tunneling. Below a critical distance both H_2Pc and CoPc molecules have a tendency to lift from the surface and jump to contact with the tip. After the jump, the conductance only weakly varies with the distance. On Cu(111) typical conductances of 0.1 G_0 were found while on Co/Cu(111) the conductance is higher by a factor of 3. STS measurements in the tunneling regime revealed strong vibrational modes located on the organic side groups of Pc which are most likely responsible for the jump to contact.

O 8.9 Mon 14:00 MA 041

Low dimensional electronic structure of a metal/organic interface — •Isabel Fernández Torrente[1], Nora González Lakunza[2], Katharina Jennifer Franke[1], Nicolás Lorente[3], Andrés Arnau[2], and José Ignacio Pascual[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [2]Unidad de Física de Materiales, Centro Mixto CSIC-UPV/EHU, San Sebastián, Spain — [3]Institut de Ciencias de Materials de Barcelona-CSIC, Barcelona, Spain

The TTF-TCNQ charge donor-acceptor complex is a prototypical organic metal. In bulk, it crystallizes in a monoclinic structure built up from parallel stacks of TTF and TCNQ, showing anisotropic conduction along the molecular rows. Our aim is to study the interface of a TTF-TCNQ organic film with a metal. By means of Low Temperature Scanning Tunneling Microscopy and Spectroscopy (LT-STM and STS) we characterise the structure and electronic properties of sub-monolayer films of TTF-TCNQ grown on Au(111). Both molecular species adsorb with a planar configuration. Nevertheless there is a strong donor-acceptor recognition and TTF and TCNQ self-assemble in alternating one-dimensional rows. This arrangement modifies strongly the electronic properties of the molecular entities and the surface state inducing the formation of a resonance with one-dimensional nature delocalised along the TCNQ rows. Ab-initio calculations explain the origin of the detected resonances by a strong modification of the surface state of the underlying metal upon hybridisation with TTF on the mixed TTF-TCNQ phase.

O 8.10 Mon 14:15 MA 041

Electron-phonon coupling in C_{60} as revealed by scanning tunneling spectroscopy — •Katharina J. Franke[1], Thomas Frederiksen[2], Sergio Monturet[3], Gunnar Schulze[1], Andres Arnau[2], Nicolas Lorente[4], and Jose Ignacio Pascual[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]Donostia International Physics Center, Donostia, Spain — [3]Universite Paul Sabatier, Toulouse, France — [4]Centro de Investigaciones en Nanociencia y Nanotecnologia, Bellaterra, Spain

Electron-phonon coupling is of major importance for charge transport through single molecule tunneling junctions. In most experimental implementations of molecular junctions the electronic coupling of the molecular orbitals with substrate states leads to a significant broadening, thus obscuring electron-phonon coupling effects. Here, we investigate the electronic structure of single C_{60} molecules adsorbed on top of a self-assembled pattern of alternating tetraphenyladamantane and C_{60}. Scanning tunnelling spectroscopy reveals that these molecules exhibit properties similar to the free molecule, such as a large gap of 3.7 eV and a narrow LUMO resonance of only ≈60 meV line width. The LUMO resonance is followed by a broad weaker peak at about 240 meV higher energy. By density functional calculations including the Jahn-Teller effect, we show that this broad feature is induced by a complex coupling of the C_{60} vibrational eigenmodes with the LUMO resonance.

O 8.11 Mon 14:30 MA 041

Electronic and Vibrational Properties of $Ce_2@C_{80}$ Metallofullerenes — •Bert Voigtländer[1], Anna Strózecka[1], Josef Mysliveček[1,2], Kaliappan Muthukumar[3], and J.Andreas Larsson[3] — [1]Institute of Bio- and Nanosystems (IBN 3), and cni – Center of Nanoelectronic Systems for Information Technology, Research Centre Jülich, 52425 Jülich, Germany — [2]Department of Surface and Plasma Physics, Charles University in Prague — [3]Tyndall National Institute, University College Cork, Lee Maltings, Prospect Row, Cork, Ireland

The electron transport properties of the fullerenes have been investigated by the study of the properties of single-molecule STM junctions over an endohedral metallofulerene $Ce_2@C_{80}$ on Cu(111). In comparison to single-molecule STM junctions over C_{60} molecules the controlled contacts to the metallofullerene show an order-of-magnitude lower conductivity. We ascribe this effect to the encapsulation of metal ions inside the fullerene cage. The STM based inelastic vibrational spectroscopy on $Ce_2@C_{80}$ shows, apart from features related to the cage phonons also a low frequency mode at 9 meV. Based on theoretical calculations of the vibrational structure of the molecule, the feature can be assigned to the movement of Ce-Ce unit. The electronic spectroscopic measurements on $Ce_2@C_{80}$ molecules reveal an unusually high increase in the differential conductance of this molecule at low bias voltages. The experiments indicate that the effect is related to the excitation of highly efficient vibrational modes and not to e.g. to a Kondo resonance that represents another common zero-bias anomaly.

O 9: Plenary Talk Sankar Das Sarma

Time: Monday 13:00–13:45 Location: H 0105

Computing with Quantum Knots: Non-Abelian Anyons and Topological Quantum Computation

O 10: Semiconductor Substrates: Epitaxy and Growth

Time: Monday 13:15–16:45 Location: MA 042

O 10.1 Mon 13:15 MA 042

Thickness-dependent structural investigation of thin GaN films by Photoelectron Diffraction — •Christoph Raisch, Alexey Sidorenko, Heiko Peisert, and Thomas Chassé — University of Tübingen, Institute of Physical Chemistry

Thin films of hexagonal gallium nitride have been grown on 6H-SiC by ion-beam assisted MBE. The thickness ranges from submonolayers to bulk-like samples of more than 100 monolayers. The samples were characterised by XPS, LEED and XPD. During growth, two different types of wetting layers were observed (i) a Ga metal wetting layer on the SiC substrate and (ii) a Ga metal wetting layer on top of the growing GaN film. They prove essential for the spreading wetting growth mechanism and were used to derive interface electronic parameters of the Ga/SiC and Ga/GaN Schottky barriers.

The substrate and the films have been examined by x-ray photoelectron diffraction XPD, a method capable of determining the local atomic structure of crystalline materials. By choosing different photoemission lines, the environments of gallium and nitrogen have been investigated separately and are compared to each other. The differences between Ga2p and Ga3d emission have been evaluated, with Ga3d photoelectrons being bulk sensitive while Ga2p photoelectrons are probing the surface. Features evolving with thickness are identified and interpreted. The experiments are supported by multiple scattering cluster calculations, showing clear trends with increasing film thickness. The simulations also allow the determination of the polarity of the films, which is found to be Ga-terminated for all samples.

O 10.2 Mon 13:30 MA 042

Morphological and chemical characterization of thin heteroepitaxial Praseodymium sesquioxide films on Si(111) — •Andreas Schaefer[1], Volkmar Zielasek[1], Thomas Schmidt[2], Anders Sandell[3], Joachim Wollschläger[4], Jens Falta[2], and Marcus Bäumer[1] — [1]Institut für Angewandte und Physikalische Chemie, Universität Bremen — [2]Institut für Festkörperphysik, Universität Bremen — [3]Department of Physics, University of Uppsala — [4]Fachbereich Physik, Universität Osnabrück

Among the rare earths Praseodymium oxides possess the highest oxygen mobility and a high oxygen storage capability. Due to this fact they are promising candidates for catalytic applications exploiting the variable valency of Pr. A simplified two dimensional model system of the oxide catalyst can be prepared on silicon substrates in an UHV environment to study the atomic details of oxygen transport and transfer when exposed to adsorbed molecules. Here we report on the growth and morphology of heteroepitaxial Pr_2O_3 films at a low deposition rate on Si(111) which were investigated using Spot Profile Analysis of Low-Energy Electron Diffraction. In the initial stages of growth the specular diffraction spot exhibits a pronounced threefold symmetry most likely reflecting the formation of highly ordered islands of triangular shape as shown by STM. A roughening of the substrate surface is observed during growth of the initial Praseodymium oxide layer. Beyond these morphological studies, preliminary results of a first chemical characterization of the films with and without adsorbates (CO and oxygen) by XAS and XPS will be presented.

O 10.3 Mon 13:45 MA 042

Combined electrical and chemical characterization of BaO thin films on Si(001) — •Dirk Müeller-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

In context with the search for alternative gate oxides on SiO_2 in CMOS technology, we have grown high-k BaO films at a thickness between 5 and 20 nm on clean Si(001) using molecular beam epitaxy of Ba metal in ambient oxygen pressure. Interface states and color centers were characterized by XPS and EELS while varying temperature and oxygen partial pressure during growth. For the electrical measurements, Si(001) has been pre-structured by optical lithography and BaO was only generated on small squares using a tungsten mask. After preparation, the films were capped with 250nm of Au and electrically characterized ex situ.

From capacity-voltage measurements on known areas of BaO windows, a dielectric constant of 30 was calculated. This means that for a 5nm BaO film corresponds to an equivalent oxide thickness (EOT) of 0.65 nm of SiO_2. These measurements also show very low hysteresis (<5mV), and flatband voltages are close to that of the workfunction difference between Si and Au (+0.65eV). These results are encouraging in terms of the concentrations of fixed and mobile oxide charges both in the bulk and at the interface. The influence of different defects at the interface and within the BaO films will be discussed.

O 10.4 Mon 14:00 MA 042

Photoelectron spectroscopy (XPS) studies on the system zirconium oxide on Si(100) — •Frank Schönbohm[1,2], Christian Flüchter[1,2], Daniel Weier[1], Sven Döring[1,2], Patrick Mehring[1], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Fakultät Physik - Technische Universität Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany — [2]DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, 44227 Dortmund, Germany

Because of the importance for industrial manufacturing we studied ultrathin ZrO_2 films on a Si(100)(2×1) reconstructed surface. We carried out XPS measurements of the Si 2p- and the Zr 3d-level and calculated the film thickness by the damping of the signal strength. Further XPS investigations were performed in order to examine the systems heat stability. The thermal behavior was investigated by annealing the sample at temperatures ranging from 500°C up to 750°C. A ZrO_2 film thickness of 11 Å on the Si(100)surface was thermally stable for temperatures up to 600°C. Above this temperature a new compound was found in the XPS spectra, chemically shifted by 3.7 eV. For temperatures higher than 750°C the ZrO_2-signal disappeared completely from the surface and the structure of the new $ZrSi_2$ compound was then examined by a combined LEED, SEM and XPD investigation. The experiments indicated that $ZrSi_2$ forms islands on the surface. The experimental diffraction data were compared to simulations resulting in a first structure model of the islands.

O 10.5 Mon 14:15 MA 042

The Influence of Carbon Contaminations in Silicon Epitaxy — •Oliver Senftleben, Peter Iskra, Tanja Stimpel-Lindner, Dorota Kulaga-Egger, Ignaz Eisele, and Hermann Baumgärtner — Universität der Bundeswehr München, Werner-Heisenberg-Weg 39, 85577 Neubiberg

Thermal desorption of the native oxide is a well-known process but leads to an increase in surface roughness and to the formation of SiC. HF treatment, however, leads to a strong carbon contamination of the surface. Both treatments influence subsequent epitaxial overgrowth differently, which will be shown troughout this contribution.

The influence of carbon contaminations on silicon epitaxy strongly depends on its distribution on the silicon surface. A rather homogenous distribution still allows epitaxial layers of good quality. This will be shown by STM and SIMS. An even higher degree of carbon contamination after HF treatment still allows epitaxial layers of good electrical quality, evaluated by I-V measurements of CVD grown pin diodes with a very high amount of carbon at the interface, measured by SIMS.

Thermal desorption of the native oxide covered by carbon contaminats at temperatures between 800 °C and 900 °C lead to the formation of SiC, which acts as a nucleation site for the Si-monomer and to the formation of stable pyramidal structures with heights up to several 10 nanometers as well as polysilicon, which is demonstrated by STM, SEM and AES measurements. This causes a reduction of the epitaxial quality of subsequent layers.

O 10.6 Mon 14:30 MA 042

Influence of an Ehrlich-Schwoebel barrier on growth oscillations during epitaxy in layer-by-layer mode — •Christian Heyn — Institut für Angewandte Physik, Universität Hamburg, Germany

We study the mechanisms behind the damping of reflection high-energy electron diffraction (RHEED) oscillations during layer-by-layer growth of GaAs and AlAs. Experimental data are compared to results of both a kinetic Monte Carlo simulation as well as a rate equations based growth model. The rate model considers in particular reversible aggregation and interlayer migration. With the rate model, we find that the height of the Ehrlich-Schwoebel barrier for interlayer migration significantly influences the oscillation damping. Under consideration of an Ehrlich-Schwoebel barrier, the rate model quantitatively reproduces experimental oscillation damping as function of growth temperature and speed. Furthermore, the presence of an Ehrlich-Schwoebel barrier explains the more strongly damped oscillations during GaAs growth in comparison to AlAs. AlAs has a higher energy barrier for surface diffusion but a lower Ehrlich-Schwoebel barrier. From a quantitative analysis we obtain values of the Ehrlich-Schwoebel barrier height for GaAs of 0.134 eV and AlAs of 0.069 eV.

O 10.7 Mon 14:45 MA 042

Investigation of a long-ranged ordered silicate adlayer on the 6H-SiC(0001) surface by LEED, AES and IPE — •Nabi Aghdassi, Ralf Ostendorf, and Helmut Zacharias — Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster

We have prepared well-ordered silicate adlayers on 6H-SiC(0001) surfaces by an ex situ hydrogen treatment at elevated temperatures. The generated surfaces appear to be fully passivated and therefore stable in ambient air. LEED patterns clearly feature a $(\sqrt{3}\times\sqrt{3})R30^\circ$ periodicity which can be attributed to a long range order of the created oxide layers. Furthermore AES spectra exhibit a distinct O_{KLL} peak as well as a Si_{LVV} peak showing a typical oxidic-like shape that is indicating the presence of Si-O bonds on the surface. The unoccupied electronic states of the SiO_2/SiC interface are studied by inverse photoemission spectroscopy (IPE).

O 10.8 Mon 15:00 MA 042

Optimized hydrogen bake as in-situ removal of residual oxide and carbon on silicon substrates for thin film deposition — •Thomas Zilbauer, Peter Iskra, Dorota Kulaga-Egger, Martin Schlosser, Helmut Lochner, Torsten Sulima, and Ignaz Eisele — Universität der Bundeswehr München, Institut für Physik, Werner-Heisenberg-Weg 39, 85577 Neubiberg

The removal of carbon impurities and the native or chemical oxide from silicon substrates is an increasingly important issue for the fabrication of nanoscale semiconductor devices. Often a last in-situ cleaning step is necessary to prepare the partly recontaminated substrate surface after thorough wet chemical cleaning for a deposition process such as CVD, ALD or MBE.

Heating the substrate to temperatures above 800 °C in a hydrogen ambient leads to quick thermal desorption of the residual oxide. However, carbon impurities on the substrate may cause formation of stable silicon carbide at these elevated temperatures.

We demonstrate results from optimizing the hydrogen bake of a commercially available cluster tool for silicon substrates with different history of wet-chemical pre-treatment. The oxygen and carbon contamination are analyzed by secondary ion mass spectrometry (SIMS). Additionally, I-V-measurements of epitaxially grown p-i-n diodes are used to evaluate the cleaning results.

O 10.9 Mon 15:15 MA 042

Impurity induced growth instabilities — •Jörg Megow and Frank Grosse — Institut für Physik der Humboldt Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

Growth instabilities can be utilized for the formation of semiconductor nanostructures, e.g. regular step bunches might be useful as templates for growth of quantum wires. A possible source for step bunching is the inclusion of small amounts of impurities during growth. The experimentally observed growth instability in the $Si_{1-x}C_x$/Si(118) system is explainable if the impurities (C) are nearly immobile and have reduced binding to the growing species (Si) [1].

We present kinetic Monte Carlo simulations for different growth scenarios. Special emphasis is given to the role of exchange processes leading to the incorporation of the impurities into subsurface sites. The resulting changes of the chemical ordering in the grown crystal are analyzed and related to changes in the step bunch distribution at the surface. The relation of the formation of three dimensional nanostructures on singular (001) surfaces and wetting behavior under different impurity concentrations is demonstrated.

[1] E.T. Croke *etal.* Appl. Phys. Lett. **77** 1310 (2000).

O 10.10 Mon 15:30 MA 042

Strain Induced Pit Formation in Ge Layers on Si(111) — •Konstantin Romanyuk[1], Vasily Cherepanov[1], Bert Voigtländer[1], and Jacek Brona[1,2] — [1]Institute of Bio- and Nanosystems (IBN 3), and cni – Center of Nanoelectronic Systems for Information Technology, Research Centre Jülich, 52425 Jülich, Germany — [2]Institute of Experimental Physics, University of Wroclaw, pl. Maxa Borna 9, PL 50-204 Wroclaw, Poland

When nanoscale Ge stripes are grown at Si step edges by step flow growth the formation of nanoscale pits in the one atomic layer thick

Ge stripes is observed. This pit formation occurs in surfactant mediated epitaxy (Bi) when a small amount of Si is deposited and attaches as a small rim at the Ge stripes. As we will explain this nanoscale pit formation is driven by both, the energy gain when Ge leaves the Ge stripe and attaches to the thin Si rim terminating the Ge stripe, and the entropy gain due to SiGe intermixing at the step edges. While the direct vertical exchange would lead to a similar final state a high exchange barrier is involved. The pathway via pit formation involves a much lower exchange barrier.

O 10.11 Mon 15:45 MA 042

Growth and arrangement of silicon and germanium nanowhiskers — •Andrea Kramer — Institut für Kristallzüchtung, Berlin

The growth of silicon and germanium nanowhiskers as well as their arrangement by pre-structuring of substrates will be discussed. Nanowhiskers are grown via vapor-liquid-solid (VLS) mechanism, which is a method based on solution growth within metal droplets, in an ultra-high vacuum chamber by molecular beam epitaxy (MBE). To obtain a defined positioning of metal droplets, and thus a regular arrangement of nanowhiskers, a reproducible process for the localization of single metal droplets in pre-structured nanopores was successfully developed. Silicon or germanium substrates are initially patterned with nanopores by focused ion beam (FIB) treatment. By adjusting metal evaporation rate and substrate temperature in the growth chamber, individual droplets are preferentially formed within the pre-structured pores. Subsequently, silicon or germanium is evaporated in order to form a solution with the metal and initiate the epitaxial growth of nanowhiskers on the substrate. The morphology of the processed samples has been investigated by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Results of whisker growth and arrangement will be presented.

O 10.12 Mon 16:00 MA 042

Structure and morphology of graphene layers on SiC(0001) — •Christian Riedl[1], Chariya Virojanadara[1], Christian Ast[1], Alexei Zakharov[2], Klaus Heinz[3], 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 — [3]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

We report on the development of graphene layers on the 4H-SiC(0001) surface by high temperature annealing under ultra high vacuum conditions focusing on two issues: firstly, we analyze the precursor stage of graphitization, the $(6\sqrt{3}\times6\sqrt{3})\mathrm{R}30^\circ$-reconstruction. By means of low energy electron diffraction (LEED) and scanning tunneling microscopy (STM) we discuss the role of three observed phases with periodicities $(6\sqrt{3}\times6\sqrt{3})\mathrm{R}30^\circ$, (6×6) and (5×5) for three different preparation conditions [1]. Secondly, the growth of epitaxial graphene is discussed in detail. Depending on tunneling bias and tip conditions STM micrographs show the graphene layers with atomic resolution and its long-range epitaxial relation to the underlying substrate [1]. We show that LEED pattern and intensities can be applied quantitatively to monitor the number of graphene layers during the preparation procedure. We correlate LEED fingerprints with angular resolved photoelectron spectroscopy (ARUPS) from HeII excitation, high resolution x-ray photoelectron spectroscopy (XPS) and low energy electron microscopy (LEEM).

[1] C. Riedl et al., Phys. Rev. B, in print

O 10.13 Mon 16:15 MA 042

Spatial variation of the Dirac-gap in epitaxial graphene — •Lucia Vitali, Christian Riedl, Robin Ohmann, Ulrich Starke, and Klaus Kern — MPI for Solid State Research, Stuttgart, Germany

The unconventional electronic properties of graphene make it a promising candidate for the realization of novel nanoelectronic circuits which was first realized using single layer graphene samples produced by mechanical exfoliation. An alternative method has been established with the epitaxial growth of graphene on SiC basal-plane surfaces by thermal decomposition of the topmost SiC bilayers. The electronic structure of mono- and few-layer graphene on SiC shows the typical linear dispersion of the π-bands at their crossing at the Dirac point. The opening of a gap as a function of the layer thickness and charge distribution can be observed by high-resolution photoemission experiments. However, the conditions and layer thickness required for the gap opening and the detailed values of gap size and Dirac energy shift are currently under debate. In the present communication we use scanning tunneling spectroscopy (STS) at low temperatures to obtain insight in the local electronic structure of mono- and bilayer graphene on SiC(0001). We show that already for the first graphene layer grown on top of the $(6\sqrt{3}\times6\sqrt{3})\mathrm{R}30^\circ$ buffer layer a gap opening is observed. The size of this gap, however, is varying with the periodicity of the interface structure, possibly due to a spatially dependent potential induced into the graphene layer. For the second layer we also observe the Dirac gap but no local spatial variation, i.e. the interface potential is too weak to modulate the electronic structure of the bilayer.

O 10.14 Mon 16:30 MA 042

Graphene band structure near the Dirac point - lifting of the degeneracy ? — Eli Rotenberg[1], Aaron Bostwick[1], Taisuke Ohta[1,2], Jessica McChesney[1,2], Thomas Seyller[3], and •Karsten Horn[2] — [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

The band structure of graphene exhibits a degeneracy of the valence and conduction bands where the linearly dispersing bands cross at the Brillouin zone boundary [1]. In contrast to previous experimental evidence which strongly supports this band crossing, recent photoemission data by Zhou et al. [2] suggest that this degeneracy is lifted in graphene layers on SiC(0001), through the influence of the substrate, and that a band gap opens at the crossing point. We discuss these results in the light of additional results and present a straightforward and rather intuitive explanation for the conflicting results in terms of the quality of the graphene films prepared on silicon carbide.

[1] J.C.Slonczewski and P.R.Weiss, Phys. Rev. 109, 272(1958). [2] A.Boswick et al., Nature Physics 3, 36(2007). [3] S.Y.Zhou et al., Nature Materials 6, 774(2007).

O 11: Time-Resolved Spectroscopy I

Time: Monday 13:30–15:00 Location: MA 043

O 11.1 Mon 13:30 MA 043

Two-photon photoemission of image-potential resonances in front of the Si(100) surface — Jens Kopprasch[1], •Christian Eickhoff[1], Irina Ostapenko[1], Cornelius Gahl[1], and Martin Weinelt[1,2] — [1]Max-Born-Institut, Max-Born-Straße 2A, 12489 Berlin — [2]Freie Universität Berlin, Arnimallee 14, 14195 Berlin

We have investigated the dangling-bond states and image-potential resonances on the Si(100) 2×1 surface by means of bichromatic two-photon photoemission. Optical parametric amplification generates 70 fs ultraviolet pulses with tunable photon energies between 4.5 and 5.5 eV. These allow us to populate unoccupied states up to the Si(100) vacuum level, probed by the IR fundamental at a fixed wavelength of 795 nm. Besides the occupied dangling-bond state D_{up}, we resolve the first two image-potential states with binding energies of $E_1 = 0.62$ eV and $E_2 = 0.18$ eV with respect to the vacuum level. Using these energies we obtain a surface dielectric-constant of $\epsilon = 11.2$ which is close to the silicon bulk-value of $\epsilon = 11.9$.

Tuning the photon energy of the pump pulse across the D_{up} to $n = 1$ and D_{up} to $n = 2$ transitions we find a significant variation of both the 2PPE peak positions and the intensities. Before resonance we observe the D_{up} initial state with the kinetic energy increasing with the pump-pulse photon-energy. Above resonance the D_{up} intensity is significantly reduced and shifted to the respective image-potential resonances at constant kinetic energy. These intensity variations indicate interference between the transition to the discrete image-potential resonance and transitions to the continuum of unoccupied bulk states.

O 11.2 Mon 13:45 MA 043

Combining density functional and density matrix theory: Optical excitation and electron relaxation at the Si(001) 2×1 surface — •Norbert Bücking[1,3], Peter Kratzer[2], Matthias

Scheffler[3], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Fachbereich Physik, 47048 Duisburg, Germany — [3]Fritz-Haber-Institut der MPG, 14195 Berlin, Germany

A theoretical two-step approach to investigate the optical excitation and subsequent phonon-assisted relaxation dynamics at semiconductor surfaces is presented and applied to the Si (001) 2×1-surface: In the first step, the electronic band structure and the Kohn-Sham wave functions are calculated by density-functional-theory (DFT) within the LDA. In the second step, dynamical equations are derived from density-matrix theory (DMT), whereby an optical field is considered via $\mathbf{A} \cdot \mathbf{p}$-coupling and phonon induced relaxation by a deformation potential coupling term. Into these equations, the numerical results of the DFT calculation (Kohn-Sham eigenvalues and wave functions) enter as coupling matrix elements. By numerically solving the dynamical equations, the time-resolved population of the excited states can be evaluated. The results for the Si (001) surface correspond to the findings of recent experiments, in particular a short (intra-surface-band scattering) and a long (bulk-surface band scattering) timescale are dominating the relaxation process. The value of the experimental short timescale is reproduced by our calculations, whereas the long timescale cannot be accurately described by our theory.

O 11.3 Mon 14:00 MA 043

The Atomistic-Continuum Modeling of Short Pulse Laser Interaction with Semiconductors — •Dmitriy Ivanov and Baerbel Rethfeld — Physics Department, Technical University of Kaiserslautern, Kaiserslautern, Germany

The understanding of fundamental mechanisms behind the sub-wave length surface modification on semiconductors is of a great importance for Information Technologies. However, strong laser-induced phase perturbations, occurring under conditions of nonequilibrium between free laser-generated carriers and phonons, make the experimental and theoretical study of short pulse laser nanostructuring on semiconductors difficult. Previously, the atomistic-continuum approach for modeling of short-pulse laser interactions with metals have been proven as an efficient tool when studying processes of laser melting, ablation, and nanostructuring on metals. In present work, a computational technique that combines the advantages of different approaches into the atomistic-continuum model for semiconductors is developed on the example of Si. In the combined model, 1) the kinetics of fast non equilibrium phase transformations is treated at atomic level with Molecular Dynamics method, and 2) the description of laser light absorption by free carriers, their transport dynamics, and strong laser-induced non equilibrium between free carriers and phonons are accounted for in the continuum part by means of free carrier dynamics model.

O 11.4 Mon 14:15 MA 043

Potential Energy Surface of Laser-Excited InSb — •Jessica Walkenhorst, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretische Physik, Fachbereich Naturwissenschaften, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel

A recent experiment [A. M. Lindenberg et al., Science **308**, 392 (2005)] performed on InSb suggests that ultrafast laser-induced nonthermal melting occurs due to a flattening of interatomic potentials. This study was based on Debye-Waller theory, applied in the time-domain and for non-equilibrium processes. We analyzed the nonthermal melting of InSb by using (i) first-principles electronic structure calculations for the interatomic potentials (ii) dynamical models to find the structure factors under different nonequilibrium conditions. Our calculations show that no dramatic flattening of the potential energy surface occurs. Instead, the softening of the transverse acoustic phonons at the X point suffices to explain the measured Gaussian x-ray intensity decay.

O 11.5 Mon 14:30 MA 043

Ultrafast electron dynamics in Pb/Si(111) investigated by two-photon photoemission — •Patrick S. Kirchmann, Martin Wolf, and Uwe Bovensiepen — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin-Dahlem

We studied the ultrafast electron relaxation dynamics of hot electrons in quantum well states (QWS) in ultrathin epitaxial Pb films on Si(111) [1] by femtosecond time-resolved two-photon photoemission spectroscopy.

Up to four unoccupied QWSs are identified, which exhibit a bi-exponential decay of the hot electron population. The slower decay is assigned to a delayed filling of the metallic QWS in the Pb adlayer by scattering from electronic states of the optically excited Si(111) substrate. The faster decay is assigned to e-e scattering within the Pb film. The overall trend of the extracted decay rates is governed by Fermi liquid theory. However, a detailed analysis reveals a well resolved dip in the decay rate which occurs precisely at the binding energy of the band bottom of the first unoccupied QWS. This local minimum of the decay rate is assigned to intra-subband scattering within the Pb film.

Thus, for a comprehensive description of the electron decay in a two-dimensional metal film not only the electron density and screening parameters as in Fermi liquid theory have to be considered. Here, we show that also the electron scattering processes in the quantized band structure have to be taken explicitly into account.

[1] P. S. Kirchmann et al., Phys. Rev. B **76**, 075406 (2007)

O 11.6 Mon 14:45 MA 043

Time-resolved Electron Diffraction studies on the ultrafast temperature response of Bi and Pb on Si(111) — •Boris Krenzer, Anja Hanisch, Simone Möllenbeck, Tobias Pelka, and Michael Horn-von Hoegen — Department of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany

Recent progress in developing ultrashort electron pulses has opened the wide field of investigating structural dynamics of surfaces upon short-pulsed laser excitations. Because the diffraction pattern is related to the atomic positions in a solid and its surface, direct investigation of transient structures on a femtosecond timescale became possible. Additionally, the diffracted intensity is affected by the thermal excitation of the solid and its surface. Thus, a time-resolved electron diffraction experiment yields information on the transient structure and the transient vibrational energy contained in the system at the same time.

Here we report on the fs-excitation of ultra-thin epitaxial Bi- and Pb-films on a Si(111)-substrate. For the Bi-film the initial temperature rise upon laser excitation is rather slow with a time-constant of 20 ps, which is in accordance to the predictions of the two-temperature model (2TM). Because Pb has a three orders of magnitude larger electron-phonon coupling constant the observed initial surface temperature rise is faster than for Bi but slower than the prediction of the 2TM. This discrepancy is attributed to the limited time-resolution of the experiment. However, the Pb/Si(111) is an ideal system to quantify the experimental temporal resolution and to test methods for improving the time-resolution.

O 12: Symposium: Size-Selected Clusters at Surfaces I (Invited Speakers: Karl-Heinz Meiwes-Broer, Heinz Hövel, Thorsten Bernhardt)

Time: Monday 13:30–16:45 Location: MA 005

Invited Talk O 12.1 Mon 13:30 MA 005

Charge transport and magnetism of deposited clusters — •Karl-Heinz Meiwes-Broer[1], Ingo Barke[1], Armin Kleibert[1], Viola von Oyenhausen[1], Joachim Bansmann[2], Kristian Sell[1], Stefan Polei[1], and Norman Wilken[1] — [1]Institut für Physik, Universität Rostock, Universitätsplatz 3, D-18051 Rostock, Germany — [2]Abteilung Oberflächenchemie und Katalyse, Universität Ulm, Albert-Einstein-Allee 47, D-89069 Ulm, Germany

Magnetism and electronic properties of clusters at surfaces are of wide interest as is documented by the current Priority Programme of the Deutsche Forschungsgemeinschaft (DFG-Schwerpunktprogramm 1153) [1]. In particular, the novel physics found on the nm-scale might lead to interesting novel objects for future applications. In this contribution 3 to 15 nm mass-filtered metal clusters are studied deposited from an ACIS source onto ultraclean solid surfaces. In the case of alloy clusters, the particles stoichiometry could independently be clarified by EDX and X-ray absorption spectroscopy, typically yielding a composition close to the target material. Low-temperature STS serves for the investigation of electronic properties. The resulting dI/dU curves are distinctly structured which results from the size-dependent density of states of the clusters as well as from the underlying substrate. Magnetic properties are interrogated with x-ray absorption (XMCD) measurements. Strongly size and substrate dependent magnetic orbital moments are found [2].

[1] Special issue on clusters at surfaces in Appl. Phys. A 82(1), 2006
[2] A. Kleibert et al., J. Appl. Phys. 101, 114318, 2007

Invited Talk O 12.2 Mon 14:00 MA 005

Supported Magic Numbers for Size-Selected Ag Clusters on Fullerene Layers — •H. Hövel[1], S. Duffe[1], L. Patryarcha[1], T. Richter[1], B. Sieben[1], C. Yin[2], B. von Issendorff[2], and M. Moseler[3,4] — [1]Technische Universität Dortmund, Experimentelle Physik I — [2]Universität Freiburg, Fakultät für Physik — [3]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg — [4]Freiburg Materials Research Center

Mass selected clusters from Ag^+_{55} to $\mathrm{Ag}^+_{561\pm5}$ were deposited on HOPG and Au(111) functionalized with monolayers (ML) of C_{60} molecules, which proved to be a new and promising choice for the investigation of mass selected clusters. Depositions at 165 K gave extremely narrow cluster height distributions in STM images measured at 77 K. Molecular dynamics simulations for the deposition suggest softlanding with minor distortions of the icosahedral cluster shape at the cluster-fullerene interface [1]. Using C_{60}/HOPG or 2 ML C_{60}/Au(111) the cluster heights are stable for more than 12 h at room temperature (RT). For 1 ML C_{60}/Au(111) the cluster height decreases and finally all clusters disappear at RT. Molecular dynamics simulations reveal a process by which the clusters decay atom by atom through 1 ML C_{60}/Au(111) at RT. A sharp maximum at 1.7 nm cluster height forms during the cluster decay, indicating that there exists some metastable 'supported magic number'. For the soft-landed clusters we measured identical spectral features for individual clusters with the same selected size using STS at 5 K.

[1] S. Duffe et al., Eur. Phys. J. D (2007), published online

Invited Talk O 12.3 Mon 14:30 MA 005

Femtosecond laser spectroscopy of clusters at surfaces — •Thorsten M. Bernhardt — Institut für Oberflächenchemie und Katalyse, Universität Ulm, 89069 Ulm, Germany

Femtosecond two photon photoemission spectroscopy is employed to investigate the electronic structure of ultra-thin magnesium oxide films and of mass-selected clusters deposited onto this substrate. Distinct changes in the electronic structure of these films induced by oxygen vacancy defects and by metal cluster deposition are identified in the photoemission spectra and help to elucidate the origin of the observed catalytic activity of supported cluster nano-systems. Furthermore, in a new experimental approach, time-of-flight mass spectrometry in conjunction with femtosecond resonance-enhanced multiphoton ionization is used to directly monitor the chemical reaction dynamics of adsorbate molecules. This new method enables the distinction of different reaction pathways through direct real-time monitoring of the mass and the kinetic energy of reaction products and intermediates.

15 min. break

O 12.4 Mon 15:15 MA 005

Mass-selected non-IPR fullerenes deposited on HOPG — •Daniel Löffler, Patrick Weis, Artur Böttcher, and Manfred M. Kappes — Institut für Physikalische Chemie, Universität Karlsruhe (TH), Germany

C_n layers, (48≤n≤68), have been created under ultra high vacuum conditions by low-energy deposition of mass-selected $\mathrm{C}_n{}^+$ clusters onto HOPG surfaces [1][2]. $\mathrm{C}_n{}^+$(48≤n≤68) ions originate from the electron-impact induced ionization and fragmentation of C_{60} and C_{70}. The resulting C_n cages represent non-IPR building blocks (Isolated Pentagon Rule) and exhibit localized reaction centers (e.g. adjacent pentagons, 2AP, heptagonal rings, HP, squares). This property leads to the formation of covalent intercage bonds, -C_n-C_n-, which are responsible for the high thermal stability of the C_n solid films. The activation energy for desorption of C_n is considerably higher than the value found for related IPR cages. The intercage binding energies found for $\mathrm{C}_n{}^+$ (62≤n≤68) are lower than those found for the corresponding $\mathrm{C}_n{}^+$ (50≤n≤58) cages. This fact indicates that the strength of the C_n-C_n bonds results from the interplay between the cage curvature (pyramidal angle) and the mean number of non-IPR reaction centers per cage. The electronic structure of the valence band, as monitored by UPS (21.2eV), varies significantly with the cage size. The surface ionization potential and the width of the HOMO-LUMO gap dependent on the cage size and on the type of non-IPR sites terminating the cage.

[1] Böttcher et al., PCCP, 7 (2005) 2816
[2] D. Löffler et al., J. Chem. Phys. 125 (2006) 224705

O 12.5 Mon 15:30 MA 005

Counting electrons in quantum-well states of Au chains on an alumina thin film on NiAl — •Maria Veronica Ganduglia-Pirovano[1], Niklas Nilius[2], Veronika Brazdova[1], Maria Kulawik[2], Joachim Sauer[1], and Hans-Joachim Freund[2] — [1]Institut für Chemie, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Low-temperature STM measurements combined with DFT calculations are employed to study the adsorption of gold on alumina/NiAl(110). The binding of Au monomers involves breaking of an oxide Al-O bond below the adatom and stabilizing the hence under-coordinated O ion by forming a new bond to an Al atom in the NiAl. The adsorption implies negative charging of the adatom. The linear arrangement of favorable binding sites induces the self-organization of Au atoms into chains. Their electronic structure is described by a series of quantum well states (QWSs) that evolve from the s-d_{z^2} orbitals of the single adatoms. The node structure of the QWSs can only be explained when considering the charge transfer through the thin alumina film into the Au adchains in the electron count.

[1] N. Nilius, M. V. Ganduglia-Pirovano, V. Brázdová, M. Kulawik, J. Sauer, and H-J. Freund, Phys. Rev. Lett. submitted.

O 12.6 Mon 15:45 MA 005

Unoccupied states of individual silver clusters and chains on Ag(111) — •Alexander Sperl[1], Jörg Kröger[1], Nicolas Neél[1], Henning Jensen[1], Richard Berndt[1], Andreas Franke[2], and Eckhard Pehlke[2] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Size-selected silver clusters on Ag(111) were fabricated by single-atom manipulation using the tip of a low-temperature scanning tunneling microscope. Unoccupied electron resonances give rise to spectral features which shift towards the Fermi level with increasing cluster size. Linear assemblies exhibit higher resonance energies than equally sized compact assemblies. Density functional theory calculations reproduce the observed energies for the linear clusters and enable an assignment of the resonances to hybridized atomic 5s and 5p orbitals with silber substrate states.

O 12.7 Mon 16:00 MA 005

Size-dependent Surface States on Strained Cobalt Nanoislands on Cu(111) — •Benjamin Heinrich[1], Mircea-Vasile Rastei[1], Laurent Limot[1], Pavel A. Ignatiev[2], Valeri S. Stepanyuk[2], Patrick Bruno[2], and Jean-Pierre Bucher[1] — [1]Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, Université Louis Pasteur, F-67034 Strasbourg, France — [2]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle/Saale, Germany

Nanoislands on metal surfaces have been a matter of intense research for decades in view of prospective applications in a vast variety of domains. One of the main challenges in this regard is to control the interplay between the physical properties, whether magnetic, electronic or chemical, and the lattice mismatch with the metal substrate, which results in changes due to strain.

In this work, we focus on the interplay between strain relaxations and the surface states of Co nanoislands on Cu(111). By low-temperature scanning tunneling spectroscopy (LT STS), taken over the islands, we show for the first time that the electronic states of the islands vary with their size: Occupied surface states exhibit a sizeable downward energy shift as the island size decreases. Atomic-scale simulations and *ab initio* calculations confirm that the driving force for the observed shift is related to size-dependent mesoscopic relaxations in the nanoislands.

O 12.8 Mon 16:15 MA 005

Thermally activated processes for mass selected Ag clusters

on 1 and 2 monolayers C_{60} on Au(111) — •S. Duffe[1], L. Patryarcha[1], T. Richter[1], B. Sieben[1], H. Hövel[1], C. Yin[2], B. von Issendorff[2], and M. Moseler[3,4] — [1]Technische Universität Dortmund, Experimentelle Physik I — [2]Universität Freiburg, Fakultät für Physik — [3]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg — [4]Freiburg Materials Research Center

We deposited at 165 K mass selected clusters from $Ag_{147\pm1}$ to $Ag_{561\pm5}$, expected to form geometrically magic icosahedra, on 1.7 ML C_{60}/Au(111). On 1 and 2 ML C_{60} we observed very narrow cluster height distributions. After annealing, the clusters on 2 ML C_{60} kept their original height for more than 12 hours at room temperature (RT). In contrast the clusters on 1 ML C_{60} decayed and disappeared at RT [1]. During the decay process we observed a metastable size with the height of 1.7 nm for different initial cluster sizes. Neither Ag_{55} with h=(1.5 ± 0.2) nm nor Ag_{147} with h=(2.0 ± 0.2) nm after deposition at 165 K corresponded to the peak at h=1.7 nm. Therefore we deposited Ag_{80} and Ag_{68} at 165 K and observed cluster heights of $\approx$ 1.5 nm on 1 and 2 ML C_{60} for both cluster sizes, probably due to their prolate shape. The subsequent annealing of the clusters up to RT caused a change of the cluster height distribution, probably due to Ostwald ripening, and the metastable size with the height of 1.7 nm was formed. Thus mass selected geometrically non-magic Ag clusters show a different behavior at RT as geometrically magic Ag clusters.

[1] S. Duffe et al., Eur. Phys. J. D (2007), published online

O 12.9 Mon 16:30 MA 005

Structure and properties of deposited size selected $Fe_{50}Co_{50}$ alloy clusters — •Wolfgang Rosellen, Furkan Bulut, Renate Kerstin Gebhardt, and Mathias Getzlaff — Institut für Angewandte Physik, Universitätsstr.1 D-40225 Düsseldorf

Size-selected $Fe_{50}Co_{50}$ alloy cluster were generated by a continuously working Arc Cluster Ion Source (ACIS). The selection is carried out by means of an electrostatic quadrupole. The typical size of the clusters is between 6-12nm. The lateral size distribution and the crystalline properties were investigate ex-situ by means of High Resolution Transmissions Electron Microscopy (HRTEM). The alloy clusters were deposited on a tungsten W(110) surface under UHV condition in order to avoid oxidation. The distribution of height and size were determined by scannning tunnelling microsopy (STM) experiments for different sizes of the incoming particles and several deposition angles with respect to the W(110) surface. Additionally, the structural properties of *individual* $Fe_{50}Co_{50}$ clusters were examined.

- [1] M. Getzlaff et al., Appl. Phys. A 82 (2006) 95
- [2] K. Gebhardt et al., Eur. Phys. J. D (submitted)

O 13: Heterogeneous Catalysis

Time: Monday 14:00–16:30 Location: HE 101

O 13.1 Mon 14:00 HE 101

Geometry of silica supported vanadium oxide particles: theoretical core excitation spectra can provide new insight. — •Matteo Cavalleri and Klaus Hermann — Fritz-Haber-Institut der MPG, Berlin, Germany

The characterization of vanadia units in supported vanadium oxide catalysts is of paramount importance for an understanding of the reactive behavior of these materials.

Here we compare results from density-functional theory calculations on O 1s core excitations of small model particles with experimental data from Near-Edge X-ray Absorption Fine Structure (NEXAFS) measurements of well-known reference compounds and of real catalytic materials in order to determine structural properties of silica-supported vanadia nanoparticles. This procedure provides an unambiguous discrimination of all different oxygen species inside the particles and overcomes limitations of previous studies using vibrational spectroscopy where the particle-support interaction was found to hide essential structural information.

As a result, we are able to identify unique spectroscopic features characterizing bridging V-O-V oxygen that can be used as a fingerprint of polymeric vanadia species. The O 1s excitations of the silica support are found to contribute to the NEXAFS spectrum at higher energies compared with those of the vanadia particle such that the two contributions can easily be separated in the experiment.

O 13.2 Mon 14:15 HE 101

Adsorption and dehydrogenation of ammonia at the V_2O_5(010) surface: DFT cluster studies — •Mathis Gruber and Klaus Hermann — Fritz-Haber-Institut der MPG, Faradayweg 4-6, D-14195 Berlin, Germany

Transition metal oxide catalysts are widely used for selective oxidation reactions. However, in many cases details of the catalytic reaction mechanisms are still under discussion. One prominent example is the ammoxidation of propylene to acrylonitrile at transition metal oxide surfaces (SOHIO process). This catalytic reaction includes, amongst other steps, the adsorption and dehydrogenation of NH_x, $x < 4$, at the catalyst surface. We have performed theoretical studies on these reaction steps where the catalyst is simulated by a finite section of the V_2O_5(010) surface. The calculations use density-functional theory combined with clusters modeling the surface and adsorbate system. Calculations for the clean V_2O_5(010) surface show that binding energies of the H atom are always significantly larger than of the NH_x species. Further, the substrate is found to lower corresponding dehydrogenation energies compared with values for the gas phase reaction. However, the lowering is too small to make dehydrogenation likely to happen under ammoxidation reaction conditions. This suggests that surface defects such as oxygen vacancies become important for the reaction. Therefore, the role of oxygen vacancies for the dehydrogenation of NH_x will be discussed in detail.

O 13.3 Mon 14:30 HE 101

Kinetische Monte Carlo Simulation von Oberflächenreaktionen auf Nanopartikeln — •Lothar Kunz und Olaf Deutschmann — Institut für Technische Chemie und Polymerchemie, Universität Karlsruhe (TH), Engesserstr. 20, 76131 Karlsruhe

Eine Erweiterung der kinetischen Monte Carlo Methode erlaubt die detaillierte Betrachtung von Oberflächenreaktionen auf geträgerten Nanopartikeln und deren Support. Dabei kann zwischen Adsorptionsplätzen auf Flächen, Kanten und Ecken der Partikel differenziert werden. Die Methode läßt sich als Brücke zwischen Dichtefunktionalrechnungen der Elementarprozesse und Mean-Field-Simulationen in der heterogenen Katalyse einsetzen.

Es wird die Erweiterung der Methode sowie deren Anwendungsmöglichkeiten vorgestellt. Eine generische Implementierung sowie ein Editor für die Eingabe des Gitters der Oberfläche und die Formulierung der Elementarprozesse wie Adsorption, Desorption, Diffusion und Reaktion erlauben eine effiziente Übertragung auf unterschiedliche Partikelformen und Reaktionen.

O 13.4 Mon 14:45 HE 101

Influence of the substrate on the catalytic activity of Au/TiO_2(110) model catalysts — •Stefan Kielbassa, Menhild Eyrich, Joachim Bansmann, and Rolf-Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

In recent years, oxide supported Au catalysts and, in particular, the low temperature CO oxidation have intensively been examined. However, various topics, like the influence of the support on the catalytic activity, are still controversially discussed. Here, we present results on the influence of the chemical nature of the TiO_2(110) support on the activity of Au/TiO_2(110) model catalysts. Substrates with different surface structures and (bulk) oxidation states were prepared by using different preparation cycles (such as annealing and sputtering steps). After deposition of Au nanoparticles by thermal evaporation ($\Theta = 0.5$ ML), the activity of the model catalysts was examined in a micro-flow reactor. Samples with fully oxidized substrates are nearly catalytically inactive, while for catalysts based on bulk-reduced substrates or thin TiO_2 films, the activity is up to 50 times higher. Atomic force microscopy (AFM) images of the surfaces show that, on the bulk-reduced supports, Au particle densities and sizes do not differ significantly and thus cannot be made responsible for the observed variations in the activity. A high activity of oxygen surface vacancies is discussed as origin of the enhanced activity of these catalysts.

O 13.5 Mon 15:00 HE 101

Olefin conversions on supported Pd model catalysts: Molecular origins of selectivity towards isomerization and hydrogenation — •Wiebke Ludwig[1], Björn Brandt[1], Jan-Henrik Fischer[1], Swetlana Schauermann[1], Francisco Zaera[2], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]University of California, Riverside, USA

Understanding the mechanisms governing alkene conversions, isomerization and hydrogenation in particular, is an important goal in catalytic research and significant for industrial processes.

Whereas no hydrogenation is observed on Pd single crystals, it was recently shown that hydrogenation readily occurs on small Pd particles, presumably due to the formation of weakly-bound subsurface hydrogen species [1].

Under realistic conditions, these reactions take place over catalysts covered with carbonaceous species originating from the decomposition of alkenes. The exact role of these strongly bound species is however still not clear.

In this study, we present results on the conversion of *cis-* and *trans-*2-butene with deuterium over a Pd model catalyst supported on a Fe_3O_4 oxide film. To investigate the influence of carbonaceous species on the reaction kinetics, we performed isothermal molecular beam experiments combined with TPD measurements on both clean and carbon-precovered catalysts.

[1] A.M. Doyle et al., Angew. Chem. Int. Ed. 2003, 42, 5240-5243.

O 13.6 Mon 15:15 HE 101

CO oxidation on Palladium(111): Rate hysteresis and periodic breakdowns — •Stefan Karpitschka[1], Stefan Wehner[1], Helmut Brand[2], and Jürgen Küppers[1,3] — [1]Experimentalphysik III, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Theoretische Physik III, Universität Bayreuth, 95440 Bayreuth, Germany — [3]Max-Planck-Institut für Plasmaphysik (EURATOM Association), 85748 Garching, Germany

A rate-measurement-study of the catalytic oxidation of carbon monoxide on Pd(111) surfaces in the high vacuum pressure range is presented. The total flux of the feed gas to the surface was held constant while its CO-fraction was varied. The existence of a regime in the feed gas composition in which the system exhibits bistable behavior was shown by long-time measurements. Pulse-like modulations of the feed gas revealed that the experimentally observed high CO-fraction border of the bistable region is determined by the equistability condition of both phases. This behavior could be caused by the presence of predominantly CO-covered defects exceeding the critical size for nucleation. The experimental results and their temperature dependence are well described by a simple mean field model containing no fit parameters.

Applying high CO-fractions in the feed gas just within the bistable range, we furthermore observed periodic breakdowns in the catalytic activity at a very low frequency, which were not yet reported for this surface. Growth and decay of surface oxides as well as noise have been tested as an origin of these periodic breakdowns.

O 13.7 Mon 15:30 HE 101

Methane Oxidation on Gold — •Guido Walther[1], Glenn Jones[1], Søren Jensen[2], and Sebastian Horch[1] — [1]CAMD, Department of Physics, DTU, 2800 Lyngby, Denmark — [2]MIC, Department of Micro and Nanotechnology, DTU, 2800 Lyngby, Denmark

Since transportation of methane from the sources to the consumers requires low temperature and high pressure, there is a keen interest in transforming methane into methanol. This study aims at investigating the fundamental process of methane oxidation on gold.

In a millireactor setup, methane oxidation was studied on various gold catalysts. The reaction products were analyzed using a gas chromatograph and a mass spectrometer. To study the trend in activity of gold, a couple of catalysts of different particle sizes were used. Additional experiments were performed on a few gold catalysts of the same particle size, but different support materials, to emphasize the support effect in terms of trends in stability. TEM analysis before and after catalytic reactions document changes in particle size and shape.

Partial methane oxidation could not be observed on these catalysts. This is consistent with the thermodynamics, which show that there is a strong tendency of CO_2 formation.

O 13.8 Mon 15:45 HE 101

Reactivity of Nickel on oxide surfaces: evidence of surface oxygen — •Yan-Chun Liu, Heiko Strauss, Andrea Berlich, and Harald Morgner — Wilhelm-Ostwald-Institute for Physical and Theoretical Chemistry, University of Leipzig, Linnéstraße 2, D-04103 Leipzig

The role of surface and subsurface oxygen during catalytic processes on oxide supported metal catalysts remains a ques-tion of debate in some cases [1,2,3]. Some controversy arises from the difficulties to identify the position of the oxygen. Using Metastable Induced Electron Spectroscopy (MIES) we have been able to identify adsorbed oxygen on top of the metallic Nickel deposits on NiO layers. Furthermore, detailed analysis of the MIE spectra provides evidence of an atomically adsorbed Nickel species. The reactivity of the different Ni adsorbates was evaluated by its reaction with oxygen. Results of the growth of Ni on TiO_2 by MIES are also presented.

[1]D. W. Goodman, C. H. F. Peden and M. S. Chen, CO oxidation on ruthenium: The nature of the active catalytic surface. Surface Science 601, L124-L126 (2007).

[2]H. Over, M. Muhler and A. P. Seitsonen, Comment on [1] Surface Science in Press.

[3]D. W. Goodman, C. H. F. Peden and M. S. Chen, Comment on [2] Surface Science in Press

O 13.9 Mon 16:00 HE 101

Interaction of CO, CO_2, O_2 and H_2O with Au/Rutile $TiO_2(011)$-(2x1)/Re($10\bar{1}0$) model catalysts — •Wilhelmine Kudernatsch[1], Karifala Dumbuya[2], J. Michael Gottfried[2], Hans-Peter Steinrück[2], and Klaus Christmann[1] — [1]Physikalische und Theoretische Chemie, Freie Universität Berlin, Germany — [2]Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

During the last decade, the peculiar activity of Au/titania catalysts for low-temperature CO oxidation has stimulated a wealth of studies using TiO_2 model catalyst systems. In a first step, we have studied the epitaxy and chemical properties of titanium dioxide films grown on rhenium surfaces under ultra-high vacuum (UHV) conditions. Titania films were prepared by co-deposition of Ti vapor in an O_2 atmosphere of $1x10^{-6}$ mbar at 900 K. On Re($10\bar{1}0$), this procedure results in the growth of rutile films terminated by a (2x1)-reconstructed (011) surface. Au-containing model catalyst systems were then prepared by controlled vapor deposition of Au onto these films.

In order to characterize the structural and chemical properties of our model catalyst surfaces, we have studied the adsorption of CO, CO_2, and H_2O on the clean and Au-covered $TiO_2(011)$-(2x1) films by means of temperature-programmed desorption (TPD) and low-energy electron diffraction (LEED). To obtain information about the chemical composition of the model catalysts in the presence of the reactants, CO and O_2, we performed in-situ measurements with high-pressure X-ray photoelectron spectroscopy (XPS) at pressures up to 1 mbar.

O 13.10 Mon 16:15 HE 101

LEEM, XPS, and STM Characterization of Oxygen Species Relevant for the Ethylene Epoxidation on Silver — •R. Reichelt, S. Günther, and J. Wintterlin — Ludwig-Maximilians-Universität, 80337 München, Germany

The epoxidation of ethylene on silver catalysts is an extremely complex reaction because of the complicated nature of the Ag/O interaction. Several oxygen species on Ag surfaces have been identified but until now there is no general agreement about their role for the catalytic reaction. Using LEEM, XPS and STM we have investigated oxygen species on Ag(111) that were prepared by thermal decomposition of NO2. We find that the species obtained sensitively depend on the preparation conditions which may explain part of the conflicting data from literature. Apart from the (4x4)O phase, another oxygen species, the so called O γ could be obtained by applying several preparation cycles of (4x4)O phase followed by flash annealing it slightly above 570 K. Angle-resolved XPS of O γ shows a surface-like behaviour. However XPS data surprisingly show that it is stable up to 800 K, suggesting a strongly bound species. Another species could be prepared by dosing CO2 on the (4x4)O structure which meanwhile vanishes in XPS. In STM the local decomposition of (4x4)-patches and related stripe phases evidenced a reaction of the (4x4)O adsorption layer with CO2. We can propose the formation of two surface carbonate species evidenced by two well separated CO2 desorption peaks in TDS. It is also demonstrated that after using NO2 readsorption of residual gas species can occur, an apparent cause for misinterpretations of spectra.

O 14: Surface or Interface Magnetism

Time: Monday 15:15–16:45 Location: MA 043

O 14.1 Mon 15:15 MA 043

Structure and magnetism in nanoscale FeCo alloys — •Stefanos Tzivanakis, Alejandro Diaz-Ortiz, and Helmut Dosch — Max-Planck-Institut für Metallforschung, Stuttgart, Germany

The interplay between dimensionality, ordering and magnetism has been investigated on two-dimensional Fe-Co alloys. Our first-principles density-functional calculations on free-standing and Mo supported alloys show a linear dependence of the magnetic moment with atomic concentration and lattice constant. Lattice strain and charge transfer play a fundamental role in determining the magnetism and phase stability of two-dimensional Fe-Co alloys. Cluster expansions for the energy and the magnetic moment were used to exhaustively search ground-state and large-magnetic-moment configurations.

O 14.2 Mon 15:30 MA 043

Spin-resolved photoemission from antiferromagnets: Cr films on Fe(110) — •Peter Bose[1], Peter Zahn[1], Jürgen Henk[2], and Ingrid Mertig[1] — [1]Martin Luther University Halle-Wittenberg, Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

Layer-wise antiferromagnetic films grown on ferromagnets are well-suited systems for investigating exchange coupling, especially for studying exchange bias. Mn and Cr films have a profound effect on the spin-dependent transport in magnetic tunnel junctions, leading in particular to magnetoresistance oscillations with a period of 2 ML (e. g. [1]). Another recent example are 2-ML oscillations of the spin polarization in spin- and angle-resolved photoemission from Cr films on Fe(110) [2].

To understand the origin of the oscillations in Cr/Fe(110) we performed first-principles relativistic electronic structure and photoemission calculations. In particular the Cr-thickness dependence of the spin polarization at normal emission will be addressed and compared with experiment [2]. Further, magnetic linear dichroism will be discussed.
[1] P. Bose, I. Mertig, J. Henk, Phys. Rev. B **75** (2007) 100402(R).
[2] Yu. S. Dedkov, Eur. Phys. J. B **57** (2007) 15.

O 14.3 Mon 15:45 MA 043

A possible source of spin-polarized electrons: The inert graphene/Ni(111) system — •Yury Dedkov[1], Mikhail Fonin[2], and Clemens Laubschat[1] — [1]Institut für Festkörperphysik, Technische Universität Dresden, Germany — [2]Fachbereich Physik, Universität Konstanz, Germany

We report on an investigation of spin-polarized secondary electron emission from the chemically inert system: graphene/Ni(111). An ordered passivated graphene layer (monolayer of graphite, MG) was formed on Ni(111) surface via cracking of propylene gas. The spin-polarization of the secondary electrons obtained from this system upon photoemission is only slightly lower than the one from the clean Ni surface, but does not change upon large oxygen exposure. These results suggest to use such passivated Ni(111) surface as a source of spin-polarized electrons which is stable against adsorption of reactive gases.

O 14.4 Mon 16:00 MA 043

Morphology and magnetism of compact 3d-metal nanoclusters on surfaces — •Violetta Sessi[1], Jian Zhang[1], Klaus Kuhnke[1], Axel Enders[2], Jan Honolka[1], and Klaus Kern[1] — [1]Max-Planck Institut für Festkörperforschung - Stuttgart — [2]Dept. of Physics and Astronomy - University of Nebraska - Lincoln

Systems of isolated 3d-metal clusters with nanometer size are known to behave as a superparamagnetic ensemble in which each cluster is a ferromagnetic entity. Only below a certain temperature (blocking temperature TB) thermal fluctuations are suppressed and cluster spins are aligned on the time scale of an experiment. Blocking can be enhanced either by increasing the surface induced magnetic anisotropy energy or by cluster-cluster interactions e.g. RKKY type interactions mediated through the substrate.

In order to study these effects we fabricated small, compact metal clusters by buffer layer assisted growth (BLAG [1]). Using this method the cluster formation takes place on a surface-supported noble gas buffer layer and the cluster growth is totally independent of the substrate.

We analyzed Co and Fe clusters supported on Ag(111) and Pt(111) by STM and by XMCD. The sample preparation using the same BLAG procedure lead to very different magnetic properties for unstrained 3D nano-clusters on Pt(111) and Ag(111) substrates, which can be attributed to the strong spin-orbit coupling of the Pt with respect to Ag. The results will be compared to ab initio calculations.

[1] J.H. Weaver, G.D. Waddill, Science 251, 1444 (1991)

O 14.5 Mon 16:15 MA 043

Bottom-up creation and adsorption of hybrid organic-inorganic magnetic molecules on metal substrates — •Daniel Wegner[1], Mark Pederson[2], Ryan Yamachika[1], Yayu Wang[1], Bart M. Bartlett[3], Jeffrey R. Long[3], and Michael F. Crommie[1] — [1]Department of Physics, University of California, Berkeley, and Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA — [2]Center for Computational Materials Science, Naval Research Laboratory, Washington, DC, USA — [3]Department of Chemistry, University of California, Berkeley, CA, USA

Charge-transfer compounds of the type M[TCNE]$_x$ (M: transition-metal, TCNE: tetracyanoethylene) form an important group of molecule-based ferromagnets with potential applications due to their high Curie temperatures. Despite extensive studies the origin of magnetic coupling is not well understood due to a lack of sufficient structural characterization, largely attributed to disordered growth. Using a bottom-up approach, we have used a scanning tunneling microscope to arrange single V atoms and TCNE molecules to form charge transfer complexes of different sizes and geometries. By tunneling spectroscopy we prove chemical bonding as well as the emergence of magnetic properties. Special attention is given to the influence of the metallic substrate on the properties of TCNE and the implications for future organic-inorganic nanoscopic devices.

O 14.6 Mon 16:30 MA 043

Optical and magnetic properties of Ni films grown on Cu(110)-(2x1)O and Cu(110)-(2x3)N — •Richard Denk, Michael Hohage, Lidong Sun, and Peter Zeppenfeld — Atomic Physics and Surface Science Division, Institute for Experimental Physics, Johannes Kepler Universiät Linz, Austria

In the last years many studies concerning the growth and magnetic properties of thin ferromagnetic layers on nonmagnetic metallic substrates have been reported. While Ni on Cu(001) is one of the most prominent and best studied model systems, significantly less attention has been given to the Cu(110) surface, due to the less favourable growth mode of Ni on the bare Cu(110) surface. We have utilised Reflectance Difference Spectroscopy (RDS), to investigate the growth and the magnetic properties of thin Ni-films on two Cu(110) templates, namely Cu(110)-(2x1)O and Cu(110)-(2x3)N. The regular RDS signal allows for real time monitoring of the film growth and for film characterization. In addition, the sensitivity of the RD-spectrometer to the polar Magneto-Optical Kerr Effect (RD-MOKE) [1] has been used, in combination with an in situ magnet, to study the magnetic properties of the Ni films. Further characterization of the films was performed with STM and LEED/AES. Finally we report on adsorbate-induced (CO) quenching and spin reorientation of the magnetism of the Ni films. References: [1] Th. Herrmann, K. Lüdge, W. Richter, K.G. Georgarakis, P. Poulolоulos, R. Nünthel, J. Lindner, M. Wahl and N. Esser, Phys. Rev. B 73, 134408 (2006)

O 15: Methods: Other Experimental Techniques I

Time: Monday 15:30–16:45 Location: MA 041

O 15.1 Mon 15:30 MA 041

Tip-enhanced Raman Spectroscopy with a High NA Parabolic Mirror — •Dai Zhang, Catrinel Stanciu, Markus Sackrow, Kai Braun, and Alfred J. Meixner — Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 8, 72076 Tübingen

Tip-enhanced Raman spectroscopy (TERS) allows chemical information collection with a sensitivity reaching single molecule level and a spatial resolution in the range of 10 nm. The efficient excitation and collection of the plasmon-enhanced optical signals of species present in the tip-sample nano-gap between the tip apex and the substrate are crucial for TERS. The optical excitation field has to be polarized along the gap and the field emerging form the gap has to be observed from the side. These geometrical restrictions require the side-illumination and light collection using a low-NA lens, limiting the sensitivity of the measurements. We present a novel method to overcome this problem based on a confocal optical microscope with a high NA parabolic mirror for the excitation and the detection instead of the objective lens. The sample is arranged co-axially with the axis of the parabolic mirror and the gap is centered in the focus. Hence localized plasmons can be efficiently excited parallel to the surface we illuminate the parabolic mirror with a radially polarized doughnut mode and the field developed from the gap can effectively be collected by the rim of the parabolic mirror and directed to the detection system. Examples about tip-enhanced imaging and spectroscopy of nanomaterials and biological systems will be shown to demonstrate the efficiency of this modification.

O 15.2 Mon 15:45 MA 041

Static speckle experiments using white synchrotron radiation — •Tushar Sant, Tobias Panzner, and Ullrich Pietsch — Solid State Physics Group, University of Siegen, 57068 Siegen, Germany

Static speckle experiments were performed using coherent white X-ray radiation from a bending magnet at BESSYII. Semiconductor and polymer surfaces were investigated under incidence condition smaller than the critical angle of total external reflection. The scattering pattern of the sample results from the illumination function modified by the surface undulations [1]. The periodic oscillations are caused by the illumination function whereas other irregular features are associated with sample surface. The speckle map of reflection from a laterally periodic structure like GaAs grating is studied [2]. Under coherent illumination the grating peaks split into speckles because of fluctuations on the sample surface. It is important to understand which length scales on the sample surface are responsible for the oscillations in reflectivity map. To investigate this experiments are done with a triangular shaped sample. Different parts of the sample are illuminated with the footprint on the sample larger or smaller than the actual sample length. This gives prior information about total illuminated area on the sample. Using this additional information a detailed surface profile of the sample is reconstructed.1. Pietsch U, et al. Physica B-Condensed Matter, 357 (2005) 45. 2. Panzner T, et al. Thin Solid Films, 515 (2007) 5563.

O 15.3 Mon 16:00 MA 041

TER-XSW investigation of CoPt$_3$ nanoparticle films on Si and Sapphire substrates — •Ardalan Zargham[1], Thomas Schmidt[1], Radowan Hildebrand[1], Bernhard Gehl[2], Marcus Bäumer[2], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Institute of Physical Chemistry, University of Bremen, Germany

CoPt$_3$ bimetallic colloidal nanoparticle films on Si and sapphire substrates are investigated concerning the real space distribution of Co and Pt in specifically defined layers above the substrates as well as the structural dependancy on plasma treatments. TER-XSW is considered to be a suitable method for these types of investigation because of its ability of material specification in vertical resolution. It is simultaneously possible to understand the surface morphology by means of XRR.

O 15.4 Mon 16:15 MA 041

Coherent reflectivity using white synchrotron radiation — •Tobias Panzner, Tushar Sant, and Ullrich Pietsch — Universität Siegen, Festkörperphysik, Walter-Flex-Str. 3, 57068 Siegen, Germany

Using coherent white synchrotron radiation in the hard x-ray region for reflectivity experiments one have access to sample properties on a nanometer scale in principle. To extract the wanted information from the performed measurements so called phase retrieval algorithms are necessary. The authors developed a straight forward simulation program based on a spatial limited atomic flat surface to evaluate the influence of different parameters on the coherent scattered signal in the detector plane. These simulations can explain some interesting features of the measurements and shows unexpected results for the influence of the so called illumination function.

O 15.5 Mon 16:30 MA 041

BEST - Beamline for Education and Scientific Training - A new VUV beamline at BESSY II — •Thorsten Zandt, Christoph Janowitz, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin

A high-resolution 5 m normal–incidence–monochromator beamline behind the dipole DIP 03–1B at BESSY II is described. It covers the energy range of 3–40 eV. The beamline is designed for high-resolution photoelectron spectroscopy utilizing a Scienta SES–2002 electron analyzer, which is permanently placed as an endstation at the beamline. A high precision manipulator on a closed-cycle He cryostat allows angle-resolved measurements over 2π steradian below 10 K. For BEST it is planned to introduce and qualify continuously students and young scientists into the fascinating possibilities of synchrotron radiation research. Optical design of the beamline and preliminary performance results will be discussed.

O 16: Invited Talk Ulrike Diebold

Time: Monday 17:00–17:45 Location: HE 101

Invited Talk O 16.1 Mon 17:00 HE 101

The Surfaces of Bulk Semiconducting Metal Oxides — •Ulrike Diebold — Department of Physics, Tulane University, New Orleans, La 70118, U.S.A.

Semiconducting metal oxides such as TiO2, ZnO, SnO2, and In2O3 find applications in a large number of technical fields, e.g., they are used photocatalysts, gas sensors, and electronic materials. In many of these applications, the fundamental surface properties play a major role. In the talk, we will give an overview of some of our recent research results on investigating bulk oxide single crystals with Scanning Tunneling Microscopy and related spectroscopic techniques. Many of our results are verified with DFT calculations, and the fruitful interplay between theory and experiment will be discussed.

O 17: Invited Talk Sergey Borisenko

Time: Monday 17:45–18:30 Location: HE 101

Invited Talk O 17.1 Mon 17:45 HE 101
Charge-Density Waves and Superconductivity in Two Dimensions: The ARPES View — •Sergey Borisenko — Institute for Solid State Research, IFW-Dresden

An interaction between electrons and phonons results in two fundamental quantum phenomena in solids: in three dimensions it can turn a metal into a superconductor whereas in one dimension it can turn a metal into an insulator. In two dimensions (2D) both superconductivity and charge-density waves (CDW) are anomalous. In superconducting cuprates, critical transition temperatures are unusually high and the energy gap may stay unclosed even above these temperatures (pseudogap). In CDW-bearing dichalcogenides the resistivity below the transition can decrease with temperature even faster than in the normal phase and a basic prerequisite for the CDW, the favorable nesting conditions seems to be absent. We demonstrate that the normal-state pseudogap also exists in two of the most studied 2D examples, dichalcogenides $2H-TaSe_2$ and $2H-NbSe_2$, and the formation of CDW is driven by a conventional nesting instability, which is masked by the pseudogap. On the other hand, we find a very unusual behavior of the pseudogap in underdoped Dy-BSCCO and Tb-BSCCO as a function of temperature overlooked in previous ARPES studies. The magnitude, character, anisotropy and temperature evolution of the 2D-CDW pseudogap are intriguingly similar to those seen in superconducting cuprates.

O 18: Poster Session I - MA 141/144 (Atomic Wires; Size-Selected Clusters; Nanostructures; Metal Substrates: Clean Surfaces+Adsorption of Organic / Bio Molecules+Solid-Liquid Interfaces+Adsorption of O and/or H; Surface or Interface Magnetism; Oxides and Insulators: Clean Surfaces)

Time: Monday 18:30–19:30 Location: Poster F

O 18.1 Mon 18:30 Poster F
Infrared studies of gold nanochains on the Si(557) stepped surface — •Chung Vu Hoang, Markus Klevenz, Robert Lovrincic, Olaf Skibbe, Frank Neubrech, and Annemarie Pucci — Kirchhoff-Institut für Physik der Universität Heidelberg

Gold nanochains on Si(557) will be fabricated under ultra high vacuum conditions. The terraces of the stepped surface serve as one-dimensional diffusion channels, which leads to the formation of parallel monoatomic chains. Due to the appearance of metallic chains an anisotropic change of the conductivity of the substrate surface can be expected. The chain growth process and conductivity dependence versus gold composition will be investigated in-situ by using transmittance infrared spectroscopy (IRS) with light polarized parallel and perpendicular to the chains, respectively. IRS is a well-established method to observe conductivity changes on surfaces. The temperature dependent behaviour of gold chains will be studied as well.

O 18.2 Mon 18:30 Poster F
Self-assembled Pt nanowires on Ge(001) — •Cosima Schuster and Udo Schwingenschlögl — Institut für Physik, Universität Augsburg, D-86135 Augsburg

Semiconductor surfaces attract great attention due to various effects of self-organization. For example, adsorption of Pt on the Ge(001) surface results in stable Pt nanowires. Because self-organization of adsorpted atoms relys on strong interaction with surface states, accounting for the full structural relaxation is a prerequisite for describing the electronic properties of a covered surface in an adequate manner.

In a first step, we have thus investigated the surface electronic structure of the $c(4\times2)$ reconstructed Ge(001) surface by means of DFT band structure calculations In particular, it is possible to attribute each state to either the Ge dimer bonds or the dangling surface bonds. The Ge–Pt surface is investigated in a second step. The formation of Pt chains on Ge(001) is accompanied by the partial breakup of the Ge surface dimers. We show that the surface electronic structure is significantly perturbed due to Ge–Pt interaction. Especially, we find remarkable shifts of Ge states towards the Fermi energy. As a consequence, the topmost Ge layers are subject to a metal-insulator transition.

O 18.3 Mon 18:30 Poster F
CVD synthesis of isolated carbon nanotube peapods on substrates — •Christian Spudat, Carola Meyer, and Claus Schneider — Research Centre Jülich, Institute for Solid State Research, Electronic Properties, 52425 Jülich

Carbon nanotubes filled with C_{60} Fullerenes, so-called "peapods", form a model system for studying one-dimensional molecular chains coupled to a ballistic conductor. C_{60} interacts only weakly with the surrounding SWCNT. Thus, small interactions such as phonon or spin coupling should be observable in transport measurements. In general, these peapods are synthesized by filling *bulk* material, and they are successively dispersed on a substrate from solution. The disadvantage of this method is that the nanotubes are rather short due to prior sonication and bundle together in ropes. Thus, characterisation of individual peapods including transport measurements is rather difficult. Clean and isolated SWCNTs for transport measurements can be grown using chemical vapour deposition. Here, we present a method to fill such SWCNTs with Fullerenes directly on substrates using vacuum filling in an evaporation chamber. We characterize the SWCNTs and peapods after each processing step using AFM, Raman and HRTEM. The main focus is the investigation of defects caused by thermal oxidation and the purification of the synthesized peapods.

O 18.4 Mon 18:30 Poster F
Atomic Nanowires of Self-Organized Pt on Ge(001) – Structural Elements and Electronic Properties — •Marc Wisniewski[1], Jörg Schäfer[1], Sebastian Meyer[1], Andrei Stekolnikov[2], Ralph Claessen[1], and Friedhelm Bechstedt[2] — [1]Physikal. Institut, Universität Würzburg, D-97074 Würzburg — [2]Inst. f. Festkörpertheorie u. -optik, Universität Jena, D-07743 Jena

A special class of nanowires is formed by Pt on the Ge(001) surface. Its low-energy electron states have been explored by scanning tunneling microscopy (STM). A dimerization along the chains is observed at high bias, which might suggest a charge density wave. However, dimer elements also exist with sideways orientation, thus being inconsistent with such picture and instead indicating dimerized back-bonding. Most significantly, for states near the Fermi level, such dimerization along the nanowires is no longer observed. Here a spatially rather uniform charge density is detected. The nanowires can be imaged down to the millivolt regime, indicating metallic character, and tunneling spectroscopy shows finite zero-bias conductivity at room temperature. Ab-initio simulation of the structure has been performed, and a model for the reconstruction at 0.25 ML coverage has been derived. It well reproduces the STM data for various biases. We find that Pt-Ge bonds are favored over Pt-Pt bonds. The prominent dimers along the chain are explained by Ge dimers, while a row of alternating Pt and Ge atoms is identified next to them. This novel tetramer-dimer-chain model consistently explains the wire geometry and its subtle asymmetry. It also accounts for the differential conductivity near the Fermi level.

O 18.5 Mon 18:30 Poster F
Adsorbate induced refacetting: Pb chains on Si(557) — •Annemarie Schuster, Marcin Czubanowski, Shima Akbari, Herbert Pfnür, and Chistoph Tegenkamp — Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstr. 2, 30167 Hannover

The adsorption of monolayers (ML) of Pb on Si(557) followed by annealing to 640K results in the formation of an atomic wire structure.

Recently performed transport measurements have shown, that below 78K only along the wires transport occurs, whereas in the perpendicular direction an insulating behavior is found [1]. This finding depends sensitively on the Pb chain structure. Therefore, we have investigated the structure on the atomic and mesoscopic scale by high-resolution low energy electron diffraction (SPA-LEED). Depending on Pb coverage in the range between 1.2 and 1.6ML, formation of various facets [(112), (335), (223)] is induced by the Pb layers, in agreement to recent STM results [2]. The facet orientation in general does not coincide with the macroscopic orientation of the (557) surface. After an initial annealing step to 600 K, starting with 1.2ML of Pb, this new vicinality can be tuned gradually and reversibly even at temperatures below 180K by further adsorption, but also by desorption of Pb. Superstructures of the Pb layers on the terraces were identified on the most stable (223) facets, showing a correlation of adjacent terraces. Here parts of the devil's staircase and the striped-incommensurate (SIC) phases known from Si(111) surfaces develop [3]. [1]C. Tegenkamp et.al. PRL 95 (2005) 176804 [2] H. Murikawa et.al. PRB 76 (2007) 165406 [3]Yakes et.al. PRB 69 (2004) 224103

O 18.6 Mon 18:30 Poster F

Two-dimensional electronic structure of dysprosium silicide nanowires on Si(557) — •Martina Wanke[1], Karolin Löser[1], Gerd Pruskil[1], Petar Stojanov[2], Eric Huwald[2], John Riley[2], and Mario Dähne[1] — [1]Institute of Solid State Physics, Technical University Berlin, D-10623 Berlin, Germany — [2]School of Physics, La Trobe University, Bundoora, VIC 3086, Australia

Rare earth silicide nanostructures are of high interest because of their extremely low Schottky barriers on *n*-Si(111) [1] and the formation of nanowires with one-dimensional metallicity on Si(001) [2]. In this work, the self-organized growth of monolayer-thick dysprosium silicide nanowires on Si(557) has been studied by scanning tunnelling microscopy and angle-resolved photoelectron spectroscopy. The bare Si(557) surface is characterized by (111) and (112) facets [3]. Accordingly, we observed the nanowires forming on the (111) facets. For coverages of 2 Å dysprosium, nanowire lengths exceeding 1 μm and widths around 5 nm were found. Their electronic structure shows a strong dispersion both parallel and perpendicular to the nanowires, which is assigned to the band structure of $DySi_2$ monolayers on Si(111). At higher coverages similar nanowires are observed at the (111) facets, which show characteric structural properties of the multilayer growth and also the Dy_3Si_5 multilayer band structure.

This work was supported by DFG, project number Da 408/11.

[1] S. Vandré et al., Phys. Rev. Lett. **82**, 1927 (1999).

[2] C. Preinesberger et al., J. Appl. Phys. **91**, 1695 (2002).

[3] A. Kirakosian et al., Appl. Phys. Lett. **79**, 1608 (2001).

O 18.7 Mon 18:30 Poster F

Structural influence towards transport: Pb wires on Si(557) — •Marcin Czubanowski, Annemarie Schuster, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Deutschland

The adsorption of 1.3 ML of Pb on Si(557) substrates followed by annealing at 640K leads to the formation of an anisotropic metallic structures as revealed by conductivity, STM and ARPES measurements. Those structures below 78K show metallic conductance along the Pb-chains, whereas in the direction perpendicular to the chain-structure an insulating behavior has been found. Additionally, ARPES measurements have shown that below T_c, those structures undergo complete Fermi nesting in the direction normal to the structure. In our recent LEED experiments, the chain structure has been systematically investigated as a function of temperature by means of SPA-LEED analysis. The adsorption of Pb transforms (locally) the surface into a regularly stepped (223) facet below T_c. This structure undergoes reversibly a commensurable-incommensurable phase transition at T_c = 78K as judged from changes in position of step diffraction spots in the $[\bar{1}\bar{1}\,2]$ direction and also the periodicity of domain wall reflexes in the $[1\bar{1}\,0]$ direction. Furthermore, the transition depends crucially on the Pb coverage. If the steps are decorated by excess Pb, e.g. 1.5ML, the transition is strongly suppressed.

O 18.8 Mon 18:30 Poster F

Metastable Impact Electron Spectroscopy (MIES) of intermediate nanocatalytic states — •Christopher Harding, Vahideh Habibpour, Sebastian Kunz, and Ulrich Heiz — Lehrstuhl für Physikalische Chemie, Technische Universität München,

Metastable ion electron spectroscopy (MIES) is a well established spectroscopic technique that can be applied in a new and novel way to nanocatalysts. It has several interesting benefits which include a dramatically enhanced sensitivity to electron orbitals with low ℓ-values (compared with UPS) and very low collision velocities leaving the surface virtually untouched.

Thin oxide films and mass-selected metal clusters form the basis of nanocatalysts and are thus of primary importance. In the MIES spectra high sensitivity to sub-1%ML coverages of clusters and also a strong enhancement of various spectral regions which give information on intermediate states in oxidation reactions can be seen.

According to theoretical predictions cluster-oxides intermediates are formed and play an important role in the catalysis of the CO oxidation reaction. These important and interesting predictions are made, based on size selected Pd clusters on MgO films. Using a laser vaporisation cluster source size selected clusters of Pd_9 and Pd_{30} were deposited onto MgO films and this mechanism investigated. The experimental MIES studies confirm the intermediate oxide formation and illustrates other intriguing aspects of the Pd-oxide intermediate state.

O 18.9 Mon 18:30 Poster F

Size-selected clusters on surfaces studied by local probe: An experimental setup and first results — •Markus Bieletzki[1], Marina Pivetta[1], Clemens Barth[2], and Ulrich Heiz[1] — [1]Lehrstuhl für Physikalische Chemie, Technische Universität München, Lichtenbergstr. 4, D-85748 Garching, Germany — [2]CRMCN-CNRS, Campus de Luminy, Case 913, 13288 Marseille Cedex 09, France

During the last decade it has been shown by several groups that clusters with sizes of up to about 30-40 atoms reveal distinct chemical properties which change as function of the precise number of atoms[1,2]. In these experiments the model catalysts were prepared by the deposition of size-selected clusters from the gas phase at low temperatures. Whereas there is strong indication that the clusters remain intact upon deposition, little is known about the dynamics (stability, diffusion, agglomeration) of the clusters at elevated temperatures and under reaction conditions. In order to study the stability of size-selected clusters on oxide surfaces and thin oxide films we built a cluster deposition experiment with size-selection which is coupled to an OMICRON variable temperature scanning probe microscope. In this contribution we present the technical details and specifications of the new experimental setup and show first AFM- and STM-images of cluster assembled materials.

[1] K. Judai, S. Abbet, A. S. Wörz, U. Heiz, C. R. Henry, Journal of the American Chemical Society 2004, 126, 2732.

[2] S. S. Lee, C. Y. Fan, T. P. Wu, S. L. Anderson, Journal of the American Chemical Society 2004, 126, 5682.

O 18.10 Mon 18:30 Poster F

Calculations of two-particle correlation functions at surfaces — •Yaroslav Pavlyukh and Jamal Berakdar — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Heinrich-Damerow-Str. 4, 06120 Halle

The spectra of the electron-induced electron pair from surfaces [1] carry information on the short-range charge and spin correlations.

We show in this contribution how the measured angular and energy correlation within the electron pair relates to the spin-resolved spectral density of the sample and the screened Coulomb interaction. Both quantities we inspect theoretically by means of a combination of many-body theory and quantum chemistry methods based on the configuration interaction.

[1] Schumann *et al.*, Physical Review Letters **95**, 117601 (2005)

O 18.11 Mon 18:30 Poster F

Spatially resolved bonding and antibonding states on a silver dimer on Ag(111) — •Alexander Sperl[1], Jörg Kröger[1], Nicolas Neél[1], Henning Jensen[1], Richard Berndt[1], Andreas Franke[2], and Eckhard Pehlke[2] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Individual silver dimers were fabricated by single-atom manipulation using the tip of a low-temperature scanning tunneling microscope. Combining spatially resolved scanning tunneling spectroscopy of the dimer with density functional theory calculations bonding and antibonding electron states are identified. While bonding states contribute to the local density of states mainly in the center of the dimer, antibonding states are localized at the atom sites. The evolution of monomer to dimer unoccupied resonances was monitored as a function of decreasing mutual silver atom distance and found to shift toward the Fermi level.

O 18.12 Mon 18:30 Poster F

Reaction Properties of Size-selected Silver Clusters Supported on LTA Zeolite — •Amgalanbaatar Baldansuren and Emil Roduner — Institute of Physical Chemistry, University of Stuttgart, Stuttgart, Germany

Size-selected clusters are important to fundamental investigations. Silver containing catalysts were prepared by aqueous ion exchange of Ag$^+$ against Na$^+$ cations in an LTA zeolite. A recent project deals with continuous wave and pulse EPR investigations into adsorption interactions of ethylene, oxygen, and nitrogen monoxide with supported silver clusters. EPR is quite straightforward to analyze structures and electronic properties of paramagnetic clusters. The present work is restricted to monitoring the activity of the Ag$_6^+$ cluster; however, depending on the metal loading, Ag^0, Ag$_3^0$ and Ag$_4^+$ clusters have been formed in the LTA pores as well. The aim of the project is to discern size-dependent effects by directly looking at the centre of potentially catalytic activity.

A well-defined cluster composed of 6 equivalent silver nuclei was obtained after oxidation and hydrogen reduction. As the unpaired spin density distribution is strongly affected by reactions with gas molecules, the symmetric structure of Ag$_6^+$ turns into less-compact or smaller clusters. After ethylene adsorption a weak proton hyperfine coupling was resolved by ENDOR. HYSCORE experiments determined that the unpaired spin density is mostly on the adsorbed ethylene and no longer on the cluster. Products of the catalytic conversion, e.g. the NO$_2$ formed on the cluster surface after NO adsorption, exhibits molecular motion at temperatures between 30 K and 125 K.

O 18.13 Mon 18:30 Poster F

Oxidation/Reduction of Au$_n$ (n=2-13) clusters on SiO$_2$/Si and HOPG — •Rainer Dietsche[1], Dong Chan Lim[1], Moritz Bubek[1], Thorsten Ketterer[1], Young Dok Kim[2], and Gerd Ganteför[1] — [1]Dep. of Physics, University of Konstanz, Konstanz, Germany — [2]Dep. of Chemistry, Sungkyunkwan University, Suwon, Korea

Gas phase Au clusters with less than 20 atoms show a pronounced even-odd alternation in their oxidation behaviour. This behaviour is due to the unpaired electron in case of even-numbered anions. For clusters deposited on metal oxides this pattern vanishes. In our experiment Au cluster anions are soft-landed on silica and graphite. Oxidation and reduction are studied by X-Ray Photoelectron Spectroscopy (XPS).

For Au$_n$ (n=2-13) clusters on Si wafers covered with native oxide layers the even-odd pattern in oxidation behaviour still is observed. This indicates that the cluster-substrate interaction is weak enough to preserve some of the gas phase properties of the clusters [1].

In a second step, the samples are removed from the UHV system and immersed into water or NaOH solution. The samples exposed to water still exhibit similar chemical properties, whereas treatment with NaOH solution results in an inversion of the even-odd alternation.

In case of Au$_n$ (n=2-9) clusters on sputtered HOPG an even-odd pattern is not observed. However, Au$_8$ more readily reacts with atomic oxygen compared to the other clusters. STM measurements of Au$_7$ clusters show that this cluster exhibits two layer, 3D structures [2].

[1] D.C. Lim et al., *ChemPhysChem* **7**, 1909 (2006)
[2] D.C. Lim et al., *Chem. Phys. Lett.* **439**, 364 (2007)

O 18.14 Mon 18:30 Poster F

Softlanding and STM imaging of Ag$_{309}$ clusters on 1 and 2 monolayers C$_{60}$/HOPG — •L. Patryarcha[1], S. Duffe[1], T. Richter[1], B. Sieben[1], H. Hövel[1], C. Yin[2], B. von Issendorff[2], and M. Moseler[3,4] — [1]Technische Universität Dortmund, Experimentelle Physik I — [2]Universität Freiburg, Fakultät für Physik — [3]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg — [4]Freiburg Materials Research Center

At 165 K Ag$_{309}$ clusters were deposited on HOPG functionalized with C$_{60}$ and imaged with STM at 77 K. With HOPG at room temperature (RT) during C$_{60}$ evaporation areas of some 100 nm stayed uncovered, and 2 ML islands were formed on 1 ML C$_{60}$ planes. On areas with 1 and 2 ML C$_{60}$ we observed very narrow cluster height distributions with h=(2.4 ± 0.2) nm. By annealing Ag$_{309}$/C$_{60}$/HOPG we observed that the cluster height stayed stable for more than 12 h at RT on 1 and 2 ML C$_{60}$. The clusters on free HOPG areas became mobile during annealing at 265 K and moved to the edges of the C$_{60}$ areas. The RT stability of Ag$_{309}$/C$_{60}$/HOPG is in contrast to the observations for Ag$_{561}$ and Ag$_{309}$ on 1 and 2 ML C$_{60}$/Au(111) which were deposited at 165 K and annealed up to RT. For the samples with an Au(111) substrate we observed that the cluster height on 1 ML C$_{60}$ decreased and finally all clusters disappeared [1]. Molecular dynamics calculations show that there is a low barrier height for the transport of Ag atoms through the C$_{60}$ film on 1 ML C$_{60}$/Au(111) which should be much higher for clusters on 1 ML C$_{60}$/HOPG.

[1] S. Duffe et al., Eur. Phys. J. D (2007), published online

O 18.15 Mon 18:30 Poster F

Size-dependent Photoabsorption and Photoemission of Supported Silver Clusters and Silver Cluster-Biomolecule Hybrid Systems — •Roland Mitric, Christian Bürgel, Jens Petersen, Alexander Kulesza, and Vlasta Bonacic-Koutecky — Humboldt-Universität zu Berlin, Institut für Chemie, Brook-Taylor-Str. 2, D-12489 Berlin, Germany

Silver clusters interacting with different environments such as surfaces or biomolecules exhibit fascinating absorption and emissive properties which can be exploited for biosensing and optoelectronic applications. We address theoretically size dependent structural and optical properties of silver clusters Ag$_n$ (n=2,4,6,8) suppported on MgO surface as well as optical properties of silver-cluster tryptophan hybrid systems Trp-Ag$_n^+$ (n=1-9). Our results on supported silver clusters provide insight into the mechanism responsible for absorption and emission patterns arising from interaction between the excitation within the cluster and the environment. We demonstrate that small clusters such as Ag$_4$ are good candidates for fluorescence centers in the visible regime. Furthermore, in the Trp-Ag$_n^+$ hybrid system we identified different types of charge transfer between the silver and biomolecule subunits. Remarkably, we observe a strong reduction of the photofragmentation yield in Trp-Ag$_9^+$ in comparison with free Ag$_9^+$ which may be attributed to energy dissipation by fluorescence. Thus, the unique optical properties of supported silver nanoclsuters combined with the specific bio-recognition of biomolecules will provide fundamentals for the future development of fluorescent nanocluster-based biochips.

O 18.16 Mon 18:30 Poster F

Comparing Resonant 2p X-ray Absorption of Size-selected Cobalt Clusters on Cu(100) and in a Linear Paul Trap — •Vicente Zamudio-Bayer[1], Leif Glaser[2], Konstantin Hirsch[1], Philipp Klar[1], Andreas Langenberg[1], Fabian Lofink[1], Robert Richter[1], Jochen Rittman[1], Marlene Vogel[1], Wilfried Wurth[2], Thomas Möller[1], Bernd von Issendorff[3], and J. Tobias Lau[1] — [1]Technische Universität Berlin, Institut für Optik und Atomare Physik, EW 3-1, Hardenbergstraße 36, D-10623 Berlin — [2]Universität Hamburg, Institut für Experimentalphysik, Luruper Chaussee 149, D-22761 Hamburg — [3]Albert-Ludwigs-Universität Freiburg, Fakultät für Physik/FMF, Stefan-Meier-Straße 21, D-79104 Freiburg

Its element specificity makes resonant X-ray absorption spectroscopy an ideal tool to study deposited clusters at low coverage. At the $2p$ absorption edges of small, size-selected cobalt clusters on Cu(100), two separate sets of lines are observed which can be interpreted in terms of atomic-like multiplet splitting. For very small clusters ($n = 1, 2, 3$), these absorption lines show a strong size dependence. The size evolution of $2p$ X-ray absorption will be discussed in comparison to size-selected free cobalt clusters, recorded recently on mass selected cluster ions in a linear Paul trap at BESSY. Direct comparison of free and deposited clusters under well defined conditions allows to distinguish size-specific properties from cluster–substrate interaction effects. A shift to higher photon energies in deposited clusters indicates screening by substrate valence electrons.

O 18.17 Mon 18:30 Poster F

EUV/XUV-Radiation: a New and Versatile Tool for Structural and Chemical Surface Analysis — •Armin Bayer, Frank Barkusky, Stefan Döring, Christian Peth, Michael Reese, and Klaus Mann — Laser-Laboratorium Göttingen e.V., Hans-Adolf-Krebs-Weg 1, 37077 Göttingen

One of the most distinct features of EUV/XUV radiation in the regime of 2...20 nm is the strong interaction cross section to almost every material giving rise to penetration depths of about a few hundred nanometers for normal incidence light. Since the order of magnitude of the applied wavelength is comparable to typical dimensions of nanostructures, EUV/XUV light serves as an ideal tool for surface near probing of nanostructured samples.

The Laser-Laboratorium Göttingen e.V. has developed a laser-driven plasma source for generation of soft x-rays in the above mentioned spectral range. A Nd:YAG laser (1064 nm, 800 mJ, 6 ns) is focused into a gas-target leading to plasma formation which in turn emits characteristic soft x-ray radiation. Depending on the employed target gas, narrow-band as well as broad-band spectra can be obtained.

Based on this light source, a Θ-2Θ-reflectometry setup as laboratory metrology tool for in-band characterization of surfaces is currently being developed, enabling the future determination of both the chemical composition (reflectometry and NEXAFS experiments) and surface morphology (scatterometry and diffractometry experiments).

In this contribution we present the experimental concept, possible measurement techniques, numerical simulations as well as first results.

O 18.18 Mon 18:30 Poster F

Probing correlated electron-pair emission from a W(001) surface — •Milton Muñoz-Navia, Carsten Winkler, Michael Birke, Ram Shanker Patel, Frank Oliver Schumann, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

An electronic system which is excited by a photon can respond by the simultaneous emission of an electron-pair also called Double Photoemission (DPE). It has been established theoretically that a non-zero DPE intensity requires electron-electron interaction. Besides the simultaneous ejection of two electrons upon photon absorption, another possible pathway of pair emission is that the photon is absorbed by a single electron which scatters from another electron. To study their relative contributions we have analysed the pair emission from a W(001) surface excited by 25 eV and 29.5 eV photons in comparison with 20 eV and 25 eV electrons. The experiments were performed with a coincidence time-of-flight setup with two channelplate detectors in back-reflection geometry. In the (γ,2e) experiments BESSY II synchrotron facility operated in single-bunch mode was used as pulsed light source, while for the (e,2e) experiments, a pulsed electron gun was employed. We find that the 2D-energy distributions for photon absorption or electron excitation are markedly different. Qualitatively this difference can be understood by the selection rule for DPE. Hence, the (γ,2e) intensity has a significant contribution due to the DPE process.

O 18.19 Mon 18:30 Poster F

Aluminum oxide etching with hydrogen — •Markus Reinl, Andreas Assmuth, Rudolf Nüssl, Tanja Stimpel-Lindner, Torsten Sulima, Hermann Baumgärtner, and Ignaz Eisele — Universität der Bundeswehr, Institut für Physik, Werner-Heisenberg-Weg 39, 85577 Neubiberg, Germany

In modern semiconductor production Al is still used as material for the probing and bonding pads. It is widely spread that the difficulties during probing are caused by the native Al_2O_3 on top of the Al pads. In order to improve the probing performance different hydrogen processes to remove the native oxide were investigated on sputtered Al.

The first experiments were implemented in an UHV chamber. The Al was exposed to H* radicals to investigate the etching behavior. Therefore pure hydrogen was piped through a 1900 K hot tantalum tube into the process chamber. With this configuration a dissociation rate of 90 % can be achieved. The in-situ analysis was done by an x-ray photoelectron spectroscopy (XPS).

The hydrogen plasma experiments were performed in a modular UHV cluster tool with Ar as plasma gas and H_2 as etching component. In the purpose of analysis with secondary ion mass spectrometry (SIMS) the cleaned surface needs to be covered with a protective layer in order to avoid a recontamination respectively re-oxidation. Therefore a cap of pure Al was deposited.

As expected the results show that the pure chemical reaction does not lead to a sufficient etching rate. In fact ion bombardment is necessary to achieve a significant etching effect.

O 18.20 Mon 18:30 Poster F

About the existence of the Au(110) surface state at the $\bar{Y}$ point — •Andreas Nuber[1], Frank Forster[1], Friedrich Reinert[1], and Kenya Shimada[2] — [1]Universität Würzburg, Experimentelle Physik II, Am Hubland, 97074 Würzburg, Germany — [2]Hiroshima Synchrotron Radiation Center, Hiroshima University, Japan

Presently there are some discussions and inconsistent results about the existence of the Shockley-type surface state at the $\bar{Y}$ point of the surface Brillouin zone on the (1×2) reconstructed Au(110) surface. We investigated this surface by high-resolution angle-resolved photoelectron spectroscopy (ARUPS). In our investigation we could not find any evidence of a surface state on the clean Au(110) surface, neither at the $\bar{\Gamma}$ point nor at the $\bar{Y}$ point. Furthermore we deposited thin films of Xe and Ag in order to investigate the changes of the surface electronic structure. With about 2 ML of Ag adsorbed, a surface state at $\bar{Y}$ shows up with $E_0 = 450$ meV which is surprisingly a lot higher than the reported binding energy of the surface state on a clean Ag(110) surface. Adsorbing noble gases on the clean (1×2) reconstructed Au(110) surface induced a coverage dependent backfolding effect.

O 18.21 Mon 18:30 Poster F

Inelastic Electron Tunnelling Spectroscopy in studies of complex metal-organic interfaces: The case of PTCDA/Ag(111) — •Adam Lassise[1], Ruslan Temirov[2], and Stefan Tautz[2] — [1]Jacobs University, Bremen, Germany — [2]Forschungszentrum Jülich, Jülich, Germany

Recently it has been proposed that the STM-based Inelastic Electron Tunnelling Spectroscopy (STM-IETS) can solve the long standing problem of the STM chemical insensitivity. However, due to the problems with the interpretation of the IETS data, the potentials of this method in application to the large organic adsorbates are not yet well understood. Here we apply STM-IETS to the well studied model case of complex organic adsorption - PTCDA/Ag(111). We analyse the IETS data obtained on PTCDA molecules in different adsorption states and show that the variations of the local electronic structure of the molecule mostly affect the intensity of IET spectral features but not their energetic positions. Finally, we use the IET imaging in order to identify the strongest vibrational modes observed in IET spectra.

O 18.22 Mon 18:30 Poster F

Ferrocene-1,1-dithiol (FDT) between perfect and defective Ag electrodes — Thomas Bredow[1], Jörg Meyer[2], Volodymyr Maslyuk[3], •Gernot Gardinowski[4], Christoph Tegenkamp[4], Herbert Pfnür[4], and Ingrid Mertig[3] — [1]Institut f. Physikalische und Thoeretische Chemie, Universität Bonn, Germany — [2]Fritz-Haber-Institut - Abtl. Theorie, Berlin, Germany — [3]Fachbereich Physik, Martin-Luther-Universität Halle-Wittenberg, Germany — [4]Institut f. Festkörperphysik, Leibniz Universität Hannover, Germany

The role of surface defects on the energetic and electronic structure of a molecule between two electrodes is of high intrest. We present a theoretical study of the interaction of ferrocene-1,1-dithiol (FDT) with two perfect or defective (vacancies, steps, etc.) parallel Ag(111) surfaces using DFT. We demonstrate, that the adsorption geometry has a strong effect on the electronic levels and conductivity. Furthermore, we show that the presence of point defects strongly enhances the molecule-surface interaction but has a suprisingly small effect on the density of states. Ferrocene dithiolate preferably binds to low-coordinated Ag atoms, which leads to significant shifts of the molecular orbitals and to a decrease of the electronic conductivity compared to the adsorption at perfect surfaces due to increased splitting of molecular levels. The latter leads to a decrease of the overlap with the metal levels near Fermi energy, and therefore to a reduction of the conductivity. Finally, we conclude that highly conducting molecules need collective stabilization by a significant amount of FDT molecules saturating the energetically favorable, but less conducting sites on an Ag electrode.

O 18.23 Mon 18:30 Poster F

C_{68} deposits on Cu(111): Topography and Electronic Properties — •Albert F. Takacs[1,2], Timofey Balashov[1], Wulf Wulfhekel[1,2], Daniel Löffler[3], Artur Böttcher[3], and Manfred M. Kappes[2,3] — [1]Physikalisches Institut, Universität Karlsruhe, D-76131, Germany — [2]CFN-DFG Centrum für Funktionelle Nanostrukturen — [3]Institut für Physikalische Chemie, Universität Karlsruhe, D-76131, Germany

Non-IPR fullerenes (Isolated Pentagon Rule) have very recently attracted attention as stable building blocks for carbon-based nanotechnology. In contrast to classic fullerenes, the smaller C_n cages, n<70 and n>60, are functionalised by terminating reactive sites. We focus here on the C_{68} species which is the largest fullerene to have only non-IPR cage isomers. Ultraviolet photoionization spectroscopy reveals the HOMO-LUMO gap of the C_{68} layers of 1.7 eV and thermal desorption spectroscopy evidences a high intercage binding energy of $\approx$2 eV. We also used scanning tunnelling microscopy(STM) to determine the geometry and electronic properties of C_{68} deposits on Cu(111). The STM images confirm that C_{68} deposits comprise cages linked in polymeric chains as determined by the geometry of the reaction centers terminating individual cage. By proper positioning and approaching of the STM tip over an individual molecule we have investigated the conductance across the cage-substrate interface. The resulting current-voltage (I-V) and differential conductance (dI/dV) characteristics reveal two distinct trends which indicate the unique role of the non-IPR sites as responsible for the strong interactions with the substrate.

O 18.24 Mon 18:30 Poster F

Characterization of FDT molecules and its binding properties on metallic surfaces — •Jedrzej Schmeidel, Gernot Gardinowski, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Universität Hannover, Abteilung Oberflächen, Appelstrasse 2, 30167 Hannover, Germany

Recently performed VASP calculations concerning the adsorption of ferrocene-1,1'-dithiol (FDT) molecules on perfect and defective Ag(111) surfaces show that details of the chemical bond have a large influence on the DOS near Fermi energy, i.e the transport behavior. Furthermore, at defect sites the thiolate bonded FDT is energetically favored. We have experimentally investigated FDT on metallic surfaces, to gain insight into this subject. FDT molecule was chosen due to its large conductance and a high structural flexibility with respect to rotation of the two cyclopentadienyl (Cp) rings. As substrate Au(111) and epitaxially grown Ag/Si(111) were used. On both surfaces the adsorption process and the stoichiometry of the FDT was controlled and checked by XPS/UPS. On Au surfaces, self assembled monolayer (SAM) structures have been investigated by means of STM, where assembled structures have been partly seen in form of parallel oriented lines with average spacings of 1.7nm. Submonolayer coverages, generated by thermal evaporation, have been investigated on Ag $\sqrt{3}\times\sqrt{3}$/Si(111). First results about the preferred adsorption at characteristic defect sites (grain boundaries, steps) will be presented and their electronic structure, obtained by STS, correlated with theoretical results.

O 18.25 Mon 18:30 Poster F

Single molecule manipulations: PTCDA on Ag(111) — •Olga Neucheva[1], Ruslan Temirov[1], Adam Lassise[2], Sergey Soubatch[1], and Stefan Tautz[1] — [1]Forschungszentrum Jülich, Jülich, Germany — [2]Jacobs University, Bremen, Germany

Manipulations of atoms and molecules with the low temperature scanning tunneling microscope open new opportunities for creating nanodevices. The size of molecules and type of their interaction with the substrate play an important role in manipulation process. For PTCDA molecules chemisorbed on Ag(111) surface, we developed a protocol of controllable and reproducible manipulation which includes a creation of stable contact between a molecule and STM-tip, tearing it from the substrate and transporting to a chosen position, and finally locating it on the surface. The reproducibility of these stages is controlled by measuring the I(t) spectra. Using this protocol, we formed different types of molecular corrals and chains in order to modify the Ag(111) surface state. Performed experiments allow us to study substrate-molecule interaction in more details.

O 18.26 Mon 18:30 Poster F

X-ray absorption spectroscopy of spin-crossover complexes on metallic surfaces. — •D. Ball[1], M. Bernien[1], M. Piantek[1], J. Miguel[1], J. Kurde[1], W. Kuch[1], H. Wende[2], M. Haryono[3], S. Hain[3], and A. Grohmann[3] — [1]Freie Universität Berlin, Inst. f. Experimentalphysik, Arnimallee 14, D-14195 Berlin — [2]Universität Duisburg-Essen, Fachbereich Physik, Experimentalphysik - AG Wende, Lotharstr. 1, D-47048 Duisburg — [3]Technische Universität Berlin, Inst. f. Chemie, Straße des 17. Juni 135, D-10623 Berlin

Many six-coordinate iron(II) complexes with an Fe–N$_6$ core show a spin-crossover (SCO) behaviour. The transition between an antiparallel alignment of the electron spins (low spin) and a parallel alignment (high spin) is triggered by temperature, pressure, or optical excitation. We present Near Edge X-ray Absorption Fine Structure (NEXAFS) measurements of mono-molecular layers of Fe(II) 2,6-bis(pyrazol-1-yl)pyridine and 2-phenyl-4,6-di(pyridin-2-yl)-1,3,5-triazine SCO complexes deposited from solution onto Au(111) surfaces. The binding of these complexes to the surfaces is established via different linker groups such as SH, SAc, and SCN. The resulting degree of order and the adsorption geometry are determined by angle-dependent NEXAFS measurements at the C- and N-K edges. The nature of the S–Au bond is studied by X-ray Photoelectron Spectroscopy. The electronic properties of the Fe center are probed by NEXAFS at the Fe L$_{2,3}$ edges. Their spin state is deduced by comparing these spectra to measurements of bulk samples. We find that the interaction with the surface significantly influences the switching behaviour.

O 18.27 Mon 18:30 Poster F

Investigation of the interface between aromatic thiolate SAMs and the Au(111) surface — •Daniel Weier[1], Axel Beimborn[1], Christian Flüchter[1,2], Frank Schönbohm[1], Ulf Berges[1,2], Sven Döring[1,2], Tobias Lühr[1] und Carsten Westphal[1,2] — [1]Fakultät Physik - Universität Dortmund, Otto-Hahn-Str.4, D 44221 Dortmund, Germany — [2]DELTA - Fakultät Physik - Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D 44227 Dortmund, Germany

SAMs (Self-assembled-monolayers) of aromatic thiolates have been intensively studied in the last three decades. The amphiphilic molecules with a chainlike structure consist of a hydrophobic head group and a hydrophilic carbon chain part. The structure of the molecules allows molecular chemisorption in close packed arrays onto well prepared surfaces due to the high affinity of the sulphur head group to the Au surface. An important trait of the molecules is their strong interaction with x-ray radiation and electrons. The problem of radiation damage within the focus of an undulator beamline is well known. In this project the photon flux density was reduced by moving the sample behind the focus. The out-of-focus measurements showed a significant reduction in the radiation damage at the adsorbed molecules and long data acquisition times became possible. We present first full angle photoelectron diffraction data of the sulphur 2p peak of SAM thiolates on Au(111). The diffracted S 2p signal clearly displays intensity variations. We compare the experimental data with the results of a first simulation of a structure model of the thiolate/Au(111) interface.

O 18.28 Mon 18:30 Poster F

Growth and electronic characterization of TMTTF-TCNQ on metal surfaces — •Dagmar Kreikemeyer Lorenzo, Isabel Fernández Torrente, Katharina Jennifer Franke, and Jose Ignacio Pascual — Institut für Experimentalphysik, Freie Universität Berlin, Berlin, Germany

Here we investigate the adsorption properties and growth of the Bechgaard salt TMTTF-TCNQ on a Au(111) surface by means of Low Temperature Scanning Tunneling Microscopy. TMTTF (tetramethyltetrathiafulvalene) is a charge donor and TCNQ (7,7,8,8- tetracyanoquinodimethane) is an acceptor. The bulk structure is formed by parallel chains of TMTTF and TCNQ, giving rise to one-dimensional conduction bands along the molecular rows. The electronic structure of TMTTF is essentially the same as the well known donor TTF, but the addition of the four methyl groups gives it more three-dimensional shape and increases the decoupling between the chains. The submonolayer growth of pure TMTTF on Au(111) shows a repulsive interaction between molecules as a consequence of its charged state [1]. On the contrary, pure TCNQ self-assembles in close-packed islands. When co-deposited on a metal surface, TMTTF and TCNQ show a strong tendency to mix in ordered domains with alternating rows of each molecule, similar to bulk. By Scanning Tunneling Spectroscopy we identify the molecular resonances of TMTTF and TCNQ and a depopulation of the surface state. Our data indicates that donor-acceptor interactions are still present on a metallic surface. [1] Torrente et al, Phys. Rev. Lett. 99, 176103 (2007)

O 18.29 Mon 18:30 Poster F

Scanning tunnelling microscopy study of nitrobiphenylthiol self-assembled monolayers on Au(111) — •Heiko Muzik, Andrey Turchanin, and Armin Gölzhäuser — Department of Physics, Physics of Supramolecular Systems, University of Bielefeld, D-33615 Bielefeld

Electron beam/extreme UV patterning of 4*-nitro-1,1*-biphenyl-4-thiol self-assembled monolayers (NBPT SAM) on gold surfaces results in the transformation of the terminal nitro groups into amino groups and in the crosslinking of the underlying aromatic cores [1,2]. Such chemical nanolithography has a great potential for nanobiotechnological applications (e.g. fabrication of protein chips[3]), where the post-processing of amino-terminated and pristine areas results in the formation of complex supramolecular assemblies with lateral dimensions of periodic structures down to 30 nm. The understanding of the formation of NBPT SAM at the molecular level is important for a further implementation of chemical nanolithography in different areas. In this contribution we show the first results of a UHV scanning tunneling microscopy (STM) study of NBPT SAMs on Au(111). We present a detailed data evaluation procedure for a non-orthogonal Multiscan-type scanner (Omicron Nanotechnology). The structural polymorphism of

NBPT SAMs will be discussed subjecting to the preparation conditions of the samples and their subsequent temperature treatment in UHV. [1] W. Eck et al., Adv. Mater. 2000, 12, 805 [2] A. Turchanin et al., Small 2007. [3] A. Turchanin et al., Adv. Mater. 2007.

O 18.30 Mon 18:30 Poster F

Methanethiolate diffusion on Au(100) and Au(111) — •Andreas Franke and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel

Alkanethioles on unreconstructed Au(111) and Au(100) surfaces are studied as model systems for the bonding and diffusion of organic molecules on metal surfaces. Unreconstructed (111) and (100) surfaces of Au exist under certain electrochemical conditions [1]. We have extend our work on CH_3S/Au(111) in a twofold way: In accordance with other studies [2] at low coverages we found CH_3S–radicals to bind as $Au(SCH_3)_2$ complexes to the Au(111) surface with a binding energy of 2.38 eV per CH_3S. We here present an *ab initio* study of the diffusion barriers for these complexes and bare CH_3S. To this purpose, we employ the nudged elastic band method (NEB) as implemented in the VASP code. Furthermore, we compare the diffusion of the bare CH_3S–radical on the (100) and (111) surface. On Au(100) the adatom formation and subsequent adsorption of two CH_3S–radicals at the adatom is slightly less favorable than chemisorption of individual radicals on the defect free surface. The most stable adsorption position for CH_3S is a tilted hollow-bridge geometry (for one radical per (4×4) surface unit cell) with a binding energy of 2.27 eV. The radical is tilted to the surface normal by 54°. Transition states along the minimum energy path with barrier heights of 620 meV and 640 meV have been calculated.

[1] M. A. Schneeweiss, et al., Appl. Phys. A **69**, 537 (1999).

[2] P. Maksymovych, et al., Phys. Rev. Lett. **97**, 146103 (2006).

O 18.31 Mon 18:30 Poster F

The adsorption of PTCDA on coin metal surfaces: a correlation between the adsorption height and the chemisorptive nature of the adsorbate-substrate bonding — •Oliver Bauer[1], Annegret Hauschild[1], Serguei Soubatch[2], Stina K. M. Henze[3], Ruslan Temirov[3], Adam Lassise[3], Frank Stefan Tautz[2], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn — [2]Institut für Bio- und Nanosysteme 3 (IBN3), Forschungszentrum Jülich GmbH, 52425 Jülich — [3]School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen

The vertical bonding distance of the adsorbate to the underlying surface can be regarded as a quantity of the strength and the chemisorptive character of the bond. The Normal-Incidence X-ray Standing Wave (NIXSW) technique has been used to determine the adsorption heights of perylene-3,4,9,10-tetracarboxylic acid dianhydride (PTCDA) on various single-crystalline coin metal surfaces. In addition we have recently investigated the adsorption heights as well as the adsorption geometry of PTCDA in the submonolayer regime on the Ag(100) and Ag(110) surfaces by NIXSW: We find vertical bonding distances of 2.66(4) Å and 2.59(1) Å respectively. For PTCDA/Ag(100), the carboxylic and anhydride oxygen atoms are located 2.57(7) Å and 2.79(10) Å above the substrate surface respectively. Based on the experimental findings bonding models which include a synergetic effect of adsorbate-substrate bonding and back-bonding are discussed for PTCDA adsorption on coin metal surfaces. Supported by the DFG and the ESRF.

O 18.32 Mon 18:30 Poster F

STM/STS Analysis of Molecular Chains Consisting of Mn_6Cr Single Molecule Magnets and Single Molecules on Highly Ordered Pyrolytic Graphite (HOPG) — •Aaron Gryzia[1], Armin Brechling[1], Wiebke Hachmann[1], Marc D. Sacher[1], Ulrich Heinzmann[1], Maik Heidemeier[2], and Thorsten Glaser[2] — [1]Molecular and Surface Physics, Bielefeld University — [2]Anorganic Chemistry I, Bielefeld University

We report on the preparation and characterization of Mn_6Cr-Single Molecule Magnets on a HOPG(0001) surface.

The Mn_6Cr-molecules show 1D molecular arrangements with many interesting features, such as the occurrence of discrete kink angles in the molecular chains of 30 deg., only two different molecular orientations, the orientation of the chains along the main crystal axis of HOPG and much larger molecule-molecule distances than expected from the van der Waals radii of the molecules. By STS we characterized Mn_6Cr, thus gaining information on the electronic levels of the molecule and the shift of the levels whether it is part of a chain or not. One of our goals is to obtain data about the exact orientation of the molecule in respect to the surface; thus we can make a statement for the physical interaction why the molecules are assembling in chains. First results of these measurements will be presented.

O 18.33 Mon 18:30 Poster F

High-Density Zig-Zag Dimer-Chain of Trimesic Acid at Graphite-Phenyloctane Interface — Ha N. T. Nguyen[1,3], •Thiruvancheril G. Gopakumar[1], Markus Lackinger[2], and Michael Hietschold[1] — [1]Institute of Physics, Solid Surfaces Analysis Group, Chemnitz University of Technology, D-09107, Chemnitz, Germany. — [2]Institute of Crystallography and Applied Mineralogy, Ludwig-Maximilians-University Munich, Munich, Germany. — [3]Department of Applied Physics, Faculty of Physics ,University of Natural Science, 227 Nguyen Van Cu, Hochiminh city, Viet Nam.

Trimesic acid (TMA) is well known for its self-assembly via hydrogen bonding, especially in fatty acids at solid-liquid interface. The well known open structures are the planar chicken wire and flower structures[1]. It has never been observed for TMA in any of the studied solvents a high density structure with molecules adsorbing parallel to the substrate at solid-liquid interface. We have observed a stable adsorption of TMA in phenyloctane (C14H22), a non-polar solvent, with high packing density at room temperature. The packing density is 1.3 molecules/nm2, which is the highest observed for any of planar adsorption of TMA structures at solid-liquid interface. The molecules interact through the carboxylic functional groups with a dimer motif leading to dimer-chain. In adjacent rows the molecules have inverted symmetry (3-fold), which provides the molecules to interact and close pack themselves in a zig-zag fashion. The high density is expected due to high concentration of TMA in phenyloctane by sonication.

[1] Markus Lackinger, et al., Langmuir 2005, 21, 4984-4988.

O 18.34 Mon 18:30 Poster F

FT IRRAS Studies of Potential-Controlled Transformations of a Monolayer of Dibenzylviologen adsorbed on a Cu(100) Electrode Surface — •Melanie Röefzaad, Duc Thanh Pham, Peter Broekmann, and Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Universität Bonn

Fourier transform infrared reflection absorption spectroscopy (FT IRRAS) has been combined with cyclic voltammetry (CV) to monitor the potential induced transformations of a monolayer formed by the redox-active 1,1′-dibenzyl-4,4′-bipyridinium (dibenzyl-viologens or DBV) on a chloride pre-covered Cu(100) electrode surface. Both the dication (DBV^{2+}) and the radical cation ($DBV^{+\cdot}$) could be detected. The DBV^{2+} has been found to adsorb at positive electrode potentials with its main molecular axis parallel to the surface in a nearly face-on orientation. Lowering the potential beyond the thermodynamic reduction potential results in a phase transition with the $DBV^{+\cdot}$ molecule in a more side-on orientation. These results are well consistent with previous in situ STM studies [1] where a distinct phase transition from a “cavitand” phase to a polymeric stacking phase has been observed. Spectra of this polymeric phase showed also the same characteristic bands as were detected after dibenzyl-viologen adsorption at potentials where isolated dimers $(DBV^{+})_2$ on the surface have been observed. This indicates that the formation of both phases is based on the same π-π- and spin paring interactions so that dimers and polymers can be hardly distinguished by IR-spectroscopy only.

[1] Pham et al., New J. Chem., 30 (2006), 1439

O 18.35 Mon 18:30 Poster F

Potential induced phase transition of a Cu monolayer on a Au(1 0 0) surface — •Christian Schlaup, Peter Broekmann, and Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, D-53115 Bonn

Underpotential deposition of Cu on Au(h k l) electrodes has been studied extensively over the past. For underpotential deposition of Cu on Au(1 0 0) electrodes in sulfuric acid electrolytes, these in situ STM studies revealed a commensurate Cu(1 × 1) structure in which Cu adatoms occupy 4-fold hollow sites [1]. Additional quasi-hexagonal Cu adlayer structures with an intermediate coverage identified by STM were traced back to chloride contaminations caused by the reference electrode [1]. However, our own experiments revealed a reversible phase transition between the commensurate Cu(1 × 1) structure at potentials near to Cu bulk deposition and a stripe structure at more positive potentials, near to the dissolution of the Cu upd layer. This phase transition of the Cu adlayer was also observed after exchanging the deposition electrolyte for a blank sulfuric acid solution, pointing to a constant Cu coverage during the phase change. Within a single stripe of the anodic phase, the Cu-Cu distances are shortened perpendicular to the stripe direction whereas between different stripes the Cu-Cu distances are elongated. The potential depended appearance of the two phases points to a stabilisation of the reconstructed phase by (bi)sulfate anions.

[1] F.A. Möller, O.M. Magnussen, R.J. Behm, *Phys. Rev. B* **1995**, *51*, 2484.

O 18.36 Mon 18:30 Poster F

SXPS studies of viologens adsorbed on a halogenide precovered Cu(100) electrode — •Stephan Breuer[1], Thanh Pham Duc[1], Sascha Hümann[2], Peter Broekmann[3], Ralf Hunger[4], Thomas Mayer[4], and Klaus Wandelt[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn — [2]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf — [3]BASF AG, G-CAE/WED - M320, 67056 Ludwigshafen — [4]Institut für Materialwissenschaften, TU Darmstadt, c/o BESSY, Albert-Einstein-Str. 15, 12489 Berlin

We have studied the redox-chemistry of Dibenzyl(DBV)- and Diphenyl(DPV)-Viologenes adsorbed on a chloride and iodide precovered Cu(100) single crystal electrode using cyclic voltametry (CV), in-situ electrochemical scanning tunneling microscopy (ECSTM) and ex-situ X-ray photoelectron spectroscopy with synchrotron radiation at BESSY II (SXPS). From ECSTM it is known, that DBV undergoes a structural phase transition on the anion modified Cu(100) surface as a function of electrode potential. While a checkerboard like cavitand-structure at positive potentials is formed by DBV^{2+}- dications a stripe-phase at negative potentials consists of $DBV^{+\cdot}$-radical cations. This assignment is supported by the N1s-electron binding energies of 402 eV (dications) and 400,7 eV (radical cations) as measured by SXPS. DPV forms only a stripe-phase of radical-cations consistent with a N1s energy of 400,6 eV. No additional chloride or iodide anions are intercalated within the respective viologene layer, as concluded from the Cl2p and I4d signals, respectively.

O 18.37 Mon 18:30 Poster F

Adsorbate-adsorbate interactions at electrochemical interfaces: S/Cu(001) in HCl solution — •Andriy Taranovskyy, Tunay Tansel, and Olaf Magnussen — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel, Germany

Following up our previous high-speed scanning tunneling microscopy study of sulfide tracer diffusion on Cu(001) in 0.01M HCl solution [1], we here present an analysis of the mutual motion of sulfide dimers in this system at room temperature. From the experimental video data histograms of the changes of the atomic configurations in subsequent frames were obtained. By fitting those to a theoretical model of dimer motion, based on solution of master equations, the hopping rates of S_{ad} in the presence of a neighboring S_{ad} were extracted. The pair interaction potential obtained from these rates shows an oscillatory distance dependence indicating anisotropic interactions. Also an influence of the electrode potential on the adsorbate interactions was observed.

[1] T. Tansel and O. Magnussen, Phys. Rev. Lett. 96, 026101 (2006).

O 18.38 Mon 18:30 Poster F

In-situ atomic-scale studies of the mechanisms and dynamics of bismuth electrodeposition by Video-STM — •Hisayoshi Matsushima[1], Erwin S. Lin[2], Sylvie Morin[2], and Olaf M. Magnussen[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, Kiel, Germany — [2]Chemistry Department, York University, Ontario, Canada

We present direct studies of mechanisms and dynamics of underpotential (UPD) and overpotential (OPD) electrodeposition of bismuth on Au(111) in 0.1 M HClO4 solution by in-situ high-speed scanning tunneling microscopy (Video-STM). Nucleation of Bi second layer islands in the OPD regime occurs heterogeneously at domain boundaries of the UPD layer, starting by trapping of isolated Bi adatoms. High-resolution images of the anisotropic (needle-like) growth [1] reveal the motion of bilayer kinks along the needle edges, indicating parallel growth of both layers.

[1] C. A. Jeffrey, D. A. Harrington and S. Morin, Surf. Sci., 512, L367 (2002)

O 18.39 Mon 18:30 Poster F

X-ray reflectivity studies of the liquid mercury-vapor and the liquid mercury-electrolyte interface — •Annika Elsen, Bridget Murphy, Jochim Stettner, and Olaf Magnussen — Institut für experimentelle und angewandte Physik der Universität Kiel, Leibnizstraße 19, 24118 Kiel

Although the liquid mercury-electrolyte interface is one of the most studied electrochemical systems, almost no structural data on this interface exists up to now. We recently started first investigations of this interface by synchrotron x-ray reflectivity. Here we discuss a new liquid mercury electrochemical cell design, for combined reflectivity and electrochemical measurements on the mercury surface covered with an electrolyte solution. The cell allows the insertion of a degassed mercury sample as well as dearated electrolyte solution under a high purity inert gas atmosphere. Preliminary electrochemical data and results of x-ray-reflectivity measurements on the liquid mercury-vapor and the liquid mercury-electrolyte interface using a laboratory source will be presented

O 18.40 Mon 18:30 Poster F

Au model anodes for Li-ion batteries studied by in-situ X-ray diffraction — •Frank Uwe Renner[1,2] and Hiroyuki Kageyama[2] — [1]MPI für Eisenforschung, Düsseldorf, Germany — [2]AIST, UBIQEN, Ikeda, Osaka, Japan

We present first results of experiments on the electrochemically-driven alloying and de-alloying of Au substrates with Li-ions from organic electrolytes studied by in-situ X-ray diffraction employing Synchrotron radiation. Au(111) single crystals, 111-textured thin Au films and nanometer-sized Au particles on HOPG have been examined using a specially designed in-situ X-ray cell. Starting from single crystalline Au systems we could follow the structural degradation and pulverization under different electrochemical conditions. Reciprocal lattice space maps show the occurrence of powder-like intensity associated with different Li-Au alloy phases. The diffraction data from the bulk Au crystals is compared with the Au(111) thin films and the behavior of the Au nano-particles on HOPG.

O 18.41 Mon 18:30 Poster F

Confined electronic state in small Co islands on Cu(100) — •Timofey Balashov[1], Albert F. Takacs[1], Markus Däne[2], Arthur Ernst[2], Patrick Bruno[2], and Wulf Wulfhekel[1] — [1]Physikalisches Institut, Universität Karlsruhe, Wolfgang-Gaede Strasse 1, 76131 Karlsruhe, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

We investigated the electronic structure of 3ML Co islands on Cu(100) with scanning tunneling microscopy and spectroscopy. A standing wave pattern was observed on the islands in the energy region from -50 to 100 meV with respect to the Fermi energy. We were able to extract the dispersion curve for this state by comparing the state energy on islands of different sizes, with different wavelengths of the standing wave pattern. The observed dispersion corresponds well to a minority Co band in theoretical band structure calculations.

O 18.42 Mon 18:30 Poster F

Mn/Cu(111): alloying, electronic and magnetic properties — Marko Kralj[1], Christian Breinlich[2], Sanja Krajinovic[1], Petar Pervan[1], Conrad Becker[2], and •Klaus Wandelt[2] — [1]Institute of Physics, Bijenicka 46, HR-10000 Zagreb — [2]Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn

Spin-split two-dimensional (2D) states which can, for instance, be realized in magnetically stabilized surface alloys, are of immense technological interest for new spintronic devices. For example, Mn/Cu(100)-c(2x2) is considered as a prototypical 2D magnetic alloy [1]. We have studied the interaction of manganese with a Cu(111) surface using different surface sensitive techniques. While the electronic structure and perfectness of a periodic root-3 alloy were characterized by ARPES and LEED, the electronic characteristics of the surface occupied by single Mn atoms were studied by STM and STS. STS at low temperature indicates no observable Kondo-effect for single Mn atoms. Increasing the temperature, leads to incorporation of Mn atoms into and below the surface layer and the appearance of very specific surface defect structures. Formation of this surface alloy first leads to the quenching of the Cu(111) surface state. Only after annealing higher than 500 K, when Mn atoms are incorporated several layers deep, leading to complex changes in the LEED pattern, ARPES indicates the appearance of a modified surface state. All this seems to indicate none or very weak magnetic and spin-splitting effects for Mn/Cu(111).

[1] M. Wuttig, Y. Gauthier, S. Blügel, Phys.Rev.Lett. 70 (1993) 3619.

O 18.43 Mon 18:30 Poster F

Co multilayers on diamond surfaces: Results from ab-initio studies — •Bernd Stärk, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster

In recent years there has been an ever increasing interest in the development and understanding of metal-semiconductor hybrid systems. They may 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 our work structural, electronic and magnetic properties of Co multilayers on diamond surfaces are investigated within the framework of density functional theory employing the local-spin-density approximation together with Gaussian orbital basis sets and norm-conserving pseudopotentials.

For one Co monolayer on a C(111)-(1×1) surface we find that Co adsorption in on-top positions is energetically most favorable. The attached Co monolayer has a weak magnetic moment of $0.69\,\mu_B$, much smaller than that of an isolated Co(0001) monolayer, which we find to be $1.88\,\mu_B$. This behavior can be attributed to the strong covalent bond forming between Co and C atoms. Adsorption of further Co(0001) layers results in a monotonous increase in the magnetic moment M_{top} of the topmost Co layer. In the case of four Co adlayers M_{top} is already close to the magnetic moment at the clean Co(0001) surface. The evolution of the magnetic moment with increasing number of Co adlayers will be discussed on the basis of the respective electronic structure.

O 18.44 Mon 18:30 Poster F

Crystal-induced surface state of Ni(111) modified by a h-BN overlayer — •Karen Zumbrägel[1], Christian Eibl[1], Kathrin Wulff[1], Matthias Hengsberger[2], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Münster, Germany — [2]Physik-Institut, Universität Zürich, Switzerland

The physics of electronic states at surfaces and interfaces is a highly relevant topic in the context of miniaturised electronic devices. We have studied the influence of a monolayer boron nitride (BN) on Ni(111) with spin-resolved inverse photoemission. While interface states have already been identified and thoroughly studied with respect to their dispersion and spin polarization [1], the behaviour of the crystal-induced surface state of clean Ni(111) [2] upon BN adsorption remains controversial. Our spin-resolved results will be discussed along with theoretical and experimental work available in the literature.

[1] K. Zumbrägel, K. Wulff, Ch. Eibl, M. Donath and M. Hengsberger (to be published) [2] M. Donath, F. Passek, and V. Dose, Phys. Rev. Lett. **70**, 2802 (1993).

O 18.45 Mon 18:30 Poster F

Potential der Mehr-Elektronen-Einfang-Spektroskopie zur Untersuchung des Oberflächenmagnetismus — •Marco Busch, Stephan Wethekam und Helmut Winter — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstraße 15, D-12489 Berlin

Unipan et al. [PRL 96 (2006) 177601; PRA 74 (2006) 062901] haben eine Methode zum Studium des Oberflächenmagnetismus vorgestellt. Sie beruht auf dem Zerfall autoionisierender He**-Zustände, die bei der Streuung von He^{2+}−Ionen an Oberflächen durch resonanten Elektroneneinfang formiert werden. Die relative Besetzung von Singulett- und Triplett-Zuständen wird zur Bestimmung der lokalen Spin-Polarisation von Ni(110) verwendet. Ausgehend von $T = 300$ K wird bei Erhöhung der Temperatur bis zu T_C auf eine Verringerung der Spin-Polarisation von -90% (bei 300 K) auf 0% geschlossen. In vergleichbaren Experimenten beobachten wir an Ni(110) eine ausschliessliche Besetzung von Singulett-Zuständen, die etwa 0,7 eV unterhalb E_F liegen, während der Triplett-Zustand (2,4 eV unterhalb E_F) nur sehr geringfügig besetzt wird. Eine signifikante Triplett-Population konnte am sauberen Ni(110) nicht nachgewiesen werden, sondern erst nach Adsorption von O_2 ($\ll$1 L) bei 300 K verbunden mit einer Erhöhung der Austrittsarbeit um bis zu 0,5 eV. Bei anschliessender Erhöhung der Temperatur bis zu T_C desorbiert der Sauerstoff vollständig und die Besetzung des Triplett-Zustandes nimmt wieder ab. Unsere Befunde legen daher nahe, dass die von Unipan et al. beobachteten Effekte auf Verunreinigungen des Ni(110) sowie deren thermische Desorption zurückzuführen und nicht mit dem Oberflächenmagnetismus korreliert sind.

O 18.46 Mon 18:30 Poster F

Magnetic properties of thin Fe films grown on GaAs(110) in a two-step process — Lars Winking, Martin Wenderoth, •Swante Sievers, Jan Homoth, and Rainer G. Ulbrich — IV. Phys. Inst., Georg-August-Universität Göttingen

Thin Fe films grown on GaAs at room-temperature (RT) or above in general suffer from As outdiffusion and the formation of nonmagnetic compounds at the heterointerface [1]. To avoid such a interdiffused interface we deposited thin Fe films of up to 5 ML thickness on in-situ cleaved GaAs(110) at 130 K and subsequently annealed them within 2 hours to RT in the second step. At RT we studied the in-plane magnetic anisotropy (IPMA) of the Fe films in UHV by means of the Magneto-Optical Kerr Effect (MOKE). Most noticeable and in contrast to Fe films grown at RT or above is the presence of a clear hysteresis already at 3.5 ML film thickness as well as an IPMA in [001] [2]. Recent results on the LT growth of thin Fe films on GaAs(001) suggest that these properties are due to the suppression of As outdiffusion [1]. This is substantiated by the square hysteresis loops. The absence of gradual magnetization reversals indicates single domain Fe films nearly free of defects or precipitates [3]. From these experimental results we deduce that reactions at the heterointerface can be efficiently suppressed by the two-step growth process. This work was supported by the DFG-SFB 602 TP A7

[1] J.-M. Lee et al., PRB 76, 052406 (2007) [2] M. Gester et al., JAP 80, 347 (1996) [3] Y. Chye et al., APL 80, 449 (2002)

O 18.47 Mon 18:30 Poster F

Mechanochemistry of thiolates on gold surfaces — •Jordi Ribas, Nisanth N. Nair, and Dominik Marx — Lehrstuhl fuer Theoretische Chemie, Ruhr Universitaet Bochum, 44780 Bochum

The capability to manipulate molecules on the atomic scale by Atomic Force Microscopy techniques has recently made it possible to induce and control chemical reactions and to construct new nanoscale architectures by applying external mechanical forces. The system consisting of thiolate molecules adsorbed on gold surfaces is not only well accessible to such experiments but previous theoretical work [1] has shown that it is possible to draw gold nanowires when alkylic thiolates are pulled off a stepped gold surface or off small gold clusters.

In this contribution we will present the results of the computational studies we have carried out to explore which nanostructures are generated and which chemical phenomena take place when other more complex thiolates rather than the alkylic ones are pulled off a gold surface. Specifically, we will compare the mechanochemical behavior of alkylic and aromatic thiolates and we will explore the mechanochemistry of bidentate and tridentate thiolates. These simulations have been performed by means of DFT static calculations and *ab initio* molecular dynamics calculations. Overall, our results have implications for the stability and degradation of molecule/metal junctions as used, for instance, in coatings and molecular electronics.

[1] (a) Krüger, D.; Fuchs, H.; Rousseau, R.; Marx, D.; Parrinello, M. *Phys. Rev. Lett.* **2002**, 89, 186402; (b) Krüger, D.; Rousseau, R.; Fuchs, H.; Marx, D. *Angew. Chem Int. Ed.* **2003**, 42, 2251.

O 18.48 Mon 18:30 Poster F

Optically monitored wet chemical preparation of SEIRA active metallic nanostructures — •Dominik Enders[1,2], Tadaaki Nagao[1,2,3], Tomonobu Nakayama[1,2], and Masakazu Aono[1,2,3] — [1]National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba, Ibaraki, 305-0044, Japan — [2]Nanoscale Quantum Conductor Array Project, ICORP, JST, 4-1-8 Honcho, Kawaguchi, Saitama, 332-0012, Japan — [3]WPI Center for Materials Nanoarchitectonics (MANA), 1-1 Namiki, Tsukuba, Ibaraki, 305-0044, Japan

The use of wet chemical methods for the preparation of surface enhanced infrared absorption (SEIRA) active nanostructures has gained much interest in the last years because of its easiness, simplicity, and the low time consumption compared to the known ultra high vacuum based methods. We present a two-step wet-chemical preparation method of plasmonic SEIRA active nanostructures. While in the first step spherical Au nanoparticles are deposited on the SiO_2/Si surface, these nanoparticles are grown in the second step to form elongated tabular islands close to the percolation threshold. In situ monitoring of the preparation process by IR spectroscopy ensures the control of film morphology during the preparation process and enables the reproducible fabrication of highly sensitive SEIRA films [1].

A comparison of our Au films with SEIRA inactive Au films shows, that in IR spectra of octadecanethiol, the CH stretching vibrational peaks are enhanced by several orders of magnitude.

[1] D. Enders, T. Nagao, T. Nakayama, and M. Aono, *Jpn. J. Appl. Phys. (in press).*

O 18.49 Mon 18:30 Poster F

Microscale structure formation at the surface of the intercalation system $TaS_2 : Rb$

— Jens Buck[1], •Eric Ludwig[1], Florian Kronast[2], Kai Rossnagel[1], Hermann Dürr[2], and Lutz Kipp[1] — [1]IEAP, Uni Kiel — [2]BESSY, Berlin

Several effects at the surface of the transition metal dichalcogenide TaS_2 occuring under deposition of Rubidium have already been studied in the past, among them nanowire network formation and the well-known metal-insulator transition. Results from spatially resolved experiments such as PEEM reveal a variety of new surface structures at the microscale. The evolution of such structures at increasing Rb concentration was examined stepwise with regard to chemical composition and topography. In contrast to preliminary results, no creation of surface cracks could be observed. It is therefore suggested that crack formation strongly depends on the preparation conditions and the sample history. The PEEM measurements were performed at beamline UE49-PGMa at BESSY,Berlin.

O 18.50 Mon 18:30 Poster F

Electron confinement in nanostructures on Cu(111)

— •Sebastian Wedekind, Guillemin Rodary, Dirk Sander, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle(Saale)

The deposition of 0.7 ML Co onto the clean Cu(111) surface at room temperature leads to the formation of various nanostructures such as hexagonal and triangular vacancy islands on Cu(111), triangular Co islands and elongated rectangular stripes of Cu bounded by parallel dislocation lines. We study the electron confinement within these nanostructures by the means of scanning tunnelling microscopy (STM) and spectroscopy (STS) at 7 K and observe pronounced spatial modulation patterns in the electron local density of states (LDOS) of the nanostructures. We extract the wave-vector (k) of these LDOS modulation patterns in the electron energy range from -1 to $+1$ eV to obtain the electron dispersion relation. We obtain a discontinuous, step-like dispersion relation, which indicates wave-vector quantization according to $k_n = n\pi/d$, where d is the characteristic length of the nanostructure, and n integer [1]. A parabolic fit through the discrete k-states gives the surface state band edge $E_0 = -0.43 \pm 0.01$ eV and the electron effective mass $m^*/m_e = 0.39 \pm 0.01$, where m_e is the electron mass. For the Co islands we find $E_0 = -0.08 \pm 0.02$ eV and $m^*/m_e = 0.42 \pm 0.01$. The step-like dispersion relation also identifies the complete eigenstate-spectrum of the confined system.

[1] G. Rodary, D. Sander, H. Liu, H. Zhao, L. Niebergall, V. Stepanyuk, P. Bruno, and J. Kirschner, Phys. Rev. B **75**, 233412 (2007)

O 18.51 Mon 18:30 Poster F

Direct Writing of Nanostructures with an Electron-Beam in Ultra High Vacuum: Concepts, Results and Rerspectives

— Michael Schirmer, Thomas Lukasczyk, Marie-Madeleine Walz, Florian Vollnhals, Miriam Schwarz, Hans-Peter Steinrück, and •Hubertus Marbach — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, D-91058 Erlangen

The engineering of nanostructures with controlled shape and chemical composition is of pivotal importance for a large number of technological applications as well as for fundamental research. In this work we discuss the generation of nanostructures by using an electron-beam in an ultra high vacuum (UHV) environment. The presented approaches are based on the capability of a high energy electron beam to locally modify adsorbed precursor molecules or the properties of the substrate. Our main method is the electron-beam induced deposition (EBID). The novel aspect is to work in an ultra clean environment, i.e., UHV, which allows us to overcome a hitherto existing limitation concerning the rather poor cleanliness of the deposits and the size limitation due to electron-beam spread in bulk substrates. The successful generation of clean metallic and oxidic nanostructures with lithographic controlled shapes and with lateral dimensions partially smaller than 10 nm on different substrates are reported. The underlying processes, the perspectives and applications of EBID in UHV as well as alternative methods to exploit an electron-beam for lithographic nanostructuring will be discussed. Supported by DFG grant MA 4246/1-1.

O 18.52 Mon 18:30 Poster F

Investigation of the low dimensional surface system Pt(110) by angle-resolved UV-photoemission

— •Peter Amann, Mariana Minca, Michael Cordin, Alexander Menzel, and Erminald Bertel — Institute of Physical Chemistry, University of Innsbruck, Innrain 52a, A-6020 Innsbruck, Austria

Photoemission of low dimensional systems is of major importance for the investigation of correlation. The Pt(110) system provides quasi one dimensional d-derived surface resonances which bear a divergent DOS at the Fermi level due to a 2D saddle point topology. Therefore one can expect maxima in the response function at wave vectors connecting the saddle points. Furthermore a strong temperature anomaly of the adsorbate covered system Br/Pt(110) is observed. As the c(2x2) phase is cooled down from RT to 50K it undergoes a phase transition and two new phases, the (3x2) and the p(2x1), additionally appear [1]. The various surface systems as well as possible driving mechanisms (e.g. Fermi-surface nesting) for the transitions are discussed. Additionaly a detailed investigation of the saddle point topology is done by temperature dependent Fermi-surface measurements.

[1] E. Dona et. al. Phys. Rev. Lett. 89, 186101 (2007)

O 18.53 Mon 18:30 Poster F

Leed spot profile analysis of a quasi-one-dimensional system as a function of temperature

— •Michael Cordin, Peter Amann, Enrico Doná, and Erminald Bertel — Institute of Physical Chemistry, University of Innsbruck, Innrain 52a, A-6020 Innsbruck, Austria

We employ low-energy electron diffraction (LEED) to investigate phase transition on the quasi-one-dimensional c(2x2)-Br/Pt(110) surface. Lowering the temperature yields a transition from a fluctuating, long range ordered phase at room temperature into an inhomogeneous state. From the LEED spot profile analysis we determine the temperature dependence of the fluctuations and the unusual reduction of the long range order parameter with falling temperature. Furthermore we observe the appearance of additional LEED spots corresponding to a primitive (2x1) and a (3x2) overstructure. The transition from the long-range ordered c(2x2) room temperature state to the inhomogeneous low-temperature state is completely reversible. The correlation length in the system is strongly anisotropic. The results agree with STM data showing the formation of striped disorder and local (2x1) and (3x2) domains at 60 K. DFT calculations yield a degeneracy of the three structures at 0 K. The formation of a long-range ordered state at 300 K out of a low-temperature disordered state seems in apparent contradiction with entropy considerations, but can be rationalised by assuming temperature-dependent interactions in the system. A possible explanation is a Peierls interaction in a surface resonance.

O 18.54 Mon 18:30 Poster F

Fundamental concepts for the structure formation of metalorganic networks based on oligopyridines and copper

— •Achim Breitruck[1], Harry E. Hoster[1], Christoph Meier[2], Ulrich Ziener[2], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm — [2]Institute of Organic Chemistry III, Ulm University, D-89069 Ulm

We studied the structures of metalorganic coordination networks formed by Cu co-deposited with Bis-terpyridine (BTP) molecules on graphite (HOPG). BTP molecules have been shown to form highly ordered adlayers stabilized by C-H···N type hydrogen bonds.[1] Using these adlayers as precursors, subsequent deposition of Cu leads to a partial lift of the hydrogen bonds to allow for the formation of even more stable Cu···N-pyridine interactions.[2] Depending on the deposited amount of Cu and BTP and also on the sample temperature during and after Cu deposition we find a high variety of ordered metalorganic 2D structures. Despite this large variety, similar characteristic building blocks were observed, in which Cu centers are surrounded by BTP molecules to form chiral units like Cu_nBTP_m (n = 1, 2; m= 3, 4)[2] out of achiral BTP's.

[1] H.E. Hoster, M. Roos, A. Breitruck, C. Meier, K. Tonigold, T. Waldmann, U. Ziener, K. Landfester, R.J. Behm, Langmuir 23, 11570-11579 (2007)

[2] A. Breitruck, H.E. Hoster, C. Meier, U. Ziener, R.J. Behm, Surf. Sci. 601, 4200-4205 (2007)

O 18.55 Mon 18:30 Poster F

Electron-Beam Induced Deposition (EBID) for the Generation of Nanostructures on Inert Metal Single Crystal Surfaces

— •Marie-Madeleine Walz, Michael Schirmer, Thomas Lukasczyk, Hans-Peter Steinrück, and Hubertus Marbach — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie

II, D-91058 Erlangen

Nanoelectronic devices, quantum computing and the generation of specific catalytically active structures are some applications in the fast growing field of nanotechnology. The prerequisite in this field is the generation of nanostructures of high purity and defined shapes. For this purpose electron-beam induced deposition was applied under ultra high vacuum (UHV) conditions. With this method, adsorbed precursor molecules are locally cracked, mainly by secondary electrons resulting from the impact of a high energy primary electron-beam from a scanning electron microscope (SEM). After the successful generation of clean metallic and oxidic nanostructures on semiconductor and reactive metal substrates, this contribution focuses on inert metal surfaces as substrates. Thereby, unwanted processes, like the catalytic decomposition of the precursor molecules without electron exposure, should be reduced. The generation of metallic or oxidic nanostructures was performed with various organometallic precursor molecules. One example is the fabrication of titanium oxide nanostructures on a Au(111) surface using Ti(^{i}OPr)$_4$ as precursor molecule. The chemical composition was studied by local Auger electron spectroscopy (AES). The work is supported by DFG grant MA 4246/1-1.

O 18.56 Mon 18:30 Poster F

Deviation from pure s-wave scattering of surface-state electrons from adatoms — •Tobias Sonnleitner and Jascha Repp — Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg

Surface state electrons on the close-packed surfaces of noble metals form a two-dimensional nearly-free electron gas. The scattering of the electrons off adatoms generates standing wave patterns in the electron density, which can be directly observed with the scanning tunneling microscope. Analysis of the standing wave patterns provides a direct way to determine the scattering properties of the adatoms. So far it has been widely accepted that metal adatoms act as s-wave scatterers due to the efficient screening of the adatom potential by bulk electrons. However, a deviation from a pure s-wave scattering would only express itself in the fraction of the standing wave pattern arising from multiple scattering events. This fraction is rather small since adatoms act as ideal absorbing black scatterers. Therefore, it is not obvious from the experimental point of view, that the assumption of a pure s-wave scattering is justified. To this end we have studied isolated pairs of copper adatoms on a clean Cu(111) substrate surface. The standing-wave patterns around these pairs have been analyzed in numerous different arrangements in order to average out effects from other scattering centers far away. In comparison to calculated patterns the fraction of these patterns arising from multiple scattering events has been extracted.

O 18.57 Mon 18:30 Poster F

Non-linear Optical Properties of Nanostructured Metal Surfaces — •Heike Arnolds[1], Natalia Garcia[1], Simon J. Henley[2], and J. David Carey[2] — [1]Surface Science Research Centre, University of Liverpool, Oxford Street, Liverpool, L69 3BX, UK — [2]Nano-Electronics Centre, Advanced Technology Institute, School of Electronics and Physical Sciences, University of Surrey, Guildford GU2 7XH, UK

Nanosecond pulsed-laser irradiation of Ag and Ni thin films was employed to produce nanostructured Ag/SiO$_2$ and Ni/SiO$_2$ substrates. By tailoring the laser fluence, it is possible to controllably adjust the mean diameter of the resultant near-spherical metal droplets [1]. We have investigated the nonlinear optical properties of these nanostructured films and find a strong enhancement of femtosecond infrared-visible sum and difference frequency yields by two to three orders of magnitude, depending on the exact size and shape of the metal droplets. The likely cause of the enhancement is the excitation of plasmons in the infrared and visible regions of the spectrum and the concomitant electric field enhancement near the metal droplets. We discuss the use of these films for plasmon-enhanced photochemistry.

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O 18.58 Mon 18:30 Poster F

STM analysis of the fluctuations at 2D phase boundaries between ordered and disordered organic adlayers — •Thomas Waldmann, Harry E. Hoster, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

The dynamic equilibrium between distinct 2D phases of organic molecules on Ag(111)-oriented films on Ru(0001) at room temperature are studied by time resolved STM. As recently found, the parallel chain structure (PCS) [2] formed by a bis(terpyridine) derivative (2,4'-BTP)[1] can be produced coexistent with a disordered 2D molecular adlayer [2]. At the boundaries between both phases a continuous exchange of molecules takes place with equal rates. At room temperature, these fluctuations are too fast for direct STM-observation, even at scan rates of 5 images s^{-1}. Adapting the approach previously applied to analyse the step dynamics at metal surfaces [3], we evaluated the displacement of the phase boundary in single scan lines as a function of time. The results are discussed in comparison with 2D phase equilibria observed at other coverages [4] and with metal step fluctuations.

[1] C. Meier, U. Ziener, K. Landfester, P. Weihrich, J. Phys. Chem. B 109, 21015 (2005)

[2] M. Roos, H.E. Hoster, A. Breitruck, R.J. Behm, Phys. Chem. Phys. 9, 5672 (2007)

[3] M. Giesen, S. Baier, Atomic transport processes on electrodes in liquid environment, J. Phys.: Condens. Matter 13, 5009 (2001)

O 18.59 Mon 18:30 Poster F

Modes in dielectric loaded surface plasmon polariton waveguides — •Jan Renger[1], Maria Ujué González[1], Sukanya Randhawa[1], Romain Quidant[1], Sébastien Massenot[2], Jonathan Grandidier[2], Alexandre Bouhelier[2], Gerard Colas des Francs[2], Laurent Markey[2], Jean-Claude Weeber[2], and Alain Dereux[2] — [1]ICFO-Institut de Ciencies Fotoniques, 08860 Castelldefels (Barcelona), Spain — [2]Institut Carnot de Bourgogne, UMR 5209 CNRS-Université de Bourgogne, F-21078 Dijon Cedex, France

Surface plasmon polaritons (SPPs) existing at metal/dielectric interfaces feature a high confinement of the electromagnetic field, which make them very promising for small photonic devices and biochemical sensors. Dielectric loading of the metal surface by thin dielectric layers, such as SiO$_2$, can be used to alter the SPP effective mode index n$_{eff}$. In this way, optical elements can be designed by patterning the dielectric layer to get areas with different n$_{eff}$. In particular, SPP waveguides can be obtained by depositing thin SiO$_2$ stripes on top of gold films. We analysed the SPPs on dielectric loaded waveguides having a width down to 100 nm by leakage radiation microscopy. The imaginary part of n$_{eff}$ - therewith the propagation length - was measured in the object plane; the real part of n$_{eff}$ was determined in the Fourier plane. The measured propagation length for very narrow dielectric stripes is close to the SPP propagation length at the bare metal interface. For increasing width of the dielectric stripes, the additional modes contribute and the propagation length is reduced to the value at an infinite extending dielectric loaded metal film.

O 18.60 Mon 18:30 Poster F

Ab initio study of oxygen adsorption and initial incorporation in Pd-Pt alloy — •Arezoo Dianat, Manfred Bobeth, and Wolfgang Pompe — Institut fuer Werkstoffwissenschaft, Technische Universitaet Dresden, Germany

In order to get insight into the catalytic behavior of the bimetallic alloy Pd-Pt, the adsorption of oxygen on the alloy surface as well as the initial oxygen incorporation have been studied by means of density-functional theory. Due to segregation processes the composition of the near-surface layers of the alloy is in general different from the bulk composition. In this work, ordered bulk phases (L1$_0$,L1$_2$) of Pd$_x$Pt$_{1-x}$ with compositions $x = 0.25$, 0.5, 0.75 as well as different compositions and atom configurations of the two outermost layers have been investigated. Adsorption energies for oxygen adsorbed *on* the (111) alloy surface and for oxygen in sub-surface position have been calculated for different oxygen coverages (0.25 to 1 ML). In the case of oxygen adsorption *on* the surfaces, the highest adsorption energy at low oxygen coverage ($\leq$ 0.25 ML) has been found for the Pd$_{0.5}$Pt$_{0.5}$ composition o f the two outermost layers, whereas at higher coverage the oxygen binding energy is highest for a Pd-rich first monolayer and Pt-rich second monolayer. Interestingly, on the latter layer system the oxygen adsorption energy is higher than on pure Pd(111). Oxygen occupation of sub-surface sites starts at a coverage of 0.5 ML for all alloy models considered. The calculated oxygen adsorption energy depends only weakly on the bulk composition. It increases slightly with Pt bulk concentration, but it differs less than 50 meV.

O 18.61 Mon 18:30 Poster F

Growth and characterization of single-wall carbon nanotubes for electronic and optical applications — •Hans Kleemann, Philipp Zeigermann, Michael Blech, Mathias Steglich, and Bernd Schröter — Universität Jena, Institut für Festkörperphysik, Max-Wien-Platz 1, 07743 Jena, Deutschland

A controlled growth of carbon nanotubes with particular structural and electronic properties at predefined positions on solid substrates is a prerequisite to utilize them in electronic or nanooptical devices. We grow single-wall nanotubes by thermal chemical vapour deposition (CVD) on various substrates like silicon, fused silica and sapphire as well as on silicon carbide. Metal films are vacuum-evaporated to catalyze the growth of high-purity single-wall nanotubes by CVD using methane as precursor gas. The quality of nanotubes is tested by raman and x-ray spectroscopy: residual catalyst amount and contamination is in general lower than the detection limits of these techniques. The morphology and orientation of the nanotubes is characterized by scanning electron and atomic force microscopy. A preferred orientation is observed on the (single-crystalline) surface of sapphire.

O 18.62 Mon 18:30 Poster F

Self-selection and Error Correction in Multi-ligand Supramolecular Networks at Surfaces — •Steven L. Tait[1], Alexander Langner[1], Nian Lin[1], Chandrasekar Rajadurai[2], Mario Ruben[2], and Klaus Kern[1,3] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart — [2]Forschungszentrum Karlsruhe GmbH — [3]Ecole Polytechnique Fédérale de Lausanne, Switzerland

Supramolecular networks stabilized by metal–organic coordination can be designed to self-organize in regular, two-dimensional lattices at surfaces, whose dimensions and properties can be controlled by selection of the organic ligand components. This approach offers a natural and highly efficient alternative to current nano-fabrication methods and provides a model system for (bio-)molecular assembly. With high-resolution scanning tunneling microscopy of such networks, we demonstrate structural error correction during assembly achieved by active molecular self-selection. Experiments were made by deposition of Fe atoms and organic ligands at the Cu(100) surface. Binary mixtures of complementary ligands allow for constructions of highly-ordered 2D arrays of compartments, whose shape and size can be predictably programmed by modular ligand replacement. Redundant mixtures of ligands of different sizes demonstrate the ability of the system to correct structural errors and achieve a high degree of order by sorting themselves into rows according to molecule size. We contrast this with a ligand mixture where the energy landscape of the intermolecular interactions does not activate an error correction mechanism, but rather provides a route for structural error tolerance.

O 18.63 Mon 18:30 Poster F

Growth of SiGe nanoislands on prestructured silicon subtrates — •Marlen Schulze, Anne-Kathrin Gerlitzke, and Torsten Boeck — Institute for Crystal Growth in the Forschungsverbund Berlin e. V.

Coherently strained and highly ordered silicon-germanium nanoscale pyramids on silicon, grown by liquid phase epitaxy (LPE) via the Stranski*Krastanov growth mechanism are very interesting objects to reduce the size of semiconductor devices. Generally, LPE is very well appropriate to study fundamental atomistic processes at the liquid-solid interface because it operates very close to thermodynamical phase equilibrium.

A patternlike array of SiGe nanostructures has been realised on prestructured silicon substrates. Si (100) substrates have been patterned by squarelike oxide stripes using local oxidation nanolithography in an atomic force microscope (AFM). The width of the stripes is precisely controlled by progress of the lateral oxidation. Subsequently, LPE was employed to grow SiGe nanoislands on the prepatterned substrates. The truncated pyramids are arranged within the oxide-free cavities directly along the stripes. The final island size significantly probes an effectively lowered lattice mismatch, i.e. a locally expanded crystal lattice in noncovered areas of the silicon substrate.

O 18.64 Mon 18:30 Poster F

Surface- induced handedness in adsorbed layers — •Philipp Schmidt-Weber[1], Thorsten Kampen[1], Arantzazu Mascaraque[2], Rocio Cortez[2], Jan-Hugo Dil[1], and Karsten Horn[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Universidad Autonoma de Madrid, Spain

Molecules that are achiral in the gas phase may acquire a chiral character through the loss of symmetry elements, which has a strong influence on their arrangement in long-range ordered structures. We have studied stilbene and its derivates, using STM, LEED and photoemission with the aim of identifying such ordering processes. Dicarboxystilbene (DCSB) loses its carboxyl hydrogen atom when adsorbed on Cu(110), and acquires a handedness on the surfaces which is readily seen in STM images. The two enantiomers then arrange in different long-range ordered structures (”herringbone” and ”parquet” patterns), which themselves possess a handedness, i.e. they exist in a dextro- and laevo- form. Using STM images in which both the substrate and the adsorbate are imaged with atomic resolution, we were able to identify two distinct types of adsorption sites as basic building blocks of the long-range structures. One of these (the ”parquet” pattern) is enantiomerically pure, while the other (”herringbone”) is a racemic structure. The fact that the latter is the thermodynamically stable one can be understood from general thermodynamic principles.

O 18.65 Mon 18:30 Poster F

Comparative study of the structure formation by two different bis(terpyridine)derivates (BTP) on HOPG — •Michael Roos[1], Christoph Meier[2], Daniel Caterbow[2], Harry E. Hoster[1], Ulrich Ziener[2], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — [2]Institute of Organic Chemistry III, Ulm University, D-89069 Ulm, Germany

Depostition of BTP molecules on HOPG by evaporation in UHV or from solution leads to large domains of highly ordered structures, which are stabilized by C-H···N type hydrogen bonds [1-3]. The energetically most favorable molecule-molecule configuration can be modified by varying the position of the N-atoms within the BTP molecules. Furthermore, depending on the deposited amount and the deposition conditions (solvent and concentration), a large variety of ordered structures is obtained. The possibility to describe these structures as a sum of localized molecule-molecule and molecule-substrate interactions is discussed. In addition, the role of dynamic effects like molecule mobility and rotation for the stability of the different phases is considered.

1. H. E. Hoster et al., Langmuir 23, 11570 (2007).
2. A. Breitruck et al., Surf Sci 601, 4200 (2007).
3. C. Meier et al., J Phys Chem B 109, 21015 (2005).

O 18.66 Mon 18:30 Poster F

SERS and single-molecule SERS in metallo-dielectric structures — •Manuel Rodrigues Gonçalves, André Siegel, and Othmar Marti — Ulm University, Institute of Experimental Physics, Albert-Einstein-Allee 11, D-89081 Ulm, Germany

Surface enhanced Raman scattering (SERS) refers to a technique to enhance the Raman scattering cross section of few molecules adsorbed on metallic surfaces, in order to achieve high enhanced spectra. Despite its success as a chemical identification technique at very low molecular concentrations, its main drawbacks are the extreme sensitivity to the electromagnetic enhancements of the metallic structures, the poor reproducibility, and the fabrication of structures with defined strong field enhancements at specific wavelengths.

Single-molecule SERS requires very high field enhancements, of the order of 10^{14}. The Raman spectra of very few, or single molecules present a blinking behaviour. It is commonly accepted that the blinking is characteristic of the Raman spectra of single molecules, adsorbed at metallic clusters or structures with extreme enhancements.

We have fabricated metallo-dielectric structures suitable for SERS using colloidal crystals as templates. The fabrication of the structures is reproducible. FEM and FDTD calculations indicate that very high field enhancements can be expected. Experiments using a confocal Raman microscope find blinking SERS at the predicted locations. This is an indication of a low number of molecules in the detection volume.

O 18.67 Mon 18:30 Poster F

Nanosecond-laser interference pattering at 266nm wavelength — •Mike Hettich, Stephen Riedel, Paul Leiderer, and Johannes Boneberg — University of Konstanz, Departement of Physics, D-78457 Konstanz, Germany

Direct laser interference patterning by ns-laser pulses allows producing periodic surface structures in a single illumination step. For that purpose thin metallic films (Au, Ta) or Si wafers are irradiated by two or more interfering laser beams. The local intensity variations achieved in this way induce lateral flow of material. We show that this enables achieving structures with a periodicity down to 150nm, if the fourth harmonic of a ns-Nd:YAG-laser is used. Upon moving the substrate laterally between the first and subsequent illumination steps, structure periods below $\lambda/2$ can be realized.

O 18.68 Mon 18:30 Poster F

SERS on micro-fabricated sharp-etched nanostructures — •Henrik Schneidewind[1], Uwe Hübner[1], Dana Cialla[2], Roland Matthes[1], Jörg Petschulat[3], Siegmund Schröter[1], and Jürgen Popp[1,2] — [1]Institute of Photonic Technology (IPHT), Albert-Einstein-Straße 9, 07745 Jena, Germany — [2]Friedrich-Schiller-University Jena, Department of Physical Chemistry, Jenaer Biochip Initiative (JBCI), Helmholtzweg 4, 07743 Jena, Germany — [3]Friedrich-Schiller-University Jena, Institute of Applied Physics, Center for Ultra-Optics, Max-Wien-Platz 1, 07743 Jena, Germany

We introduce highly reproducible metallic nanostructure arrays which can be used as active substrates for the Surface Enhanced Raman Spectroscopy (SERS). The arrays were prepared by means of e-beam lithography, vacuum deposition, and ion-beam etching. The sharp-edged gold nanostructures with corner radii smaller than 20 nm are arranged in arrays with a periodicity of 200 nm. Sharp-edged structures were chosen instead of round dots, which are easier to prepare, in order to achieve large enhancement factors by using the lightning rod effect. The resonance frequency of the arrays was determined by using UV-Vis-spectrometry in order to select the excitation wavelength for SERS experiments. The arrays showing uniform SERS-signals across the whole field size of 0.2 mm in edge length are ready for practical use, which will be shown using a dye as test substance.

O 18.69 Mon 18:30 Poster F

In-situ Etching of self-organized InAs/GaAs (001) Quantum Dots — •Theresa Lutz[1], Takayuki Suzuki[1], Lijuan Wang[1], Suwit Kiravittaya[1], Armando Rastelli[2], Oliver G. Schmidt[2], Giovanni Costantini[1], and Klaus Kern[1,3] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]Leibniz Institute for Solid State and Materials Research, Dresden — [3]Ecole Polytechnique Fédérale de Lausanne, Switzerland

It is well known that the epitaxial growth of InAs on GaAs(001) leads to the development of strain induced nanoscale islands with high crystalline quality. Because of the enormous potential for device applications there is a great interest in understanding the growth process in detail. Even though there are a lot of experimental results concerning the growth of quantum dots, the physics behind it is not completely understood yet. Recently, it has been shown that during growth a transition takes place from small shallow faceted pyramidal islands to bigger and steeper islands, so-called domes. We use selective InAs in-situ etching to systematically modify the island size. The result is a backward transition of the islands as a function of the etching time. The details of the shape transition are discussed taking into account the non-uniform composition of the islands. This demonstrates that the shape of the quantum dots depends on their size and composition, which is typical for processes close to thermodynamic equilibrium.

O 18.70 Mon 18:30 Poster F

Fabrication of Cobalt clusters by pulsed laser deposition — •Markus Trautmann, Christian Pansow, Matthias Büenfeld, Veit Grosse, Frank Schmidl, and Paul Seidel — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, D-07743 Jena

Besides Fe and Ni (and different Fe-/Ni-compounds) Co is a catalyst material used in synthesis of carbon nanotubes (CNTs). Clusters can be formed for example by annealing of thin Co films which are usually produced by sputtering technique or electron beam evaporation. To get applicable clusters for the growth of CNTs thin films of about 1 nm are required. In this work we use pulsed laser deposition (PLD). This method enables low deposition rates of less than 0,04 monolayers per pulse using a 99,99 % Co target and a KrF excimer laser. We present our experimental set up for PLD under different vacuum conditions to produce Co layers on SiO_2-coated Si-substrates. First results of surface and film analysis using different methods as atomic force microscopy (AFM), x-ray diffraction (XRD), scanning electron microscopy (SEM) and Auger electron spectroscopy (AES) will be presented.

O 18.71 Mon 18:30 Poster F

Production of patterned metal clusters using Focused Ion Beams (FIB) — •Farhad Ghaleh[1], Niklas Grönhagen[1], Heinz Hövel[1], Lars Bruchhaus[2], Sven Bauerdick[2], Jürgen Thiel[2], and Ralf Jede[2] — [1]Technische Universität Dortmund, Exp. Physik I, Dortmund — [2]Raith GmbH, Dortmund

Nanometer sized pits on HOPG substrates can be used as nucleation centers to produce clusters with a narrow size distribution. In previous experiments [1] nanometer sized pits were produced by sputtering and oxidizing the sample. As a result we get nanopits which are a few nanometers wide and only one monolayer deep, distributed at random locations on the surface.

In the present study a focused beam of gallium ions is used to produce nanopits in a given pattern on the substrate. The FIB instrument (Raith ionLiNE) is capable of a resolution below 10 nm [2]. Using the nanopits as nucleation centers we are able to produce patterned gold islands as well as patterned silver clusters by depositing metal atoms.

Furthermore the nanopit distribution on the surface in combination with Monte Carlo simulations helps investigating the ion beams, e.g. ion distribution, recoils as well as the penetration depth of the ions [3]. In this respect the oxidation of HOPG-samples provides a method to study the ion impact effects.

[1] H. Hövel, Appl. Phys. A 72, 295 (2001)

[2] J. Gierak et al.: Appl. Phys. A 80, 187 (2005)

[3] F. Ghaleh, R. Köster, H. Hövel, L. Bruchhaus, S. Bauerdick, J. Thiel, R. Jede: J. Appl. Phys. 101, 044301 (2007)

O 18.72 Mon 18:30 Poster F

In-situ Scanning Tunneling Microscope studies of the ripening process of InAs Quantum Dots on GaAs during Growth in the MOVPE — •M. Guderian, R. Kremzow, M. Pristovsek, and M. Kneissl — TU Berlin, Institut für Festkörperphysik, EW 6-1, Hardenbergstr. 36, D-10623 Berlin, Germany

Quantum dots (QD) are highly interesting for a number of different applications, like single photon emitters or semiconductor lasers. For industrial applications these optoelectronic devices are mainly grown by metal organic vapour phase epitaxy (MOVPE) systems which allows mass fabrication. QD growth has been studied intensely, but the understanding of the mechanisms responsible for the formation of the QDs and especially of the ripening process is still poor. In order to investigate the dynamics of the ripening process and to clarify the theory of QD ripening we employed our novel in-situ scanning tunnelling microscope (STM) technique which allows measurements directly during MOVPE growth. In this presentation we will discuss the ripening process of InAs QDs on GaAs(001):Si at 475°C where the development of the surface was analysed directly with the in-situ STM. Ex-situ AFM measurements showed a big scattering of the data, due to different substrates and varying cooling rates, while the in-situ measurements showed clear trends in RMS roughness and size distributions. E.g. the dot density decreased proportional to e^{-1} while the average dot size increased. In comparison of different ripening theories our experimental result follows the classical Ostwald ripening theory for the InAs on GaAs(001):Si system.

O 18.73 Mon 18:30 Poster F

Melting behaviour of metallic nanostructures — •Daniel Benner, Anja Habenicht, Paul Leiderer, and Johannes Boneberg — Universität Konstanz, Fachbereich Physik, LS Leiderer, 78457 Konstanz

Triangular flat metallic nanostructures and metallic films of identical thickness on inert substrates (e.g. glass, silicon) are illuminated by single intensive nanosecond laser pulses with fluences at and above the melting threshold and the melting behaviour of these two systems is compared.

For the metallic thin films we determine the melting threshold by nanosecond time-resolved reflectivity measurements which can be used to deduce the melting time. Upon melting of the nanostructures a dewetting process sets in which also reduces the reflected intensity. Our measurements show that the dewetting process of the nanostructures sets in at laser intensities well below the melting threshold of the films. For the dimensions of the nanostructures used here (thickness ~50nm, lateral dimensions ~ 200nm) reduced melting temperatures are not expected. Therefore we assign that behaviour to the increased absorption cross section of the nanostructures.

O 18.74 Mon 18:30 Poster F

Preparation and Characterization of Gold Nanocrystals on the native Oxide Layer of Si-Surfaces — •Jawad Slieh, Andreas Winter, Aaron Gryzia, Armin Brechling, Wiebke Hachmann, and Ulrich Heinzmann — Molecular and Surface Physics, Bielefeld University

We report on the fabrication of gold crystals in the size range between one hundred nm and several μm, using a combination of a sputter and an annealing technique. Gold was deposited on the native oxide layer of freshly cleaned silicon wafer pieces (10×10 mm^2) in an inert gas sputtering chamber at a rate of 5 nm/min. Subsequently the samples were transferred into a UHV chamber and annealed for several hours at temperatures between 800°C and 1000°C. The deposited gold layer thickness and the annealing temperature and time have been studied systematically. After preparation, the gold crystals were characterized by means of different techniques such as Atomic Force Microscopy (AFM), Transmissions Electron Microscopy (TEM), Scanning Electron Microscopy (SEM), X-Ray Diffraction (XRD) and Laue Diffraction.

These different sized gold crystals will be used in a diffraction experiment (Laue configuration) with a micro focus x-ray tube (Oxford Instruments UltraBright) in order to estimate the minimal crystal size for the observation of diffraction spots of individual gold crystals. First results of these experiments will also be discussed.

O 18.75 Mon 18:30 Poster F

Mass selected Co clusters in contact with semiconductor surfaces — •Viola v. Oeynhausen, Kristian Sell, Ingo Barke, and Karlheinz Meiwes-Broer — Institut für Physik, Universität Rostock, Universitätsplatz 3, 18051 Rostock

Metal-semiconductor structures are of substantial technical relevance since Schottky-barrier based devices are fundamental elements of high-speed electronic applications. Metal nanoparticles on semiconductor surfaces can be seen as a model system for such devices. The Scanning Tunneling Microscope (STM) provides insight in transport properties on nanometer scale and at low temperature. Furthermore, it reveals the geometric structure and shape of clusters, an important prerequisite for understanding the detailed electronic and magnetic properties. We produce mass-selected Co clusters with an Arc Cluster Ion Source (ACIS) and deposite them onto Si(111)7x7 and Ge(001) under UHV conditions. These are ideal substrates due to their well-known electronic structure and simple preparation under UHV conditions. They serve as a reference in STS measurements, thus minimizing tip-induced artefacts. Macroscopic Cobalt surfaces show dominant, highly localized d-states near the Fermi level . Such states are proposed to cause interesting effects like Kondo interaction and spin modulation of captured surface state electrons.

O 18.76 Mon 18:30 Poster F

Study of supported metal Clusters and nano Dots with time and energy resolved PEEM — •Martin Rohmer[1], Christian Schneider[1], Michael Bauer[2], Heinz Hövel[3], Farhad Ghaleh[3], and Martin Aeschlimann[1] — [1]Technische Universität Kaiserslautern, 67663 Kaiserslautern — [2]Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24118 Kiel — [3]Experimentelle Physik I, Universität Dortmund, 44221 Dortmund

The ultrafast dynamics associated with collective (plasmon) excitations as well as single electron excitations in supported clusters is addressed with high lateral resolution by means of the time- and energy resolved two-photon Photoemission Electron Microscopy (TR-2PPEEM). Experiments performed at different cluster and nanostructured systems show that this setup is capable to map even very small particle to particle variations in the hot electron lifetime of the order of a few femtoseconds [1]. The high temporal sensitivity of time-resolved PEEM to these inhomogenities arises from the parallel data acquisition mode intrinsic to this technique. It significantly reduces the resolution limiting influence of systematic error arising from temporal fluctuations in the experimental parameters. Here we report about the potential and our progress in measuring electron live times in silver clusters and nano dots.

[1] Mapping the femtosecond dynamics of supported clusters with nanometer resolution, M. Rohmer, F. Ghaleh, M. Aeschlimann, M. Bauer, H. Hövel; Eur. Phys. J. D, Online First

O 18.77 Mon 18:30 Poster F

Image-potential states at (001) surfaces of alkaline-earth metal oxides — •Björn Baumeier, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

We present the results of a comparative *ab initio* study of the atomic and electronic structure of MgO, CaO, SrO and BaO and their relaxed (001) surfaces. Based on density functional theory, we use self-interaction-corrected pseudopotentials which permit a reliable description of electronic properties, in particular. The calculated bulk and surface geometric structures are consistent with well established literature data. The bulk electronic structure turns out to be in very good agreement with the results of quasiparticle calculations and experiment. Concerning surface electronic properties, the calculations reveal, in particular, that MgO(001), CaO(001) and SrO(001) exhibit negative electron affinity while BaO(001) does not. As a consequence, not only bound surface states which are localized at the surface occur in the former three cases but also a salient band of image-potential states appears in sections of the surface Brillouin zone which reside in vacuum in front of the surface. Such image-potential states do not arise at the BaO(001) surface.

The image-potential states at MgO(001) are compared to traditional image-potential states at Cu(001) and to traditional surface states at MgS(001), respectively. This exemplary comparision reveals details of the peculiar nature of the image-potential states at (001) surfaces of alkaline-earth metal oxides.

O 18.78 Mon 18:30 Poster F

Tensor LEED study of the surface relaxation of $SrF_2(111)$ — •Stephan Härtel, Jochen Vogt, and Helmut Weiss — Chemisches Institut der Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, D-39106 Magdeburg

The knowledge about the surface relaxation of other insulators than the alkali halides is comparatively weak yet. Experimental work was carried out for instance for $CaF_2(111)$ and $BaF_2(111)$ [1] which both crystallize in the fluorite structure. Very often those two compounds are treated together with the homologous material SrF_2 but up to now there are no quantitative experimental results available for the surface relaxation of this alkaline earth fluoride. In the present work the $SrF_2(111)$ surface was investigated by means of LEED in an energy range from 80 to 320 eV. The recorded I(E) data were analyzed using the tensor LEED approach. The topmost F^- layer in the first F-Sr-F triple layer is shifted inward by $0{,}13\pm0{,}07$ Å whereas the Sr^{2+} layer does not exhibit a significant shift. The following F^- layer is also relaxed towards the bulk by $0{,}07\pm0{,}07$ Å which is in the range of the measuring accuracy. No significant changes of the ion positions in the deeper triple layers were observed. The results are in qualitative good agreement with a theoretical calculation [2] for $SrF_2(111)$.

[1] Vogt, J. et al., Surf. Sci. **578** (2005)

[2] Jockisch et al., J. Phys.: Cond. Matt. **5** (1993)

O 18.79 Mon 18:30 Poster F

Exploring Optical Properties of MgO Films with an STM — •Hadj Mohamed Benia, Philipp Myrach, Niklas Nilius, and Hans-Joachim Freund — Fritz-Haber-Institut, Berlin, Germany

Electron injection from the tip of an STM is used to stimulate local photon emission from the surface of a thin MgO film on Mo(001). Depending on the excitation energy, several emission regimes are identified on the basis of the energy and the spatial distribution of the emitted photons. At low excitation bias, tip-induced plasmons are preferentially excited in the tip-sample gap, carrying little information on the oxide. With increasing tip bias, radiative electron transitions between field-emission resonances dominate the optical response. Their dependence on the local work function allows mapping of this quantity across the oxide film. Intrinsic optical modes of the MgO, e.g. radiative decays of excitons, are only observed when operating the STM in the field emission regime.

O 18.80 Mon 18:30 Poster F

Diffraction of fast atoms and molecules during grazing scattering from a LiF(001) Surface — •Andreas Schüller, Stephan Wethekam, and Helmut Winter — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstraße 15, 12489 Berlin

Neutral atoms and molecules with energies from 300 eV up to some 10 keV are scattered under a grazing angle of incidence from a clean and flat LiF(001) surface. For scattering along low index directions in the surface plane ("axial surface channeling") we observe defined patterns in the intensity distributions for scattered atoms which can be attributed to diffraction effects [1, 2]. The data can be understood by diffraction of fast atoms at the surface where the symmetry of the crystal lattice and of the interaction potential between atom and surface determine the diffraction pattern. The periodicity of the surface potential follows the geometrical arrangement of surface atoms and determines the angular position of diffraction peaks. The corrugation of the surface potential determines the characteristic intensity modulations of these diffraction peaks which can be observed also for fast and for heavy atoms, where diffraction based on the periodicity of the crystal lattice can not be resolved. Such so called "supernumerary rainbows" allows one to derive the corrugation of atomic interaction potentials in the eV regime with high accuracy.

[1] A. Schüller, S. Wethekam, and H. Winter, Phys. Rev. Lett. 98, 016103 (2007).

[2] P. Rousseau, H. Khemliche, A.G. Borisov, and P. Roncin, Phys. Rev. Lett. 98, 016104 (2007).

O 19: Evening Talk Gerhard Ertl

Time: Monday 20:00–21:00 Location: Urania

Reaktionen an Festkörper-Oberflächen: Vom Atomaren zum Komplexen

O 20: Plenary Talk James Hudspeth

Time: Tuesday 8:30–9:15 Location: H 0105

How hearing happens

O 21: Invited Talk Stefan Blügel

Time: Tuesday 9:30–10:15 Location: HE 101

Invited Talk O 21.1 Tue 9:30 HE 101

Electrons at Surfaces Taking an Unexpected Turn — •Stefan Blügel — Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

Electrons in the vicinity of surfaces are in a space asymmetric environment. This causes a number of interesting phenomena, like the Rashba spin-orbit effect [1], spin-depending scattering [2] and spin-polarized electrons [3] at non-magnetic surfaces, which little attention had been paid to in the past. For electrons at magnetic surfaces, thin films and nanostructures also time-inversion symmetry is broken. This can give rise to an unidirectional exchange interaction, known as Dzyaloshinsky-Moriya (DM) interaction. Although this interaction, favoring spatially rotating spin structures, is known for nearly 50 years, its consequences for the magnetic structure in low-dimensional magnets remained basically unexplored. We show by *ab initio* calculations that the DM interaction can cause homochiral magnetic phases at achiral surfaces – phases, which had been overlooked during the past 20 years – but have been observed recently in terms of a left rotating cycloidal spiral for Mn on W(110) [4]. Theoretical models [5] display a rich phase diagram of possible magnetic phases. At the end, I will present arguments motivating the search for the existence of a lattice of nano-skyrmions.

[1] Yu. M. Koroteev *et al.*, Phys. Rev. Lett. **93**, 046403 (2004).
[2] J.I. Pascual *et al.*, Phys. Rev. Lett. **93**, 196802 (2004).
[3] T. Hirahara *et al.*, Phys. Rev. Lett. **97**, 146803 (2006).
[4] M. Bode *et al.*, Nature **447**, 190 (2007).
[5] M. Heide *et al.*, submitted to Phys. Rev. B.

O 22: Invited Talk Johannes Pollmann

Time: Tuesday 10:15–11:00 Location: HE 101

Invited Talk O 22.1 Tue 10:15 HE 101

Adsorption Processes on SiC Surfaces: First-Principles Theory — •Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster

The surface atomic structure, the topology of surface dangling bonds, and the high directionality of adsorbate-substrate interactions play a crucial role in the chemical activity of semiconductor surfaces. This has been well appreciated in many adsorption studies using silicon surfaces as prototype substrates. In this respect, the ionic compound semiconductor SiC offers particularly interesting new degrees of freedom because of its comparatively small lattice constant and its rich variety of surface reconstructions which give rise to very amazing and unusual adsorption processes in certain cases, as observed in experiment. For example, atomic hydrogen adsorbed on the fairly open SiC(001)-(3×2) surface does not lead to surface passivation but induces surface metallization. Likewise, molecular hydrogen readily adsorbes at room temperature dissociatively on the SiC(001)-c(4×2) surface while it does not react with SiC(001)-(3×2) although both surfaces are characterized by similar surface dimers. Interestingly, adsorption of hydrocarbons on SiC(001)-(3×2) versus Si(001)-(2×1) shows salient substrate-related differences, as well. In this talk adsorption of atomic and molecular hydrogen, acetylene, ethylene and benzene, as well as silicon-oxynitride adlayers on SiC surfaces will be discussed. Scrutinizing a number of reaction scenarios within first-principles theory allows us to identify the physical origin and nature of the peculiar adsorption behaviour of SiC surfaces.

O 23: SYNF: Ferroic Materials and Novel Functionalities I (FV: MA+O+MM+DF+DS+HL+TT)

Time: Tuesday 10:30–13:15 Location: A 151

See SYNF for details about the program.

O 24: SYSA: Tayloring Organic Interfaces: Molecular Structures and Applications I (Invited Speaker: Fernando Flores; FV: DS+CPP+HL+O)

Time: Tuesday 9:30–10:45 Location: H 0105

See SYSA for details about the the program.

O 25: SYSA: Tayloring Organic Interfaces: Molecular Structures and Applications II (Invited Speakers: Norbert Koch, Antoine Kahn; FV: DS+CPP+HL+O)

Time: Tuesday 10:45–13:00 Location: H 0105

See SYSA for details about the program.

O 26: Methods: Electronic Structure Theory

Time: Tuesday 11:15–12:30 Location: MA 042

O 26.1 Tue 11:15 MA 042

Improved description of correlation energies within an ab-initio framework — •Judith Harl and Georg Kresse — Vienna University, Sensengasse 8/12, 1090 Vienna, Austria

A well known shortcoming of the standard exchange-correlation functionals (LDA and GGA) used in density functional theory is that they do not include long-range correlation and therefore fail to describe Van-der-Waals bonded systems accurately.

The adiabatic connection fluctuation-dissipation theorem (ACFDT) [1,2] provides an exact expression for the correlation energy depending on the system's response function when switching from the Kohn-Sham to the full many-body Hamiltonian. ACFDT calculations for real systems, mostly within the random phase approximation (RPA), have become feasible recently (e.g. [3,4]).

In this work, we apply the ACFDT within the RPA to rare-gas solids and to a set of insulators and metals. Lattice constants and bulk moduli are improved compared to gradient corrected functionals with relative errors reduced by roughly a factor 2.

[1] D.C.Langreth, J.P.Perdew, Solid State Commun. **17**, 1425 (1975).

[2] O.Gunnarsson, B.I.Lundqvist, Phys. Rev. B **13**, 4274 (1976).

[3] F.Furche, Phys. Rev B **64**, 195120 (2001).

[4] A.Marini *et al.*, Phys. Rev. Lett. **96**, 136404 (2006).

O 26.2 Tue 11:30 MA 042

Long-range electronic correlation quantified in rare gas/metal adsorption: Xe/Cu(111). — •Mariana Rossi, Xinguo Ren, Andrea Sanfilippo, Paula Havu, Volker Blum, and Matthias Scheffler — Fritz-Haber-Institut, Berlin, Germany

The adsorption of rare gases on metal surfaces should be a classic example of physisorption, but the underlying electronic binding mechanism remains under debate. Here, we revisit Xe/Cu(111), where empirical potentials predict binding, but the wrong adsorption site (fcc hollow instead of top); in constrast, standard DFT finds the right binding site, but either overbinds significantly (LDA) or hardly binds at all (GGA). To create a systematic picture of binding in this system, we apply the recent local xc correction scheme of Hu, Reuter and Scheffler [1] and a hierarchy of electronic structure approaches of increasing sophistication: LDA, GGA (PBE and BLYP), hybrid functionals, semiempirical C6 corrections for Van der Waals, and MP2, all carried out within the same computational framework, the all-electron code FHI-aims [2]. The inclusion of MP2 is critical to recover the correct Xe binding distance (d=3.6 Å). [1]Q. Hu, K. Reuter, and M. Scheffler, Phys. Rev. Lett. **98**, 176103 (2007); **99**, 169903(E) (2007). [2] V. Blum *et al.*, The FHI-aims project, www.fhi-berlin.mpg.de/aims/

O 26.3 Tue 11:45 MA 042

On the accuracy of DFT exchange-correlation functionals for H bonds in small water clusters: Benchmarks approaching the complete basis set limit — •Biswajit Santra[1], Angelos Michaelides[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany. — [2]London Centre for Nanotechnology and Department of Chemistry, University College London, London WC1E 6BT, UK.

The ability of DFT exchange-correlation functionals to describe H bonds between H_2O molecules remains an important open question. Here, we address this issue through a series of studies of small gas phase water clusters. Using Møller-Plesset perturbation theory (MP2) as our reference, we have assessed the abilities of 16 DFT xc functionals to describe the energetics of the low energy isomeric structures of water dimers, trimers, tetramers, and pentamers. Errors from basis set incompleteness have been minimized in both the MP2 reference data and the DFT calculations, thus, enabling a systematic evaluation of the true performance of the tested functionals. Among the functionals considered, the hybrid X3LYP and PBE0 functionals are the best: predicting H bond strengths within 10 meV (∼0.3 kcal/mol) of MP2. Of the nonhybrid GGA functionals, mPWLYP and PBE1W perform the best. The popular BLYP and B3LYP functionals consistently underbind. PBE, PW91, and TPSS display rather variable performance with cluster size, leading us to conclude that results from dimers and trimers alone are insufficient to determine the general abilities of a given functional.

O 26.4 Tue 12:00 MA 042

Constrained adiabatic DFT modeling nonadiabatic behavior - simple and effective — •Matthias Timmer and Peter Kratzer — Fachbereich Physik, Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

Non-adiabatic effects, in our case the creation of electron-hole pairs, become more and more accessible in theoretical calculations, and they have long been observed experimentally in, e.g., the detection of chemicurrents. We present a new method to calculate the excitation spectrum of electron-hole pairs in adsorption on metals for adatoms which have an initial spin magnetic moment. To accomplish this we use a mapping of the system onto a bosonic Hamiltonian. Starting from adiabatic DFT calculations we calculate the classical trajectory of the adatom. This trajectory can be used to calculate the nonadiabatic occupations of the adiabatic Kohn-Sham states. Nonadiabaticity is originating from spin relaxation effects. In order to describe this relaxation, the spin degree of freedom is treated explicitly within the density matrix formalism. A projection on the adsorbate orbitals is then used to change the occupation of the adiabatic KS states in a way that guarantees the obtained spin polarization localized at the adatom. By treating the spin up and spin down case separately, and by using the density of states, we get separate energy spectra for the spin up and spin down case, and for electrons and holes, which is novel for these computationally fast adiabatic DFT calculations. As an example, we apply our method to the system H on Al(111). We compare our results to previous TDDFT and model calculations.

O 26.5 Tue 12:15 MA 042

Electronic properties of PbTe/CdTe(100) interfaces — •Roman Leitsmann and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller Universität Jena

Previously studied semiconductor interfaces often consist of chemically different materials with the same crystallographic structure. Usually they are influenced by lattice-constant mismatch and the polarity of adjacent surfaces. Here we investigate the electronic structure of interfaces between highly ionic crystals with different crystal structure but nearly identical cubic lattice constants by first principles total energy calculations in the repeated slab approximation. The interfaces are strongly influenced by electrostatic fields. As a prototypical example we investigate the structural well defined polar PbTe/CdTe(100) interfaces [1,2,3].

We develop four different different slab models to calculate the band offsets and projected interface band-structures. These models are used to investigate the electronic properties. The occurrence of interface states is studied versus the different approaches. Moreover we discuss the reliability of the four approaches for the description of different experimental situations.

[1] W. Heiss et al., APL 88, 192109 (2006) [2] R. Leitsmann et al., New J. Phys. 8, 317 (2006) [3] R. Leitsmann et al., PRB 74, 085309 (2006)

O 27: Time-Resolved Spectroscopy II

Time: Tuesday 11:15–12:45 Location: MA 043

O 27.1 Tue 11:15 MA 043

Unoccupied band-structure and hot electron lifetimes in Pb and Bi quantum-wells — Andreas Ruffing[1], •Stefan Mathias[1], Martin Wiesenmayer[2], Luis Miaja-Avila[3], Frederik Deicke[1], Henry Kapteyn[3], Margaret Murnane[3], and Michael Bauer[2] — [1]Department of Physics, TU Kaiserslautern, 67663 Kaiserslautern — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany — [3]JILA, University of Colorado, Colorado 80309-0440, USA

The two-dimensional electronic structure of metallic quantum wells (QW) enable an unique access to peculiarities of solid state band structures by means of momentum resolved photoelectron spectroscopy, such as avoided crossings, band gaps or modifications due to interactions at interfaces. With respect to ultrafast dynamical processes in metals these features are highly interesting as they enable for instance insights into the relevance of band-structure details for the decay of hot electrons. Momentum and time-resolved two-photon photoemission (2PPE) performed with a two-dimensional electron analyzer for parallel energy (E) and momentum ($k_{||}$) detection provide the required sensitivity for such experiments. In this contribution we will present and discuss first results obtained for ultrathin Pb and Bi quantum wells grown on a Cu(111) substrate. The 2PPE experiments enable us to directly map the unoccupied band structure of these systems and the according momentum resolved hot electron lifetime $\tau(E, k_{||})$.

O 27.2 Tue 11:30 MA 043

Photoelectron microscopy of the Mott-Hubbard transition at inhomogeneously Rb adsorbed 1T-TaS$_2$ surfaces — •Dirk Rahn[1], Hans Starnberg[2], Martin Marczynski-Bühlow[1], Tim Riedel[1], Jens Buck[1], Kai Rossnagel[1], and Lutz Kipp[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel, Germany — [2]Department of Physics, Göteborg University and Chalmers University of Technology, SE-41296 Göteborg, Sweden

Layered 1T-TaS$_2$ is of particular interest because it shows a rich phase diagram including various charge-density-wave phases and a first-order metal-insulator transition at about 180K which is widely understood as a Mott-Hubbard-type localization. Using angle-resolved photoemission, it has been shown that a similar metal-insulator transition at the surface of 1T-TaS$_2$ can be induced already at room temperature by simple adsorption of Rb [1]. To further investigate this emerging transition we have tried to prepare sharp Rb domains at the surface of 1T-TaS$_2$. Photoelectron microscopy measurements at beamline BL 31 at MAX-lab (Lund) and photoelectron spectroscopy measurements at beamline BW 3 at HASYLAB (Hamburg) show that it is indeed possible to prepare such a sharp Rb domain and that the Mott-Hubbard transiton is taking place in the Rb adsorbed region. Photoelectron microscopy images of the inhomogeneously Rb adsorbed surface will be presented as well as photoelectron spectra at sites with different alkali metal concentrations. This work is supported by the DFG Forschergruppe FOR 353 and the European Community - Research Infrastructure Action. [1] Rossnagel et. al. Phys. Rev. Lett. 95, 126403 (2005).

O 27.3 Tue 11:45 MA 043

Spectroscopy of TaS_2 through the metal-insulator transition — •Martin Beye, Alexander Föhlisch, Urs Hasslinger, Annette Pietzsch, and Wilfried Wurth — Institut für Experimentalphysik, Universität Hamburg, Deutschland

Soft X-ray spectroscopies allow the analysis of the electronic structure of matter. They are specific to different elements, to their chemical surroundings and to individual orbitals, resolving their polarization. In combination with the newly available pulsed soft X-ray sources, they constitute an ideal tool to locally probe ultra-fast electron dynamics of phase transitions.

The layered material $1T - TaS_2$ for example is at room temperature in a Mott insulating phase and exhibits a transition to a metallic state at liquid nitrogen temperatures, connected with the evolution of a charge density wave and a slight shift in atomic positions. This is well established around the Ta-atoms but should show effects on the electronic structure at S-centers as well. At the synchrotron sources MAX-lab and BESSY, we have studied the occupied and unoccupied electronic states. We observe large differences at both atomic centers depending on sample temperature and on polarization.

In a next step, we will drive the phase transition through excitation with a short-pulsed optical laser and study the electron dynamics on a femtosecond timescale at the free electron laser in Hamburg (FLASH).

We acknowledge the help of the BESSY and MAX-lab staff, in particular Franz Hennies, the group around Kai Rossnagel (University Kiel) who provided the samples and the GrK 1355.

O 27.4 Tue 12:00 MA 043

Ultrafast laser-induced phase transitions in group-V elements — •Nils Huntemann, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretische Physik, Fachbereich Naturwissenschaften, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

A number of pressure-induced phase transitions exist in Arsenic, Antimony, and Bismuth [U. Häussermann et al., J. Am. Chem. Soc. **124**, 15359 (2002)]. These transitions occur in thermodynamical equilibrium. In the last years different nonthermal, ultrafast structural changes have been induced in solids by means of femtosecond laser pulses [See, for example, A. Cavalleri et al., Phys. Rev. Lett. **87**, 237401 (2001)]. These structural transitions take place under extreme nonequilibrium conditions, primarily because laser light interacts very strongly with electrons but not with ions, and secondarily because the electrons thermalize relatively slowly with the ions (typically on a timescale of roughly 10 ps). As a consequence, laser-driven phase transitions are induced while the electrons are very hot, but the ions are still cold.

Based on first-principles electronic structure calculations we explored the possibility of inducing nonthermal structural changes in the above-mentioned group-V elements by ultrashort laser pulses. For this purpose, we determined the potential energy surface (electronic free energy) as a function of the lattice parameters and atomic coordinates for different electronic temperatures, which simulates the ultrafast laser heating of the electrons.

O 27.5 Tue 12:15 MA 043

Kinetic Approach for Laser-Induced Heating of Metals — •Banaz Omar and Baerbel Rethfeld — Technical University of Kaiserslautern, Department of Physics, Erwin Schroedinger Str. 46, D-67663 Kaiserslautern, Germany.

Non-equilibrium distribution functions of electron gas and phonon gas are calculated for metals irradiated with an ultrashort intense laser pulse. The excitation during femtosecond irradiation and the subsequent thermalization of the free electrons, as well as the dynamics of phonons can be described by a kinetic equation. The microscopic collision processes, such as absorption by inverse Bremsstrahlung, electron-electron, and electron-phonon interaction are considered with complete Boltzmann collision integrals. In contrast to aluminum, with a free-electron like conduction band considered in [1], the d-band in gold lies within the conduction band at about 2.5 eV below the Fermi surface of free electrons in s-band. Therefore, secondary electrons may be excited strongly, originating also from the d-band. We apply our kinetic approach to the case of gold by taking the electron density of states into account, and compare with the case of excitation of aluminum.

[1] B. Rethfeld, A. Kaiser, M. Vicanek, and G. Simon, Phys. Rev. B 65, 214303 (2002)

O 27.6 Tue 12:30 MA 043

Electron Transfer & Solvation Dynamics at the NH$_3$/Cu(111) Interface: Determination of Tunneling Barriers — •Julia Stähler, Michael Meyer, Uwe Bovensiepen, Daniela O. Kusmierek, and Martin Wolf — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

Understanding the fundamental processes of heterogeneous electron transfer (ET) is highly important for a variety of different fields, as e.g. the development of nanoscale molecular electronic devices or photovoltaic cells. Here, we investigate ET and solvation dynamics at the interface of amorphous NH$_3$ and Cu(111) using femtosecond time-resolved two-photon photoelectron spectroscopy. After photoexcitation with UV light, metal electrons are injected into the adsorbate layer. They localize at favorable sites and are stabilized by reorientations of the surrounding solvent molecules. Concurrently, they decay back to the metal substrate. Two different regimes are observed for both, electron solvation and electron back transfer: Initially, electron decay and stabilization occur on fs-timescales. The dynamics slow down abruptly after 250 fs leading to electron transfer and solvation on ps-timescales. The lifetime of this second species of solvated electrons depends exponentially on the ammonia layer thickness, showing that ET is mediated by distance-dependent tunneling through an interfacial barrier. The acquired data allows for an estimate of the temporal evolution of this transient potential barrier, yielding profound insight into the ET mechanisms at molecule-metal interfaces.

O 28: Symposium: Size-Selected Clusters at Surfaces II (Invited Speakers: Steven Buratto, Stefan Vajda, Matthias Arenz)

Time: Tuesday 11:15–13:00 Location: MA 005

Invited Talk O 28.1 Tue 11:15 MA 005
Size-selected Au and Ag nanoclusters on rutile TiO2 (110) (1x1) surfaces probed by UHV-STM — Xiao Tong, Lauren Benz, Steeve Chretien, Paul Kemper, Michael Bowers, Horia Metiu, and •Steven Buratto — University of California, Santa Barbara, CA USA

Catalysis of the oxidation of CO and small olefins by Au and Ag nanoclusters on oxide supports is known to be strongly dependent on the size of the cluster and its interaction with the oxide surface. In our group we have probed this size dependence by depositing size-selected clusters of Agn+ and Aun+ (n = 1-7) from the gas phase onto single crystal rutile TiO2 (110) (1x1) surfaces at room temperature under soft-landing (< 2 eV/atom) conditions. We analyze the clusters on the surface using ultra-high vacuum scanning tunneling microscopy (UHV-STM) and compare the resulting structures with theory. In the case of Aun+ , Ag+ and Ag2+ clusters deposited under soft-landing conditions we observe large, sintered clusters indicating high mobility for these species on the surface. For Aun+ (n > 1) and Agn+ (n > 2) clusters deposited under soft-landing conditions, however, we observe a high density of intact clusters bound to the surface indicating that these species have very limited mobility on the surface. We have also shown that the sintering of Au+ soft-landed on TiO2 (110) occurs only for a surface covered with hydroxyl groups. On a pristine surface with an oxygen vacancy density near 10%, Au atoms remain intact on the surface.

Invited Talk O 28.2 Tue 11:45 MA 005
Towards the understanding of size/shape and function relationship in catalysis of complex reactions — •Stefan Vajda[1], Sungsik Lee[1], Larry A. Curtiss[1], Jeffrey P. Greeley[1], Paul C. Redfern[1], Peter Zapol[1], Michael J. Pellin[1], Jeffrey W. Elam[1], Byeongdu Lee[1], Sönke Seifert[1], Randall E. Winans[1], Yu Lei[1,2], Randall J. Meyer[2], Arantxa Fraile-Rodríguez[3], Luis M. Molina[4], Maria J. López[4], Julio M. Alonso[4], Kristian Sell[5], Ingo Barke[5], Armin Kleibert[5], Viola von Oeynhausen[5], and Karl-Heinz Meiwes-Broer[5] — [1]Argonne National Laboratory, Argonne, USA — [2]University of Illinois at Chicago, USA — [3]Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland — [4]Universidad de Valladolid, Valladolid, Spain — [5]Institut für Physik, Universität Rostock, Rostock, Germany

This contribution focuses on partial oxidation reactions catalyzed by sub-nanometer to several ten nanometer large size-selected clusters. Catalytic performance and changes in cluster shape are studied under realistic reaction conditions, allowing to elucidate the size/shape/composition and function relationship in catalysis. Here we show 1) gold and silver clusters which promote with high selectivity the direct oxidation of propylene to propylene oxide, and 2) sub-nanometer platinum clusters catalyzing the oxidative dehydrogenation of propane with high selectivity and activity. Theoretical calculations and modeling provide a detailed insight of the catalytic process. The findings stress the important role of small clusters in promoting reactions with high selectivity and activity.

Invited Talk O 28.3 Tue 12:15 MA 005
Cluster Catalysis: Size dependent reactivity induced by reverse spill-over — •Matthias Arenz, Martin Röttgen, Christopher Harding, Sebastian Kunz, Vahideh Habibour, Viktoria Teslenko, and Ulrich Heiz — Technische Universität München, München, Germany

In heterogeneous, the routes whereby molecules come and go from active sites can substantially affect their reactivity. In the presented work, the CO oxidation rate on size selected Pd clusters supported on thin MgO films is investigated in pulsed molecular beam experiments. By varying the cluster coverage independent of the cluster size, we were able to change the ratio of direct and diffusion flux (reverse spill over) of CO onto the cluster catalyst and thus probe the influence of reverse spill-over on the reaction rate for different cluster sizes (Pd8 and Pd30). The experimental results show, that the change in reaction rate as a function of cluster coverage is different for Pd8 and Pd30. In order to explain these findings, the CO flux onto the clusters is modeled utilizing the collection zone model for the given experimental conditions. The results indicate that for small clusters (Pd8), the reaction probability of an impinging CO molecule is independent of whether it is supplied by diffusion or direct flux. By contrast, for larger clusters (Pd30) a reduced reaction probability is found for CO supplied by reverse spill over compared to CO supplied by direct flux.

O 28.4 Tue 12:45 MA 005
Deuteration of mass-selected C_n clusters deposited on HOPG — •Artur Böttcher, Daniel Löffler, Patrick Weis, Manfred Kappes, Angela Bihlmeier, and Wilhelm Klopper — Institut für Physikalische Chemie, Universität Karlsruhe (TH), D-76128 Karlsruhe, Germany

We studied the size-selectivity in the deuteration of carbon clusters, C_n (n=48-70) deposited on HOPG. In contrast to the weakly stabilized molecular solids of classical fullerenes, the non-IPR fullerenes form strongly bound $[C_n]_m$ oligomers stabilized by covalent bonds between the non-IPR sites in C_n cages. The deuteration procedure has been performed under ultra high vacuum conditions by exposing the deposited layers to atomic deuterium. The adoption of deuterium atoms raises the inter-cage cohesion of the C_{60} and C_{70} films what has been attributed to the formation of D-induced polymeric chains likely comprising covalently interlinked cages. Deuteration of non-IPR films results in considerable weakening of the intercage bonds as revealed by lower sublimation enthalpies found for all C_nD_x films [1]. DFT calculations indicate a considerable reduction of the inter-cage bonds accompanying the progressing D-adoption. This process ends with D-induced scission of oligomers and formation of weakly interacting C_nD_x cages. The contrary reaction trends are triggered by the presence of the non-IPR sites which act as decisive reaction centers. The size of the C_n cages appears of minor relevance for the reaction path.

[1] D. Löffler et al. J. Chem. Phys. Smalley Issue(2007)

O 29: Symposium: Surface Spectroscopy on Kondo Systems I (Invited Speakers: Wolf-Dieter Schneider, Fakher Assaad, Serguei Molodtsov)

Time: Tuesday 11:15–13:30 Location: HE 101

Invited Talk O 29.1 Tue 11:15 HE 101
From single magnetic adatoms to two-dimensional Kondo lattices: A local view — •Wolf-Dieter Schneider — EPFL, Institut de Physique des Nanostructures, CH-1015 Lausanne, Switzerland

The unique ability of scanning tunneling microscopy and spectroscopy to address an individual atom on a surface has contributed considerably to our understanding of fundamental excitations and interactions at the atomic level. Here we present a few case studies from our laboratory. These include the detection of the Kondo effect at magnetic adatoms [1], the observation of very-low-energy adsorbate vibrations [2] revealing a surprising similarity with the spectroscopic signatures of Kondo scattering and spin-flip excitations, the manifestation of local disorder within a Ce-adatom superlattice on Ag(111) in its two-dimensional (2D) electronic bandstructure, and the 2D melting via a hexatic phase of a Ce-adatom superlattice on Cu(111). In such superlattices, depending on the relative strength of Kondo scattering versus RKKY interactions, ferromagnetic or antiferromagnetic adatom pairs at different separations may be formed leading to exciting magnetic properties of such artificial nanostructures. These results provide illustrative examples in the emerging fields of nanoscience and nanotechnology for the characterisation and the controlled engineering of physical properties at the single atom level.

[1] J. Li, W.-D. Schneider, R. Berndt, and B. Delley, Phys. Rev. Lett. 80, 2893 (1998).

[2] M. Pivetta, M. Ternes, F. Patthey, and W.-D. Schneider, Phys. Rev. Lett. 99, 126104 (2007).

Invited Talk O 29.2 Tue 11:45 HE 101

The Kondo Lattice in two dimensions: numerical studies of the Fermi surface. — •Fakher F. Assaad, Kevin S.D. Beach, and Lee C. Martin — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The Kondo lattice model on a square lattice is the simplest model capturing the physics of heavy fermion materials. Below the coherence temperature and in the paramagnetic phase, it describes the heavy fermion metallic state which is characterized by a large Fermi surface with Luttinger volume incorporating both the conduction electrons and the localized moments. In this talk we will review recent results aimed at understanding the evolution and breakdown of this Fermi surface as function of temperature, magnetic field as well as across a magnetic order-disorder transition. Our results stem from large scale Quantum Monte Carlo simulations in the framework of the Dynamical Cluster Approximation.

Invited Talk O 29.3 Tue 12:15 HE 101

ARPES Study of Hybridization Phenomena in Heavy-Fermion Lanthanide Compounds — •Serguei Molodtsov — Dresden University of Technology, Germany

High-resolution angle-resolved photoemission spectra of various heavy-fermion Ce and Yb systems reveal strong momentum (k) dependent splittings of the 4f signals around the expected intersection points of the 4f final states with valence bands in the Brillouin zone [1]. The obtained dispersion of the interacting 4f states both in the region of the Fermi level and at higher binding energies is explained in terms of a simplified periodic Anderson model by a k dependence of the electron hopping matrix element disregarding clearly interpretation in terms of the single-impurity Anderson model for single-crystalline samples. The obtained data show that the heavy-fermion behavior depends crucially on properties of the electronic bands not necessarily located in the immediate vicinity of the Fermi energy.

[1]. S. Danzenbaecher et al. Phys. Rev. B 72 (2005) 033104; Phys. Rev. Lett. 96 (2006) 106402; D.V. Vyalikh et al. Phys. Rev. Lett. 96 (2006) 026404; Phys. Rev. Lett. (2007), accepted.

O 29.4 Tue 12:45 HE 101

k- and spin-dependent hybridization effects in Ce monolayer — •Yury Dedkov[1], Denis Vyalikh[1], Mikhail Fonin[2], Yury Kucherenko[3], Serguei Molodtsov[1], and Clemens Laubschat[1] — [1]Institut für Festkörperphysik, TU Dresden, Germany — [2]Fachbereich Physik, Universität Konstanz, Germany — [3]Institute for Metal Physics, Kiev, Ukraine

Here we present applications of the periodic Anderson model (PAM) to consideration of wave vector (**k**)- and spin-dependent hybridization effects in Ce metal. It was shown that **k**-dependent splitting of the $4f$ ionization peak of Ce/W(110) are correctly described in the framework of the PAM (Coulomb repulsion between two f electrons localized on the same lattice site $U_{ff} \to \infty$). Our results show that the wave vector is conserved upon hybridization. In case of the magnetically ordered Ce monolayer, spin- and angle-resolved resonant photoemission spectra reveal spin-dependent changes of the Fermi-level peak intensities (which reflect the hybridization strength). That indicate a spin-dependence of $4f$ hybridization and, thus, of $4f$ occupancy and local moment. The phenomenon was also described in the framework of PAM by $4f$ electron hopping into the exchange split Fe $3d$ derived bands that form a spin-gap at the Fermi energy around the $\overline{\Gamma}$ point of the surface Brillouin zone.

O 29.5 Tue 13:00 HE 101

High-Resolution Photoemission Spectroscopy on an Ordered Pt_5Ce Surface Alloy: Kondo-Resonance, Band Structure and Fermi Surface — •Christina Albers[1], Markus Klein[1], Kevin Beach[2], Fakher Assaad[2], and Friedrich Reinert[1] — [1]Universität Würzburg, Experimentelle Physik II, 97074 Würzburg — [2]Universität Würzburg, Theoretische Physik I, 97074 Würzburg

We present a detailed investigation of the electronic structure of an ordered Pt_5Ce-film by means of angular resolved ultraviolet photoemission spectroscopy (ARUPS). An *in situ* prepared, ordered Pt_5Ce surface alloy, consisting of alternating layers of Pt_2Ce and kagome-nets of Pt, forms stable and reproduceable films on the Pt substrate. We investigated in detail the $4f$ Kondo resonance, other renormalization effects on the k-dependent band structure, and the temperature-dependence of the spectral features. In particular we studied the $4f$-states by a comparison of the data on Pt_5Ce and Pt_5La. The experimental results will be discussed together with DMFT calculations.

O 29.6 Tue 13:15 HE 101

FeSi - Kondo insulator or itinerant system? — •Dirk Menzel[1], Markus Klein[2], Damian Zur[1], Klaus Doll[3], Friedrich Reinert[2], and Joachim Schoenes[1] — [1]Technische Universität Braunschweig, Institut für Physik der Kondensierten Materie — [2]Universität Würzburg, Lehrstuhl für Experimentelle Physik II — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart

The claim that FeSi is the first Kondo insulator containing no f-electrons [1] resulted in an intense discussion about the nature of this material. However, recent theoretical and experimental investigations have generated more and more arguments for an interpretation of apparently uncommon electronic properties in an itinerant band model. We have performed angle-resolved high-resolution photoemission spectroscopy on FeSi single crystals using a He spectral lamp as well as synchrotron radiation. The photoemission spectra agree qualitatively with the bandstructure derived from single-particle GGA calculations. However, we could also observe strong renormalization effects near the valence band maximum. A quantitative consistency can be obtained when an interaction among the Fe-d-electrons is added to the calculations in the form of self energy corrections. The resulting spectral function is in surprisingly good accordance to the experimental data. These results support the interpretation of FeSi as an itinerant material with d-correlations without the necessity of including Kondo interactions.

[1] G. Aeppli and Z. Fisk, Comments Cond. Mat. Phys. **16**, 155 (1992).

O 30: Phenomena at Semiconductor Surfaces

Time: Tuesday 12:00–14:00 Location: MA 041

O 30.1 Tue 12:00 MA 041

Vibrational relaxation of CO stretching excitation on Si(100): DFT study — •Sung Sakong and Peter Kratzer — Fachbereich Physik, Universität Duisburg-Essen, Duisburg, Germany

On semiconductor and insulator surfaces, the vibrational lifetime of adsorbates can be very long and the vibrational energy is predominantly dissipated to phonons, because electron-hole pair excitations are not allowed. Recently, the lifetime of the CO stretch vibration on Si(100) has been measured to be 2.3 nano seconds (Laß *et al.*, J. Chem. Phys. **123** 051102 (2005)).

We have performed density functional theory calculations within the framework of the generalized gradient approximation for the energy dissipation of the CO vibrational mode on the Si(100) surface. In this scheme, the vibrational relaxation is controlled by the anharmonic coupling between vibrational modes and the interaction between vibrations and phonons. In DFT, vibrational excitations of the adsorbate are accurately described by the multi-dimensional potential energy surface which includes anharmonic coupling between vibrations. And the phonon properties of the underlying Si substrate are calculated with the force field method to treat a large slab. From this information, the coupling between anharmonic vibrations and the phonon continuum is calculated within perturbation theory, thus the transition rate is derived by Fermi's Golden Rule. The calculated lifetime is in qualitative agreement with the experiments and the suggested microscopic decay channels of the stretching mode of C-O into lateral shift/bending quanta and a phonon satisfy energy conservation.

O 30.2 Tue 12:15 MA 041

Cyclopentene (C5H8) on InP(001)(2x4): adsorption structure — •R. Passmann[1,2], P. Favero[3], T. Bruhn[1,2], W. Braun[4], W. G. Schmidt[5], M. Kneissl[1], W. Richter[6], N. Esser[1,2], and P. Vogt[1] — [1]TU Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany — [2]ISAS - Institute for Analytical Sciences, Department Berlin, Albert-Einstein-Str. 9, 12489 Berlin, Germany — [3]Instituto de Física da Universidade de Brasília, Brazil — [4]BESSY GmbH, Albert-Einstein-Str. 15, 12489 Berlin, Germany — [5]Universität Paderborn, Warburger Str. 100, 33098 Paderborn, Germany — [6]Universita Tor Vergata, Via della Ricerca Scientifica 1, 00133 Roma, Italy

In this study we report on the modification of the InP(001)(2x4) surface upon C5H8 exposure, observed by reflectance anisotropy spectroscopy (RAS), synchrotron based PES (SXPS) and LEED. The samples were prepared in ultra high vacuum and the reconstruction formation was controlled by LEED and RAS. The characteristic features at 1.8 eV in the RAS spectra related to the InP(2x4) surface is reduced during the deposition of the molecules and shifted towards higher photon energies. SXPS measurements of the C1s, In4d and P2p core level confirm a covalent bonding of the C5H8 molecules to the top In-P mixed dimer. The molecules can be desorbed at 400°C and the (2x4) reconstruction can be restored. The comparison to DFT total energy calculations supports an interaction between C5H8 and the top-layer dangling bonds. From these results a structural model for the absorption of C5H8 on the InP(2x4) surface is proposed.

O 30.3 Tue 12:30 MA 041

Adsorption of small organic ring molecules on GaAs(001) c(4x4) - Structural and electronic properties — •T. Bruhn[1,2], R. Passmann[1,2], C. Friedrich[1], G. Gavrila[3], T.A. Nilsen[5], W. Braun[4], D.R.T. Zahn[3], B.O. Fimland[5], W. Richter[6], M. Kneissl[1], N. Esser[1,2], and P. Vogt[1] — [1]TU Berlin, Institut für Festkörperphysik, Hardenbergstr.36, 10623 Berlin, Germany — [2]ISAS Berlin, Albert-Einstein-Str.9, 12489 Berlin, Germany — [3]TU Chemnitz, Institut für Physik, 09107 Chemnitz, Germany — [4]BESSY GmbH, Albert-Einstein-Str.15, 12489 Berlin, Germany — [5]NUST, NO-7491 Trondheim, Norway — [6]Universita Tor Vergata, Via della Ricerca Scientifica 1, 00133 Roma, Italy

For a selective implementation of functional organic units in semiconductor devices, a detailed understanding of the electronic and structural properties of the interface is indispensable. In a first step, we have investigated the influence of the adsorption of small ring molecules (Cyclopentene (C_5H_8) and 1,4-Cyclohexadiene (C_6H_8)) on the GaAs $c(4\times4)$ surface. The samples were prepared in UHV and investigated with reflectance anisotropy spectroscopy (RAS), soft x-ray photoelectron spectroscopy (SXPS) and scanning tunneling microscopy (STM). Measurements of the C 1s, Ga 3d and As 3d core levels exhibit a covalent bonding of the molecules to the topmost As dimers. A significant influence on the surface band bending could be observed. Furthermore, the results indicate that the adsorption process depends on functional units of the adsorbed molecules. A structure model of the interface formation is suggested for the first time.

O 30.4 Tue 12:45 MA 041

Terephthalic acid (TPA) on Si(111)-7×7 and Si(111)-$\sqrt{3}\times\sqrt{3}$-Ag surfaces — •Takayuki Suzuki, Theresa Lutz, Giovanni Costantini, and Klaus Kern — Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart

We have carried out STM measurements of terephthalic acid (TPA) deposited on Si(111)7×7 and Si(111)-$\sqrt{3}\times\sqrt{3}$-Ag surfaces. Due to a strong molecule-substrate interaction, TPA molecules do not form any ordered molecular layer but adsorb randomly on the Si(111)7×7 surface with several binding motifs. On the contrary, the interaction of TPA with the Si(111)-$\sqrt{3}\times\sqrt{3}$-Ag surface is much weaker allowing for the formation of an ordered layer stabilized by intermolecular hydrogen bonds. The TPA overlayer is characterized by a modulation of about 2nm in period along the $\langle\bar{1}\bar{1}2\rangle$ direction. This periodicity is not uniform but appears wider in some places and narrower in the others. The wide and the narrow regions have a parallelogram $\begin{pmatrix} 3 & 0 \\ -2 & 7 \end{pmatrix}$ and a rectangular $\begin{pmatrix} 3 & 0 \\ -3 & 6 \end{pmatrix}$ unit cell comprising 5 and 4 TPA molecules, respectively. This study demonstrates the viability of silver passivated silicon surfaces as optimal substrates for supramolecular self-organisation.

O 30.5 Tue 13:00 MA 041

Bistability of single cyclooctadiene molecules on Si(001) induced by inelastic electron tunneling — •Christophe Nacci, Jérôme Lagoute, Xi Liu, and Stefan Fölsch — Paul Drude Institute for Solid-State Electronics, Hausvogteiplatz 5-7, 10117 Berlin, Germany

The tip-induced switching of single 1,5 cyclooctadiene molecules (COD) on Si(001) was studied by low-temperature scanning tunneling microscopy. COD (C_8H_{12}) is a cyclic alkene with a twisted boat double-degenerate configuration which adsorbs in two different structures: the so-called bridge structure and the upright structure, with the bridge structure being the prevalent conformation [1]. Time spectroscopy of the tunnel current with the tip positioned over the molecule adsorbed in the bridge structure reveals fluctuations between two levels of current reminiscent to statistical telegraph noise. This behavior is interpreted as a reversible dynamic switching of the adsorbed molecule between two degenerate conformations triggered by inelastic single-electron excitation. First measurements on COD adsorbed in the upright structure reveal a significantly different noise response with an enhanced quantum yield and a lifted degeneracy of the current level population probabilities.

[1] J. H. Cho et al. Phys. Rev. B **64**, 241306 (2001)

O 30.6 Tue 13:15 MA 041

Investigations of Ga atom wire formation on Si(112) — •Moritz Speckmann[1], Thomas Schmidt[1], Jan-Ingo Flege[1,2], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, 28334 Bremen — [2]National Synchrotron Light Source, Brookhaven National Laboratory, Upton, New York 11973, USA

High index surfaces are of strong interest in today's research because they are supposed to be a candidate for self-assembling systems, e. g. nano wires. In this work the adsorption of Ga on Si(112) has been investigated with different surface sensitive techniques. The stepped silicon surface consists of (111)- and (337)-facets. Because of the lower surface energy at the step edges growth of metals, e.g. Ga or Al, results in quasi-1D metal quantum wires along the direction of the step edges.

STM and LEED images clearly reveal a Ga:Si(112)-(6 × 1)-reconstruction with Ga atom rows along the step edges in [1$\bar{1}$0]-direction. Using XPEEM experiments performed at NSLS, Brookhaven and comparing with the Ga:Si(111)-($\sqrt{3}\times\sqrt{3}$)-reconstruction we were able to determine the coverage of the Ga:Si(112)-(6 × 1)-reconstruction. Our results correspond to 10 Ga atoms per (6×1) unit cell and therefore confirm the model by Snijders et al. (Phys. Rev. B, **72**, 2005). Furthermore we performed x-ray standing waves experiments at HASYLAB, Hamburg. The obtained positions of the Ga atoms again show a strong agreement with the proposed positions in the model.

O 30.7 Tue 13:30 MA 041

Self-assembled films of Lead Phthalocyanine on GaAs(001) surfaces — •V. Rackwitz[1], R. Passmann[1,2], M. Kneissl[1], N. Esser[1,2], and P. Vogt[1] — [1]TU Berlin, Institute of Solide State Physics, Hardenbergstr. 36, 10623 Berlin, Germany — [2]ISAS Berlin, Albert-Einstein-Str. 9, 12489 Berlin, Germany

The influence of the atomic surface structure on the adsorption process of organic molecules on semiconductor surfaces is not yet fully understood. However, the interface arrangement of such hybrid systems is crucialy important for applications in sensors and electronic devices.

In this work we present our results on the adsorption of the nonplanar lead phthalocyanines (PbPc) on the three main GaAs(001) reconstructions the c(4×4), (2×4) and (4×2). The interface formation is investigated by Reflections Anisotropy Spectroscopy (RAS), Atomic Force Microscope (AFM) and Auger Electron Spectroscopy (AES). The results shows that intra-molecular contributions resulting from the PbPc dominate the RAS spectrum upon deposition on the c(4×4) and (4×2) but not on the (2×4). The film thickness in all three cases is approximately 20nm as determined by AFM. We interpret the anisotropies of the PbPc layers as resulting from the inital atomic structure of the GaAs(001) surfaces.

O 30.8 Tue 13:45 MA 041

Investigation of crucial interfaces for III-V multi-junction solar cells — •Ulf Seidel, Henning Döscher, and Thomas Hannappel — Hahn-Meitner-Institut, Glienicker Str. 100, 14109 Berlin, Germany

Currently high efficiency III-V multi-junction solar cells are grown epitaxially on Ge(100)-substrates, which are simultaneously utilized for the low band gap subcell. Our concept is the replacement of Ge in these devices by a more efficient InGaAsP/InGaAs tandem solar cells integrated on Si(100) substrates. According structures contain many different layers of III-V semiconductors, which were prepared in this work via MOVPE. For the best performance of the solar cells sharp hetero-interfaces are necessary. Here, the investigation of two interfaces is presented in detail: (1) InGaAs/GaAsSb that is needed in the tunnel junction of our low band gap multi-junction solar cell and (2) Si/GaP that is needed for the epitaxy of our III-V solar cells on silicon(100) substrates instead of InP(100). Both interfaces were characterized in-situ during the MOVPE-growth with reflectance difference spectroscopy (RDS) and after a contamination free transfer in ultra high vacuum with X-ray photoelectron spectroscopy (XPS), low energy electron diffraction (LEED) and scanning tunnelling microscopy. Additionally AFM micrographs were recorded.

O 31: Prize Talk Bernard Barbara (Gentner-Kastler Prize)

Time: Tuesday 13:00–13:45 Location: H 0105

Quantum Tunnelling and Coherence in Magnetic Molecule and Ions

O 32: Oxides and Insulators: Clean Surfaces

Time: Tuesday 13:00–16:45 Location: MA 042

O 32.1 Tue 13:00 MA 042

Structure of the rutile TiO_2(011)-(2x1) surface — •Navid Khorshidi[1], Andreas Stierle[1], Vedran Vonk[1], Claus Ellinger[1], Helmut Dosch[1], Ulrike Diebold[2], Xueqing Gong[3], and Annabella Selloni[3] — [1]Max-Planck-Institut für Metallforschung, Stuttgart, Germany — [2]Tulane University, New Orleans, USA — [3]Princeton University, Princeton, USA

TiO_2 has various applications in technology and is one of the most investigated metal oxides. It is used in solar cells and its photocatalytic activity makes an understanding of the structure of diverse surface orientations desirable. Although there are many studies on TiO_2 surfaces, the (011) surface has been rarely investigated. First principal DFT calculations predict the (011)-(1x1) face to have the third lowest energy and in a Wulff Construction a large part of the surface is (011) oriented. TiO_2 nano particles exhibit preferentially (011) oriented facets. Therefore a structure model of this surface is required to understand the photocatalytic processes on an atomic scale.

We have investigated the TiO_2(011)-(2x1) surface using Surface X-Ray Diffraction (SXRD), Scanning Tunnelling Microscopy (STM) and Low Energy Electron Diffraction (LEED). From our data we are able to derive a novel model for the (011) surface in combination with DFT calculations. The new model has a much lower surface energy than the one suggested previously and fits the X-Ray data very well.

O 32.2 Tue 13:15 MA 042

Structure determination of clean V_2O_3(0001) and TiO_2(110) surfaces — •Werner Unterberger[1], Emily A. Kröger[1], Tsenolo J. Lerotholi[2], Francesco Allegretti[2], David I. Sayago[1], Matthew Knight[2], and Phillip Woodruff[1,2] — [1]Fritz-Haber-Institute — [2]Physics Department, University of Warwick

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 the clean surfaces of TiO_2(110) and thin epitaxial films of V_2O_3 on Pd(111).

For V_2O_3(0001) key questions are termination and relaxation of the clean surface; current understanding is based only on theoretical calculations and STM imaging. While the PhD technique is more naturally suited to studies of adsorbate structures, here we report its application to the clean surfaces of V_2O_3 and TiO_2. The TiO_2(110) surface is in principle well-known, and so provides a valuable test of the methodology, although the sign and magnitude of the relaxation of the bridging O atoms has been the subject of recent controversy. The PhD analysis for this surface yields relaxation parameter values in good agreement with the most recent results giving some confidence in the method. For the V_2O_3(0001) surface the results clearly favour the "half-metal"termination with a strongly relaxed outermost layer, as found in published theoretical total energy calculations. However, the PhD results prove inconclusive regarding the presence or absence of surface vanadyl (V=O) species favoured by theory.

O 32.3 Tue 13:30 MA 042

Direct Observation of d^2L^2 Charge Transfer States in TiO_2 thin films by Resonant Photoelectron Spectroscopy — •Sebastian Müller and Dieter Schmeisser — Brandenburgische Technische Universität Cottbus, Angewandte Physik - Sensorik, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany

We investigate the electronic structure of TiO_2 thin films by SR-PES, NEXAFS and ResPES. The films are prepared in a combined in-situ/ex-situ process that leads to stoichiometric thin films ($\approx$ 10 nm) in Rutile structure. We focus on ResPES at the Ti 2p edge. When the photon energy is close to the Ti 2p absorption edge we observe additional features about 13 eV below the valence band main features. These features show clear spectator auger decay at the resonance leading to d^0 final state. From this, we deduce the existence of the d^2L^2 initial charge transfer state as this is the only possible channel that enables the corresponding spectator auger decay. These features have the same origin as the satellite structures observed in core level spectra, esp. 2p and 3p.

O 32.4 Tue 13:45 MA 042

Tensor LEED study of the surface relaxation and lattice dynamics of RbI(100) and RbBr(100) — •Stephan Härtel, Jochen Vogt, and Helmut Weiss — Chemisches Institut der Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, D-39106 Magdeburg

During the last decade the surfaces of several alkali halides were investigated by LEED and other experimental techniques. In good agreement with theoretical predictions for many compounds a rumpling as well as a contraction of the first interlayer distance was found. Up to now no LEED data of the rubidium halides were available. In the present work RbI(100) and RbBr(100) were investigated by means of LEED in an energy range from 30 to 220 eV. The recorded I(E) data were analyzed using the tensor LEED approach. RbI(100) exhibits a slight rumpling where the Rb^+ are shifted inward by 0,07±0,03 Å and the I^- outward by 0,02±0,01 Å. There is no significant contraction of the interlayer distance. In contrast to theoretical calculations [1] the lattice amplitudes of the ions of the two topmost layers are not enlarged significantly compared to the bulk values. For RbBr(100) also a rumpling was observed which is however smaller than that of RbI. The first interlayer distance is reduced by about 1.5%. Different from RbI the lattice amplitudes in the two topmost layers are enlarged by a factor of 1.3 for Rb^+ and 1.25 for Br^-.

[1] de Wette, F.W. et al.: New surface mode on the (001) surfaces of RbBr and RbI, Physical Review B, **35**, 5 (1987)

O 32.5 Tue 14:00 MA 042

Lattice Dynamics of Cu_2O: Bulk and (110) Surface — •Klaus-Peter Bohnen[1], Rolf Heid[1], Aloysius Soon[2], and Catherine Stampfl[2] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik — [2]School of Physics, The University of Sydney

A number of theoretical studies have been carried out in the past to investigate the stability of various surface oxides for the O/Cu system however despite the fact that catalytic processes usually proceed at elevated temperatures stability at finite temperatures has never been studied for these systems. Modern ab-initio methods however allow for the determination of the lattice dynamics and the phononic contribution to the free energy. Using density functional perturbation theory we have studied the lattice dynamics of Cu_2O-bulk as well as Cu_2O(110). In calculating the free energy as function of lattice constant we obtained for the bulk a negative thermal expansion up to roughly 300 K in excellent agreement with experiments. This is due to anomalous mode Grüneisen parameters for vibrational modes in the low energy regime. Due to the anomalous behavior of the mode Grüneisen parameter the bulk system is highly unstable against variations of the lattice constant by more than 2%. To investigate the stability of the O/Cu surfaces we have investigated the lattice dynamics of Cu_2O(110) as a prototype. Despite a large number of low lying modes no instability has been found. These calculations allow also for the O/Cu system for the first time for a realistic estimation of the surface free energy which is important for the determination of surface thermodynamic properties.

O 32.6 Tue 14:15 MA 042

Electronic structure and thermodynamic stability of cubic $La_xSr_{1-x}MnO_3$ (001) surfaces: First-principles calculations by means of hybrid density-functional theory — •Sergejs Piskunovs[1], Eckhard Spohr[1], and Timo Jacob[2] — [1]Lehrstuhl fuer Theoretische Chemie, Universitaet Duisburg-Essen, Campus Essen, S05 V06 E15, Universitaetsstr. 5, D-45141 Essen, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin-Dahlem, Germany

Surface properties of $La_xSr_{1-x}MnO_3$ (LSM) are of high scientific and technological interest due to potential application of these materials in magnetoresistive devices, spintronics, and high-temperature fuel cells. Using the hybrid exchange-correlation functional within density functional theory, we calculated the electronic structure for a wide range of cubic LSM(001) surfaces at low doping $x \sim 1/8$. The layered antiferromagnetic structure is found to be the most energetically favorable for all LSM(001) surfaces under study. Stability of the considered LSM surfaces has been predicted by means of the atomistic thermodynamics. Our calculations show that segregation of Sr at La(Sr)-terminated surface does not lead to its stabilization and thus is thermodynamically unlikely. On the other hand, MnO_2-terminated LSM(001) can be stabilized through adsorption of atomic oxygen atop of Mn sites.

O 32.7 Tue 14:30 MA 042

Preparation of model single crystalline aluminium oxide films suitable for scanning tunnelling microscopy — •Sergiy Borodin and Michael Rohwerder — Max-Planck-Institut für Eisenforschung, Düsseldorf, Deutschland

Self assembly of organic molecules on aluminium or aluminium alloys is of increasing technical importance, e.g. for adhesion promotion and corrosion protection. For the performance of the SAMs in many cases their defect structure is of importance. However, it is difficult to obtain detailed information about the nanoscopic defect structure, as it is difficult to prepare suitable atomically flat samples that can be scanned by STM.

In this work a model thin film aluminum has been prepared under UHV conditions, whose surface is suitable for a scanning tunneling microscopy investigation, e.g. of phosphonate self-assembly on aluminium. This surface is stable even upon contact at high water exposures and hence much superior to model aluminium oxide surfaces prepared on NiAl.

O 32.8 Tue 14:45 MA 042

Work function measurements with a combined AFM/STM setup under ultrahigh vacuum conditions at 5K on thin MgO films grown on Ag(001) — •Thomas König, Georg Hermann Simon, Violeta Simic-Milosevic, Markus Heyde, and Hans-Joachim Freund — Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, 14196 Berlin, Germany

For many years metal supported thin oxide films have been investigated in the research field of heterogeneous catalysis. The properties of the thin films depend strongly on both the support and the film thickness. While thick films approach the properties of bulk material thin films exhibit their own characteristics. It has been proposed by Pacchioni et al. [1] that charging can occur by depositing metal atoms on ultrathin MgO films grown on metal supports. The charging of Au atoms on top of a thin MgO film grown on Ag(001) has been confirmed by STM measurements done by Sterrer et al. [2]. The MgO film on top the metal support leads to a compression of the metal electrons which for a free metal spill over into the vacuum. The compression results in a reduction of the surface dipole and thus to a decrease of the work function. Here we present work function measurements on different MgO film thicknesses grown on Ag(001). The measurements have been done with our combined AFM/STM setup operating under UHV conditions at 5K. The results will be discussed and compared with theoretical calculations.

[1] L. G. Giordano et al., Phys. Rev. B 73, 045414, 2005. [2] M. Sterrer et al., Phys. Rev. Lett. 98, 096107, 2007.

O 32.9 Tue 15:00 MA 042

Stress of CoO(111) on Ir(100) — •Zhen Tian, Dirk Sander, and Juergen Kirschner — Max-Plank Institute of Micrsostructure Physics

An important aspect of epitaxial oxide films is that the growth of (111) oriented films with rock salt structure leads to polar surfaces, where adjacent layers are composed of either anions or cations only. Considerable repulsive Coulomb interaction within the oxide (111) layers are therefore expected [1]. We measured the stress change during the formation of CoO(111) on Ir(100) by post-oxidation of Co films [2]. Combined structural investigations by LEED and stress measurements by the crystal curvature technique are performed. The formation of the CoO(111)-c(10×2) structure by post-oxidation of 2 monolayers Co induces a compressive surface stress change of −0.5 N/m. The epitaxial Co film prior to oxidation is under a tensile stress of +16 GPa, which is induced by the lattice misfit between fcc-Co and Ir. The formation of the CoO(111) film induces a tensile stress change of +2.1 N/m, as compared to the clean Ir(100) surface. This stress change is quantitatively ascribed to the anisotropic misfit between the c(10×2) structure of CoO(111) and Ir(100) of +0.22 % and +4.2 % along Ir[110] and Ir[$1\bar{1}0$], respectively. Our stress measurements indicate that charge depolarization effects [3] might be operative on the CoO(111)-c(10×2) film.

[1] C. Noguera, J. Phys.: Condens. Matter 12 (2000) R367-R410.

[2] C. Giovanardi, L. Hammer, and K. Heinz, Phys. Rev. B 74, 125429 (2006).

[3]C. Tusche, H. L. Meyerheim, and J. Kirschner, Phys. Rev. Lett. 99 (2007) 026102.

O 32.10 Tue 15:15 MA 042

Metal-insulator transition on the V_2O_5(001) surface: Theory and experiment — •Maria Veronica Ganduglia-Pirovano[1], Remy Fortrie[1], Joachim Sauer[1], Ralf-Peter Blum[2], Horst Niehus[2], Carsten Hucho[3], Shamil Shaikhutdinov[4], and Hans-Joachim Freund[4] — [1]Inst. für Chemie, HU-Berlin — [2]Inst. für Physik, HU-Berlin — [3]Paul-Drude-Institut Berlin — [4]FHI Berlin

Several vanadium oxides undergo a metal-to-insulator transition (MIT) in the bulk, e.g., V_2O_3 at ∼150 K, VO_2 at 340 K, whereas V_2O_5 is a semiconductor. Experimental evidence for a thermally induced *surface* insulator-metal transition (MIT) at the V_2O_5(001) surface at 350-400 K is presented. This surface exposes vanadyl (V=O) double rows along the [010] direction. Using density functional theory (DFT) in combination with statistical thermodynamics, the facile reduction along the rows was predicted.[1] The experimentally observed MIT transition expands preferentially in the direction of these rows. We then used the Monte Carlo method to simulate the reduced V_2O_5(001) surface at a given temperature and defect concentration. We typically find areas with a random distribution of isolated defects and others with up to 5 sites forming [010] oriented trenches. Using calculated band gaps for reduced V_2O_5 structures as obtained with DFT+U, we construct band gaps maps which agree with those derived from scanning tunneling spectroscopy data; only the areas with defective rows are metallic. [1] M. V. Ganduglia-Pirovano and J. Sauer, PRB **70**, 045422 (2004). [2] R.-P. Blum, H. Niehus, C. Hucho et al., PRL. in press.

O 32.11 Tue 15:30 MA 042

Structural arrangement of room temperature ionic liquids at a hard wall — •Heiko Schröder, Markus Mezger, Sebastian Schramm, Harald Reichert, John Okasinski, and Helmut Dosch — Max-Planck-Institut für Metallforschung, Stuttgart

Interfacial phenomena in physical, chemical, and biological systems are of increasing relevance in many of today's technological applications. In order to access solid-liquid interfaces and extract microscopic details of their local structure with high resolution, we have employed high energy x-ray microbeam reflectivity. Here, we discuss the analysis and interpretation of reflectivity data recorded at the interface between different room temperature ionic liquids (RTIL) and a hard wall (sapphire). Real space structures could be resolved with Å-resolution. Although crucial for the understanding of solvent properties, only little is known about the structural arrangement of anions and cations in RTILs at solid interfaces. We systematically examined different parameters altering the interfacial properties. By choosing different combinations of anions and cations, the ion-ion and ion-substrate interaction as well as the size ratio of the involved ions could be varied. By modifying the temperature, the ratio between entropy and interfacial energy can be tuned as well, favoring a disordered liquid or interfacial layering, respectively. This results in different structural arrangements at the molecular level.

O 32.12 Tue 15:45 MA 042

The Au(111) Electrolyte Interface: A DFT Investigation — Sudha Venkatachalam[1], Felice C. Simeone[1], Dieter M. Kolb[1], and •Timo Jacob[1,2] — [1]Institut für Elektrochemie, Universität Ulm, D-89081 Ulm — [2]Fritz-Haber-Institut der MPG, D-14195 Berlin

Density functional theory calculations have been performed to derive a detailed model of the electric double layer for Au(111) in contact with an aqueous H_2SO_4 electrolyte. At potentials of $E \geq +0.8$ V vs. SCE various surface sensitive techniques found evidence for a $(\sqrt{3} \times \sqrt{7})$R19.1° (bi)sulfate structure, but the nature of coadsorbates remains still unclear. Focusing on a sulfate adlayer, the coadsorption of H_3O^+ and/or H_2O has been studied [1]. The calculated binding energies show that the coadsorption of a single H_3O^+ per sulfate (stabilizing the adlayer by hydrogen bonds) is the most stable configuration. In addition, the charge density distribution within the adlayer well agrees with effective barrier heights deduced from recent distance tunnelling spectroscopy measurements [2].

Afterwards we studied the interfacial structure that forms at negative electrode potentials and found that water arranges near the electrode in an ice-like hexagonal structure with hydronium ions being located in the second water layer and non-specifically adsorbed. Again the calculated charge density distribution shows a perfect correspondence to distance tunnelling spectroscopy measurements.

[1] S. Venkatachalam, T. Jacob, Z. Phys. Chem., **221**, 1393 (2007).

[2] S. Venkatachalam *et al.*, Angew. Chem. Int. Ed., DOI: 10.1002/anie.200702868.

O 32.13 Tue 16:00 MA 042

Surface Stress Variation as a Function of Charge for the Metal at Metal - Electrolyte Interface — •Maxim Smetanin[1], Raghavan N Viswanath[1], Dominik Kramer[1], and Joerg Weissmueller[1,2] — [1]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, Karlsruhe, Germany — [2]Universität des Saarlandes, Saarbruecken, Germany

During the last decade, there has been considerable progress in measuring and understanding the capillary forces on metal surfaces. The present work revisits the question, what is the magnitude of the surface stress charge coefficient(SSCC) for the gold in an electrolyte near the potential of zero charge, in particular in respect to comparison to numerical computation. We report in-situ measurements of f(q) for planar gold electrodes in weakly adsorbing electrolytes, using a cantilever bending technique with optical detection. We used 40 nm thick, (111)-textured gold films on 100 *m thick (100)-oriented silicon wafers in aqueous NaF and HClO4. The films were characterized in respect to roughness (using a scanning probe microscopy) and to contamination (using Auger microscopy). Their pzc value was determined in 7 mM NaF using the minimum of the differential capacitance, it is ca. 0.20 V vs. SCE. The wafer bending results testify to an essentially linear f(q) near the pzc and electrode charging occurs mainly within the diffuse double layer at minimum influence of specific ions adsorption. SSCC was found to be of the order of -1.95 V for 7 mM NaF and -2.02 V for 10 mM HClO4.

O 32.14 Tue 16:15 MA 042

STM of superstructures and surface transformations on Pt(111) in a sulfuric acid electrolyte — •Björn Braunschweig and Winfried Daum — Institut für Physik und Physikalische Technologien, TU-Clausthal, Leibnizstrasse 4, D-38678 Clausthal-Zellerfeld

Imaging of weakly chemisorbed species on Pt surfaces with the STM in electrochemical environments and with molecular resolution is a challenge to the experimenter as these electrode surfaces are very susceptible to contaminations at a level well below the sensitivity of cyclic voltammetry. We have investigated the surface structure of Pt(111) in a 0.1 M H_2SO_4 electrolyte in the potential range of sulfate adsorption. In agreement with a previous study [1] we observe a disorder-order transitions at a potential of 0.5 V versus the reversible hydrogen electrode (RHE). For potentials between 0.5 and 0.8 V RHE we identified two distinctly different sulfate superstructures: the well-known $(\sqrt{3} \times \sqrt{7})$R19.1° superstructure and a new (3x1) superstructure. We were able to simultaneously image the sulfate and the Pt surface lattice and to determine the registry of the sulfate anions with the substrate. The structure in the unit cell of the (3x1) superstructure indicates the presence of an additional molecular component, possibly hydronium or water molecules. For potential sweeps to 0.8 V RHE and above the ordered sulfate overlayer changes instantaneously to a more disordered structure presumably due to adsorption of OH^- ions.

[1] A.M. Funtikov, U. Linke, U. Stimming and R. Vogel; Surf.Sci. 324, L343 (1995) and J. Electroanal. Chem. 428, 147 (1997)

O 32.15 Tue 16:30 MA 042

The quest for ZnO($11\bar{2}0$) surface states – an ARPES study — •Christian Pettenkofer and Stefan Andres — Hahn-Meitner-Institut, Glienicker Str. 100, D-14109 Berlin

We present angle resolved photoemission data from differently prepared ZnO($11\bar{2}0$) single crystals and epitaxially grown thin films. ZnO($11\bar{2}0$) single crystal surfaces were prepared by both cleaving in vacuum and sputtering-annealing cycles of pre-polished crystals. ZnO($11\bar{2}0$) thin films were grown heteroepitaxially on the r-face of sapphire by MOMBE using diethylzinc and water as precursor molecules. The ARUPS-spectra were recorded at the TGM7 beamline at BESSY-II synchrotron light facility in Berlin.

The band dispersion along $k_{\parallel}$ and $k_{\perp}$ is discussed in accordance with theoretical band structure calculations of the bulk electronic states within the GGA-DFT framework. An excellent agreement between the theoretically and experimentally determined band structure is achieved for the upper valence bands. Furthermore the surface electronic structure of both the epitaxially grown thin films and the single crystals coincide very well with each other.

It is shown, that despite the very different nature of the surface preparation methods no surface states could be observed. Therefore different effects such as hydrogen adsorption, surface defects and lattice relaxation will be discussed with regard to the specific surface preparation method.

O 33: Symposium: Frontiers of Surface Sensitive Electron Microscopy I (Invited Speakers: James Hannon, Raoul van Gastel, Thomas Schmidt)

Time: Tuesday 13:45–16:15 Location: MA 005

Invited Talk O 33.1 Tue 13:45 MA 005

Dynamics at Strained Surfaces — •James B. Hannon — IBM T.J. Watson Research Center, Yorktown Heights, NY 10598, USA

It has long been recognized that surface stress influences surface morphology and kinetics. For example, stress can drive the spontaneous formation of periodic patterns. Analysis of the equilibrium configuration of stress domains can be used to determine surface thermodynamic parameters [1]. However, in many (if not most) systems, reaching equilibrium in experiment can be difficult. In this talk, I will describe experiments in which surface thermodynamic parameters are determined by analyzing the motion of stress domains far from equilibrium. In the first example, step motion on Si(100) is used to determine the strain pattern of a dislocation that intersects the surface [2]. In the second example, the rapid growth of isolated 7x7 domains on Si(111) is described. I show how certain generic features of the domain growth (e.g., faceting) are related to the orientational dependence of the domain boundary free energy.

Work performed with R.M. Tromp (IBM) and V.B. Shenoy (Brown Univ).

[1] Science 295 (2002) 299; Nature Materials 3 (2004) 95.

[2] Science 313 (2006) 1266.

Invited Talk O 33.2 Tue 14:15 MA 005

The role of long-range interactions in determining surface morphologies: a combined LEEM/SXRD study — •Raoul van Gastel — MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

LEEM has been used to study long-ranged elastic interactions that occur in metal heteroepitaxy. The elastic interactions are used to achieve shaping and sizing of nanostructures. Pb/Cu(111) is first used as an example to illustrate how LEEM is applied to quantify the thermodynamic parameters that are driving the self-assembly of two phases, a surface alloy phase and an overlayer phase. We show how those parameters can be manipulated to induce size and shape changes of individual domains.

For the similar Bi/Cu(111) system we have combined surface X-ray diffraction (SXRD) and LEEM to investigate the atomic structure and pattern formation. We investigate the structure of the different surface phases and pinpoint the origin of the morphological changes to the atomic structure of the different phases. The pattern formation and the dramatic changes that occur during the transitions are analyzed and the thermodynamic parameters that control the rich phase behavior in this system are quantified. Finally, a brief illustration is given of how electrostatic interactions can lead to similar effects in the self-assembly of organic molecules on metal substrates.

O 33.3 Tue 14:45 MA 005

Real Time Imaging of Surface Diffusion Fields during Island decay — •Dirk Wall[1], Kelly R. Roos[1,2], Kimberly L. Roos[1], Ingo Lohmar[3], Joachim Krug[3], Michael Horn-von Hoegen[1], and Frank-J. Meyer zu Heringdorf[1] — [1]Department of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE) Universität Duisburg-Essen, D-47057 Duisburg, Germany — [2]Department of Physics, Bradley University, Peoria, IL 61625, USA — [3]Institut für Theoretische Physik, Universität zu Köln, 50937 Köln, Germany

Photoemission Electron Microscopy (PEEM) is used to study the thermal decay (650°C - 850°C) of Ag islands grown epitaxially on flat and vicinal Silicon surfaces. During island decay, bright quasi static Ag-reconstructed zones are formed around each of the islands. Micro Low Energy Electron Diffraction (μ-LEED) reveals that the photoemission contrast is caused by different reconstructions due to a coverage gradient that extends outward from the edge of the islands. A simple continuum model is presented explaining the dynamic decay of the islands. We additionally studied the diffusion anisotropy on numerous vicinal Silicon surfaces. The degree of diffusion anisotropy of the system is thereby revealed by the shape of the zones. We demonstrate that the imaging of these reconstructed "isocoverage-zones"constitutes a unique experimental method for directly imaging diffusion fields and diffusion anisotropy in epitaxial systems. The general applicability of this imaging technique is demonstrated by the decay of Indium islands on Silicon.

O 33.4 Tue 15:00 MA 005

Structural imaging of surface oxidation and oxidation catalysis on transition metal surfaces — •Jan Ingo Flege and Peter Sutter — Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY, United States

The oxides of 4d late transition metals (TM), such as ruthenium and rhodium, are a class of materials with desirable functional properties, e. g., for catalysis. However, the mechanism of initial oxidation of these materials and the nature of the structures produced by facile oxygen uptake into sub-surface layers have been notoriously difficult to investigate experimentally, primarily because of a lack of spatially resolving and structurally sensitive techniques adequate for identifying the initial nanometer-sized oxidation products under reaction conditions.

Here we use spatially and temporally resolved structural fingerprinting in connection with multiple scattering calculations to characterize surface oxidation as well as the catalytic properties of the resulting oxygen-rich structures on Ru(0001) and Rh(111). We will show that for both Ru and Rh the initial oxidation proceeds by initial formation of a O-TM-O trilayer. However, while in the case of Rh the thicker oxide structures emerge from the trilayer surface oxide, the bulk oxide RuO$_2$(110) islands grow independently from the trilayer, competing for surface area. Furthermore, individual phase-specific chemical reactivities for CO oxidation and cooperative effects during the catalytic cycle induced by the nanoscale heterogeneity will be discussed.

O 33.5 Tue 15:15 MA 005

Photoemission electron microscopy investigation of organic thin films — •Maria Benedetta Casu[1], Indro Biswas[1], Mathias Nagel[1], Peter Nagel[2], Stefan Schuppler[2], and Thomas Chassé[1] — [1]Institute of Physical and Theoretical Chemistry, University of Tuebingen, 72076 Tübingen, Germany — [2]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe, Germany

Organic electronic devices offer an interesting alternative to inorganic semiconductor electronics due to low-cost deposition methods, flexible substrates, and simple packaging. The organic molecules can be vapour deposited under vacuum, spin coated, dip coated or printed on the proper substrate. All these techniques are relevant for low cost electronics and their potentiality is still enormous. To favour further technical developments, the full understanding of electronic, structural, and morphological properties of organic materials plays a paramount role. Diindenoperylene (DIP) is a perylene-based molecule that shows a very high hole mobility already in thin films, good film forming properties and thermal stability, thus it may be considered as a promising molecule for electronics. In this work we present the results of photoemission electron microscopy (PEEM) investigations on DIP thin films deposited on polycrystalline gold. We focused on the different phases that may occur while growing a film on a given substrate. Based on the synergy of PEEM, X-ray photoemission, and nano near-edge X-ray absorption fine structure spectroscopy results, we propose a model for the growth of DIP thin film deposited with a relative low deposition rate (0.3 nm/min) on polycrystalline gold kept at room temperature.

O 33.6 Tue 15:30 MA 005

Characterization of nanosize buried defect in Mo/Si multilayer structure by EUV photoemission electron microscopy — •jingquan lin[1], jochen maul[2], nils weber[3], matthias escher[3], michael merkel[3], gerd schoenhense[2], and ulf kleineberg[1] — [1]Ludwig Maximilians University,Garching,Germany — [2]Mainz University, Mainz, Germany — [3]Focus-GmbH, Huenstetten-Kesselbach, Germany

Extreme ultraviolet lithography (EUVL) is one of the leading next-generation lithography candidates for the 32 nm node and below. The fabrication of defect-free masks including their inspection is a significant challenge for the implementation of EUVL. Here, we report experimental results of EUVL mask blank defects and patterned absorber inspection using photoemission electron microscopy (PEEM) technique. With EUV-PEEM, bump-type and pit type defects that buried under EUVL multilayer were investigated. In the case of bump-type defect we have demonstrated its sensitivity to a phase defects with lateral size of 35 nm and height of 4 nm. We also investigated artificial microstructures with lateral size of several 100 nm in /on top of Mo/Si multilayer structure. The inspection results show that EUV-PEEM has ability of detecting an absorbing micro-structure and a closely-situated tiny defect in the multilayer structure simultaneously. In addition, a comparison detection of phase defect sample with different working wavelength was conducted.

Invited Talk O 33.7 Tue 15:45 MA 005

SMART - Spectromicroscopy with aberration correction for high resolution surface characterization — •Th. Schmidt[1,2], F. Maier[1], H. Marchetto[2], P. Lévesque[2], U. Groh[1], R. Fink[3], H.-J. Freund[2], E. Umbach[1,7], and SMART- Collaboration[1,2,3,4,5,6] — [1]University of Würzburg, EP II — [2]Fritz-Haber-Institute, Berlin — [3]University of Erlangen, PC — [4]TU Darmstadt — [5]TU Clausthal — [6]Carl Zeiss NTS GmbH — [7]Forschungszentrum Karlsruhe

Combining high-brilliance synchrotron radiation with a parallel imaging LEEM or PEEM allows a comprehensive characterization of surfaces, adsorbates, and ultrathin films. The SMART (Spectro-Microscope with Aberration correction for many Relevant Techniques), installed at BESSY, aims at a lateral resolution of 2 nm and an energy resolution of 100 meV, which can only be achieved by aberration correction and energy filtering. The actual lateral resolution of 3.1 nm is already the best for this kind of microscope. Using different sources (polarized x-rays, UV-light, electron gun) the SMART excels as a versatile instrument by imaging photo-emitted (XPEEM, UV-PEEM) and reflected electrons (LEEM) to study the morphology, chemical distribution, electronic state, molecular orientation, atomic steps, etc. Fast switching enables spectroscopy (nano-XPS, nano-NEXAFS, etc.) and (b) diffraction from small object areas (nano-PED = photoelectron diffraction, valence band mapping, LEED, etc). First experiments on the growth properties of organic thin films show the potential of the instrument and will be briefly presented. Funded by the BMBF, contract 05 KS4 WWB/4.

O 34: Metal Substrates: Adsorption of Organic/Bio Molecules II

Time: Tuesday 13:45–16:30 Location: MA 043

O 34.1 Tue 13:45 MA 043

Conformations vs. Interaction energy: adsorption of flexible (bio)molecules on inorganic substrates — •Luca M. Ghiringhelli and Luigi Delle Site — Max-Planck-Institute for Polymer Research, Ackermannweg 10, D 55021 Mainz, Germany

We present a first principle density functional study of phenylalanine interacting with three different classes of surfaces, namely a purely repulsive hard-wall, mildly interacting close packed surfaces of group 11 metals (Cu(111), Ag(111), and Au(111)), and strongly interacting close packed surfaces of group 10 metals (Ni(111), Pd(111), and Pt(111)). In particular, we characterize, by changing the substrate, the passage from the statistical behavior of a flexible molecule in the presence of the topological confinement of a hard-wall to a purely chemical behavior where the molecule, highly deformed compared to the free state, strongly binds to the surface and statistical conformations play no more a role. Such a comparative study allows to characterize some of the key aspects of the adsorption process for a prototype of flexible amino acids on experimentally and technologically relevant metal surfaces.

O 34.2 Tue 14:00 MA 043

Spectroscopic mapping of chirality at the molecular level: PVBA on Cu(111) — •Robin Ohmann, Lucia Vitali, and Klaus Kern — Max-Planck-Institute for Solid State Research, Stuttgart, Germany

Chirality is a fundamental aspect of molecular biology and biochemistry, and is of central importance in pharmaceutics, yet directly imaging chirality of molecules proves to be challenging. Here, we present a combined scanning tunneling microscopy (STM) and spectroscopy (STS) study of 4-[trans-2-(pyrid-4-yl-vinyl)] benzoic acid (PVBA) adsorbed on a Cu(111)-surface. The molecules, deposited in ultra high vacuum (UHV) via molecular beam epitaxy, have been measured at low temperature (6 K). Single PVBA molecules (monomers), which become chiral upon adsorption on the surface, dimers and linear as well as triangular ensembles consisting of more than two molecules are observed. The contribution of different molecular orbitals to the local density of states has been measured for monomers and dimers by acquiring conductance maps. This allows directly visualizing the chirality of the adsorbed molecules. In the case of dimers we found homochiral and heterochiral species, which show respectively point-symmetric and mirror-symmetric spectroscopic features. Furthermore the interaction of monomers and dimers with the surface, as revealed by the scattering of the standing waves, will be discussed.

O 34.3 Tue 14:15 MA 043

Entropy driven stabilization of oligopyridine mono- and multilayer phases on HOPG - a thermal desorption study — •Michael Roos, Harry E. Hoster, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University

As shown in recent STM investigations, bis(terpyridine)derivates (BTP) form highly ordered hydrogen bonded networks on HOPG at both the solid/liquid [1] and the solid/gas [2,3] interface. In this study, we systematically investigate and compare the thermal desorption behavior for varying initial coverages of BTP molecules. We can clearly distinguish between two peaks corresponding to the mono- und multilayer regime. Surprisingly, the activation energies for desorption are about equal for both phases. Therefore, the different stabilities of mono- and multilayers must be associated with large differences in the preexponential factors, which are $\nu = 1{\cdot}10^{24}\ s^{-1}$ for the zero order-like desorption from the multilayer and $\nu = 1{\cdot}10^{18}\ s^{-1}$ for the submonolayer regime. In this coverage range, we find a repulsion-dominated desorption behaviour, indicated by a pronounced down-shift of the onset of desorption, which is in contradiction to the expected attractive influence of the increasing number of C-H···N bonds. The thermal desorption results can be explained in terms of transition state theory, keeping in mind the large moment of inertia of the BTP molecules.

1. C. Meier et al., J Phys Chem B 109, 21015 (2005).
2. H. E. Hoster et al., Langmuir 23, 11570 (2007).
3. A. Breitruck et al., Surf Sci 601, 4200 (2007).

O 34.4 Tue 14:30 MA 043

Analysis of structural and electronic properties of complex molecular phases: Tetracene on Ag(111) — •Sergey Soubatch, Ruslan Temirov, and Stefan Tautz — Forschungszentrum Jülich, Jülich, Germany

Formation and properties of disordered and ordered phases of tetracene on Ag(111) surface have been studied using LT-STM. At submonolayer coverage, tetracene forms a disordered phase due to repulsive interactions between flat-laying molecules on the metal surface. As the coverage rises, the tetracene phase starts to order. This process is driven by a balancing of intermolecular repulsion, attraction between molecules and the substrate, and competition between the positional and rotational entropy. Two long range ordered phases can appear at the surface. The alpha-phase represents a compact monolayer of flat-lying molecules, those electronic properties are strongly affected by interaction with the metal. It is revealed by significant shift of LUMO level registered by differential conductance spectroscopy. The beta-phase has more complex structure including interfacial layer and additional layer and molecular chains on top. Whilst the molecules in more planar configuration at the interface are strongly coupled to metallic electron states of the substrate, the molecules tilted out of the metal surface and/or separated from the metal by interfacial layer are found to be decoupled. For such molecules strong effect of local environment and intermolecular interaction on the energy of LUMO level is observed. The structural model for complex tetracene beta-phase has been proposed.

O 34.5 Tue 14:45 MA 043

The Influence of Alkanespacers on the Structure of Biphenylalkanethiol SAMs on Au(111) Surfaces — •Michel Kazempoor and Gerhard Pirug — Institut für Bio- und Nanosysteme (IBN3) and Center of Nanoelectronic Systems; Forschungszentrum Jülich GmbH, D-52425 Jülich

We prepared self assembled monolayers of ω-(4'-methylbiphenyl-4-yl)-alkanethiols (BPn, n = number of CH_2 units) on Au(111) surfaces and analyzed the unit cell size by means of Low Energy Electron Diffraction (LEED). The structural dependency on the number of CH_2 units (n = 2 - 6) in the alkane chain has been studied systematically. The samples were prepared in a separate preparation chamber by gas phase deposition and subsequently transferred into the UHV analysis chamber. The formation of ordered phases after annealing for at least 12 h to temperatures between 298 K and 410 K was studied. All investigated molecules show commensurate structures on the Au(111) surface which are at variance to unit cells derived from repeating units seen by STM. The odd numbered molecules (BP3 and BP5) show the same ordered $(2\sqrt{3} \times \sqrt{91})$ structure. In comparison the even numbered BPn molecules exhibit different phases clearly distinguished by their LEED patterns. While BP2 and BP6 show only one, but not the same dominant structure, BP4 forms three temperature dependent phases. Structure models will be presented based on the unit cells determined by LEED and the molecular packing seen by STM. Different unit cell sizes imply that the stress between the Au-S interface and the biphenyl overlayer is compensated within the alkane spacer.

O 34.6 Tue 15:00 MA 043

Why a 'decoupled' switch doesn't switch. Self-assembled monolayers of Azobenzenethiol on gold — •Roland Schmidt[1], Daniel Brete[1,2], Wolfgang Freyer[1], Cornelius Gahl[1], and Martin Weinelt[1,2] — [1]Max-Born-Institut, Max-Born-Straße 2A, 12489 Berlin — [2]FU-Berlin, Arnimallee 14, 14195 Berlin

We have investigated well oriented, self-assembled monolayers of alkanethiols on gold, functionalized by the molecular switch azobenzene ($HS-(CH_2)_n-O-C_6H4-N_2-C_6H_4-CF_3$, $n=3,6,10$). Using X-ray absorption spectroscopy the tilt angle between the backbone of the azobenzene group and the surface normal was shown to be $\sim 15°$, with only slight dependence on the length of the alkane chain n. The evaluation of autoionization spectra of the $N1s^{-1}\pi^{*+1}$ state in terms of the core-hole-clock approach gave a charge-transfer time τ_{CT} of the LUMO of several 10 fs. Also τ_{CT} showed no significant dependence on the length of the alkane chain n. Hence the switches are significantly decoupled from the substrate. However, a strong quenching of the SAM's $\pi-\pi^*$-excitation is observed in UV-Vis spectroscopy, pointing out that lateral interactions among the azobenzene chromophores in the crystal-like layer dominate both the charge transfer and the geometrical structur of the SAM. This is supported by the energy dependence of τ_{CT} that is atypical for tunnelling into the substrate. We suppose that the ultrafast delocalization of the S_2 excitation causes the observed inefficiency of photochemical switching of alkanethiol based SAMs.

O 34.7 Tue 15:15 MA 043

Molecular Switches at Solid Surfaces: A DFT Study of Azobenzene on Coinage Metals — •Erik McNellis, Abbas Dehghan Baghi, and Karsten Reuter — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin (Germany)

Following the rapidly advancing miniaturization in microelectronics and sensing, molecules that may be switched between defined conformational states are envisioned as fundamental storage and logic units in a future “molecular nanotechnology”. Considering contacting and defined integration into a larger framework, it is more precisely the molecular function when the molecule is stabilized at a solid surface that is of key interest. A necessary prerequisite for an atomic-scale understanding of this function of the adsorbed switch is a detailed structural and electronic characterization of the stable (or meta-stable, long-lived) molecular states. For this, we use density-functional theory and study the prototypical cis-trans isomer azobenzene (C_6H_5-N=N-C_6H_5) at coinage metal surfaces. Treating electronic exchange and correlation (xc) at the generalized gradient approximation (GGA) level, we obtain an essentially zero net binding of both conformational isomers at Ag(111) and Au(111). This is significantly different at Cu(111), where the bonding particularly of the cis isomer is strong enough to even reverse the gas phase energetic order of the two isomers. We are able to rationalize these findings as a competition between the covalent bonding of the central azo (-N=N-) bridge to the substrate on the one side, and the surface interaction of the two closed-shell phenyl (-C_6H_5) rings on the other side.

O 34.8 Tue 15:30 MA 043

The role of surface-molecule interaction in the isomerisation of Azobenzene molecules — •Nils Henningsen[1], Riccardo Rurali[2], Katharina J. Franke[1], Isabel Fernandez Torrente[1], Gunnar Schulze[1], Beate Priewisch[3], Karola Rück-Braun[3], and Nacho Pascual[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [2]Departament d'Enginyeria Electrònica, Universitat Autònoma de Barcelona, Spain — [3]Institut für Chemie, Technische Universität Berlin, Germany

Azobenzene is a prototype molecular switch in the gas phase and in solution. Upon adsorption on a surface, the switching properties are largely influenced. By means of scanning tunnelling microscopy (STM) and density functional theory (DFT) we investigate the switching behaviour of an azobenzene derivative (DMC: di-meta-cyano-Azobenzene) on several noble metal surfaces, Au(111), Ag(100) and Cu(100). STM reveals that, after vacuum deposition, DMC adsorbs exclusively as trans-isomers. By applying voltage pulses with the STM tip, we are able to induce a conformational change into the cis-configuration on Ag(100) and on Cu(100). DFT calculations show that the stabilization of the cis isomers is mediated by a strong hybridization of the azo-group with the substrate. We argue that the larger the hybridization with the substrate the more stable is the cis configuration. This causes that the cis isomer is very stable on Cu(100), while the reversible switching into the trans state is possible on Ag. On Au(111) almost no hybridization is present thus we observe that only the trans molecules is a stable state on the surface.

O 34.9 Tue 15:45 MA 043

Adsorption studies of azobenzene molecules on Cu(001) and Au(111) — •Marten Piantek, Matthias Bernien, Jorge Miguel, and Wolfgang Kuch — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14145 Berlin

Mono- and multilayers of Dimetacyano-azobenzene (DMC) have been evaporated under ultra high vacuum conditions on Au(111) and Cu(001) substrates in order to investigate the influence of the substrate on their physical properties. The electronic properties as well as the adsorption geometry of the molecules were studied by angle-dependent near-edge X-ray absorption fine structure (NEXAFS) spectroscopy. DMC molecules adsorb in their planar trans conformation flat on the Au(111) surface. X-ray photoemission spectroscopy (XPS) of the monolayer on Au(111) yielded the same spectra as for the multilayer. Thus we conclude that there are no additional chemical bonds formed between the molecule and the metallic surface. On Cu(100) the molecules in the first monolayer present an out-of-plane geometry with respect to the substrate. From the change in the π^* resonances at the N K-edge NEXAFS we conclude that a molecular nitrogen π-bond breaks, while the angular dependence of NEXAFS shows that the benzonitrile moieties are tilted out of the molecular plane. The XPS N1s peaks of a monolayer of DMC on Cu(001) are shifted compared to those of the multilayer sample, due to an additional bond formation to the substrate.

O 34.10 Tue 16:00 MA 043

Reversible switching of tetra-*tert*-butylazobenzene on Au(111): A vibrational analysis — •László Óvári[1,2], Martin Wolf[1], and Petra Tegeder[1] — [1]Fachbereich Physik, Freie Universität Berlin — [2]Reaction Kinetics Research Laboratory, Chemical Research Center of HAS, Szeged, Hungary

High resolution electron energy loss spectroscopy (HREELS) is employed to analyze reversible changes in the geometrical structure of the molecular switch 3,3',5,5'-tetra-*tert*-butylazobenzene (TBA) adsorbed on Au(111), which are induced by UV-light and thermal activation. TBA was chosen because the four lateral *tert*-butyl-groups act as "spacer-legs"to increase the separation between the surface and the azobenzene π-system, and therefore leading to a reduced electronic coupling. From angular dependent measurements, *viz.* specular and off-specular scattering geometry, it could be proved that TBA adsorbs in the planar trans configuration in the submonolayer regime. UV-light exposure at 355 nm (3.5 eV) leads to pronounced changes in the vibrational structure of the TBA molecules in direct contact with the Au(111) surface, which we assign to a trans to cis isomerization. The reverse process, that is, the cis to trans isomerization, can be stimulated by thermal activation. An intensity decrease of vibrational modes as a function of photon dose allows calculation of an effective cross section of $\sigma \approx 2*10^{-21}$ cm^2 for the trans to cis isomerization.

O 34.11 Tue 16:15 MA 043

Switching of Spiropyran molecules on a Au(111) surface — •Gunnar Schulze, Michael Karcher, Katharina Franke, Christoph Rüdt, Paul Fumagalli, and Jose Ignacio Pascual — Inst. für Experimentalphysik, Freie Universität Berlin, Berlin, Germany

The photon and electron mediated conversion of the molecule 3-methyl-6-nitro-spiropyran (SP) into its merocyanine isomer were investigated on a Au(111) surface by means of low temperature scanning tunnelling microscopy (STM) and by photo-absorption spectroscopy. STM resolves that the structure of SP molecular assemblies strongly depend on parameters like temperature and molecular density. The electronic properties of SP molecules on a metal surface, as obtained by scanning tunnelling spectroscopy (STS) and by photo-absorption spectroscopy, were compared to the electronic properties in solution. The alignment of these molecular states is specially important when inducing the SP to MC conversion.

O 35: Symposium: Atomic Wires at Surfaces II
(Invited Speakers: Erio Tosatti, Serge Lemay, Shuji Hasegawa)

Time: Tuesday 14:00–16:45 Location: HE 101

Invited Talk O 35.1 Tue 14:00 HE 101

Magnetic phenomena, spin orbit effects, and electron transport in*nanowire contacts, particularly in Platinum — •Erio Tosatti[1,2], Alexander Smogunov[2,1], Andrea Dal Corso[1], Anna Delin[3], and Ruben Weht[4] — [1]SISSA and Democritos, Trieste, Italy — [2]ICTP, Trieste, Italy — [3]KTH Stockholm, Sweden — [4]CNEA San Martin, Argentina

Nanocontacts between metal tips take in some instances the shape of ultra-thin suspended nanowires. Ballistic electron conductance through nanowire contacts is calculated based on plane wave/ultrasoft pseudopotential code developed to handle magnetism and spin orbit. As an application, the effect of magnetism on conductance will be demonstrated for monatomic contacts of 3d metals such as Ni and Co [1] with results in good agreement with break junction data.[2] Next, I will describe a new form of nanomagnetism, consisting of the spontaneous appearance of local magnetism at the nanocontact even in transition metals that are nonmagnetic in bulk such as Pt or Pd. The presence of nanomagnetism should in principle affect the conductance, as is demonstrated by direct calculation. Due to strong spin orbit, magnetism in a monatomic Pt nanowire or nanocontact should provide a novel case of "colossal magnetic anisotropy".[3] [1] A. Smogunov et al., Phys.Rev.B 70, 045417 (2004); Phys. Rev. B 74, 045429 (2006). [2] C. Untiedt, et al., Phys. Rev. B 69, 081401 (2004). [3] A. Delin and E. Tosatti, Phys. Rev. B 68, 144434 (2003); A. Delin, et al., Phys. Rev. Lett. 92, 057201 (2004); A. Smogunov, A Dal Corso, A. Delin, R. Weht and E. Tosatti, to be published.

O 35.2 Tue 14:30 HE 101

One-dimensional low energy plasmons in Au atom chains — •Tadaaki Nagao — World Premier International(WPI) Research Center, International Center for Materials Nanoarchitectonics(MANA), National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba 305-0044 JAPAN

Sound-wave-like collective excitation in dense one-dimensional (1D) electron systems confined to Au atom chains on the Si(557) surface is investigated [1]. Electron energy loss spectroscopy using a highly collimated slow electron beam has detected a characteristic low-energy 1D plasmon (wire plasmon) that Tomonaga has mentioned in his theory [2]. This plasmon freely propagates along the Au atom chain and appears as that of 1D free electron gas. However, theoretical analysis adopting a quantum-mechanical scheme beyond the free-electron model indicates a significant dynamic exchange-correlation effect due to strong 1D confinement. By cooling to below 100 K, we detected for the first time a significant change in the plasmon dispersion in the tiny momentum and energy region, which definitely reflects a tiny gap opening due to a metal-to-insulator transition of the atom chains. We also detected similar 1D charge excitations on different silicon surfaces.

\noindent [1] T. Nagao, S. Yaginuma, T. Inaoka, T. Sakurai, Phys. Rev. Lett. 97, 116802 (2006).

\noindent [2] S. Tomonaga, Prog. Theor. Phys. 5, 544(1950).

O 35.3 Tue 14:45 HE 101

Atomic structure and electronic properties of rare earth-silicide nanowires on Si(001) — •Martina Wanke[1], Christian Preinesberger[1], Gerd Pruskil[1], Denis Vyalikh[2], Sergeij Molodtsov[2], Steffen Danzenbächer[2], Clemens Laubschat[2], Petar Stojanov[3], Eric Huwald[3], John Riley[3], and Mario Dähne[1] — [1]Institute of Solid State Physics, Technical University Berlin, D-10623 Berlin, Germany — [2]Institute of Solid State Physics, Technical University Dresden, D-01219 Dresden, Germany — [3]School of Physics, La Trobe University, Bundoora, VIC 3086, Australia

Scanning tunneling microscopy (STM) and angle-resolved photoemission (ARPES) are used to investigate the self-assembly and electronic structure of rare earth silicide nanowires on Si(001) surfaces. Two types of self-assembled nanowires can be formed depending in particular on annealing temperature and material exposure. In high resolution STM images we found closed-packed thin nanowires and free-standing, broad nanowires with similar properties on planar and vicinal Si(001) surfaces. Using ARPES at BESSY II for electronic characterization we discovered three strongly dispersing bands crossing the Fermi energy along the nanowire direction for the free-standing nanowires. A beginning weak dispersion of electronic states is also found for the thin nanowire type. In perpendicular direction both types only show a periodic intensity variation at the Fermi energy, but negligible dispersion. The Fermi surface shows one-dimensional electronic features. This project was supported by DFG, project number Da 408/11.

O 35.4 Tue 15:00 HE 101

ELS-LEED investigations of Dy-silicide nanostructures on Silicon — •Svend Vagt[1], Eddy Patrick Rugeramigabo[1], Tadaaki Nagao[2], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — [2]National Institute for Materials Science, Tsukuba, Japan

Dysprosium silicide nanostructures have been grown by depositing up to 1ML of Dy on Si(111) and on vicinal Si(001) substrates. Ultra-high vacuum conditions ($p \leq 1\times10^{-10}$ mbar during Dy deposition) are prerequisite to avoid Dy oxidation. The atomic and electronic properties have been investigated using ELS-LEED, which allows the simultaneous study of geometric and electronic properties at the same point in k-space with both high momentum and energy resolution.

Deposition of 1ML of Dy on Si(111) at RT followed by annealing at 500°C results in a flat monolayer with $DySi_2$ stoichiometry. The diffraction pattern revealed the typical 1×1 structure. A 2D-Plasmon dispersion is reported for the first time with a $\sqrt{q_{||}}$ behavior up to $q_{||}$=0.08 Å^{-1} in k-space. High quality arrays of parallel nanowires have been grown on 4°-vicinal Si(001) at 500°C for a Dy coverage around 0.4ML. A $n\times2$ periodicity has been found, with n shifting from 10 to 7 for increasing coverage up to 0.75ML. The energy loss disperses only in the direction along the nanowires, whereas in the perpendicular direction the plasmon can not be excited. The plasmon dispersion turned out to be a quasi-1D-plasmon. It has been accurately simulated by explicitely taking into account the finite width of the $DySi_2$ nanowire structures. Interactions between adjacent nanowires play a minor role.

15 min. break

Invited Talk O 35.5 Tue 15:30 HE 101

Simultaneous electrical transport and scanning tunneling spectroscopy of carbon nanotubes — Brian J. LeRoy, Iddo Heller, Vijay K. Pahilwani, Jing Kong, Cees Dekker, and •Serge G. Lemay — Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands

Using scanning tunneling spectroscopy, we demonstrate that current directly injected into a freely suspended individual single-wall carbon nanotube can be used to excite, detect and control a specific vibrational mode of the molecule. Electrons tunneling inelastically into the nanotube cause a non-equilibrium occupation of the radial breathing mode, leading to both stimulated emission and absorption of phonons by successive electron tunneling events. We exploit this effect to estimate a quality factor of well over 10,000 for this nanomechanical oscillator. We further employ the suspended geometry to perform scanning tunneling spectroscopy measurements on single-walled carbon nanotubes with independently addressable source and drain electrodes in the Coulomb blockade regime. This three-terminal configuration allows the coupling to the source and drain electrodes to be quantitatively measured, which we exploit to demonstrate that electrons were added to spin-degenerate states of the carbon nanotube. Unexpectedly, the Coulomb peaks also show a strong spatial dependence. By performing simultaneous scanning tunneling spectroscopy and electrical transport measurements we show that the probed states are extended between the source and drain electrodes and that the observed spatial dependence thus reflects a tip-induced modulation of the contact resistance.

Invited Talk O 35.6 Tue 16:00 HE 101

Transport at Atomic Wires on Silicon Surfaces — •Shuji Hasegawa — University of Tokyo, Tokyo, Japan

Owing to new techniques of microscopic four-point probes with four-tip scanning tunneling microscope (4T-STM) and monolithic four-point probes, electronic transport through single-atomic layers as well as atomic chains and nanowires on semiconductor crystals can be now measured directly. Interesting transport properties of such atomic-scale structures have been revealed; the instability and atomic-scale defects intrinsic to atomic wires play decisive roles in transport. I will introduce and summarize several topics in the talk such as metal-insulator transition, hoping conduction due to defects, inter-chain transport and so on. Recent advancements with metal-coated carbon-nanotube tips in 4T-STM are also introduced.

O 35.7 Tue 16:30 HE 101

Structural influence towards transport: Pb wires on Si(557) — •Marcin Czubanowski, Annemarie Schuster, Christoph Tegenkamp, and Herbert Pfnür — Institut of Solid State Physics, Surface Science Department, Hannover, Germany

The adsorption of 1.3 ML of Pb on Si(557) substrates followed by annealing at 640K leads to the formation of an anisotropic metallic structures as revealed by conductivity, STM and ARPES measurements. Those structures below 78K show metallic conductance along the Pb-chains, whereas in the direction perpendicular to the chain-structure an insulating behavior has been found. Additionally, ARPES measurements have shown that below T_c, those structures undergo complete Fermi nesting in the direction normal to the structure. In our recent LEED experiments, the chain structure has been systematically investigated as a function of temperature by means of SPA-LEED analysis. The adsorption of Pb transforms (locally) the surface into a regularly stepped (223) facet below T_c. This structure undergoes reversibly a comensurable-incomensurable phase transition at $T_c = 78$K as judged from changes in position of step diffraction spots in the $[\overline{11}\,2]$ direction and also the periodicity of domain wall reflexes in the $[1\overline{1}\,0]$ direction. Furthermore, the transition depends crucially on the Pb coverage. If the steps are decorated by excess Pb, e.g. 1.5ML, the transition is strongly suppressed.

O 36: Surfaces and Films: Forces, Structure and Manipulation

Time: Tuesday 14:15–16:45 Location: MA 041

O 36.1 Tue 14:15 MA 041

Low-Temperature STM Study of the $(\sqrt{3}\times\sqrt{3})30^\circ$ Reconstructed Ni_2P (0001) Surface - Atomic Resolution and Geometric Model — •Georg Hermann Simon[1], Thomas König[1], Markus Heyde[1], Hans-Joachim Freund[1], Kumiko Kinoshita[2], Yuta Nakagawa[2], Shushi Suzuki[2], and Kiyotaka Asakura[2] — [1]Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, D-14195 Berlin, Germany — [2]Catalysis Research Center, Hokkaido University, Sapporo 001-0021, Japan

New catalysts have to be found to follow the demanding legislation around the world for the reduction of sulfur contents in transportation fuels. A promising candidate is Ni_2P [1], which is fairly new to surface science. Despite several wet-chemical studies, simulation, spectroscopic and the first room-temperature STM characterization [2] there are many open questions to this material. In surface studies (0001) oriented single crystals have been analyzed so far. In our ultrahigh vacuum low-temperature STM study we worked on a deeper understanding of the surface termination, its preparation and mircostructure. We present atomically resolved images of a previously unreported $(\sqrt{3}\times\sqrt{3})30^\circ$ reconstruction of the (0001) surface. We put forward considerations for a geometrical model that is being developed in our cooperation based on the Ni_3P_1 termination of Ni_2P (0001).
[1] X. Wang, P. Clark, S.T. Oyama, J. Catal. 208 (2002) 321.
[2] M.G. Moula, S. Suzuki, W.-J. Chun, S. Otani, S.T. Oyama, K. Asakura, Surf. Interface Anal. 38 (2006) 1611.

O 36.2 Tue 14:30 MA 041

Force measurement with a scanning tunneling microscope — •Kai-Felix Braun[1,2] and Saw-Wai Hla[2] — [1]Physikalisch Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig — [2]Clippinger Laboratories, Ohio University, Athens, Ohio 45701, USA

We present a method to measure the interaction force between single atoms with a scanning tunneling microscope [1]. During experiments for atomic manipulation with a scanning tunneling microscope the tip height curve is recorded. It is shown here that the amplitude of the manipulation curve is a measure for the interaction force between the microscopes tip and a single atom adsorbed on a surface. A simple formula is derived and tested. Extensions of this scheme to different surfaces shall be discussed.

[1] K.-F. Braun and S.W. Hla, Physical Review B 75 (2007), 033406

O 36.3 Tue 14:45 MA 041

The Force to Move an Atom — •Markus Ternes[1], Christopher P. Lutz[1], Cyrus F. Hirjibehedin[1], Franz J. Giessibl[2], and Andreas J. Heinrich[1] — [1]IBM Research Division, Almaden Research Center, San Jose, USA — [2]Institute of Experimental and Applied Physics, University of Regensburg, Regensburg, Germany

Atomic manipulation of single atoms and molecules by scanning probe microscopy enables the assembly of structures at the single-atom scale – the ultimate lower size limit. However, it has been difficult to answer the simple question: How much force does it take to manipulate atoms and molecules on surfaces? To address this question, we used a combined atomic force and scanning tunneling microscope to simultaneously measure the force and the current between an adsorbate and a tip during atomic manipulation.

We found that the force it takes to move an atom depends crucially on the binding between adsorbate and surface. Our results indicate that for moving metal atoms on metal surfaces, the lateral force component plays the dominant role. In contrast, we found that the forces to manipulate molecular adsorbates, such as carbon monoxide (CO), were markedly different.

Measuring the forces during manipulation yielded the full potential energy landscape of the tip-sample interaction. Surprisingly, the potential energy barriers are comparable to diffusion barriers, which are obtained in the absence of a probe tip.

O 36.4 Tue 15:00 MA 041

Lateral Resolution in Piezoresponse Force Microscopy — Tobias Jungk, Akos Hoffmann, and •Elisabeth Soergel — Institute of Physics, University of Bonn, Wegelerstrasse 8, 53115 Bonn, Germany

Among the methods for visualization of ferroelectric domains piezoresponse force microscopy (PFM) has become a very common technique mainly due to its high lateral resolution without any need for specific sample preparation. Although domain structures are easily imaged with this method, the lateral resolution and thus the observed domain wall width is still under discussion. The reported values for the width of 180° domain walls scatter noticeably. These inconsistencies can be explained by the PFM background inherent to the experimental setup that can broaden the observed domain wall widths. In this contribution, we present a quantitative study of the resolution in PFM depending on the tip radius, the type of sample and the thickness of the sample. For bulk single crystals the measured linear dependency of the width of the domain wall on the tip radius using PFM is validated by a simple theoretical model. Independent on the crystal type (BaTiO3, KNbO3, KTP, LiNbO3, LiTaO3, PGO and SBN) the same lateral resolution was measured. Using a Ti-Pt-coated tip with a nominal radius of 15 nm the so far highest lateral resolution in bulk ferroelectric crystals of only 17 nm was obtained.

O 36.5 Tue 15:15 MA 041

Morphology and electronic structure of epitaxially grown $CuInS_2$ films — •Carsten Lehmann[1], Volker Eyert[2], and Christian Pettenkofer[1] — [1]Hahn-Meitner-Institut, SE6, Berlin, Germany — [2]Universität Augsburg, Inst. f. Physik, Augsburg, Germany

The ternary compound semiconductor $CuInS_2$ with a direct band gap of 1.53 finds application as absorber material in modern thin film solar cells. For a better understanding of the parameters determining the properties of a junction detailed information on the electronic structure is necessary. We report on ARUPS measurements on thin epitaxial $CuInS_2$ films prepared on sulfur passivated GaAs(100) and GaAs(111)B. Samples were prepared in a combined UHV GSMBE deposition and analysis system with an organic sulfur precursor. The bandstructure mapping was performed at the beamline TGM7 at BESSY II. The experimentally obtained electronic structure for CuInS$_2$(001) shows good agreement with augmented spherical wave (ASW) calculations based on density functional theory (DFT) and the local density approximation (LDA). For CuInS$_2$(112) films deposited on GaAs(111)B substrates we observe a LEED pattern with a sixfold symmetry which is not in accordance with a simple chalcopyrite (112) structure. We will discuss the observed structure within a domain model of the surface and its implications on our obtained spectra.

O 36.6 Tue 15:30 MA 041

3D force field measurements using non-contact atomic force microscopy on KBr: Theory and Experiment — •Kai Ruschmeier[1,2], Regina Hoffmann[3], and André Schirmeisen[1,2] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Wilhelm-Klemm Str. 10, 48149 Münster — [2]CeNTech, Center for Nanotechnology, Heisenbergstr. 11, 48149 Münster — [3]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe

Atomic force microscopy is capable of characterizing surfaces with atomic resolution. Here, we use an ultrahigh vacuum atomic force microscope in non-contact mode to measure the three-dimensional force field [1,2] of a KBr(001) surface at room temperature. On a predefined grid we measure the force distance curves over a wide range of tip-sample distances, from attractive to repulsive forces. Atomic resolution surface scans before and after the 3D force curve measurements showing single atomic defects assured an unmodified atomically sharp tip. The subtraction of long-range van-der-Waals and electrostatic forces allows us to extract the short-range chemical forces. The results show good agreement with site-specific atomistic simulations of short-range tip-sample forces for a K$^+$-terminated tip [3] and thus allow us to identify the tip apex atom polarity as well as the lattice sites in our AFM images. Furthermore we calculate the lateral tip sample force from the potential energy landscape and compare these results with theoretical predictions.

[1] H. Hölscher et al., APL 81, 4428 (2002) [2] A. Schirmeisen et al., PRL 97, 136101 (2006) [3] R. Hoffmann et al., PRL 92, 146103 (2004)

O 36.7 Tue 15:45 MA 041

Single crystal microcalorimetry: Measuring molecule-surface interactions — •Jan-Henrik Fischer[1], Jason Farmer[2], Jens Hartmann[1], Swetlana Schauermann[1] und Hans-Joachim Freund[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Department of Chemistry, University of Washington, Seattle

Determination of the strength of adsorbate-surface interaction is an important fundamental issue in surface science and an essential prerequisite for understanding real catalytic processes. The strength of adsorbate-surface bonding and of lateral adsorbate-adsorbate interactions can be addressed by measurement of heats of adsorption as a function of surface structure, coverage and presence of other co-adsorbates.

Traditional experimental techniques for probing the energetics of adsorption, such as e.g. thermal desorption spectroscopy, provide reliable results only for reversible adsorption systems and cannot be correctly applied for processes including dissociation, clustering, diffusion into the bulk or reaction with other coadsorbates. These restrictions can be overcome by using a direct calorimetric measurement of adsorption energies on surfaces. For this purpose we set up a new microcalorimetry experiment at Fritz-Haber-Institut, which is based on a method previously developed by King and Campbell [1]. The method relies on the measurement of a temperature change upon adsorption of gaseous molecules on ultrathin ($1-10\,\mu$m) single crystals, which is realized by application of a pyroelectric detector and an independent laser-based energy calibration.

[1] Campbell et al., Rev. Sci. Instr. **75**, 11 (2004)

O 36.8 Tue 16:00 MA 041

Investigating surface dynamics with inelastic X-ray scattering — •Bridget Murphy[1], Martin Müller[1], Jochim Stettner[1], Herwig Requardt[2], Jorge Serrano[2], Michael Krisch[2], and Werner Press[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]ESRF, BP 220, F-38043 Grenoble Cedex 9, France

Inelastic x-ray scattering in grazing incidence conditions provides a new tool to selectively study either surface or bulk lattice dynamics in a single experiment. It is possible to study acoustic and optical surface phonon modes currently with a 3meV resolution over a wide range of momentum space and make a direct comparison between surface and bulk dispersion. In particular $2H-\mathrm{NbSe}_2$ and $2H-\mathrm{TaSe}_2$will be discussed. For these materials a Kohn anomaly has been previously reported. Our data demonstrate that the softening of the Kohn anomaly at the $2H-\mathrm{NbSe}_2$ surface is significantly greater that that reported for the bulk [1]. This is an indication of a relaxation in the top most layers of the crystal. Temperature dependent studies will be presented.

[1] B. M. Murphy, H. Requardt, J. Stettner, J. Serrano, M. Krisch, M. Müller, W. Press, Phys. Rev. Lett. 95, 256104 (2005)

O 36.9 Tue 16:15 MA 041

Variations of the electrochemical potential at monoatomic steps resolved by scanning tunneling potentiometry — •Mark Kaspers[1], Alexander Bernhart[1], Bastian Weyers[1], Evgeny Zubkov[1], Rolf Möller[1], Christian Bobisch[2], Jan Homoth[3], Martin Wenderoth[3], Thomas Druga[3], Lars Winking[3], and Rainer-G. Ulbrich[3] — [1]University of Duisburg-Essen, Department of Physics, Duisburg, Germany — [2]University of California, Irvine, USA — [3]Georg-August-University, Physical Institute, Göttingen, Germany

On macroscopic scale the energy dissipation of electrons scattering at phonons, atomic steps, grain boundaries etc. contribute to the total resistivity. To gain access to these effects on the nanoscale scanning tunneling potentiometry was performed on a Si(111)-($\sqrt{3}\times\sqrt{3}$)-Ag surface superstructure. The experimental data show how the variations of the electrochemical potential are correlated to the topography. E.g. the potential drops at step edges on a lengthscale of about 1.2nm.

Our setup consists of an optimized Omicron Nanoprobe equipped with three independent STM-units. Two STM-tips were used to apply a constant lateral current through the Ag adlayer. The third tip maps the topography as well as the local potential simultaneously.

Our experiment gives access to the spatial variations of the potential inside the structure itself right across the obstacles. This provides a new insight in the elementary processes of the electric resistance observed in macroscopic experiments.

O 36.10 Tue 16:30 MA 041

Photoemission experiments using soft x-ray standing waves — •Sven Döring[1,2], Daniel Weier[1,2], Ulf Berges[1,2], Charles S. Fadley[3,4,5], and Carsten Westphal[1,2] — [1]DELTA, TU Dortmund, Maria-Goeppert-Mayer-Str. 2, 44221 Dortmund, Germany — [2]Experimentelle Physik 1, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany — [3]Materials and Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA — [4]University of California, Davis, CA 95616, USA — [5]Forschungszentrum Jülich, IFF-9, 52425 Jülich, Germany

A high depth resolution can be obtained by creating a soft x-ray standing wave field on the sample surface and performing photoemission experiments in this field. A high reflectivity is necessary for a sufficient standing wave modulation. Multilayer samples are used which provide a strong first order Bragg reflection. The standing wave field can be moved through the sample surface by a sample rotation around the Bragg angle. The shape and modulation of these rocking curves contain information about the sample. First measurements on various samples were performed at the TU Dortmund's synchrotron light source DELTA and at higher energies at BESSY II in Berlin. Results from different samples will be presented in the talk: rocking curves from bare multilayers will be shown as well as a first test measurement of a thin layer of MgO on a wedge of Fe on top of a multilayer. The data show depth profiles obtained of the internal interface. Different chemical states of the same element can be identified by their chemical shift in the XPS spectrum and allocated to certain layers.

O 37: SYNF: Ferroic Materials and Novel Functionalities II (Invited Speakers: Jochen Mannhart, Warren Pickett, Yoshinori Tokura, Ramamoorthy Ramesh, Agnes Barthelemy, Evgeny Tsymbal; FV: MA+O+MM+DF+DS+HL+TT)

Time: Tuesday 14:30–17:30 Location: A 151

See SYNF for details about the program.

O 38: SYSA: Tayloring Organic Interfaces: Molecular Structures and Applications III (Invited Speaker: Alberto Salleo; FV: DS+CPP+HL+O)

Time: Tuesday 14:30–16:30 Location: H 2013

See SYSA for details about the program.

O 39: SYSA: Tayloring Organic Interfaces: Molecular Structures and Applications IV (Poster; FV: DS+CPP+HL+O)

Time: Tuesday 14:30–20:00 Location: Poster A

See SYSA for details about the program.

O 40: SYSA: Tayloring Organic Interfaces: Molecular Structures and Applications V (Invited speaker: Henning Sirringhaus; FV: DS+CPP+HL+O)

Time: Tuesday 16:30–18:30 Location: H 2013

See SYSA for details about the program.

O 41: Invited Talk Christian Frischkorn

Time: Tuesday 17:00–17:45 Location: HE 101

Invited Talk O 41.1 Tue 17:00 HE 101
Nonadiabatic Processes in Surface Femtochemistry at Metals — •Christian Frischkorn — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

A fundamental understanding of chemical reaction dynamics relies on the Born-Oppenheimer approximation, a key concept in chemical physics which assumes that the reaction evolves electronically adiabatically on the ground or an excited potential energy surface. Thereby, nonadiabatic coupling effects between nuclear motions and electronic degrees of freedom are neglected. However, in surface femtochemistry, where a chemical reaction on a surface is initiated by an ultrashort laser pulse, exactly this nonadiabatic coupling between electron-hole pair excitations in the metal substrate and nuclear (vibrational) degrees of freedom of the adsorbed reactants provides the base to describe the evolving reaction dynamics. The appeal of surface femtochemistry is to switch on this nonadiabaticity directly in the time domain. Various time-resolved spectroscopic techniques are used to obtain microscopic-level information on the underlying reaction mechanism, coupling times and energy partitioning between different degrees of freedom of the reaction product as will be illustrated by several examples of femtosecond-laser induced surface reactions.

O 42: Invited Talk Gil Alexandrowicz

Time: Tuesday 17:45–18:30 Location: HE 101

Invited Talk O 42.1 Tue 17:45 HE 101
Lateral Interactions on Surfaces: An Empirical Perspective — •Gil Alexandrowicz[1], Pepijn R. Kole[1], Everett Y. M. Lee[1], Holly Hedgeland[1], Riccardo Ferrando[2], Andrew P. Jardine[1], William Allison[1], and John Ellis[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge, UK — [2]Dipartimento di Fisica, Università di Genova, Genova, Italy

Lateral forces between surface atoms and molecules play a critical role in a wide variety of surface related phenomena. Examples include thin film growth, industrial catalysis, and the assembly of nanostructures. Direct experimental data for the nature and the magnitude of these forces was typically unavailable, and simplifying assumptions were made both to deduce these interactions from indirect macroscopic measurements and to include them in numerical models of surface systems.

The recently developed helium spin echo spectrometer[1], has the unique capability to measure both surface motion and lateral interactions on an atomic length scale and on a pico to nano-second time scale[2]. In this talk I will describe how this instrument is used to measure lateral interactions and present recent results obtained for the strongly interacting surface system CO/Pt(111). Surprisingly, we find that the standard surface science approximations completely fail to describe this prototypical system and that the interactions between the CO molecules are of a complex many body nature. [1] AP Jardine et. al. Science 305, 1790 (2004). [2] G Alexandrowicz et. al. Phys. Rev. Lett. 97, 156103(2006).

O 43: Poster Session II - MA 141/144 (Surface Spectroscopy on Kondo Systems; Frontiers of Surface Sensitive Electron Microscopy; Methods: Scanning Probe Techniques+Electronic Structure Theory+Other; Time-Resolved Spectroscopy of Surface Dynamics with EUV and XUV Radiation; joined by SYNF posters)

Time: Tuesday 18:30–19:30 Location: Poster F

O 43.1 Tue 18:30 Poster F
The Kondo-resonance in photoemission spectra on ordered

Ce surface alloys — •Markus Klein[1], Christina Albers[1], Juarez Da Silva[3], Kevin Beach[2], Fakher Assaad[2], and Friedrich Reinert[1] — [1]Universität Würzburg, Experimentelle Physik II, Am Hubland, 97074 Würzburg, Germany — [2]Universität Würzburg, Theoretische Physik I, Am Hubland, 97074 Würzburg, Germany — [3]National Renewable Energy Laboratory, 1617 Cole Blvd., Golden, CO 80401, USA

The physical properties of Kondo systems are determined by interactions between localized f-states and conduction electrons. Of particular interest are low-dimensional systems as they can serve as elementary model systems. Due to its surface sensitivity angle-resolved photoelectron spectroscopy (ARUPS) is an excellent tool to study directly the electronic structure of a two-dimensional Kondo system. This requires highly ordered and ultra thin singlecrystalline films. We have prepared singlecrystalline Ce surface-alloys by *in situ* deposition of Ce on noble metal surfaces. Our ARUPS results show a temperature and wave-vector dependent Kondo-resonance and other hybridization effects. We discuss our spectroscopic results with the help of data from isostructural La films, LDA+U, and DMFT calculations.

O 43.2 Tue 18:30 Poster F

Temperature Dependence of the Single Particle Spectral Function of the 2D Kondo Lattice Model using the Dynamical Cluster Approximation — •Lee Martin and Fakher Assaad — Universität Würzburg, Germany

We apply the dynamical cluster approximation, with a quantum Monte Carlo cluster solver using various cluster sizes, to the two-dimensional Kondo lattice model to investigate the evolution of the conduction electron single particle spectral function as a function of temperature. In the hole doped, paramagnetic metallic phase the problem contains two energy scales: the Kondo temperature, T_K, and the lower scale, the coherence temperature T_{coh}. With decreasing temperature, moving from the local moment to Kondo screened regime, we look for signatures of T_K in the spectral function before finally observing the formation of the coherent heavy fermion state at and below T_{coh}.

O 43.3 Tue 18:30 Poster F

Evidence for quantum confinement in lognormal size distributed nanodiamonds — •Thomas Berg[1], Edit Marosits[2], Jochen Maul[1], Peter Nagel[3], Ulrich Ott[2], Florian Schertz[1], Stefan Schuppler[3], Christa Sudek[2], and Gerd Schönhense[1] — [1]Institut für Physik, Staudingerweg 7, D-55128 Mainz, Germany — [2]Max-Planck-Institut für Chemie, Becherweg 27, D-55128 Mainz, Germany — [3]Forschungszentrum Karlsruhe, IFP, 76021 Karlsruhe, Germany

Quantum confinement (QC) in semiconductor nanoparticles was discovered more than two decades ago and received increasing interest during the recent years. In the case of nanodiamonds evidence for QC was reported by [1], but the discussion on the extend of these effects in nanosized diamonds is still ongoing [2,3,4].

We report on NEXAFS-PEEM measurements of the Carbon K-edge of meteoritic nanodiamonds. The NEXAFS spectrum of this nanodiamond population shows a broadened and asymmetric exciton which was assigned to the particles size distribution in recent publications but a detailed explanation is still missing. We present quantitative analysis of the modified peak shape in respect to energy shifts of the exciton and the onset of the carbon K-edge caused by the well known size distribution of this nanodiamond population as a consequence of QC. This project is supported by DFG (SCHO 341/10-1).

[1] Chang et al., Phys. Rev. Lett. 82, 5377 (1999) [2] Lley et al., Phys. Rev. Lett. 84, 5679 (2000) [3] Pong et al., Phys. Rev. Lett. 84, 5680 (2000) [4] Willey et al., Phys. Rev. Lett. 95, 113401 (2005)

O 43.4 Tue 18:30 Poster F

Setup and Characterization of a Standing-Wave PEEM for EUVL mask inspection — •Jochen maul[1], Jingquan Lin[2], Andreas Oelsner[1], Dima Valdaitsev[1], Nils Weber[3], Matthias Escher[3], Michael Merkel[3], Ulf Kleineberg[2], and Gerd Schoenhense[1] — [1]Institut fuer Physik, Staudinger Weg 7, Johannes Gutenberg-Universitaet, D-55128 Mainz — [2]Ludwig Maximilian-Universitaet, Am Coulombwall 1, 85748 Garching — [3]Focus GmbH, Neukirchner Str. 2, D-65510 Huenstetten-Kesselbach

Extreme ultraviolet lithography (EUVL) is one of the promising possibilities for driving the critical dimensions of semiconductor devices to the ultimate limit. One central issue for chip production using EUVL is the quality of reflective masks with patterned absorbers, employed for the structuring of semiconductor elements. Here, the density and the properties of defects are essential. For multilayer optics, two different types of defects are generally distinguished: amplitude defects and phase defects (or "buried defects") distorting the standing electrical wave inside the multilayer and leading to variations in the field strength at the surface. We show that standing-wave PEEM is a very powerful method as a spatially resolving detector for "at-wavelength (13.5 nm)" metrology. A setup has been designed that allows the study of masks with a size of six square inches. The present detection limit of our method for phase defects is 35 nm.

This work is supported by the European Union (6th Framework program) within the project "Exploring new limits to Moores law- More Moore".

O 43.5 Tue 18:30 Poster F

Optical magnetic circular dichroism in two-photon photoemission — •Kerstin Hild, Jochen Maul, Gerd Schoenhense, and Hans-Joachim Elmers — Institut fuer Physik, Staudinger Weg 7, Johannes Gutenberg-Universitaet, D-55128 Mainz

Magnetic circular dichroism in two-photon photoemission (2PPE) was demonstrated based on frequency-doubled femtosecond laserlight (pulse length ~150fs). Thin films of Ni2MnGa and Co2FeSi Heusler alloys showed magnetic asymmetries in the integrated photoemission intensity of 0.35% and 0.43%. Thereby, 2PPE was excited by perpendicular incident polarization-modulated light, while the sample magnetization was orientated parallel and antiparallel to the laser beam by an external magnetic field. Asymmetries were measured by a phase-sensitive detection. Furthermore a magnetite thin film was investigated by frequency-tripled laser light in one-photon photoemission showing a magnetic asymmetry of 0.47%, which is much larger than the value 0.08% measured under two-photon-photoemission. The results are compared with earlier work using linearly polarized UV light [1] and circularly polarized laser light [2].

[1] G.K.L. Marx, H.J. Elmers, G. Schönhense, Phys. Rev. Lett. 84 (2000) 5888. [2] T. Nakagawa, T. Yokoyama, Phys. Rev. Lett. 96 (2006) 237402.

O 43.6 Tue 18:30 Poster F

Transmission photoemission electron microscopy for lateral mapping of the X-ray absorption structure of a metalloprotein in a liquid cell — •Daniel Panzer[1], Christian Beck[2], Jochen Maul[1], Marco Möller[2], Heinz Decker[2], and Gerd Schönhense[1] — [1]Institut fuer Physik, Staudinger Weg 7, Johannes Gutenberg-Universitaet, D-55099 Mainz — [2]Institut fuer Molekulare Biophysik, Welderweg 26, D-55099 Mainz

The mechanism of oxygen incorporation in respiratoty proteins is subject of intensive discussion. We use photoemission electron microscopy in an X-ray transmission mode for full-field imaging of the X-ray absorption structure of copper in the respiratory metalloprotein hemocyanin KLH1. It contains 160 oxygen bonding sites. Each site reversibly binds one molecule oxygen between two copper atoms. In our setup, hemocyanin is dissolved in aqueous solution and enclosed in an ultra-high vacuum compatible liquid sample cell with silicon nitride membranes. The local X-ray absorption structure of the liquid sample is converted into photoelectrons at the microscope side of the cell acting as a photocathode. In this way, different copper valences are laterally distinguished under in vivo-like conditions, attributed to Cu(I) in the deoxy-state and Cu(II) in the oxy-state.

This project was funded by the DPG (SCHO 341/7).

O 43.7 Tue 18:30 Poster F

Time and energy resolved mulitphoton-photoemission microscopy of organic materials — •Florian Lindla, Gerhard Lilienkamp, and Winfried Daum — Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstraße 4, 38678 Clausthal, Germany

Polystyrene (PS) microspheres and PS films on oxidized Pt surfaces were investigated by a photoemission-electron-microscope (PEEM) with 400nm (3.1eV) fs laser excitation. For pump-probe measurements the illumination system was equipped with a delay-line consisting of thin film polarizer plates as beam splitter/combiner.

Energy resolved measurements on PS microspheres (300nm in diameter) resulted in an energy distribution showing one peak, which slightly shifts to higher electron energies at higher laser intensities.

For further investigation first time resolved measurements were performed on an oxidized Pt surface with partial PS coverage (around 100nm thickness), revealing the expected 2-photon-photoemission

(2PPE) signal for the Pt substrate, while the signal of the PS coating is independent of probe delay, presumably due to an highly filled intermediate state proposed before.

O 43.8 Tue 18:30 Poster F

Characterization of W-Tips used in Tuning-Fork Non-Contact Atomic Force Microscopy by Field Ion Microscopy — •Daniel-Alexander Braun[1], Jens Falter[1,4], Thomas König[2], André Schirmeisen[1,4], Hendrik Hölscher[4], Udo D. Schwarz[3], and Harald Fuchs[1,4] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [3]Department of Mechanical Engineering, Yale University, New Haven, CT, USA — [4]Center for Nanotechnology (CeNTech), University of Münster, Münster, Germany

The atomic force microscope (AFM) is capable to image surfaces with atomic resolution. However, the interpretation of the atomic scale contrast is often difficult and inconclusive. This deficiency is partly caused by the unknown structure of the probing tip, as the chemical interaction between tip and surface and therefore the image contrast is largely determined by the exact configuration of the tip apex. Field ion microscope (FIM) images, on the other hand, enable a complete reconstruction of the atomic geometry of a sharp metallic tip. In this work, we present a special tip holder which can be used in both our home-built AFM and FIM. This combination allows to characterize the exact atomic structure of both interaction partners, the sample and the tip. First results are presented, where the apex radii of electrochemically etched tungsten tips are determined by FIM and subsequently correlated to force distance curves.

O 43.9 Tue 18:30 Poster F

Self-actuating self-sensing cantilever for dynamic AFM — •Henning von Allwörden, Alexander Schwarz, C. Julian Chen, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Jungiusstraße 11, 20355 Hamburg

Conventional AFM force sensors consist of a flexible cantilever beam made from silicon. For operation in the dynamic mode they are actuated by a driver piezo. Common methods for detection of the cantilever oscillation are optical techniques like beam deflection or interferometry. Hence, force sensor, its actuation and its detection are three separated devices. Combining them into a single device would make AFM instruments much simpler in design and handling. The qPlus sensor [1] is a tuning fork based on z-cut quartz. One arm is glued to a substrate, the other serves as a cantilever. The cantilever oscillation is detected by utilizing the piezoelectric effect of quartz via a pair of electrodes. However, excitation is still done externally. Furthermore, these sensors have large spring constants, resulting in a low force sensitivity. It is not possible to choose from a large variety of spring constants and resonance frequencies. Our idea is to place two pairs of electrodes, one for actuation and one for detection on a cantilever made from a single piece of x-cut quartz. Hence, we would have a self-actuating self-sensing cantilever [2]. Eigenfrequency and spring constant can be adjusted by choosing appropriate dimensions. The general concept of this sensor will be discussed and properties of prototypes will be presented.

[1] Giessibl, Appl. Phys. Lett. **73**, 3956 (1998)
[2] patent pending

O 43.10 Tue 18:30 Poster F

Strategies for measuring interfacial friction by lateral manipulation of nanoparticles using atomic force microscopy techniques — •T. Mönninghoff[1], D. Dietzel[1,2], L. Jansen[1,3], H. Fuchs[1,2,3], U. D. Schwarz[4], and A. Schirmeisen[1,2] — [1]Institute of Physics, University of Münster, Germany — [2]Forschungszentrum Karlsruhe (FZK), Germany — [3]Center for Nanotechnology (CeNTech), University of Münster, Germany — [4]Department of Mechanical Engineering, Yale University, New Haven, CT, USA

A promising approach for quantifying interfacial friction is to measure lateral forces during the manipulation of nanoparticles with the atomic force microscope. This technique allows addressing many current issues in the field of nanoscale friction, like the influence of contact size and interface crystallinity, which are not fully accessible with conventional friction force microscopy. We present different manipulation strategies that have been developed to either enable the defined and repeated manipulation of single nanoparticles or to gather statistical data on a larger ensemble of particles found within a particular scan area. Especially the latter approach allows fast and statistically significant data. In all cases, the particle-surface interfacial friction can be extracted from the additional torsional signal of the cantilever during the pushing process in contact mode operation [1]. As a model system for the demonstration of the different manipulation strategies, antimony nanoparticles with different diameters and crystallinity grown on a HOPG substrate have been chosen. [1] Dietzel et al., J. Appl. Phys.102, 084306 (2007)

O 43.11 Tue 18:30 Poster F

Design of an UHV-STM for applications at low temperatures and high magnetic fields — Daniel Haude[1], •Matthias Menzel[1], Kirsten von Bergmann[1], Matthias Bode[2], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, University of Hamburg, Germany — [2]Center for Nanoscale Materials, Argonne National Laboratory, USA

We constructed a Scanning Tunneling Microscope (STM) for spin-polarized studies of magnetic adatoms on metallic surfaces. This STM is mounted in a commercial ^{3}He-Flow-Cryostat, which allows measurements in UHV conditions and at a magnetic field up to 9 T perpendicular to the sample. With ^{4}He in the gas loop we already reached a temperature of 1.16 K leading to an estimation of a temperature of 700 mK with ^{3}He in the cycle. Since the STM is fixed at the bottom of the cryostat insert, tip and sample are transferred without visibility using a magnetic drive for linear and rotary motions. The cryostat is mounted via a transfer chamber to an existing UHV system which has been described elsewhere [1].

Tips and samples can be transferred throughout the pre-existing UHV system thus allowing us to investigate the same samples with different STM's. With an electron beam evaporator we can deposit different magnetic materials onto the cold substrate enabling studies of magnetic properties of single atoms or clusters of few atoms.

[1] O. Pietzsch *et al.*, Rev. Sci. Instrum. **71**, 424 (2000)

O 43.12 Tue 18:30 Poster F

Einfluss der elektronischen Struktur der Tunnelspitze auf spektroskopische Messungen — •Oliver Ferdinand, Kirsten von Bergmann, André Kubetzka, and Roland Wiesendanger — Institut für Angewandte Physik, Universität Hamburg, D-20355 Hamburg

Die Raster-Tunnel-Spektroskopie (RTS) misst die lokale differentielle Leitfähigkeit. Diese ist bei kleinen Spannungen in erster Näherung proportional zur lokalen Zustandsdichte (LDOS) beider Elektroden, Probe und Tunnelspitze, und mathematisch eine mit dem Transmissionskoeffizienten gewichtete Faltung beider LDOS. Gerade wenn der relevante Bereich um das Fermi-Niveau E_F konzentriert ist, wie z.B. bei Kondo-Systemen oder inelastischen Prozessen, wirken sich daher Oberfläche und Spitze in gleichem Maße auf die gemessenen Spektren aus, so dass eine möglichst strukturlose LDOS der Tunnelspitze erforderlich ist.

Es wird gezeigt, dass sich verschiedene Spitzen-Materialien unterschiedlich auf die Spektren auswirken. Dazu wurden Wolfram, Iridium und Gold verwendet und sowohl in-situ als auch ex-situ [1] Präparationsverfahren ausprobiert.

[1] A. J. Melmed, J. Vac. Sci. Technol. B **9**, 601 (1991)

O 43.13 Tue 18:30 Poster F

Spin-dependent Image Potential States Studied By SP-STS — •Anika Emmenegger, Stefan Krause, Gabriela Herzog, André Kubetzka, Daniel Haude, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Germany

An electron approaching a metal surface feels the attractive force of the polarization charge it induces in the surface region of the solid. If the surface has a band gap near the vacuum level, the electron gets trapped by its own image, confined by the surface on the one side and the slowly decaying Coulombic potential on the other side. These image-potential induced surface states (IPS) form a Rydberg-like series close to the vacuum level. Though located relatively far away from the surface, they are still sensitive to the local elctronic, atomic and magnetic surface structure.

Consequently, spin-polarized scanning tunneling spectroscopy (SP-STS) of IPS allows to investigate the magnetic surface properties on a local scale but at tip-sample distances larger than in normal tunneling experiments, thereby reducing the probability of accidental tip-sample collisions [1]. However, STS performed by commercial scanning tunneling microscopes (STM) is usually limited to a maximum bias voltage of 10V. Going beyond this limit we are able to investigate spin-dependent IPS of higher order at further increased tunneling distances.

First measurements in a high voltage regime will be presented and discussed.

[1] A. Kubetzka *et al.*, Appl. Phys. Lett. **91**, 012508 (2007).

O 43.14 Tue 18:30 Poster F

Signature of a nanoparticle in the evanescent heat transfer measured by NSThM — •Uli F. Wischnath, Joachim Welker, and Achim Kittel — Univ. Oldenburg, Energy and Semiconductor Research, D-26129 Oldenburg, Germany

The Near-field Scanning Thermal Microscope (NSThM) allows the investigation of the heat transfer by evanescent fields in the direct vicinity of a sample that is at a distance between 1 and 100 nm. It is based on a variable-temperature ultra high vacuum scanning tunneling microscope (VT-UHV STM) with a probe designed as a thermocouple in order to measure thermal properties. The STM abilities of the microscope are used for the spatial control of the temperature probe.

For the work presented here nanoparticles were deposited on a flat surface by dip coating and scanned with the NSThM in constant current mode. They show a typical feature in the heat transfer image: higher values compared to the one on the flats are surrounding the particles whereas right on top of the particle the values are lower than the ones on the flats.

These findings might be explained by calculations which have been made by theoreticians for a similar case: A maximum in the heat transfer is found for a sphere (representing the probe) scanned in a constant height over a surface with a sphere on top at the position where the two spheres start to overlap.

O 43.15 Tue 18:30 Poster F

Dynamic Force Microscopy: Fundamental mechanism of energy dissipation for organic molecules — •Markus Fendrich[1], Kai Ruschmeier[2], Christian Weiss[1], Manfred Lange[1], Tobias Kunstmann[1], André Schirmeisen[2], and Rolf Möller[1] — [1]Fachbereich Physik, Universität Duisburg-Essen, D-47048 Duisburg — [2]CeNTech Center for NanoTechnology, Heisenbergstr. 11, D-48149 Münster

In frequency modulation atomic force microscopy (FM-AFM), the damping signal reveals information about energy dissipation processes within the tip-sample system with high lateral resolution.[1] However, the mechanisms of energy dissipation are still not fully understood; especially for organic molecular systems, few results have been achieved so far. We present experimental data on the topography and dissipation of 3,4,9,10 perylene-tetracarboxylic dianhydride (PTCDA) on Ag(111). The molecules are known to form stable islands at submonolayer coverage.[2] We achieved molecular resolution in the topography and the damping signal alike. The damping signal of the PTCDA molecules shows a sub-molecular contrast, revealing two peaks at the ends of each molecule. The origin of this dissipation signal is still under debate; a tip-induced switching of the functional groups of each molecule might act as a channel for energy dissipation.

[1] S. Morita et al., Noncontact Atomic Force Microscopy, Springer (2002) [2] K. Glöckler et al., Surf. Sci. 405, 1 (1998)

O 43.16 Tue 18:30 Poster F

Development of an UHV variable temperature STM — •Thomas Eelbo, Mike Gyamfi, Stefan Meckler, Oswald Pietzsch, and Roland Wiesendanger — Institute of Applied Physics and Microstructure Advanced Research Center Hamburg, University of Hamburg, Jungiusstraße 11, 20355 Hamburg, Germany

The design of a new VT-STM is presented together with a numerical simulation for the temperature behaviour of the system. The microscope will be installed into a two chamber ultra high vacuum system for studying local electronic and magnetic states of self-assembled nanostructures at atomic length scale.

The microscope is equipped with an inertial drive for Slip-Stick based tip-coarse approach. A mechanism for in-situ tip and sample exchange has been integrated, being crucial for spin polarized experiments using magnetically coated tips.

During the development of the microscope special attention was paid on the minimization of the base temperature. Therefore a numerical simulation was written, which describes the thermal anchoring of various parts to the flow cryostat and the chamber system.

O 43.17 Tue 18:30 Poster F

A New Scanning Tunneling Microscope for Spin-Sensitive Measurements in Ultrahigh Vacuum, at Low Temperatures, and in High Magnetic Fields — •Mike Gyamfi, Stefan Meckler, Oswald Pietzsch, and Roland Wiesendanger — Institute of Applied Physics and Microstructure Advanced Research Center Hamburg, University of Hamburg, Jungiusstrasse 11, 20355 Hamburg, Germany

To study the spin dependent local electronic structure of single magnetic nanowires and nanoislands a new scanning tunneling microscope with spin sensitivity has been developed.

The microscope is operated in a liquid helium bath cryostat with a base temperature of 5K and a superconducting magnet that provides a magnetic field in arbitrary direction to the sample. It is equipped with an inertial drive for tip coarse approach and an additional one for sample rotation. The latter one allows the preparation of samples directly in the microscope at cryogenic conditions. Furthermore, a tip exchange mechanism has been integrated that enables spin dependent measurements with magnetically coated tips.

The microscope, the ultrahigh vacuum system with the magnet cryostat, and first measurements are presented to demonstrate the functionality of the recently installed system.

O 43.18 Tue 18:30 Poster F

Interferometric detection methods for scanning near-field optical microscopy — •Christoph Zeh, Susanne C. Schneider, and Lukas M. Eng — Institute of Applied Photophysics, TU Dresden, D-01062 Dresden

Scanning near-field optical microscopy (SNOM) is a scanning probe technique which allows optical examination of nanostructures with a resolution ways below the classical diffraction limit. Hence, it finds many applications in nano science. Basically, there are two types of SNOM: the aperture-type, utilizing a tapered optical fibre for local illumination and/or detection, and the (apertureless) scattering type, in which light is scattered from a small particle, e.g. an AFM tip. Both types suffer from weak signal strengths, due to coupling losses at the fibre tip, or due to the small scattering cross sections. In order to amplify the optical near field signal, detection systems based on heterodyne or homodyne interferometry are very appropriate. Furthermore, the heterodyne detection method allows us to separate the near field's optical amplitude and phase, since the near-field signal is compared with a well known, but frequency shifted, reference signal. In this work we compare interferometric detection schemes with respect to their resolution limit and signal-to-noise ratio, for both free-beam version as well as fibre-based version.

O 43.19 Tue 18:30 Poster F

Eddy current microscopy — •Marion Meier, Tino Roll, and Marika Schleberger — Universität Duisburg-Essen, Fachbereich Physik, Lotharstraße 1, D-47048, Germany

Eddy current microscopy (ECM) provides a unique method to gain qualitative insight into the local electrical conductivity of nano structures. ECM is based on the well established method of non-contact scanning force microscopy. The basic principle is as follows: Either the time-dependent magnetic field of an oscillating magnetic probe induces eddy currents within conducting materials or the magnetic stray fields of magnetic domains induce eddy currents within a conducting probe. In any case, the induced currents lead to an electrodynamic interaction between the probe and the sample. Therefore, the oscillation of the probe is damped according to Lenz's rule, leading to a contrast in either the phase or in the damping signal. This technique, thus, provides standard force microscopy with a material sensitive contrast in addition to the conventional topography signal. Since not much is known yet about the experimental limitations of the technique, we used several reference samples such as magnetic recording tapes, conducting wires written by e-beam lithography, and SNOM samples. The latter samples offer the advantage of a high difference in conductivity. We will present results from ex situ as well as from in situ measurements. The method will be applied to nanostructured samples such as thin films and metallic islands on silicon, in order to characterize the influence defects and size effects on the resistivity.

O 43.20 Tue 18:30 Poster F

High-Resolution Combined Low-Temperature Scanning Tunneling/Atomic Force Microscope for 3D Force Spectroscopy — Boris J. Albers[1], Todd Schwendemann[1], Mehmet Z. Baykara[1], Nicolas Pilet[1], •Marcus Liebmann[1], Markus Heyde[2], and Udo D. Schwarz[1] — [1]Deptartment of Mechanical Engingeering, Yale University, New Haven, USA — [2]Lawrence Berkeley National Laboratory, University of California, Berkeley, USA

We present the design and first results from a new home-built low-temperature scanning probe microscope enabling high-resolution experimentation in both scanning tunneling microscopy (STM) and non-contact atomic force microscopy (NC-AFM) modes. An exchangeable tuning fork based Q-plus style sensor is used to allow for flexibility in choosing probe tip materials. The system features an on-top cryostat, where the microscope is enclosed in a double set of thermal shields. Tip as well as sample can be changed in-situ at low temperatures to keep turn-around times low. By opening the front shutters of the shields, unrestricted access from dedicated flanges permits the direct deposition of molecules or atoms on either tip or sample while they remain cold. As examples for the microscope's performance, we present data measured on Cu(111) in STM mode as well as on graphite in NC-AFM mode, featuring atomic resolution with corrugations of 4-5 pm and corrugations below 1 pm could be measured. In addition, atomic resolution data obtained by means of three-dimensional force spectroscopy is shown.

O 43.21 Tue 18:30 Poster F

Energy dissipation of ballistic injected electrons and holes through individual molecules — •Alexander Bernhart[1], Mark Kaspers[1], Bastian Weyers[1], Evgeny Zubkov[1], Christian Bobisch[2], and Rolf Möller[1] — [1]Department of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]University of California, Irvine, USA

Ballistic Electron Emission Microscopy (BEEM) not only represents an ideal technique to study the electronic transmission at the Schottky-interface between a metal and a semiconductor, but moreover it allows to analyze the ballistic transport through adsorbates on top of a metal. Bismuth (Bi) films with a thickness of 3-4nm were grown on n-doped and p-doped Si(100) and Si(111). Recently we could analyze the ballistic transport of electrons through two different molecular adlayers, PTCDA and C_{60}, deposited on top of the Bi film. In addition the ballistic transport of holes through an adlayer of C_{60} was studied. All experiments were performed by a modified "Nanoprobe"system (Omicron) providing four STM units which may be operated independently on the same sample. In this case one STM unit was used to contact the metal layer, and other one is operated as a conventional STM at negative or positive tip bias, hence injecting electrons or holes into the sample surface.

O 43.22 Tue 18:30 Poster F

surface velocity of shear quartzes for high speed friction measurements — •fengzhen zhang[1], othmar marti[1], stefan walheim[2], and thomas schimmel[2] — [1]Uni Ulm — [2]Uni Karlsruhe/FZK

Investigations of the friction properties with the relative low speeds(micrometer/s) have been carried out with Atomic Force Microscopy(AFM). Technologically relevant friction processes operate at speeds of several m/s. Due to the limitation of the piezo scanners in standard AFM, a new oscillation setup is required for the microscopic research on high speed friction. We have measured the surface velocity of shear quartzes. In this presentation we show the calibration setup and results of the surface speed for 3MHz quartzes. We discuss the influence of surface inhomogeneities on the accuracy of the velocity measurement. As a first application we present friction measurements obtained on structured films deposited on shear quartzes.

O 43.23 Tue 18:30 Poster F

Scanning tunneling microscopy measurements of graphene on an insulating substrate. — •Viktor Geringer[1], Sven Runte[1], Marcus Liebmann[1], Tim Echtermeyer[2], Reinhard Rückamp[1], Max Lemme[2], and Markus Morgenstern[1] — [1]II. Physikalisches Institut, RWTH Aachen and JARA-FIT, Otto-Blumenthal-Straße, 52074 Aachen — [2]Advanced Microelectronic Center Aachen (AMICA), AMO GmbH, Otto-Blumenthal-Str. 25, 52074 Aachen

We present scanning tunneling microscopy (STM) measurements of single and few layer graphene examined under ultrahigh vacuum conditions. The samples were prepared on a silicon dioxide surface by mechanical exfoliation of a graphite crystal and contacted by depositing gold electrodes around the graphene flake. An instrumental challenge in STM investigations of small graphene flakes is the tip positioning with respect to the sample. We solved this technical problem by using an optical long-distance microscope and a x-y-positioning drive for the STM sample stage. A lateral pre-positioning precision of 5-10 μm has been achieved.

We show atomically resolved and large-scale topographic images of the graphene surface as well as first scanning tunneling spectroscopy (STS) results.

O 43.24 Tue 18:30 Poster F

A UHV-STM system for measurements at 300 mK and 14 T — •Stefan Becker, Marcus Liebmann, and Markus Morgenstern — II. Physikalisches Institut B, RWTH Aachen and JARA-FIT, Otto-Blumenthal-Straße, 52074 Aachen

We have designed an ultrahigh vacuum (UHV) system featuring a homebuilt scanning tunnelling microscope (STM) inside of a 300 mK cryostat with a 14 T solenoid magnet exhibiting a single-shot time of 100 h. Two independent chambers hold various instruments for sample and STM tip preparation, including sample heaters, a sputter gun, evaporators and a combined LEED/Auger system. The STM body is compact and rigid (Ø 30 mm) for stability and high resonance frequencies. It has an *in situ* tip exchange mechanism and a sample positioning stage. The whole system is supported by air damping legs inside an acoustically insulating room.

O 43.25 Tue 18:30 Poster F

Development of TERS System with Scanning Capability — •Seth White, Dietrich Wulferding, Alexander Doering, Hongdan Yan, Pushpendra Kumar, and Peter Lemmens — IPKM, TU-Braunschweig

The combination of Tip-Enhanced Raman Spectroscopy with real-time surface characterization in one experimental setup shows great promise as a method for precise local measurement of spatially confined systems. After employing an AFM with an etched [1] nano-apex scanning tip made of Ag or Au[2] to gain structural information one can immediately use the same tip to substantially increase Raman activity at a particular point of interest. Single molecules trapped near the surface of nano-porous oxidized silicon and alumina can be investigated using this finely tunable, highly directed approach.

O 43.26 Tue 18:30 Poster F

Use of a "needle-sensor" for non-contact scanning force microscopy and simultaneous measurement of the tunneling current — Bert Voigtländer[1] and •Irek Morawski[1,2] — [1]Institute of Bio- and Nanosystems (IBN 3), and cni – Center of Nanoelectronic Systems for Information Technology, Research Centre Jülich, 52425 Jülich, Germany — [2]Institute of Experimental Physics, University of Wrocław, pl. Maxa Borna 9, PL 50-204 Wrocław, Poland

A simultaneous measurement of forces and tunneling current during imaging of surfaces is of great interest. We present AFM/STM images of graphite and metal surface obtained by means of the quartz needle-sensor with an attached tungsten tip at ambient conditions. The needle sensor is an extensional mode quartz oscillator operating at a frequency of 1 MHz and one is similar to a tuning fork sensor more frequently used in scanning force microscopy. This sensor has been operated with a phase locked loop (PLL) control extended with an additional electronic circuit, namely an attenuator, two band-pass amplifier stages, providing both: sub-angstroms mechanical oscillation amplitude and high signal/noise ratio. Dependences of the frequency shift against a tip-surface displacement measured for mentioned surfaces are presented. A "feedback circuit enabled"method of a calibration of the needle-sensor vibration amplitude is proposed and discussed.

O 43.27 Tue 18:30 Poster F

Construction of a Fibre-Tip SNOM for Investigation of Soft Organic Materials — •Philipp Lange[2], Omar Al-Khatib[1], Dörthe M. Eisele[1], Mario Dähne[2], Jürgen P. Rabe[1], and Stefan Kirstein[1] — [1]HU-Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin — [2]TU Berlin, Institut für Physik, Hardenbergstr. 36, 10623 Berlin

The setup of a fibre-tip scanning near field optical microscope (SNOM) is presented that was specially designed for the investigation of soft organic materials in air providing low tip-sample interaction, low thermal drift, and high topographic resolution. For topographic scanning the shear force of a fibre probe is detected. For this a tapered glass fibre probe is mounted on a tuning fork piezo which is forced to oscillate above the resonance frequency. The phase shift induced by the tuning fork is taken as a sensitive signal for damping of the tip oscillation due to tip-sample interaction and used for distance control. A dye laser is coupled into the fibre for near field optical excitation of the sample. The scanning unit is mounted on top of an inverted fluorescence microscope that allows comfortable adjustment and micro-positioning of tip and sample, preselection of scan areas of prior interest, and very efficient far-field detection of the luminescence. First images of fluorescent nano-particles and dye aggregates on solid surface are presented.

O 43.28 Tue 18:30 Poster F

The nanoscale electrochemical potential of a current carrying surface state resolved with Scanning Tunneling Potentiometry — •Jan Homoth[1], Martin Wenderoth[1], Thomas Druga[1], Lars Winking[1], Rainer G. Ulbrich[1], Mark Kaspers[2], Alexander Bernhart[2], Bastian Weyers[2], Evgeny Zubkov[2], Rolf Möller[2], and Christian Bobisch[3] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen — [2]University of Duisburg-Essen, Department of Physics, Duisburg, Germany — [3]University of California, Irvine, USA

Charge transport through the surface state of the $Si(111)\sqrt{3}\cdot\sqrt{3}-Ag$ surface has been investigated with a lateral resolution of Angstroms. Across line defects like monatomic terrace steps the electrochemical potential $\mu_{ec}(x,y)$ varies strongly. Transport across such defects occurs as tunneling through a quantum mechanical barrier. We demonstrate that the variation in μ_{ec} responds linearly to the applied current density and does not depend on the local current direction. Furthermore, the variation of μ_{ec} does not coincide with the topography data: A lateral shift is observed and the widths differ. Using a variety of tip configurations we analyze the experimental widths and lateral shifts in detail. Comparing these results with STM-calculations, we conclude that the change of μ_{ec} is unaffected by tip convolution artefacts and cannot be described with a step-like change in μ_{ec}. A qualitative model describing the spatially dependent electron distribution and the variation of μ_{ec} is derived, extending the early approach of Datta. This work was supported by the DFG, SFB 602 Tp A7.

O 43.29 Tue 18:30 Poster F

Analyzing and determination of the different shear force interactions — •Kai Braun, Catrinel Stanciu, Dai Zhang, and Alfred J. Meixner — Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle, 72076 Tübingen

Shear-force feedback is among the most common used mechanisms for distance control in scanning near-field optical microscopes (SNOM). A reliable SNOM measurement requires extremely precise tuning of the distance between the tip and the sample. Although being widely used, the nature of the shear-force interaction is still not fully understood. The oscillating probe is usually modelled as a driven harmonic oscillator, influenced by different forces due to the interaction of the tip with the sample. We present here an extensive study of this interactions for different combinations of substrates (Au, Si, HOPG and glass) and tips (Au, W and glass). We measured the amplitude and phase of the tip oscillation as a function of the tip-sample distance in the non-contact range. The measurements allow us to distinguish the different forces between the tip and the substrate. The dominating nature of the interactions strongly depends on the material of both the tip and the substrate and also with the distance. In particular, gold tips on gold samples, of actual interest in tip-enhanced microscopy, undergo mainly elastic interaction for larger distances, with an attractive component evident for smaller distances. These results can help for a better understanding of optical near-field measurements, in particular for avoiding artefacts when measuring heterogeneous samples.

O 43.30 Tue 18:30 Poster F

Design of a vacuum system for the local study of molecules — •Matthias Prostak, Germar Hoffmann, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg

Molecules are a fascinating class of materials and have a large potential impact for the design of novel, molecule-based devices. One major advantage is the possibility of low temperature preparation in industrial processes. Therefore, the precise control of growth parameters is relevant for the preparation of clean and homogeneous molecular structures.

Here, we will present the design of a new, very versatile and compact vacuum system for such a preparation study. The vacuum system is equipped with a scanning tunneling microscope, a LEED optics and an Auger spectrometer for surface analysis. In this vacuum system, flexible exchange of molecule evaporators through the load-lock and the preparation of metal-insulator-molecule sandwiches is possible. Since commercially available samples of molecules are often not sufficiently clean for high-quality investigations, the vacuum system is additionally equipped with an extra side chamber to degas molecular samples for purification over several hours and days. We will discuss the design and the first realization.

O 43.31 Tue 18:30 Poster F

Towards a quantitative determination of charge distribution and local potential by Phase-Electrostatic Force Microscopy: theory and applications — •Cristiano Albonetti, Paolo Annibale, and Fabio Biscarini — CNR-Institute for the Study of Nanostructured Materials (ISMN), Bologna, Italy

The cantilever phase signal of the atomic force microscope, in conjunction to lift-mode operation, is used to map the electrostatic interaction between the cantilever's tip and the sample with a lateral resolution less than 50 nm. The detection of the phase, sensitive to tip-sample force gradient, allows to gain a higher resolution with respect to more conventional electrostatic probes based on force detection. Relevant organic and inorganic samples, with well-defined morphology, were measured by modeling the tip-sample electrostatic interaction in the prolate spherical coordinates reference system. Layered α-sexithiophene ultra-thin films grown on Si/SiO_x substrate show a monotonic decrease of the local surface potentials with the increase of the surface coverage, consistently with the predicted confinement at the first few monolayers of the charge accumulation layer (organic sample). Silicon oxide nano-stripes, made by scanning probe lithography, show a variable electrostatic contrast due to a different amount of charges trapped in the oxide, thus yielding significant information about the mechanism of the oxidation process (inorganic sample). The application of this technique to operating thin film organic field effect transistors allows to correlate local surface potential with the morphology of the transistor channel.

O 43.32 Tue 18:30 Poster F

Design criteria for scanning tunneling microscopes to reduce the response to external disturbances — •Maximilian Assig[1], Alexandra Ast[2], Christian R. Ast[1], and Klaus Kern[1] — [1]MPI für Festkörperforschung, Stuttgart, Germany — [2]ITM, Universität Stuttgart, Germany

In a scanning tunneling microscope (STM) the tip-sample distance is the crucial aspect of the measurement process as the tunneling current depends on it exponentially. Since it is *a priori* impossible to distinguish in the tunneling current the actual signal from external disturbances, care must be taken to isolate the measurement setup as effectively as possible from the outside environment. Here we present an approach to reduce the response of the tip-sample distance to external disturbances, which are unwanted in the tunneling current. The idea is to optimize the design of the STM itself, so that the response of the tip and the sample to external disturbances is minimized. A design criterion has been developed based on experimental measurements of the tip-sample transfer function as well as a simple theoretical model.

O 43.33 Tue 18:30 Poster F

The x-ray experimental endstation of beamline BL9 at DELTA — •Michael Paulus, Christian Sternemann, Christina Krywka, Andreas Schacht, and Metin Tolan — Experimentelle Physik I/DELTA, Technische Universität Dortmund, Maria-Goeppert-Mayer Str.2, 44221 Dortmund, Deutschland

The Dortmund Electron Accelerator DELTA is a synchrotron radiation source located at the TU Dortmund, Germany, and is operated a 1.5 GeV with a maximum electron current of 120 mA and lifetimes of about 10 hours. The beamline BL9 is attached to a superconducting asymmetric wiggler which supplies radiation in the energy range between 4 keV and 30 keV. The incident radiation is monochromatized by means of a Si (311) double crystal monochromator with sagittally bend second monochromator crystal. The experimental endstation of BL9 is equipped with a Huber six-circle diffractometer and is dedicated to (grazing incidence) x-ray diffraction and x-ray reflectivity studies on solid surfaces, thin films and liquid - solid interfaces. Recently, the end station was extended to perform small and wide angle x-ray scattering experiments making use of an image plate scanner. Moreover, a spectrometer in Rowland geometry is accessible to perform resonant inelastic x-ray scattering experiments.

O 43.34 Tue 18:30 Poster F

Positron annihilation induced Auger electron spectroscopy on Si single crystals — •Jakob Mayer[1], Klaus Schreckenbach[1,2], and Christoph Hugenschmidt[1,2] — [1]Technische Universität München, Physikdepartment E21, James-Franck-Str., 85748 Garching — [2]ZWE FRM II, Lichtenbergstr.1, 85747 Garching

Positron annihilation induced Auger electron spectroscopy (PAES) is a powerful technique for the element selective investigation of surfaces. Due to the different hole creation process compared to conventional EAES, i.e. ionisation by means of positron electron annihilation instead of collision, the impact energy of the positrons can be chosen very low and hence the secondary electron background ends at this low energy. Furthermore only the topmost atomic layer is examined, due to the positron diffusion back to the surface. The main challenge in PAES is the low positron current, which is on the order of pA. Even at the high intensity positron source NEPOMUC at the FRM II the measurement times are on the order of hours. In order to reduce the acquisition time a new electron energy analyser with a higher efficiency has been installed. First measurements on polycrystalline Cu and Si single crystals will be presented and compared to previous measurements.

O 43.35 Tue 18:30 Poster F

Order-N scaling of the Full-potential Linearized Augmented Plane Wave method

— •Frank Freimuth, Daniel Wortmann, and Stefan Blügel — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany

Density functional theory codes based on the Full-potential Linearized Augmented Plane Wave (FLAPW) method have been highly successful due to their generality and wide applicability. In particular, in the field of surfaces, open structures and complex magnetic materials with many chemical elements, the FLAPW method sets the standart for precision among the *ab initio* methods. On the other hand, the computational effort of the FLAPW method is relatively high, obeying a cubic scaling law with system size, making the applicability to larger systems increasingly more difficult.

We will present new ideas to combine the Green-function embedding method and the transfer-matrix formalism [1] with the LAPW basis set to construct a computer code with a (roughly) linear scaling of the computational effort with increase of system size in one dimension. The total problem is decomposed into layers which can be calculated individually and are joint together with the help of the embedded Green function technique. This opens new perspectives in the calculation of complex nanoferronic junctions. Support by the DFG-SPP 1243 is gratefully acknowledged.

[1] D. Wortmann, H. Ishida, and S. Blügel, Phys. Rev. B **66**, 075113 (2002).

O 43.36 Tue 18:30 Poster F

Topology-dependent life-time of surface states

— •Koray Köksal and Jamal Berakdar — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Heinrich-Damerow-Str. 4, D-06120 Halle(Saale), Germany

On the ground of analytical and numerical calculations we show that the life time of surface states of noble metals can be tuned by the appropriate topology of surface. Results are presented for curved Cu(111) surface. We also discuss how the predicted effect can be realized experimentally and measured by means of scanning tunneling spectroscopy [1] and two-photon photoemission [2,3].

- [1] L. Limot, E. Pehlke, J. Kröger, and R. Berndt, Phys. Rev. Lett. **94**, 036805 (2005)
- [2] R. W. Schoenlein, J. G. Fujimoto, G. L. Eesley, and T. W. Capehart, Phys. Rev. Lett. **61**, 2596 (1988)
- [3] A. Winkelmann, F. Bisio, R. Ocaña, W.-C. Lin, M. Nývlt, H. Petek, and J. Kirschner, Phys. Rev. Lett. **98**, 226601 (2007)

O 43.37 Tue 18:30 Poster F

Multilayer-Optiken für die fs-Röntgendiffraktometrie

— •Jörg Wiesmann und Carsten Michaelsen — Incoatec GmbH, Geesthacht, Germany

An mehreren Orten auf der Welt befinden sich gepulste Synchrotron-Röntgenquellen im Bau, so genannte Freie Elektronen Laser. In Vorbereitung hierauf beschäftigt sich eine zunehmende Zahl von Forschergruppen mit vorbereitenden Laborexperimenten, wobei lasergenerierte Plasmaquellen zur Erzeugung von gepulster Röntgenstrahlung im sub-Pikosekunden Bereich verwendent werden. Derartige Laborquellen erfordern die Entwicklung von Röntgenoptiken, die auf der einen Seite ein großes Lichtsammelvermögen besitzen, und die auf der anderen Seite die Brillanz und die Zeitstruktur der Röntgenstrahlung aufrechterhalten. In diesem Beitrag werden verschiedene Röntgenoptiken im Hinblick auf diese Erfordernisse anhand jüngster experimenteller Ergebnisse vorgestellt.

O 43.38 Tue 18:30 Poster F

An XUV- Split and Delay Line at the Free Electron Laser in Hamburg

— •Torben Beeck[1], Mitsuru Nagasono[1,2], Holger Meyer[1], Sven Gieschen[1], Martin Beye[1], William F. Schlotter[1], Florian Sorgenfrei[1], Alexander Föhlisch[1], and Wilfried Wurth[1] — [1]Institut für Experimentalphysik Universität Hamburg, Germany — [2]XFEL Project Head Office, RIKEN, Hyogo, Japan

At the Free Electron Laser in Hamburg (FLASH) we are integrating a soft x-ray beam split and delay line to the plane grating monochromator beamline (PG2). This system will enable pump-probe spectroscopy of ultrafast dynamics. Pulse to pulse timing jitter is circumvented by the controlled synchronisation of the delay line. The wavefront of the incoming beam is divided by illuminating the edge of a mirror. By controlling the optical path length for each beam, pulse delays as short as 10 fs or as long as 20 ps can be generated.

The system employs four mirrors to split and mix the beam and four mirrors to control the delay. Each mirror is a silicon single crystal with a diamond like carbon coating. The four delay mirrors are arranged at grazing incidence forming a parallelogram. Together with the beam splitters this forms an adjustable path Mach-Zehnder interferometer. For stability the delay mirrors are fixed to a rigid support structure. Simply translating the structure imparts a delay between the pulses.

This work is supported by the BMBF in the framework of the Forschungsschwerpunkt 301, "FLASH: Matter in the light of ultrafast and extremely intense x-ray pulses".

O 43.39 Tue 18:30 Poster F

Transient surface temperature of ultralthin Bi(111) heterolayers on Si(001) upon fs-laser excitation

— •Anja Hanisch, Boris Krenzer, Simone Möllenbeck, Tobias Pelka, Paul Schneider, and Michael Horn-von Hoegen — Department of Physics, Universität Duisburg-Essen, D- 47048 Duisburg, Germany

The transient temperature rise of ultrathin epitaxial Bi(111) films on Si(001) substrates upon excitation with fs-laser pulses is studied by ultrafast time resolved reflection high energy electron diffraction (RHEED). Spot intensities taken at different time delays between pumping laser pulses and probing electron pulses are converted to the transient surface temperature using the Debye-Waller Effect.[1]

A rapid increase of the surface temperature from 80 K up to 190 K is followed by a slow exponential decay with a time constant of 640 ps for a 5.5 nm thin Bi film.[2] The slow cooling is determined by the thermal boundary resistance at the interface between Bi and Si. We observe a linear dependence of the decay constant with the film thickness for films thicker than 6 nm, which is in agreement with the general theory of the thermal boundary resistance. In contrast films thinner than 6nm show an enhanced thermal boundary resistance with a decay constant up to two times larger than expected. In order to explain this deviation, we suggest that for thinner films the discretisation of the phonon dispersion compared to the bulk-like behaviour of thicker films plays an important role.

[1] A. Janzen et al., Rev. Sci. Inst. 78, 013906 (2007).

[2] B. Krenzer et al., New J. Phys. 8, 190 (2006).

O 43.40 Tue 18:30 Poster F

Influence of Laser Heating on the X-ray Diffraction Intensity of InSb

— •Jessica Walkenhorst, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretische Physik, Fachbereich Naturwissenschaften, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel

Hillyard et al. have measured the x-ray diffraction intensity of the (111) peak of InSb after intense laser excitation, which provides insight in the first stages of laser-induced ultrafast melting. They found that the diffraction peak follows a Gaussian decay. This time-dependence has been analyzed using the Debye model for the atomic vibrations, assuming the laser heating to produce a uniform softening of all phonon frequencies. We performed (i) first principle electronic structure calculations, (ii) molecular dynamic simulations to calculate the phonon frequencies at the Γ-, X- and L-point and the resulting x-ray intensity. We found, that dramatic phonon softening does not occur at all the investigated k-points but instead the softening of the transverse acoustic phonons at the X-point suffices to explain the measured Gaussian x-ray intensity decay and perfectly reproduces the decay's measured time constant.

O 43.41 Tue 18:30 Poster F

Time-, energy- and ANGLE-resolved photoelectron spectroscopy of surface dynamics using femtosecond XUV pulses — •Stefan Mathias[1], Luis Miaja-Avila[2], Margaret Murnane[2], Henry Kapteyn[2], Martin Aeschlimann[1], and Michael Bauer[3] — [1]Department of Physics, TU Kaiserslautern, 67663 Kaiserslautern, Germany — [2]JILA, University of Colorado, Colorado 80309-0440, USA — [3]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany

The *angle* resolved photoelectron spectroscopy (ARPES) has emerged as a leading technique in identifying static key properties of complex systems such as adsorbed molecules, ultrathin quantum-well films or high temperature superconductors. We present an experimental setup combining the ARPES technique with a pump-probe scheme for time-resolved measurements using a 1 kHz femtosecond XUV source [1]. The performance of the system with respect to time-, energy- and momentum-resolution will be discussed on the basis of ARPES spectra recorded with ultra short photon pulses of an energy of 42 eV. Furthermore, the potential of time-resolved ARPES to study surface dynamics in future experiments is considered.
[1] S. Mathias, L. Miaja-Avila, M. Murnane, H. Kapteyn, M. Aeschlimann, M. Bauer, Rev. Sci. Instrum. 78, 083105 (2007)

O 43.42 Tue 18:30 Poster F

first test of a beam splitter and delay line for the XUV at FLASH — •Rolf Mitzner[1], Björn Siemer[1], Marco Rutkowski[1], Sebastian Roling[1], Matthias Neeb[2], Tino Noll[2], Kai Tiedtke[3], Wolfgang Eberhardt[2], and Helmut Zacharias[1] — [1]Physikalisches Institut, Westfälische Wilhels-Universität, 48149 Münster — [2]BESSY GmbH, Albert Einstein Str. 15, 12489 Berlin — [3]HASYLAB, DESY, 22603 Hamburg

In order to do jitter-free X-ray pump and probe experiments at the Free Electron Laser in Hamburg (FLASH) as well as to characterize the temporal structure of its high power pulses a novel beam splitter and delay unit (autocorrelator) has been designed and constructed [1]. Based on geometrical beam splitting by a mirror edge the apparatus covers the XUV energy range up to photon energies of 200 eV providing a total delay of about 20 picoseconds with femtosecond resolution. Using 13.5 nm radiation from the FEL the beam has been split in two beams delayed to each other. The shape of the split beams as well as its fluctuations has been recorded for different delays up to several picoseconds. Overlapping the split beams under a small angle 10 m behind the autocorrelator lateral interference fringes have been observerved at zero delay between the two beams. When changing the path difference the fringes have been disappeared thus demonstrating the proper function of the delay line in the XUV. The visibility of the fringes as a function of the delay (path length difference) should allow the direct determination of the average coherence time of the FEL pulses. [1] R. Mitzner et.al., Proc. Of SPIE 592000D (2005)

O 43.43 Tue 18:30 Poster F

A femtosecond X-ray/optical cross-correlator: Free-electron laser X-ray pulse induced transient optical reflectivity — •Cornelius Gahl[1,4], Armin Azima[3], Martin Beye[2], Martin Deppe[2], Kristian Döbrich[1], Urs Hasslinger[2], Franz Hennies[2,5], Alexej Melnikov[1], Mitsuru Nagasono[2], Annette Pietzsch[2], Martin Wolf[1], Wilfried Wurth[2], and Alexander Föhlisch[2] — [1]Fachbereich Physik, Freie Universität Berlin — [2]Institut für Experimentalphysik, Universität Hamburg — [3]HASYLAB/DESY, Hamburg — [4]Max-Born-Institut Berlin — [5]MAX-lab, Lund Universitet, Sweden

Due to their short pulse duration and high brilliance over a wide range of photon energies free-electron-laser (FEL) based femtosecond x-ray pulse sources make possible completely new classes of experiments. Since it is extremely difficult to precisely synchronize a FEL with an external femtosecond laser source, one has to measure the relative arrival time of x-ray and optical pulse to perform pump-probe experiments with optimal time resolution. At the Free-Electron-Laser in Hamburg (FLASH) we exploited the high peak brilliance for this purpose by measuring the x-ray induced transient change in optical reflectivity at a GaAs surface. The ultrafast drop in reflectivity on the time scale of the pulse duration enables us to determine the temporal overlap of x-ray and optical pulses as well as the statistical timing jitter and a systematical drift within a pulse train. Therefore this easy to implement technique denotes an important step towards delay control for femtosecond time-resolved experiments and opens up the field of femtosecond X-ray induced dynamics.

O 43.44 Tue 18:30 Poster F

An angle-resolved time-of flight spectrometer for low-energy photoelectron spectroscopy — •Laurenz Rettig, Patrick S. Kirchmann, Uwe Bovensiepen, and Martin Wolf — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

We developed and constructed a two-dimensional position-sensitive time-of-flight spectrometer (pTOF) for the angle-resolved analysis of low-energy electrons photoemitted from a metal surface by femtosecond laser pulses. The spectrometer design combines a field-free drift tube with 22° acceptance angle and a microchannel plate stack with a delay-line anode [1] for position encoding. The pTOF spectrometer allows to determine both surface in-plane electron momentum components p_x and p_y along with the kinetic energy. The pTOF concept is optimized to study the electron scattering dynamics of laterally anisotropic electronic systems such as self-assembled quasi-1D atomic nano-wires or stepped surfaces.

Here, we present the working principles as well as the hard- and software implementation of the pTOF, which includes real-time analysis of multiple electron hits per laser pulse. This multihit capability is crucial for pulsed laser spectroscopy with repetition rates of $\sim$ 100 kHz. To demonstrate the performance of the spectrometer measurements on a Cu(111) single-crystalline surface were performed using UV femtosecond laser pulses of 6.20 eV photon energy.

[1] O. Jagutzki, A. Cerezo, A. Czasch, et al., IEEE Trans. Nucl. Sci. **49**, 2477 (2002).

O 43.45 Tue 18:30 Poster F

Spectral Line Shape Variations in Time-Resolved Photoemission from a Solid — E.E. Krasovskii[1,2], •Karsten Balzer[2], Sebastian Bauch[2], and Michael Bonitz[2] — [1]Insititute of Metal Physics, National Academy of Science of Ukraine, 03142 Kiev, Ukraine — [2]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität Kiel, Leibnizstrasse 15, 24098 Kiel, Germany

Time resolved photoemission with (sub)femtosecond UV pulses is of hight current interest [1] and is, here, studied by solving the time-dependent Schrödinger equation for a one-dimensional model crystal [2]. Without the laser field the shape and the energy location of the spectrum is determined by the energy dependence of photoemission cross section. In the presence of the laser field, the time growth of the population of the final state is predicted to cause extremely sharp variations of spectral width as a function of release time. This can help enhance resolution of the measurements. A simple phenomenological model to describe the line shape is proposed and shown to accurately reproduce the numerical results.

[1] M. Hentschel et al., Nature 414, 509 (2001).

[2] E.E. Krasovskii, and M. Bonitz, accepted for publication in Phys. Rev. Lett. (2007).

O 43.46 Tue 18:30 Poster F

Spin-dependent electron lifetimes in $3d$ ferromagnet thin films — •Andreas Goris[1,3], Ilja Panzer[1,3], Martin Pickel[2], Anke B. Schmidt[2], Fabian Giesen[1], Jürgen Braun[4], Markus Donath[2], and Martin Weinelt[1,3] — [1]Max-Born-Institut, Max-Born-Strasse 2A, 12489 Berlin — [2]Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Strasse 10, 48149 Münster — [3]Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [4]Institut für Mathematik und angewandte Informatik, Universität Hildesheim, Samelsonplatz 1, 31141 Hildesheim

The experimentally found values of the lifetime ratio (τ_{maj}/τ_{min}) of hot electrons in $3d$ ferromagnetic thin films are by a factor of 4-5 smaller than predicted by values of modern *ab initio* calculations [1,2].

We have measured the spin-dependent hot-electron lifetime for varying excitation density in a 20 ML Co film on Cu (001) with spin-resolved two-photon photoemission. We identify three contributions to the time resolved spectra: the off-resonant excitation of the image-potential state, the hot electron decay, and the signature of a spin flip exchange-scattering process with an occupied surface-resonance state. In this process a minority hole is filled in the surface-resonance while a majority electron is in turn lifted above the Fermi energy . These results are supported by recent self-consistent LSDA + DMFT calculations of the Co bandstructure. For comparison the lifetime ratio of hot electrons in Ni is discussed.

[1] Aeschlimann et al., Phys. Rev. Lett. **79**, 5158 (1997)

[2] Zhukov et al., Phys. Rev. Lett. **93**, 096401 (2004)

O 44: Plenary Talk André Geim

Time: Wednesday 8:30–9:15 Location: H 0105

Graphene: Exploring Carbon Flatland

O 45: Plenary Talk Knut Urban

Time: Wednesday 9:15–10:00 Location: H 0105

The new paradigm of electron microscopy on the way to the ultimate limits of optics

O 46: Invited Talk Stefan Mayr (Gaede Prize)

Time: Wednesday 13:30–14:15 Location: HE 101

Prize Talk O 46.1 Wed 13:30 HE 101

Structure formation, kinetics and mechanics in thin films and solids: from nanoscale to macroscopic properties in experiments and simulations. — •Stefan Georg Mayr — I. Physikalisches Institut, Georg-August-Universität Göttingen — Träger des Gaede-Preises

Macroscopic properties of functional thin films and solids, including structure and mechanics, are frequently dominated by processes at the atomic level, while the growing demand for miniaturization in science and technology has strongly triggered interest in nanoscale phenomena. Fine tuning and creation of new materials can thus greatly benefit from a detailed understanding across time and length scales. To achieve this, we employ a complimentary approach of experiments, atomistic computer simulations and analytical modelling, which we exemplify in two instances: We report about our studies on i) the mechanisms of self-organized structure formation at surfaces in driven systems and on ii) the nanomechanics in disordered solids. While i) combines an external forcing (materials deposition, energetic ions, templates) with intrinsic thermodynamics / kinetics to induce pattern formation or ultrasmooth surfaces, ii) is characterized by the occurrence of a highly heterogeneous dynamics in response to stress. In both cases, i) and ii), we choose metallic glasses as model systems due to their spatial isotropy, but also investigate generalizations to non-metallic as well as crystalline systems. Recent implications for the miniaturization of functional thin films and applications are also discussed. *Funded in part by the DFG - SFB 602 (TP B3), DFG - SPP 1239(TP C4) and GIF 428-303.1.*

O 47: Invited Talk Emily Carter

Time: Wednesday 14:15–15:00 Location: HE 101

Invited Talk O 47.1 Wed 14:15 HE 101

Ab Initio Treatment of Strongly Correlated Electron Materials — •Emily Carter — Department of Mechanical and Aerospace Engineering and Program in Applied and Computational Mathematics, Princeton University, Princeton, NJ 08544 USA

Density functional theory (DFT) has been anointed as the method of choice for a quantum mechanics description of molecules and materials, but it is best used as a qualitative indicator because its quantitative accuracy is still limited by approximate electron exchange and correlation (XC). Moreover, there are cases where DFT fails completely, even in a qualitative sense. Photochemistry, strongly correlated systems, physisorption, and polymers are all at best poorly described within standard DFT. We will discuss two ab initio techniques we have been developing in order to accurately treat excited states and strongly correlated electrons in condensed matter. In particular, we will discuss our embedded configuration interaction theory, which offers a locally improved description of XC, and an ab initio version of the so-called LDA+U method for strongly correlated materials. We will discuss applications of these techniques to problems where DFT fails (for various reasons that shall be outlined in the talk): the Kondo effect (transition metal impurities in nonmagnetic metallic hosts) and properties of first row transition metal oxides.

O 48: SYSA: Tayloring Organic Interfaces: Molecular Structures and Applications VI (Invited Speaker: Ivan Stich; FV: DS+CPP+HL+O)

Time: Wednesday 14:30–17:30 Location: H 2013

See SYSA for details about the program.

O 49: Particles and Clusters

Time: Wednesday 15:15–17:45 Location: MA 005

O 49.1 Wed 15:15 MA 005

Comparing the sampling efficiency of genetic and basin-hopping algorithms in the structural optimization of Lennard-Jones clusters — •Vladimir Froltsov and Karsten Reuter — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin (Germany)

Detailed knowledge about structural properties is an indispensable prerequisite en route towards a future exploitation of the intriguing materials properties of small atomic clusters. Crucial for the corresponding global geometry optimization problem is a reliable sampling of the high-dimensional potential-energy surface (PES) to identify the (meta)stable minima. In view of the high computational cost when the PES is evaluated with predictive quality by first-principles methods, utmost efficiency with a minimum dependence on the initial starting configuration is an additional demand on the sampling scheme. With this focus we compare the efficiency of the two prevalent algorithms for PES sampling, namely genetic algorithms (GA) and the basin-hopping (BH) approach, using the determination of the ground-state structure of model Lennard-Jones clusters as criterion. We find an intriguing cross-over between the two approaches, with BH more efficient than

GA for cluster sizes up to 65, and GA more efficient for larger clusters. We rationalize this finding with the ability of the population-based GA's to explore in parallel disjunct parts of the PES, which becomes increasingly important for the increasingly high-dimensional PESs of larger clusters.

O 49.2 Wed 15:30 MA 005

Absorption spectra of small metal clusters — •George Pal[1], Yaroslav Pavlyukh[2], Hans Christian Schneider[1], and Wolfgang Hübner[1] — [1]Department of — [2]Institut für Physik,

We present results for the photoabsorption cross sections of small sodium clusters (Na_4, Na_9^+ and Na_{21}^+) calculated by means of a linear response approach for the electron-hole correlation function. Following Refs. [1] and [2], we compute the electron-hole correlation function as the functional derivative of the generalized density matrix with respect to an external field, which yields an equation of the Bethe-Salpeter type. This procedure is conserving and fulfills important sum rules by construction. The theoretical spectra are in excellent agreement with the experimental results.

[1] L. P. Kadanoff and G. Baym, Phys. Rev. **124**, 287 (1961)
[2] N.-H. Kwong and M. Bonitz, Phys Rev. Lett. **84**, 1768 (2000)

O 49.3 Wed 15:45 MA 005

Ensemble-modelling of CdSe/ZnS core-shell nanoparticles using x-ray powder diffraction data — •Franziska Niederdraenk[1], Christian Kumpf[1], Reinhard Neder[2], and Eberhard Umbach[1,3] — [1]Universität Würzburg, Experimentelle Physik II, 97074 Würzburg — [2]Universität Würzburg, Mineralogisches Institut, 97074 Würzburg — [3]Forschungszentrum Karlsruhe GmbH, D-76021 Karlsruhe

Standard methods for the analysis of powder x-ray diffraction data (like e.g. a Rietveld refinement) cannot be used efficiently for heterogenic or imperfect systems like core-shell nanoparticles, since they are usually based on bulk-crystal approaches. In particular, mixed (epitactic) structures, interface-effects, and imperfections like relaxations and stacking faults, that often occur in very small particles (<3 nm), cannot be handled. In order to overcome these limitations we developed a bottom-up approach which models the entire nanoparticle including the shell, and hence takes all structural features implicitly into account. The Debye formula is used to calculate the corresponding diffraction pattern. Furthermore a size distribution for the nanoparticles is considered by applying ensemble averaging.

We present data from CdSe particles with a diameter of ˜4 nm and a ZnS shell of nominally ˜1 nm thickness. Different shapes and different shells for the particles were tested, as well as all relevant structural parameters refined. The best model consists of an elliptical CdSe core with a non-epitaxial ZnS shell which does not cover the core-surface completely.

O 49.4 Wed 16:00 MA 005

Understanding the reversibility of graphene and carbon nanotubes covalent functionalization — •Elena Roxana Margine[1] and Xavier Blase[1,2] — [1]LPMCN Université Lyon I, France — [2]Institut Néel, CNRS and Université Joseph Fourier, Grenoble, France

The reversibility of the grafting process of functional groups on the surface of carbon nantotubes is an essential step in the recovery of the ballistic properties of metallic nanotubes after separation or assembling. We use {\it ab initio} calculations to explore activation barriers against desorption of aryl radicals from the surface of graphene and nanotubes. We provide evidence for the recently observed partial reversibility of the diazonium salts reaction with carbon nanotubes and discuss the possibility of improving the reversibility using different functional groups.

O 49.5 Wed 16:15 MA 005

Plasmon-induced chaotic photodesorption of xenon from silver nanoparticles on a thin alumina film — •Ki Hyun Kim[1], Kazuo Watanabe[1], Dietrich Menzel[1,2], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Technische Universität München, 85747 Garching, Germany

We have observed a unique action of plasmon excitations in photodesorption of xenon from silver nanoparticles (AgNPs, $\sim$8 nm particle diameter) deposited on a thin alumina film. A mass selected time-of-flight method was used to measure the kinetic energy and the total amount of desorbed atoms. The results show that xenon atoms from a xenon monolayer on AgNPs are photodesorbed nonthermally when the laser is tuned to excite the (1,0) mode of the Mie-plasmon of AgNPs (3.5 eV, *p*-polarization) at low fluences ($<\sim 2$ mJ/cm^2) where laser induced thermal desorption is negligible. Moreover, the photodesorption yield on plasmon resonance showed chaotic behavior with large bursts and intermittences. These effects were suppressed for multilayers of xenon, which indicates that the nonthermal desorption is not due to thermal heating of the AgNPs.

We suggest a new mechanism of plasmonic desorption by accumulated momentum transfer of the repetitive Pauli repulsions between the collectively oscillating surface electrons and the xenon atom in its shallow physisorption well. The chaotic behavior is ascribed to plasmon coupling which creates fluctuating hotspots and decays slowly (>300 fs) enough to accelerate xenon atoms sufficiently to desorb them.

O 49.6 Wed 16:30 MA 005

Growth mechanism of group 5 transition metal clusters elucidated by far-infrared spectroscopy — •Philipp Gruene[1], Gerard Meijer[1], Carsten Ratsch[2], and André Fielicke[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]UCLA, Los Angeles, USA

The knowledge of the electronic and geometric structure of clusters is vital for the understanding of their physical and chemical properties. However, the determination of the clusters' geometric structure is an experimental challenge. Recently, we have shown that vibrational spectroscopy in combination with density functional theory calculations can provide information on the geometric structures of free metal clusters.[1] The experimental far-infrared spectra of free metal clusters are obtained by multiple photon dissociation (MPD) spectroscopy of their complexes with rare gas atoms, using the intense and tunable radiation of a free electron laser. We have completed the investigations on clusters of group 5 elements of the periodic table, namely vanadium, niobium, and tantalum. For all three elements many cluster sizes show remarkable similarities in their vibrational features, indicating a similar growth mechanism. Furthermore, for niobium clusters both neutral and cationic clusters have been studied, which allows for an understanding of the influence of a single electron both on the vibrational properties as well as on the clusters' geometric structure.

[1] A. Fielicke, A. Kirilyuk, C. Ratsch, J. Behler, M. Scheffler, G. von Helden, and G. Meijer, Phys. Rev. Lett. **93**, 023401 (2004).

O 49.7 Wed 16:45 MA 005

Ag cluster growth on biaxially oriented PET — •Günther Weidlinger, Lidong Sun, José Manuel Flores-Camacho, Michael Hohage, Daniel Primetzhofer, Peter Bauer, and Peter Zeppenfeld — Institut für Experimentalphysik, Johannes Kepler Universität Linz, Altenberger Straße 69, A-4040 Linz

Ag was deposited on biaxially oriented polyethylene terephthalate (PET) by means of Physical Vapor Deposition under UHV conditions up to a nominal Ag layer thickness of 5 nm. Since Ag does not wet the PET surface, Ag clusters are formed on the surface rather than a continous metal film. The optical properties of these silver clusters were monitored with Reflectance Difference Spectroscopy (RDS) during metal deposition. Morphological studies of the samples reveal that the clusters are embedded in the PET substrate and that the shape of the individual clusters as well as their in-plane arrangement is isotropic. Despite the structural isotropy of the Ag clusters, an inplane anisotropy of the cluster plasmon resonance can be observed in the RD spectra. This is attributed to the anisotropic dielectric properties of the substrate and its influence on the plasmon response. At low nominal Ag thicknesses (≤ 0.3 nm), the FWHM and the energy position of the plasmon resonance show a $1/R$-dependence on the cluster radius R. A broadening and an accelerated red-shift of the resonance due to retardation effects and cluster-cluster interactions are observed for silver thicknesses above 0.3 nm.

O 49.8 Wed 17:00 MA 005

Fluorescence yield of optical emitters close to noble-metal nanoparticles — •Florian Hallermann and Gero von Plessen — I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

The intensity of fluorescence from a fluorescent emitter is modified when placed in close proximity to a noble-metal nanoparticle. This modification is partially caused by a change in excitation efficiency due to the local-field enhancement near the nanoparticle, and partially by additional radiative and non-radiative decay processes due to resonant energy transfer from the emitter to the metal. Here we calculate the total fluorescence yield of fluorescent emitters distributed uniformly around a noble-metal nanoparticle, as a function of excitation and emission wavelengths.

O 49.9 Wed 17:15 MA 005

Creation of hot electrons below the surface by highly charged ions — •Thorsten Peters[1], Chrstian Haake[1], Domocos Kovacs[2], Detlef Diesing[3], Artur Golczewski[4], Gregor Kowarik[4], Friedrich Aumayr[4], Andreas Wucher[1], and Marika Schleberger[1] — [1]Universität Duisburg-Essen, Fachbereich Physik, Lotharstrasse 1, 47057 Duisburg, Germany — [2]Experimentalphysik II, Ruhr-Universität Bochum, 44801 Bochum, Germany — [3]Physikalische Chemie, Universität Duisburg-Essen, 45117 Essen, Germany — [4]Institut für Allgemeine Physik, Technische Universität Wien, A-1040 Vienna, Austria

Highly charged ions provide a unique method for creating ultra high energy densities in the surface region of a solid. Thin film metal-insulator-metal junctions are used in a novel approach to investigate the dissipation of the energy of multiply charged ions impinging on a polycrystalline metal surface. The ion–metal interaction leads to Auger electron emission of several ten eV which again leads to excited electrons and holes within the top layer. A substantial fraction of these charge carriers is transported inwards and can be measured as an internal current in the thin film tunnel junction. In Ag–AlO_x–Al junctions, yields of typically 0.1–1 electrons per impinging ion are detected in the bottom Al layer. The separate effects of potential and kinetic energy on the tunneling yield are investigated by varying the charges state of the Ar projectile ions from 2+ to 9+ for kinetic energies in the range from 1 to 12 keV. The tunneling yield is found to scale linearly with the potential and kinetic energy of the projectile.

O 49.10 Wed 17:30 MA 005

Structure and properties of Au on nanostructured ceria — •Martin Baron, Dario Stacchiola, Shamil Shaikhutdinov, and Hajo Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

It is well established that oxide supported gold nanoparticles catalyse CO oxidation at temperatures as low as 200 K [1]. Among those reported in the literature, gold catalysts supported on the cerium oxide (CeO2) often show a superior activity, in particular when ceria is present as nanoparticles [2]. To date, there are still open questions regarding the reaction mechanism and the nature of active species. In particular, the role of cationic (Au3+, Au+) species in this reaction remains unclear. Herein, we will present combined STM, XPS, LEED and IRAS studies of gold particles deposited on both extended CeO2 films and ceria nanoparticles. Well ordered CeO2 films were grown on Ru(0001) single crystal, and the quality of the films was controlled by XPS, LEED and STM. The ceria nanoparticles were prepared on thin silica films, which are essentially inert towards Au and CO, such that Au was only nucleated on the ceria particles and CO adsorbed only on Au/ceria. The results are rationalized on the basis of highly defective surface of nanoceria, which modifies the electronic structure of gold. [1] M. Haruta, N. Yamada, T. Kobayashi, and S. Iijima, J. Catal., 115 (1989) 301 [2] Carrettin S., Concepción P., Corma A., López Nieto J.M., Puntes V.F. (2004) Angew.

O 50: Symposium: Surface Spectroscopy on Kondo Systems II (Invited Speakers: Jonathan Denlinger, Johann Kroha, Alexander Schneider)

Time: Wednesday 15:15–18:00 Location: HE 101

Invited Talk O 50.1 Wed 15:15 HE 101

ARPES Mapping of the Fermi Surfaces of Three-Dimensional Heavy Fermion Systems — •Jonathan Denlinger — Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

Angle-resolved photoemission (ARPES) on most heavy fermion f-electron systems is a very challenging task because they are typically three-dimensional, incurring effects of k_z-broadening, and may not cleave well. Also their electronic structures typically contain many overlapping bands and very small (meV) hybridization energy scales near the Fermi level thus requiring high momentum- and energy-resolution. Experimental advances in electron spectrometers, x-ray synchrotron sources and automation have enabled acquisition of large variable photon-energy ARPES electronic structure maps that permit a k_z-tomographic determination of the 3D band structures and Fermi surfaces with sufficient detail to be truly complementary to dHvA in addressing theoretical predictions for this class of materials. Progress in this direction is discussed for the systems of CeRu_2Si_2, CeCoIn_5 and YbBiPt.

Invited Talk O 50.2 Wed 15:45 HE 101

Local Kondo Physics vs. Lattice Effects in Real Solids — •Johann Kroha — Physikalisches Institut, Universität Bonn

In recent years, photoemission spectroscopy (PES) as well as scanning tunneling microscopy (STM) have been developed into powerful tools for investigating the low-energy features characteristic for strongly correlated impurity and lattice systems due to their high spectral resolution of only a few meV.

We first review briefly the physical origin of the multiple low-energy resonances in heavy-electron compounds as Kondo spin fluctuations, involving the crystal-field or spin-orbit split 4f orbitals of rare earth ions. We then discuss the different shape of STM Kondo spectra, where multiple Kondo resonances are not observed, and explain this fact by the orbital selectivity of the STM in contrast to PES. We propose a method to determine the spatial orientation of individual orbitals of Kondo impurities on a metal surface from their STM spectra.

In the second part of the talk we analyze theoretically recent PES experiments on the heavy fermion compound $\text{CeCu}_{6-x}\text{Au}_x$, which undergoes a quantum phase transition (QPT) to an antiferromagnetically ordered state at $x \simeq 0.1$. The PES spectra, taken at $T \simeq 10$ K, i.e. well above the ordering temperature, probe the local Kondo physics of the Ce atoms, and indicate a sharp drop of the Kondo temperature T_K near $x = 0.1$. By analyzing the origin of this drop theoretically, we conjecture on whether in $\text{CeCu}_{6-x}\text{Au}_x$ the Hertz-Millis scenario (persistence of quasiparticles through the QPT) or the local quantum critical scenario (breakdown of quasiparticles at the QPT) is realized.

Invited Talk O 50.3 Wed 16:15 HE 101

Local Correlation Physics of Transition Metal Atoms on Noble Metal Surfaces — •M. Alexander Schneider — Lehrstuhl für Festkörperphysik, Universität Erlangen, Staudtstr. 7, D-91058 Erlangen

Scanning tunneling spectroscopy at low temperatures has allowed experimentalists to access the properties of the single Kondo impurity at surfaces [1]. This local approach proved fruitful as it has opened the route to study systematically the coupling of an impurity to various electronic states at the surface [2] and also the coupling between Kondo impurities [3]. In my talk I will discuss the experimental findings of the properties of Co-Atoms on noble metal surfaces and multilayer substrates.

[1] J. Li, et al., Phys. Rev. Lett **80**, 2893 (1998) and V. Madhavan, et al., Science **280**, 567 (1998)

[2] M.A. Schneider, et al., Jap. J. Appl. Phys. **44 (7B)**, 5328 (2005)

[3] P. Wahl, et al., Phys. Rev. Lett. **98**, 056601 (2007)

O 50.4 Wed 16:45 HE 101

Kondo Peak Splitting in a Magnetic Field for Ti/CuN/Cu(100)-$c(2 \times 2)$ — •Harald Brune[1,2], Markus Ternes[1], Christopher P. Lutz[1], Cyrus F. Hirjibehedin[1,3], and Andreas J. Heinrich[1] — [1]IBM Almaden Research Center — [2]Ecole Polytechnique Fédérale de Lausanne — [3]London Centre for Nanotechnology

dI/dV–spectra recorded with an STM operating at 0.6 K show a Kondo peak when the tip is centered over individual Ti atoms adsorbed onto the Cu sites of CuN-$c(2\times2)$–islands on a Cu(100) surface. In the gas phase Ti has $S = 1$, however, the observed spectra are suggestive of $S = 1/2$. The peak is sufficiently narrow to observe its splitting under an out-of-plane magnetic field. We discuss the results in light of measurements of the d-state LDOS centered at 0.7 eV above E_F.

O 50.5 Wed 17:00 HE 101

Contribution of the surface state to the observation of the surface Kondo resonance — •Jörg Henzl and Karina Morgenstern — Insitut für Festkörperphysik, Leibniz Universität Hannover, Germany

Tunneling spectra obtained on and near Co atoms adsorbed on Ag(111) show at 5 to 6 K a Kondo resonance that appears as a characteristic dip around the Fermi energy. The feature is present up to 1.5 nm around Co atoms adsorbed on terraces with the surface state onset in the occupied region of the density of states. On a narrow terrace, where the surface state onset lies in the unoccupied region of the density of states, it is only present up to 0.5 nm. This difference demonstrates directly the importance of the surface state electrons in the observation of the surface Kondo resonance.

O 50.6 Wed 17:15 HE 101

Kondo effect of subsurface Fe and Co impurities in Cu(100) - a comparative STS study — •Alexander Weismann, Martin Wenderoth, Henning Prüser, and Rainer G. Ulbrich — IV. Physikalisches Institut; Georg-August Universität Göttingen, Germany

We prepared single isolated subsurface iron and cobalt atoms beneath the Cu(100) surface by co-deposition of host metal and impurity compound under UHV conditions. The STM topographies at 6K show bulk state LDOS oscillations with four-fold symmetry in the vicinity of the defects. The observed patterns are in good agreement with the results of calculations based on host metals Greens function. This allows a depth classification and an extraction of the Kondo-related scattering phase from the STM experiment. In STS measurements both species of impurities show characteristic Kondo features on distinctly different energy scales. The dI/dV spectra show Fano line shapes depending on depth of the impurity below the surface. In the case of Fe the observed resonance width is extremely narrow so that even in the topographies a significant change of the interference pattern within +/- 3mV around zero bias can be observed. This work was supported by DFG SFB 602 TPA3.

O 50.7 Wed 17:30 HE 101

Electronic structure of thin ytterbium layers on W(110) — •Yury Dedkov[1], Denis Vyalikh[1], Matthias Holder[1], Martin Weser[1], Serguei Molodtsov[1], Yury Kucherenko[2], Mikhail Fonin[3], and Clemens Laubschat[1] — [1]Institut für Festkörperphysik, TU Dresden, Germany — [2]Institute for Metal Physics, Kiev, Ukraine — [3]Fachbereich Physik, Universität Konstanz, Germany

Among the lanthanides, Yb and Ce are of fundamental interest, because of the strong interaction between $4f$ and valence-band (VB) states leading to mixed-valence and Kondo phenomena in a number of compounds [1,2]. This analogy between Yb and Ce systems has been explained on the basis of the electron-hole symmetry of the quasiatomic $4f$ shell. While the correspondence has been established for a number of compounds, no evidence for such symmetry has been reported up to now for the pure metals. Motivated by the recent work [3], we report on the results of the angle-resolved photoemission (PE) studies of thin layers of Yb (1-3 ML-thick) on W(110) surface. The clear splitting of the Yb $4f_{7/2}$ state was observed in the PE spectra measured around $\overline{\Gamma}$ point for 1 ML-thick Yb film. The measured PE spectra were analyzed by means of the simplified periodic Anderson model.

[1] C. Laubschat, G. Kaindl, W.-D. Schneider, B. Reihl, and N. Mårtensson, Phys. Rev. B **33**, 6675 (1986).

[2] F. Patthey, J.-M. Imer, W.-D. Schneider, H. Beck, Y. Baer, and B. Delley, Phys. Rev. B **42**, 8864 (1990).

[3] D. V. Vyalikh, Yu. Kucherenko, S. Danzebächer, Yu. S. Dedkov, C. Laubschat, and S. L. Molodtsov, Phys. Rev. Lett. **96**, 026404 (2006).

O 50.8 Wed 17:45 HE 101

Conductance and Kondo effect of a controlled single atom contact — •néel nicolas, kröger jörg, limot laurent, and berndt richard — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany

The tip of a low-temperature scanning tunneling microscope is brought into contact with individual cobalt atoms adsorbed on Cu(100). A smooth transition from the tunneling regime to contact occurs at a conductance G around the quantun of conductance G0. Spectroscopy in the contact regime, i. ,e., at currents in a micro-ampere range was achieved and indicated a significant change of the Kondo temperature TK. Calculations indicate that the proximity of the tip shifts the cobalt d-band and thus affects TK.

O 51: Metal Substrates: Adsorption of Organic/Bio Molecules III

Time: Wednesday 15:15–18:30 Location: MA 041

O 51.1 Wed 15:15 MA 041

Molecular 2D Ordering of Viologens Under Non-Equilibrium Condition - an EC-STM Approach — •Duc Thanh Pham, Klaus Wandelt, and Peter Broekmann — Institut f. Physikalische und Theoretische Chemie, Uni Bonn

The structural characterization of 1,1'-dibenzyl-4,4' bipyridinium molecules (dibenzyl-viologen, DBV), adsorbed on a chloride modified Cu(100) electrode is studied by means of Cyclic Voltammetry (CV) and ElectroChemical Scanning Tunneling Microscopy (EC-STM). All previous studies on this system started with the non-reactive adsorption of DBV^{2+} in the double layer regime resulting in the surface assisted organization of a cationic DBV^{2+} monolayer on top of the c(2x2) anionic chloride adlayer. However, within the electrode potential window ranging from E = -150 mV to E = -250 mV where the first reduction step from the di-cationic to the radical mono-cationic viologen form takes place, a "reactive"adsorption of viologen occurs. Preferred reaction products at the surface are metastable viologen dimer species with a viologen coverage of 0.077 ML. Once formed under kinetic control, this dimer phase exhibits an unusually high stability against changes of the potential. It can only be converted irreversibly into either the oxidized dicationic species or the more compact and thermodynamically favorable "polymeric"stacking phase of radical mono-cations by significantly more anodic or cathodic potentials sweeps, respectively.

O 51.2 Wed 15:30 MA 041

Ultra-thin films of α-sexithiophene on Au(001) at room and elevated temperature — •Anke Höfer, Klaus Duncker, Mario Kiel, Sebastian Wedekind, René Hammer, and Wolf Widdra — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg

The rodlike, π-conjugated molecule α-sexithiophene (α-6T) is widely used in organic electronics, in which the performance of the devices strongly depends on molecular order. Ultra-thin films of α-6T on Au(001) have been studied by scanning tunneling microscopy (STM) in UHV. At room temperature in the monolayer regime two different highly ordered adsorption phases coexist which are related to quenching (phase D) and conservation (phase L) of the underlying substrate reconstruction. As the molecular structure of D is identical to one found on Ag(001), the other one is similar to that observed on Au(111) [1]. Both structures show different homochiral domains necessitating chiral self-recognition of the adsorbed molecules. Thermally induced both phases disappear at 400 K, whereas the transition of L is irreversible. In-situ observations at elevated temperatures from 410 K up to 630 K show the formation of a molecular network, which is interpreted as result of thiophene polymerization. The onset temperature of polymerization differs for the surface areas with quenched and conserved reconstruction.

[1] M. Kiel, K. Duncker, Ch. Hagendorf, W. Widdra, Phys. Rev. B 75, 195439 (2007)

O 51.3 Wed 15:45 MA 041

Formation of covalently bound chains from Dibromoterfluorene molecules on Au(111) — •Leif Lafferentz[1], Hao Yu[2], Stefan Hecht[2], and Leonhard Grill[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [2]Institut für Chemie, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 2, 12489 Berlin

Supramolecular structures formed by self-assembly on surfaces have attracted a lot of interest in the last years. While the formation of arrays relying on non-covalent bonds can yield structures of high complexity, they tend to be not very robust. For nanostructures of potential interest for future applications, a more rigid connection of the molecular building blocks is required.

Recently, it has been shown in our group that it is possible to form molecular networks of predesigned architecture by directed covalent linking of porphyrin molecules [1]. We will present results on the versatility of this method using differently designed building blocks, namely Dibromoterfluorene (DBTF). Intact molecules are found on the Au(111) surface in characteristic arrays. Upon sufficient heating, these molecules become "activated" and are connected by covalent bonds to form long chains. The constructed macromolecules are characterized by scanning tunneling microscopy (STM). Furthermore, manipulation of the molecular chains by using the STM tip will be presented. [1] L. Grill, M. Dyer, L. Lafferentz, M. Persson, M. V. Peters, and S. Hecht, Nature Nanotech. 2, 687 (2007)

O 51.4 Wed 16:00 MA 041

Protection group controlled surface chemistry-organization and heat induced coupling of biphenyl derivatives on metal surfaces — •Serpil Boz[1], Meike Stöhr[1], Umut Soydaner[2], and Marcel Mayor[2] — [1]University of Basel, Department of Physics, Klingelbergstrasse, CH-4056 Basel, Switzerland. — [2]University of Basel, Department of Chemistry, St. Johannsring 19, CH-4056 Basel, Switzerland

The development of scanning probe methods enabled the investigation of molecules on surfaces with impressive resolutions. The arrangement of the molecules in ordered patterns occurs because of a delicate balance between molecule - substrate and intermolecular interactions such as van der Waals interactions, H-bonding or dipolar coupling. A very appealing concept is to profit from the order of these pre-organized structures and to interlink the molecular building blocks to macromolecules. A prominent example for this is diacetylenes which have been polymerized on surfaces either by UV-light or with aid of the STM tip. Here we would like to present our new concept to control both, the molecular self-assembly and the subsequent intermolecular coupling reactivity by protection group chemistry. We studied a BOC protected biphenyl derivative which forms a parallel and a herringbone arrangement at room temperature on a Cu (111) surface. A second phase is observed after the sample is annealed at 196°C and covalently linked dimers by splitting off the BOC groups are formed. As a result of further annealing, individual cross-shaped polymeric structures are obtained.

O 51.5 Wed 16:15 MA 041

Thermally induced polymerization of molecules on surfaces — •Manfred Matena[1], Jorge Lobo-Checa[1], Meike Stöhr[1], Kathrin Müller[2], Thomas A. Jung[2], Till Riehm[3], and Lutz H. Gade[3] — [1]Departement Physik, Universität Basel, Switzerland — [2]Paul-Scherrer-Institut, Villigen, Switzerland — [3]Institut für Anorganische Chemie, Universität Heidelberg, Germany

By utilizing the concepts of supramolecular chemistry, impressive results for molecular self-assembly on surfaces have been presented. Mostly, non-covalent interactions like metal coordination, hydrogen bonding or dipolar coupling are exploited to create extended supramolecular patterns in variable dimensions. One common approach to influencing these structures relies mainly on the sophisticated design of the molecular functional groups. Thus it makes use of properties already inherent to the molecules. In our work we have chosen a different concept. A thermally-induced surface-assisted reaction was used to modify the endgroups of a perylene derivative (TAPP) and thereby, the molecular interactions are altered.

TAPP was found to form a closed-packed assembly on Cu(111), whereas the intermolecular interactions are based upon vdW-forces. After annealing at 150°C, a metal coordinated rectangular network is obtained which is commensurate to the underlying Cu surface. In this case the organic molecules coordinate to Cu atoms through the lone pairs of their nitrogen atoms. A second annealing step at temperatures >240°C modifies the molecule on the surface and leads to covalently linked polyaromatic chains.

O 51.6 Wed 16:30 MA 041

Molecular self-assembly on an ultrathin insulating film — •Christian Bombis[1,2], Nataliya Kalashnik[1], Wei Xu[1], Erik Laegsgaard[1], Flemming Besenbacher[1], and Trolle Linderoth[1] — [1]Department of Physics and Astronomy, and iNANO, University of Aarhus, 8000 Aarhus C, Denmark — [2]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Molecular self-assembly of cyanuric acid (CA) and melamine (M) on an ultrathin NaCl film grown on Au(111) is investigated by means of STM. Since it was shown that an ultrathin insulating film of NaCl on a metallic substrate enables electronical decoupling of an adsorbed molecule from the conducting substrate, while still allowing imaging of the molecule with STM, this method gained increasing attention for reasons of practical interest. However, due to weak molecule-substrate interactions stabilization of the molecules on alkali halides is a challenging task. In the present study we present the preparation and growth of ultrathin NaCl films in submonolayer quantities on Au(111). CA and M were thermally evaporated on such a NaCl/Au(111) substrate held at room temperature. We were able to image ordered molecular islands at comparatively high temperatures between 120 and 180 K on top of the NaCl film, which are nucleated at NaCl step edges. As we could identify the same adsorption structures on the NaCl film as previously reported by Xu et al.* for CA and M on pure Au(111), we conclude that the stabilization of the molecules is facilitated by their ability to form complementary triple hydrogen bond motifs with a high intermolecular interaction strength. *small 2007, 3, No. 5, 854-858

O 51.7 Wed 16:45 MA 041

Scanning Tunneling Microscopy Study of Iron(II) Phthalocyanine Growth on Metal and Insulating Surfaces — •Alessandro Scarfato[1,2], Shih-Hsin Chang[1], Germar Hoffmann[1], and Roland Wiesendanger[1] — [1]Institute of Applied Physics and Microstructure Research Center Hamburg, University of Hamburg, Jungiusstrasse 11, D-20355, Hamburg, Germany — [2]Dipartimento di Fisica "E. R. Caianiello", Università degli Studi di Salerno e CNR-INFM Laboratorio Regionale SUPERMAT, via Salvador Allende, I-84081 Baronissi (SA), Italy

The growth behavior of iron(II) phthalocyanine (FePc) molecules on Cu(111) and on NaCl/Cu(111) surfaces up to a coverage ~ 1.5 ML has been studied by a variable-temperature scanning tunneling microscope. Molecules have been deposited at room temperature to allow for surface diffusion. At low coverage (~ 0.5 ML) no tendency of self assembling was observed, while at high coverages (> 1 ML) the second layer molecules self-organize to form long-range domains in the alpha phase. In order to tune molecule-substrate interaction insulating NaCl layers are introduced. Adsorption of FePc molecules on NaCl shows site specificity, i.e. the Fe atom adsorbs on top of a Cl^- anion. We will discuss our results on the growth morphology in terms of molecule-molecule and molecule-substrate interactions in comparison with previous findings for FePc on Au(111).

O 51.8 Wed 17:00 MA 041

STM and STS on Ultrathin Organic Layers of Fluorinated Cobalt Phthalocyanine (F16CoPc) on Crystalline Substrates — •Mahmoud Abdel-Hafiez, Marius Toader, Thiruvancheril Gopakumar, and Michael Hietschold — Institute of Physics, Solid Surfaces Analysis Group, Chemnitz University of Technology, D-09107, Chemnitz, Germany

Scanning Tunneling Microscope (STM) and Spectroscopy (STS) are used to study the adsorption geometry and electronic structure of isolated hexafluro-cobalt phthalocyanine (F16CoPc) molecules adsorbed on the basal plan of HOPG and Ag(110). Monolayers were prepared using organic molecular beam epitaxy (OMBE) under ultra high vacuum (UHV) conditions at room temperature and investigated at 45 K using Omicron VT-STM. F16CoPc forms a perfect quadratic superstructure independent of the substrate. In both cases a planar adsorption of molecules is observed with a non-commensurate superstructure with the substrate lattice. Moreover tunneling voltage polarity dependent contrast reversal at the cobalt center is observed, especially in the case of molecules on Ag(110). Adsorption geometry of molecules within the adlayer shows the influence of fluorine atoms in the packing. Tunneling spectroscopy and single molecule calculations are employed to understand the type of interactions between F16CoPc and the substrate, as well as the effects of fluorine atoms on the geometric configurations of the adsorbed F16CoPc molecules.

O 51.9 Wed 17:15 MA 041

Ordered 2D assemblies of phenoxy substituted phthalocyanines as hosts for further guest molecules — Tomas Samuely[1], Shi-Xia Liu[2], Nikolai Wintjes[1], Marco Haas[2], Silvio Decurtins[2], Thomas A. Jung[1,3], and •Meike Stöhr[1] — [1]Institute of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [2]Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, 3012-Bern, Switzerland — [3]Laboratory for Micro- and Nanostructures, Paul-Scherrer-Institute, 5232 Villigen, Switzerland

Symmetrically substituted phthalocyanines (Pcs) with eight peripheral di-(tert-butyl)phenoxy (DTPO) groups self-organize on Ag(111) and Au(111) substrates into various phases. These phases coexist due to a retardation of the thermodynamic optimization of the conformations, caused by the proximity of the Pc core to the metal substrate together with the steric entanglement between neighboring DTPO substituents. The rotational degrees of freedom allow all the DTPO substituents to be arranged above the plane of the Pc core, forming a bowl-like structure, which enables the interaction of the Pc core with the metal substrate. Moreover, this bowl-like shape predetermines such assemblies to serve as a host accommodating guest molecules. As an example, C60 molecules, upon deposition on an ordered layer of the DTPO substituted Pcs, bind to two clearly distinguishable sites, exhibiting different morphologic and electronic properties. Since Pcs are well-known electron donors and C60 molecules are good electron acceptors, such ordered guest-host systems allow addressable STM/STS investigations of individual donor-acceptor complexes.

O 51.10 Wed 17:30 MA 041

Adsorption and ordering of a triphenylene $Cr(CO)_3$ complex on noble metal surfaces — •Christoph H. Schmitz[1], Julian Ikonomov[1], Iordan Kossev[1], Carola Rang[2], Serguei Soubatch[3], Olga Neucheva[3], Frank Stefan Tautz[3], Karl Heinz Dötz[2], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Bonn — [2]Kekulé-Institut für Organische Chemie und Biochemie, Universität Bonn — [3]Institute of Bio- and Nanosystems 3, Forschungszentrum Jülich

Adsorption by physical vapor deposition of metal-organic complexes is so far known for metallocene- and phthalocyanine-derivatives. Here we report on the deposition of the chromium complex (1,2,3,4,4a,12b)-tricarbonyl-(2,3-diethyl-1,4-dimethoxytriphenylene)chromium(0) (TPHC) and the corresponding ligand 2,3-diethyl-1,4-dimethoxy-triphenylene (TPH). This complex is of interest, since a haptotropic migration of the $Cr(CO)_3$-moiety is found in solution and may also be present in adsorbed layers. We succeeded to prepare ordered layers of TPHC and TPH on silver and copper single crystal surfaces that were investigated by scanning tunneling microscopy and x-ray photoelectron spectroscopy. STM shows the formation of long range ordered structures with different unit cells for TPHC and TPH. This demonstrates that the $Cr(CO)_3$-moiety has a decisive influence on the lateral interaction of the molecules on the surface. XPS results reveal the intact adsorption of TPHC. Experiments with low energy electron diffraction, however, fail since a decomposition of the complex due to electron bombardment occurs. (Funded by DFG SFB 624)

O 51.11 Wed 17:45 MA 041

Local and Long Range Structure of Ferrocene on Au(111) Surfaces — •Gerhard Pirug[1], Michel Kazempoor[1], Josef Mysliveček[2], and Bert Voigtländer[1] — [1]Institut für Bio- und Nanosysteme (IBN3), Forschungszentrum Jülich GmbH, Germany — [2]Dept. of Surface and Plasma Science, Faculty of Mathematics and Physics, Charles University Prague, Czech Republic

The adsorption of ferrocene ($Fe(C_5H_5)_2$) on Au(111) surfaces has been studied spectroscopically applying HREELS and structurally by means of LEED and STM. The vibrational modes observed by HREELS indicate reversible molecular adsorption at temperatures of about 110 K. The corresponding frequencies are not significantly shifted with respect to IR or Raman data for solid ferrocene, indicating a weak adsorbate - substrate interaction. Multilayer adsorption can be distinguished from the physisorbed first layer based on relative intensity changes of vibrational modes. In the monolayer regime vibrational modes with a perpendicular dipole moment from more or less upright standing ferrocene molecules dominate. Dissociation into cyclopentadienyl radicals (C_5H_5) can be excluded. Molecular self assembly yields well ordered surface structures. A commensurate $(3 \times \sqrt{3})$rect (p2mg) structure has been identified from topographical STM images and LEED pattern, consistently. In addition a compressed incommensurate structure develops. Both structures are at variance with recent findings by Braun et al.[1] but can be related to the crystallographic structure of crystalline ferrocene. ([1]K.F. Braun V. Iancu, N. Pertaya, K.H. Rieder and S.-W. Hla, Phys. Rev. Lett. 96, 246102 (2006))

O 51.12 Wed 18:00 MA 041

Interaction of scanning tunneling microscopy tip with adatoms and molecules on metal surfaces: ab initio studies — •Kun Tao[1], Valeri S. Stepanyuk[1], Dmitri I. Bazhanov[2], and Patrick Bruno[1] — [1]Max-Planck-Institut fur Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — [2]Faculty of Physics, Moscow state University, 119899 Moscow, Russia

We perform ab initio calculations of the interaction of the STM tip with magnetic adatoms and molecules on metal surfaces. We apply density functional theory (DFT) based methods (SIESTA, VASP) and perform calculations in the fully relaxed geometries for the tip and the substrate. Both interactions with nonmagnetic and magnetic tips are studied. We concentrate on 3d transition metal adatoms supported on Cu(100) and Cu(111) surfaces. The interaction of the tip with molecule-metal sandwich, consisting of the benzene molecule and 3d adatom, is discussed. Our study reveals that electronic states and magnetic moments of adatoms can be drastically changed by interaction with tip. We also show that magnetic coupling between the tip and the adatom can be manipulated by approaching the tip to the substrate.

O 51.13 Wed 18:15 MA 041

Surface-selection rule for infrared spectra of adsorbate molecules violated by metal ad-atoms — •Olaf Skibbe[1], Martin Binder[1], Andreas Otto[2], and Annemarie Pucci[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, D-69120 Heidelberg — [2]Institut für Physik der kondensierten Materie, Heinrich-Heine Universiät, Düsseldorf

Copper adatoms on Cu(111) significantly modify the infrared reflection-absorption spectrum of ethylene (C_2H_4) on Cu(111). The infrared spectral changes do not involve significant shifts of vibration frequencies as they would be expected for strong distortions. But originally non-infrared active Raman modes of the centrosymmetric molecule appear in the spectra and the infrared active CH_2-wagging mode disappears already below 0.2 monolayers of Cu adatoms. High-resolution electron energy loss spectra of adsorbed ethylene for various Cu-adatom pre-coverage show the same vibration lines and indicate the change in their dipole character. Since the molecules are obviously unchanged, the Raman lines in the infrared spectra must get their dynamic dipole moment from transient electron transfer favored by atomic disorder on the metal surface, which is an experimental proof of a previous hypothesis. The completely new and surprising result of this work is the disappearing infrared active mode at sub-monolayer Cu-adatom coverage, which we explain by screening due to the background polarizability increased by Cu adatoms.

O 52: Time-Resolved Spectroscopy III

Time: Wednesday 15:15–18:30 Location: MA 042

O 52.1 Wed 15:15 MA 042

Interferometric control of spin-polarized photoemission from Cu(001) — •Aimo Winkelmann, Wen-Chin Lin, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle(Saale), Germany

We demonstrate that we can tune the spin-polarization of photoelectrons emitted in a three-photon process from Cu(001) by interferometric control of the delay between two ultrashort optical pulses in a pump-probe experiment. As a function of pulse delay, the spin polarization can be changed from ±20% to ∓40% using circularly polarized light for excitation. We differentiate between the regime of optical interference for overlapping pulses and, for longer delays, the influence of the material response. The influence of the coherent material response is detected by observing interference oscillations at twice the optical frequency. These are created by the interference of the pump pulse induced electromagnetic polarization at the surface and the subsequent probe pulse. The spin polarization of the observed electrons for delays longer than the pulse length also shows the oscillations at twice the optical frequency.

O 52.2 Wed 15:30 MA 042

Spin-dependent inter- and intraband scattering in image-potential-state bands on 3d ferromagnets — •Anke B. Schmidt[1], Martin Pickel[2], Markus Donath[1], and Martin Weinelt[2] — [1]Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany — [2]Max-Born-Institut, Max-Born-Straße 2A, 12489 Berlin and Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany

We have observed ultrafast electron-magnon scattering of image-potential-state electrons on ultrathin ferromagnetic films in three different regions of energy and momentum transfer directly in the time domain. In our spin- and time-dependent photoemission experiment we employ the dispersing image-potential-state electron as observer or primary electron, thus effectively separating low-energy losses from direct decay into d-holes. For the quasielastic processes resonant interband scattering and dephasing at the band minimum as well as intraband scattering, an energy relaxation process, we found evidence to suggest that electron-magnon scattering constitutes a significant scattering channel for excited minority-spin electrons on iron even on the femtosecond timescale.

O 52.3 Wed 15:45 MA 042

Coherent dynamics at Gd(0001) and Tb(0001) surfaces: magnon-enhanced damping of optical phonons — •Alexey Melnikov[1], Alexey Povolotskiy[2], and Uwe Bovensiepen[1] — [1]Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, D-14195 Berlin, Germany — [2]St. Petersburg State University, Laser Research Institute, St. Petersburg, 198504 Russia

Coherent lattice and spin dynamics were studied at the Gd(0001) surface by time-resolved second harmonic generation [1]. To understand the elementary processes responsible for optical excitation and damping of coherent phonons (CP) and magnons (CM), we perform temperature-dependent studies in Gd and Tb. With lowering the temperature T from the Curie point T_C to 40K amplitudes of CP and CM increase by more than an order following the increase of spin ordering and showing an essentially "magnetic" nature of the excitation. The CP damping rate Γ increases linearly with the temperature in transition metals, which is attributed to anharmonic phonon-phonon scattering [2]. In Gd we observe a monotonous increase of $\Gamma(T)$ at $T < T_C$ but near T_C it reduces significantly. We explain this by phonon-magnon scattering contributing to Γ at $T < T_C$. This contribution scales with the magnetoelastic constant mediated by the spin-orbit interaction. This conclusion is confirmed by $\Gamma(T)$ measured in Tb (L=3), where the spin-lattice coupling is much larger than in Gd (L=0): the phonon-magnon contribution to $\Gamma(T)$ is found to be 6 times larger than in Gd.

[1] A. Melnikov et al., Phys. Rev. Lett. **91**, 277403 (2003).

[2] M. Hase et al., Phys. Rev. B **71**, 184301 (2005).

O 52.4 Wed 16:00 MA 042

Observing photo-induced chemical reactions of molecules on surfaces in real-time — •Mihai E. Vaida, Peter E. Hindelang, Robert Tchitnga, and Thorsten M. Bernhardt — Institut für Oberflächenchemie und Katalyse, Universität Ulm, Albert-Einstein-Allee 47, D-89069 Ulm, Germany

Time-of-flight mass spectrometry in conjunction with femtosecond resonance-enhanced multiphoton ionization is used to monitor ultrafast chemical reactions of supported molecules. A new experimental approach enables the quick and precise in situ preparation of the surface with sub-monolayer adsorbate coverage prior to photo-induced reaction. The investigation of different reaction pathways is accomplished by direct real-time monitoring of the different reaction products and intermediates as well as their kinetic energy content. First results for methyl iodide adsorbed on ultra-thin insulating magnesia films will be presented.

O 52.5 Wed 16:15 MA 042

Reversible switching of azobenzene in direct contact with a Au(111) surface — •Sebastian Hagen, Peter Kate, Felix Leyssner, Martin Wolf, and Petra Tegeder — Freie Universität Berlin, Fachbereich Physik

Two-photon photoemission spectroscopy is employed to analyze reversible changes in the electronic structure of the molecular switch tetra-*tert*-butyl-azobenzene (TBA) adsorbed on Au(111), which are induced by light and thermal activation. Cycles of illumination and annealing steps confirm the reversibility of the switching process, which we assign to a *trans*/*cis*-isomerization of TBA molecules in direct contact with the Au(111) surface. Based on wavelength dependent measurements we propose that the optically-induced conformational change (*trans*- to *cis*-isomerization) of the adsorbed molecules is not caused by direct intramolecular excitation as in the liquid phase but rather by an indirect mechanism, *viz.* a substrate mediated process. Thereby photoexcitation of holes in the Au *d*-band followed by a charge transfer to the HOMO level drives the isomerization in the photon energy range between 2.1 and 4.6 eV. In addition, for photon energies above 4.6 eV the creation of a negative ion resonance *via* attachment of excited electrons to the molecules plays a role.

O 52.6 Wed 16:30 MA 042

Electron dynamics at the PTCDA/Ag(111) interface studied with 2PPE — •Manuel Marks[1], Christian Schwalb[1], Sönke Sachs[2], Achim Schöll[2], Eberhard Umbach[2,3], 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 — [3]Forschungszentrum Karlsruhe, D-76021 Karlsruhe

We investigated epitaxial grown PTCDA (3,4,9,10-perylene-tetracarboxylic acid-dianhydride) on the Ag(111) surface as model system for a metal-organic interface by means of time- and angle-resolved two-photon photoemission (2PPE). In the presence of thin PTCDA films, an unoccupied state with an effective electron mass of 0.39 m_e is observed in the projected band gap of Ag 0.6 eV above E_F. Its inelastic electronic lifetime is $\simeq$ 50 fs and the state has an appreciable metallic character, significantly exceeding that of the image-potential states. We assign the new state to a mixture of the former Ag(111) Shockley surface state and the LUMO+1 of the first PTCDA monolayer (ML). In contrast to this interface state, which changes only weakly with PTCDA coverage, the binding energy of the first image-potential state shows a strong dependence. It increases by 135 meV for 1 ML, compared to clean Ag(111), but with absorption of the second ML, a subsequent drop of -70 meV relative to the clean surface occurs. A similar coverage dependence can be seen in the effective electron mass, which decreases by 20% from the first to the second PTCDA layer.

O 52.7 Wed 16:45 MA 042

Strong temperature dependence of vibrational relaxation of H/Ge(100) — Xu Han, Kristian Lass, and •Eckart Hasselbrink — Department of Chemistry, University of Duisburg-Essen, D-45117 Essen, Germany

The population relaxation of vibrational excitations of adsorbates is the result of various dynamical couplings. However, the underlying microscopic mechanisms at semiconductor surfaces are not yet fully understood. Germanium provides special research interests because of its lower surface Debye temperature than silicon. On Ge(100) surface the Debye temperature is more than two times smaller than in bulk, which implies a strong anharmonicity on the surface.

IR pump-SFG probe measurements of the vibrational population relaxation on H (2×1)/Ge(100) surfaces revealed a strong temperature dependence of the vibrational lifetime. T_1 was measured to be 0.5 ns for the Ge-H symmetric stretch at RT. The relaxation of vibrational energy follows a single exponential decay. The order of measured decay constants decreases from one nanosecond to 100 picoseconds, with increasing the substrate temperature from 273 K to 400 K. The model fitting of the temperature dependence suggests that relaxation of the Ge-H stretch mode initiates simultaneous excitation of three Ge-H bending quanta and four bulk phonons above RT. Our DFT calculations suggest that the vibration-phonon coupling, via anharmonicity, dominates the vibrational decay processes. The strong temperature dependence is facilitated by the quick increase of the density of states associated with low-frequency phonons.

O 52.8 Wed 17:00 MA 042

Time-resolved investigation of laser-induced diffusion of CO on terraces of vicinal Pt(111) — •Jens Güdde, Marco Lawrenz, and Ulrich Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität Marburg, D-35032 Marburg

We report on a time-domain study of diffusion of CO on a vicinal Pt(111) surface at low substrate temperature induced electronically via substrate electrons excited by femtosecond laser pulses. Diffusion is observed by monitoring the occupation of step sites on vicinal substrates by nonlinear optical second harmonic generation (SHG). Two-pulse correlation experiments were done to study the dynamics of energy flow from the initially excited substrate electrons to the adsorbate degrees of freedom. In contrast to O/Pt(111) [1], CO has a substantially higher binding energy at the step sites than at the terrace sites. For this reason the steps can be employed as traps for adsorbed CO at low temperatures and laser-induced diffusion can be observed by SHG not only from the steps to the terraces but also from terrace to step sites. For terrace diffusion of CO with a barrier of only 0.2 eV our correlation measurements at substrate temperatures of 40 and 60 K indicate a transition from an electronically driven process at low temperatures to a phonon driven process at higher substrate temperatures.

[1] K. Stépán *et al.*, Phys. Rev. Lett. **94**, 236103 (2005).

O 52.9 Wed 17:15 MA 042

Image-potential states and resonances on the clean and Argon covered (111)-surfaces of Copper and Silver — •Andreas Damm, Kai Schubert, Jens Güdde, and Ulrich Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg, Germany

We report on a comparative 2PPE study of the influence of Ar adlayers on the properties of image-potential states of Ag(111) and Cu(111). On both surfaces only the $n = 1$ state is non resonant with bulk states. As a result of Ar adsorption a drop of the workfunction and a systematic lowering of the binding energies of the image-potential electrons is observed. On Cu(111) however the first image state is bound close to the conduction band minimum. Thus this state becomes a resonance for Ar coverages $\Theta \geq 2$ ML, whereas it remains in the band gap of the bulk states on Ag(111) for coverages up to $\Theta = 4$ ML. This leads to a strikingly different dependence of the first image state's lifetime on layer thickness for the two surfaces. On Ag(111) the lifetime of the first image state depends exponentially on the number of adsorbed Ar layers, and rises from 32 fs on the clean surface to about 6 ps for Ar coverages of 4 ML. On Cu(111) the initial lifetime increase with layer thickness is essentially the same, but at an Ar coverage of $\Theta = 2$ ML a kink occurs in correlation with that state becoming resonant with the conduction band of bulk Copper. For higher coverages the increase of lifetime shows again an exponential behavior, but surprisingly with a reduced thickness dependence compared to the non resonant case.

O 52.10 Wed 17:30 MA 042

Towards time resolved core level photoelectron spectroscopy with femtosecond X-ray free-electron lasers — •Annette Pietzsch, Alexander Föhlisch, Martin Beye, Martin Deppe, Franz Hennies, Mitsuru Nagasono, and Wilfried Wurth — Institut für Experimentalphysik, Universität Hamburg, Luruper Chaussee 149, D-22761 Hamburg

We have conducted an investigation of space-charge induced peak shift and peak broadening in W 4f core-level photoemission from a W(110) single crystal surface using femtosecond X-ray pulses from the Free-Electron Laser at Hamburg (FLASH). We have established experimentally and through theoretical modelling what should be generally applicable conditions for photoelectron spectroscopy on solids and surfaces using femtosecond X-ray pulses from free-electron laser facilities. As a next step, we have studied within this working range time-resolved core-level photoelectron spectroscopy on a surface combining a femtosecond optical laser synchronized to the femtosecond X-ray pulses. Here, side bands to the W 4f core level lines give evidence of the cross-correlation between the femtosecond x-ray and optical pulses needed for future studies of femtosecond time-resolved core-level photoelectron spectroscopy on solids and surfaces. This work is supported in the framework of the BMBF Forschungsschwerpunkt 301 FLASH: Matter in the light of ultrashort and extremely intense x-ray pulses.

A. Pietzsch et al., submitted

O 52.11 Wed 17:45 MA 042

Zeit- und ortsaufgelöste Nahfelduntersuchung an strukturierten metallischen Oberflächen — •Andreas Bitzer und Markus Walther — Molecular and Optical Physics, Institute of Physics, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Strasse 3, 79104-Freiburg, Germany

Wir präsentieren eine eigens entwickelte Methode zur zeit- und ortsaufgelösten Nahfelduntersuchung an mikrostrukturierten metallischen Oberflächen. Durch gepulste Terahertz-Strahlung werden Oberflächenladungen zu elektromagnetischen Schwingungen angeregt beispielsweise an einem Metallgitter, einem Metalldraht und an einer mikrostrukturierten Metallfolie. Anhand unserem Verfahren ist es nun möglich, direkt an der Oberfläche der Probe das Nahfeld des elektrischen Feldes sowohl zeit- als auch ortsaufgelöst zu bestimmen. Mittels einer Fourieranalyse lässt sich dabei die spektrale Feldverteilung räumlich auflösen. So konnten wir an metallischen Filmen mit periodischen subwellenlängen-großen Lochgittern, welche im THz-Frequenzbereich als Bandpassfilter eingesetzt werden, charakteristische geometrische Moden beobachten. Ein weiteres Gebiet das sich mit Hilfe unserer Methode eindrucksvoll beobachten lässt ist die räumliche und zeitliche Feldentwicklung während der Feldpropagation entlang eines Wellenleiters. Am Beispiel eines Metalldrahtes werden wir den Einkopplungsvorgang eines THz Pulses in einen solchen Wellenleiter visualisieren und anschließend demonstrieren wie sich der THz-Puls entlang des Drahtes fortbewegt.

O 52.12 Wed 18:00 MA 042

Surface States and Kramers-Kronig relations in one-dimensional Photonic Crystals — •Michael Bergmair and Kurt Hingerl — CD-Labor für oberflächenoptische Methoden, Institut für Halbleiter- und Festkörperphysik, Universität Linz, Austria

Surface states provide very interesting features such as large field enhancement and are very sensitive to the geometry and dielectric behaviour of the investigated structure. A thin metallic sheet allows to investigate the near field and permits a design of a system with negative refracting behaviour. A one-dimensional photonic crystal consisting of layers which have a resonant dielectric behaviour in the infrared (photon-phonon coupling) show very interesting surface states: due to the coupling of bulk and surface states around the resonant frequency a dispersion with negative group velocity occurs. In this region the damping remains small yielding a large figure of merit n'/n'' which is the ratio of real and imaginary part of the dielectric function. In our work we will calculate the dispersion of such coupled surface states and unveil the mechanism that leads to this small damping values. Furthermore we investigate whether and how Kramers-Kronig relations can be applied to systems where the internal structure is on the order of the wavelength.

O 52.13 Wed 18:15 MA 042

Enhanced photodesorption by vibrational pre-excitation: Quantum model simulations for Cs/Cu(111) — •Dominik Kröner — Universität Potsdam, Institut für Chemie, Theoretische Chemie, Karl-Liebknecht-Str. 24-25, D-14476 Potsdam, Germany

We present electronic and nuclear quantum model simulations for the direct, laser-induced charge transfer from a Cu(111) surface state, to an unoccupied resonance state of an adsorbed Cs-atom. An one-electron model potential for Cu(111) by Chulkov *et al.* [1] is extended by a Cs adsorbate potential to determine energies and lifetimes of electronic states of Cs/Cu(111) at low coverage. In addition, empirical nuclear potential energy surfaces of the electronic ground and the antibonding excited state along the Cs-Cu distance are constructed. For both models, electronic and nuclear, we perform open-system quantum dynamics with the goals: (i) to estimate the excitation (charge transfer) and Cs desorption probabilities [2], (ii) to optimize the charge transfer process by laser pulse shaping using optimal control theory [2], and (iii) to increase the negligible desorption yield of Cs from the Cu surface, obtained from direct UV excitation, by vibrationally pre-exciting the Cs-Cu bond using a THz-laser pulse [3].

[1] E. V. Chulkov, V. M. Silkin, P. M. Echenique, *Surf. Sci.* **437**, 330 (1999).
[2] D. Kröner, T. Klamroth, M. Nest, P. Saalfrank, *Appl. Phys. A* **88**, 535 (2007).
[3] D. Kröner, S. Klinkusch, T. Klamroth, *Surf. Sci.*, accepted (2007).

O 53: Surface Nanopatterns

Time: Wednesday 15:15–18:30 Location: MA 043

O 53.1 Wed 15:15 MA 043

Investigation of surface modifications induced by swift heavy ions in the MeV regime. Part I: Experiment — •Sevilay Akcöltekin and Marika Schleberger — Universität Duisburg-Essen, Fachbereich Physik, Lotharstrasse 1, 47048 Duisburg

Over the past few years, ion-induced track formation on various crystal surfaces have been observed in many studies. Depending on the energy and charge state of the projectile-ions as well as the target properties, track production can turn out differently. Experimental investigation of track creation on different sample surfaces with energetic heavy ^{131}Xe^{23+} (0.71 MeV/u) and ^{207}Pb^{28+} (0.51 MeV/u) projectiles in the electronic stopping regime are discussed in the present work. Focusing on two classes of target materials such as oxides (SrTiO$_3$, TiO$_2$, Al$_2$O$_3$) and highly oriented pyrolytic graphit (HOPG), we present experimental data on (AFM, STM) track formation after irradiation at varying angle of incidence from 90° down to 0.3° . Especially at grazing angle of incidence, elongated chains of nanohillocks with lengths of about several hundred nanometers can be created. A statistical analysis of the track length and distance between the neighboring hillocks shows a strong dependence on the angle of incidence. Based on these experimental results a new approach describing the track formation could be developed.

O 53.2 Wed 15:30 MA 043

Investigation of surface modifications induced by swift heavy ions in the MeV regime. Part II : Theory — •Orkhan Osmani[1,2] and Marika Schleberger[1] — [1]Universität Duisburg-Essen, Fachbereich Physik, Lotharstrasse 1, 47048 Duisburg — [2]TU Kaiserslautern, Fachbereich Physik, Gottlieb-Daimler-Straße, 67653 Kaiserslautern

In the last few years various experiments on ion-solid interactions have been performed. In a recent experiment structural chain like surface modifications with chain length up to some micrometers have been observed. These modifications are strongly dependent on the angle of incidence and believed to be created by local melting of the solid due to the energy transfer of the ion to the solid. An new model will be presented which is capable to describe the energy loss of a swift heavy ion penetrating an insulator like SrTi0$_3$ and the creation of the so called nanodots. At ion energies of several 10 MeV to 100 MeV the energy loss is due to electronic stopping only. To describe the electronic excitation induced bye the ion–electron interaction we use an approach taking the electronic density into account. Time and spatially resolved energy losses are calculated and used as sourceterms for the electrons within a Two–Temperature–Modell. Finally, the relaxation of the electrons by simultaneous phononic excitation leads to a phononic temperature distribution. In this way, it can be checked if the phononic temperature is above the melting temperature, thus leading to a thermal melting.

O 53.3 Wed 15:45 MA 043

X-ray scattering and diffraction from Xe-induced ripples in crystalline silicon — •Andreas Biermanns[1], Ullrich Pietsch[1], Souren Grigorian[1], Jörg Grenzer[2], Stefan Facsko[2], Antje Hanisch[2], Dina Carbone[3], and Hartmut Metzger[3] — [1]Universität Siegen, Germany — [2]Foschungszentrum Dresden-Rossendorf, Germany — [3]ID01 beamline, ESRF, France

The formation of surface-nanostructures with a characteristic size ranging from several nanometer up to microns has attracted significant interest in the last decades in the context of fabrication of novel opto-electronic and storage devices. One kind of those nanostructures are wave-like patterns (ripples) produced by an interplay between a roughening process caused by ion beam erosion (sputtering) of the surface and smoothening processes caused by surface diffusion. In this contribution we report on investigations of patterned Si (001) surfaces after irradiation with Xe^{+}-ions using ion-energies up to 40keV. During the sputtering, an amorphous surface-layer is formed followed by a rather sharp interface towards crystalline material, showing the same morphology as the surface. The structures of the amorphous layer and the amorphous-crystalline interface were studied by means of grazing-incidence - small angle scattering (GISAXS) and diffraction (GID) using synchrotron-radiation. We found that the crystal structure at the interface is expanded along the ripples, caused by the creation of defects inside the surface region, whereas this expansion is strongly reduced across the ripples. This different relaxation may play a driving role in pattern formation at the interface.

O 53.4 Wed 16:00 MA 043

High energy Xe^{+} ion beam induced ripple structures on silicon — •Antje Hanisch[1], Joerg Grenzer[1], Stefan Facsko[1], Ingolf Winkler[1], Andreas Biermanns[2], Souren Grigorian[2], and Ullrich Pietsch[2] — [1]Forschungszentrum Dresden-Rossendorf, Institute for Ion Beam Physics and Materials Research, Bautzner Landstrasse 128, 01328 Dresden, Germany — [2]University of Siegen, Institute of Physics, Walter-Flex-Strasse 3, 57078 Siegen, Germany

Ion beam bombardment on semiconductor surfaces leads to well-defined morphological structures in the nanoscale range. Due to the impact of ions a self-organized wave-like surface structure develops. Ion bombardment causes an amorphization of a surface-adjacent layer of several nanometers and creates a periodical structure on the surface as well as at the amorphous-crystalline interface. We investigate the dependence of the periodicity on the crystallography of (100) silicon bombarded with Xe^{+} ions, the ion beam incidence and the azimutal angle of the sample surface. So far we found that the ripple wavelength scales with the ion energy in a range of 5 to 70 keV. In order to understand the initiation of the ripple formation we also ask the question which role the initial surface structure plays. Therefore we investigate the formation of ripples on pre-structured and rough surfaces such as wafers with an intentional miscut. Therefore, we not only introduce a certain initial roughness but also vary the orientation of the (100) lattice plane in respect to the surface. We try to distinguish between ion beam induced surface effects (sputter erosion) and the influence of the crystalline Si lattice (strain) on the ripple formation.

O 53.5 Wed 16:15 MA 043

Continuum model for pattern formation on ion-beam eroded surfaces under target rotation — •Karsten Dreimann and Stefan Jakob Linz — Institut für Theoretische Physik, Universität Münster, Wilhelm-Klemm-Straße 9, 48149 Münster, Germany

A recently proposed continuum model [1] for the formation of nanostructures on semiconductor surfaces generated by low-energy ion-beam erosion under normal and oblique ion incidence is generalized to the case of additional target rotation. After transformation, this model takes on the form of a driven damped isotropic Kuramoto-Sivashinsky equation. Primary focus of our investigation [2] is the theoretical analysis of the competition of flat, hexagonal and square-like surface structures as function of the external rotation rate and the sputtering time. As a major result, we find that target rotation stabilizes the occurence of flat surfaces. Comparison with recent experimental results will also be given.

[1] S. Vogel, S.J. Linz, Europhys.Lett. **76**, 884-890 (2006)
[2] K. Dreimann, S.J. Linz, unpublished

O 53.6 Wed 16:30 MA 043

Bifurcation behavior of the anisotropic damped Kuramoto-Sivashinsky equation — Christian Rehwald, Karsten Dreimann, Sebastian Vogel, and •Stefan Jakob Linz — Institut für Theoretische Physik, Universität Münster, Wilhelm-Klemm-Straße 9, 48149 Münster, Germany

A recently proposed continuum model [1] for the formation of surface patterns on semiconductor surfaces generated by low-energy ion-beam erosion under normal and oblique ion incidence is studied in analytical and numerical details. After transformation, this model takes on the form of a damped anisotropic Kuramoto-Sivashinsky equation. Primary focus of our investigation [2] is the theoretical analysis of the competition of flat, rhombic and ripple-like surface structures and their stability and bifurcation behavior as function of the entering parameters. Comparison with recent experimental results will also be given.
[1] S. Vogel, S.J. Linz, Europhys.Lett. **76**, 884-890 (2006)
[2] C. Rehwald, K. Dreimann, S. Vogel, S.J. Linz, unpublished

O 53.7 Wed 16:45 MA 043

Electron beam stimulated thermal desorption of oxygen: a lithographic method — •Jan Rönspies, Tammo Block, Svend Vagt, and Herbert Pfnür — Leibniz Universität Hannover, Institut für Festkörperphysik, 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 windows structures are suitable for growing contigous metallic nanowires with thickness of a few monolayers.

These uncovered structures with lateral dimensions down to $10nm$ were analyzed futher by tunneling microscopy. The Auger excitation process (Knotek-Feibelman mechanism) necessary for electron-beam stimulated thermal desorption of oxygen (EBSTD) allows generation of ultra-small structures. The subsequent processing step combines thermal desorption of the remaining monoxide and simultanous etching promoted by thermally activated silicon atoms, which turns out to be a strongly anisotropic process close to step edges. 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. Thus exploitation of the quantized nature of ultrasmall structures far above liquid He temperatures becomes feasible as well as contacting of single molecules.

O 53.8 Wed 17:00 MA 043

A new approach to Electron Beam Chemical Lithography — •Nirmalya Ballav, Sören Schilp, and Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

We present a new lithographic technique - electron beam chemical lithography (EBCL) with aliphatic self-assembled monolayers (SAMs) as resist materials. The technique is based on irradiation-promoted exchange reaction (IPER). The key idea of the IPER approach is tuning the extent of the exchange-reaction between a SAM covering the substrate and a potential molecular substituent by electron irradiation, which allows to get binary mixed SAMs of variable composition depending on the dose. Since the irradiation can be performed by a focused electron beam, IPER can be directly implemented into the lithographic framework and used for the fabrication of different chemical pattern on micro- and nanometer length scales. We demonstrated a feasibility of such approach by the preparation of chemical templates for the surface-induced polymerization (SIP) of the test polymer poly-N-isopropylacrylamide. Using these templates, we fabricated polymer micro- and nanobrushes in a broad height range. The advantages of EBCL-IPER are (i) the use of commercially available aliphatic compounds; (ii) a broad variety of different chemical patterns; and (iii) much lower patterning dose as compared to aromatic resists used before for EBCL. The approach is not limited by SIP, but can be used for different applications, relying on chemical patterning, e.g. biomedical studies and sensor fabrication.

O 53.9 Wed 17:15 MA 043

Lithographic Fabrication of Clean Oxidic Nanostructures by Means of Electron-Beam Induced Deposition (EBID) — •Michael Schirmer, Thomas Lukasczyk, Florian Vollnhals, Miriam Schwarz, Hans-Peter Steinrück, and Hubertus Marbach — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstraße 3, D-91058 Erlangen, Germany

In this contribution we present a route to generate iron oxide and titanium oxide nanostructures on different surfaces. The method we use is electron-beam induced deposition (EBID) in ultra high vacuum (UHV). Hereby, the beam of a high resolution UHV scanning electron microscope (SEM, spot size < 3 nm) is exploited to locally crack certain precursor molecules resulting in a deposit of the non volatile fragments. Two pathways to generate oxidic nanostructures are explored: (a) the selective oxidation of clean metallic EBID nanostructures (FeO_x on Rh(110)); (b) the direct EBID deposition of oxide structures (TiO_x on Si(001)) using a metal- and oxygen-containing precursor molecule. The latter approach leads to deposits, which contain large amounts of carbon from the precursor molecule titanium (IV) isopropoxide. Postannealing while dosing oxygen leads to the formation of clean TiO_x nanocrystallites as verified by local Auger spectroscopy. The growth of the crystallites can be observed in situ by means of SEM. Latest results and the perspective of this method will be discussed. This work was supported by the Deutsche Forschungsgemeinschaft under grant MA 4246/1-1.

O 53.10 Wed 17:30 MA 043

Fabrication of Clean Iron Nanostructures with Arbitrary Shape via an Electron-Beam Induced Process — •Thomas Lukasczyk, Michael Schirmer, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058 Erlangen

The generation of pure metallic nanostructures with arbitrary shape is still a fundamental challenge in the fast growing field of nano science. Our approach is the technique of electron-beam induced deposition (EBID) in ultra high vacuum (UHV), in which a highly focused spot of electrons is utilized to locally crack adsorbed precursor molecules, resulting in the deposition of non-volatile fragments. An electron-column, integrated in an UHV-Chamber, in combination with a lithographic package enables the controlled fabrication of nanostructures, which can be characterized via scanning electron microscopy, scanning tunneling microscopy and Auger electron spectroscopy. The precursor iron pentacarbonyl ($Fe(CO)_5$) proved to be very effective for the generation of pure iron structures on silicon and rhodium single crystal surfaces. For both substrates the deposits are composed almost completely of iron. Interestingly, on Si(100), the deposited nanostructures are discontinuous in shape, consisting of pure iron dots smaller than 10 nm. The deposit purity and appearance is greatly influenced by the substrate temperature and the surface condition. Furthermore, it will be discussed that UHV is mandatory to achieve pure metallic deposits. This work was supported by the Deutsche Forschungsgemeinschaft under grant MA 4246/1-1.

O 53.11 Wed 17:45 MA 043

Surface nano-patterns with high structural regularity, tunable properties, and diverse applications — •Yong Lei and Gerhard Wilde — Institut für Materialphysik, Universität Münster

Ordered arrays of surface nanostructures (nanodots and nanoholes) and free-standing one-dimensional nanostructures (nanotubes and nanowires) were fabricated on flat substrates using an UTAM (ultra-thin alumina mask) surface nano-patterning technique. The nanodot and nanohole arrays were prepared using vacuum evaporation processes and focused-ion-beam etching, respectively, while the nanowire and nanotube arrays were prepared using electrochemical processes and CVD processes. The structural parameters (size, spacing, and shape) of the UTAM-fabricated surface nanostructures can be adjusted by controlling the pore size of the UTAMs. The advantages of the UTAM surface nano-patterning, such as the achievement of tunable structural parameters and properties, large pattern area, high throughput and low equipment costs, make the technique suitable for fabricating ordered surface nanostructures with a broad range of applications ranging from optical, sensing, and electronics devices.

References: 1. Y. Lei, W.P. Cai, G. Wilde, Prog. Mater. Sci., 52 (2007) 465-539. 2. Y. Lei, Z. Jiao, M.H. Wu, G. Wilde, Adv. Eng. Mater., 9 (2007) 343-348. 3. Y. Lei, et al., Chem. Mater., 17 (2005) 580-585. 4. Y. Lei, W.K. Chim, H.P. Sun, G. Wilde, Appl. Phy. Lett., 86 (2005) 103106. 5. Y. Lei, W.K. Chim, J. Weissmuller, G. Wilde, et al., Nanotechnology, 16 (2005) 1892-1898. 6. Z. Chen, Y. Lei, et al., J. Cryst. Growth, 268 (2004) 560-563.

O 53.12 Wed 18:00 MA 043

Ordered nanomasks on Si and SiO_2 surfaces for the preparation of templates on the nanoscale — •Alfred Plettl, Marc Saitner, Fabian Enderle, Achim Manzke, Christian Pfahler, and Paul Ziemann — Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm, Germany

Periodically ordered nanomasks are generated by a micellar technique [1], a miniemulsion technique [2] and an extension of a well known colloidal patterning method (Fischer pattern) to the sub100 nm regime by a new isotropic plasma etching procedure. For template preparation an ICP-RIE plasma etcher is used subsequently. CF_4/CHF_3-gas mixtures were applied for manipulation of Si [3] and SiO_2 surfaces. The order of the masks is transferred into arrays of pillars or holes from the sub10 nm scale to standard subμm scale with aspect ratios of about 10 for the smallest structures. Combining these unconventional lithography techniques with the conventional electron beam lithography offers the possibility for nonperiodic arrangements. Some examples of application will be given.

[1] G. Kästle et al., Adv. Funct.Mat. 13, 853 (2003).
[2] A. Manzke et al., Adv. Mater. 19, 1337 (2007).
[3] S. Brieger et al., Nanotechnology 17, 4991 (2006).

O 53.13 Wed 18:15 MA 043

Self-organized nano-patterning of solid surface: dependence on the target material — •Olga Varlamova[1,2], Guobin Jia[2],

and Juergen Reif[1,2] — [1]LS Experimentalphysik II, BTU Cottbus, Konrad-Wachsmann-Allee 1, 03046 Cottbus — [2]IHP/BTU Joint-Lab, Konrad-Wachsmann-Allee 1, 03046 Cottbus

Self-organized surface patterns (ripples) were induced on different materials (dielectrics, semiconductors, metals and amorphous silica)by femtosecond laser irradiation with intensity below the single-shot damage threshold. In all cases, the dependence on characteristic features like irradiation dose and laser polarization was studied in our experiments. It is shown, that general features of the surface patterns do not depend on the type of material, nor was any correlation to the atomic structure of the irradiated surface detected. Instead, in all materials a similarly strong correlation between polarization direction of the laser beam and the orientation of the ripples is observed. The main difference between the different targets, however, is the intensity dependence of typical feature sizes and a specific window of irradiation dose for each material to produce surface nano-pattering.

O 54: SYSA: Tayloring Organic Interfaces: Molecular Structures and Applications VII (Invited Speaker: Stephan Roth; FV: DS+CPP+HL+O)

Time: Wednesday 17:45–19:30 Location: H 2013

See SYSA for details about the program.

O 55: Poster Session III - MA 141/144 (Methods: Atomic and Electronic Structure; Particles and Clusters; Heterogeneous Catalysis; Semiconductor Substrates: Epitaxy and Growth+Adsorption+Clean Surfaces+Solid-Liquid Interfaces; Oxides and Insulators: Solid-Liquid Interfaces+Epitaxy and Growth; Phase Transitions; Metal Substrates: Adsorption of Inorganic Molecules+Epitaxy and Growth; Surface Chemical Reactions; Bimetallic Nanosystems: Tuning Physical and Chemical Properties; Oxides and insulators: Adsorption; Organic, polymeric, biomolecular films; etc.)

Time: Wednesday 18:30–19:30 Location: Poster F

O 55.1 Wed 18:30 Poster F

Lagrange Functions for Electronic Structure Calculations — •Christine Broelemann, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, WWU Münster

We have examined the efficiency of Lagrange functions, as compared to plane waves, for calculating electronic properties of atoms, molecules, solids and surfaces within density functional theory. Real space Lagrange functions provide – like plane waves – an orthonormal and complete basis set. Our results show that the efficiency of both methods is the same for bulk calculations. In contrast to the plane wave method, however, it is possible within the Lagrange function method to conveniently adapt the real space grid for a given system. Taking advantage of this fact, the number of grid points can be reduced in vacuum regions, in particular. Lagrange functions can be used for periodic as well as for finite systems alike. It turns out that they are particularly useful for electronic structure calculations of charged systems. Problems occuring within the plane wave method due to long-range Coulomb interactions can be avoided that way.

O 55.2 Wed 18:30 Poster F

Combined direct and inverse photoemission experiment: A thorough characterization of energy, angle and spin resolution — •Michael Budke, Tobias Allmers, and Markus Donath — Physikalisches Institut, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

We present an experimental setup that combines spin- and angle-resolved direct (PE) and inverse photoemission (IPE) in one UHV chamber [1], allowing measurements of the spin-resolved electronic structure below and above the Fermi level of the same sample preparation. The system for PE operates with a gas discharge lamp and an electron analyzer combined with a SPLEED detector. Our spectrometer for IPE [2] is home-made and comprises a spin-polarized electron source and energy-selective Geiger-Müller counters for photon detection. The achievable energy resolutions are better than 50 meV for PE and better than 200 meV for IPE. The latter value states an improvement of a factor of two compared to other state-of-the-art IPE spectrometers. The high energy resolution makes the setup especially suitable for studies in the close vincinity of the Fermi level.

In this contribution, the two spectrometers are characterized concerning energy and angle resolution by means of the Fermi-level crossing of the L-gap surface state on Cu(111). Spin-resolved measurements of Co/Cu(100) will be presented combined with a characterization of the spin polarization of the electron beam and the Sherman function of the SPLEED detector. [1] M. Budke *et al.*, RSI **78**, (in press). [2] M. Budke *et al.*, RSI **78**, 083903 (2007).

O 55.3 Wed 18:30 Poster F

Two-photon Photoemission spectroscopy of the clean and alkali-doped 1T-TiSe$_2$ transition-metal dichalcogenide — •Martin Wiesenmayer, Jens Buck, Timm Rohwer, Kai Rossnagel, Lutz Kipp, and Michael Bauer — Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24098 Kiel, Germany

The transition-metal dichalcogenide 1T-TiSe$_2$ has attracted considerable attention in the recent past due to a structural phase transition at $T \approx 200$ K accompanied by the formation of a charge density wave (CDW) state. In a two-photon photoemission (2PPE) study we investigated the electron excitation spectra of these two phases in the vicinity of the Γ point of the Brillouin zone and their modification due to the adsorption and intercalation of different alkali species. We are able to identify a characteristic excitation band as well as phase- and intercalation specific modifications in the vicinity of the Fermi edge. Our experiments are furthermore supported by time-resolved 2PPE measurements addressing the ultrafast decay dynamics of the electron excitations. Our results will be discussed under consideration of corresponding results from past photoemission and inverse photoemission studies.

O 55.4 Wed 18:30 Poster F

Atomically Resolved Kelvin Probe Force Microscopy Measurements Analysed by a nc-AFM simulator — •Thilo Glatzel[1] and Laurent Nony[2] — [1]Department of Physics, University of Basel, Klingelbergstr. 82, 4056 Basel, Switzerland — [2]L2MP, UMR CNRS 6137, Univ. d'Aix-Marseille III, 13397 Marseille Cedex 20, France

Amplitude-Modulation Kelvin probe force microscopy (AM-KPFM) experiments have shown frequently atomically resolved contact potential difference (CPD) images. In this work, we report numerical investigations performed with a modified scheme of our nc-AFM simulator [1], with the goal to address the origin of such a contrast.

For that purpose, the core of our simulator has been modified to mimic the AM-KPFM setup. In AM-KPFM, the bias voltage that is applied between the tip and the surface is modulated at a frequency that matches the one of the second eigenmode of the cantilever. The long-range, short-range and electrostatic forces used to describe the system are derived from analytical expressions. The coupling between the first and the second eigenmodes of the cantilever will also be discussed.

Our results reproduce the experimental observations, thus showing that atomic variations of the CPD that are observed experimentally very likely reveal the atomic variations of the electrostatic potential at the surface of the ionic crystal.

[1] L. Nony et al., Phys Rev B 74, 235439 (2006).

O 55.5 Wed 18:30 Poster F

Photoelectron Spectroscopy at FLASH: Limits and Perspectives — •Martin Marczynski-Bühlow, Matthias Kalläne, Stefan Hellmann, Sabrina Lang, Claas Thede, Tim Riedel, Sönke Harm, Kai Rossnagel, and Lutz Kipp — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098

The Free Electron Laser in Hamburg (FLASH) produces very brilliant, ultrashort, and coherent photon pulses in the VUV regime.

Employing high-intensity monochromatic VUV–pulses ($h\nu = 115.5$ eV, FEL 3^{rd} harmonic) delivered by the PG2 beamline of FLASH we performed angle resolved as well as core–level photoelectron spectroscopy (PES) on the transition metal dichalcogenide 1T–TaS$_2$ in the Mott insulating phase (T = 140 K). For high photon intensities strong space charge (SCE) effects have been observed. To determine the limit where PES is still feasible, the measurements are compared with simulations of SCEs based on the Barnes & Hut Treecode Algorithm originally developed for simulating planetary movements. Furthermore, the perspectives of PES with FEL light in terms of time-resolved pump-probe experiments, spatially and angularly resolved PES with photon sieves [1], and the influence of high photon intensities on the momentum resolved electronic structure as well as on the photoemission process itself will be illustrated.

This work is supported by the Innovationsfond des Landes Schleswig-Holstein.

[1] L. Kipp, M. Skibowski, R. L. Johnson, R. Berndt, R. Adelung, S. Harm and R. Seemann, Nature 414, 184 (2001).

O 55.6 Wed 18:30 Poster F

Electronic structure of the non-polar GaN(1$\bar{1}$00) surface — •Marco Bertelli[1], Peter Löptien[1], Jörg Malindretos[1], Martin Wenderoth[1], Rainer G. Ulbrich[1], Angela Rizzi[1], Maria Clelia Righi[2], and Alessandra Catellani[2,3] — [1]IV. Physikalisches Institut and Virtual Institute of Spin Electronics (VISel), Georg-August Universität Göttingen, D-37077 Göttingen, Germany — [2]CNR-INFM National Center on nanoStructures and bioSystems at Surfaces (S^3) and Dipartimento di Fisica, Università di Modena e Reggio Emilia, I-41100 Modena, Italy — [3]CNR-IMEM, Parco Area delle Scienze, 37A, I-43010 Parma, and (S^3), Italy

Cross-section scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) have been performed on the non-polar GaN(1$\bar{1}$00) surface (m-plane).

The unintentionally n-doped GaN(0001) samples were thinned down to $\sim 100\ \mu m$, cleaved along the m-plane in ultra high vacuum and measured in-situ by STM at room temperature. The experimental empty state topographies collected with sample bias from +2.9 V to +4.0 V show an unreconstructed surface.

First principle DFT-LDA calculations of the surface electronic properties were performed. In agreement with experiment, the calculations predict a relaxed surface but no reconstruction. Two surface bands appear inside the semiconductor band gap at the borders of the surface Brillouin zone, one empty band localized on the Ga-atoms and one filled band on the N-atoms. Up to now this theoretical prediction has not been confirmed by the STS experiment.

O 55.7 Wed 18:30 Poster F

Electronic structure of transition metal dichalcogenide misfit compounds — •Matthias Kalläne, Kai Rossnagel, and Lutz Kipp — Institute for Experimental and Applied Physics, University of Kiel, D-24098 Kiel, Germany

The incommensurate layered transition metal dichalcogenide (TMDC) misfit compounds are composed of alternatingly stacked slabs of hexagonally ordered TMDCs and cubic monochalcogenides, leading to a lattice mismatch in one direction parallel to the surface. In spite of the incommensurability, however, the slabs are in a very high stacking order perpendicular to the layers and the crystals show a high stability. In order to investigate the bonding perpendicular to the layers and the influence of the incommensurability on the electronic structure we have employed angle–resolved photoelectron spectroscopy on different TMDC misfit compounds. By studying the electronic structure at the Fermi surface, we could directly observe a charge transfer to the TMDC layers, while the electronic band dispersion perpendicular to the layers was found to be negligible. Therefore, the interlayer bonding seems to be dominated by ionic contributions, similar to intercalated TMDC compounds. To reveal possible incommensurability effects we have analyzed the band dispersion in different crystal directions and have found signatures of both subsystems in the electronic structure.

The photoemission experiments were carried out at the ALS in Berkeley. Work at the University of Kiel is supported by DFG Forschergruppe FOR 353.

O 55.8 Wed 18:30 Poster F

Plasma Electrochemistry in Ionic Liquids: Deposition of Copper-Nanoparticles — •Mareike Brettholle[1], Oliver Höfft[1], Sebastian Mathes[2], Sherif Zein El Abedin[1], and Frank Endres[1] — [1]Institut für Metallurgie, TU Clausthal, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Physik und Physikalische Technologien, TU Clausthal, 38678 Clausthal-Zellerfeld, Germany

Ionic liquids 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 their low vapour pressure low pressure plasmas can easily be applied. The idea is to use the free electrons of the plasma to reduce the dissolved metal atoms in the liquid and generate this way the metal particles. In ionic liquids this principle was utilized recently by Meiss et al. [2]. Here we present our results using an argon plasma as electrode for the electrochemical deposition of copper nanoparticles (5-100 nm) from a Cu solution in 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide [BMP]Tf2N and 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide [EMIm]Tf2N. XPS, REM, EDX and Dynamic light scattering (DLS) were used to characterise the particles. [1] F. Endres, S. Zein El Abedin , Phys. Chem. Chem. Phys., 8 (2006) 2101; [2] S. A. Meiss, M. Rohnke, L. Kienle, S. Zein El Abedin, F. Endres and Jürgen Janek, Chem. Phys. Chem., 8 (2007) 50

O 55.9 Wed 18:30 Poster F

Fluorescence in the presence of metallic nanoparticles — •Philipp Reichenbach, Thomas Härtling, and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany

When fluorescent molecules (being excited by incident light) are placed in the neighbourhood of metallic nanoparticles, big changes of the observed fluorescence rate can occur. On the one hand, the excitation of the molecule can be strongly enhanced as a result of the scattering of the exciting light at the nanoparticle. On the other hand, part of the fluorescent radiation will be absorbed by the nanoparticle. The dependence of these two factors from the system parameters like excitation wavelength, relative position of molecule and particle as well as surrounding medium was investigated. As a result, we are able to clearly identify set-ups for which enhanced fluorescence microscopy/spectroscopy becomes feasible.

O 55.10 Wed 18:30 Poster F

***Ab initio* study on electronic and optical properties of silicon nanocrystals embedded in SiO$_2$ matrices** — •Kaori Seino[1], Friedhelm Bechstedt[1], and Peter Kroll[2] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Jena, Germany — [2]Department of Chemistry and Biochemistry, University of Texas at Arlington, Arlington, TX, USA

Although a high control of size and arrangement of Si nanocrystals (NCs) embedded in a SiO$_2$ can be obtained experimentally, theoretical works for Si NCs embedded in SiO$_2$ are limited. We study electronic and optical properties for Si NCs embedded in an amorphous SiO$_2$ matrix by means of first-principles calculations. Many theoretical results are available for hydrogenated Si NCs. We investigate the dependence on the diameter of the Si NCs, varying in the range from 0.8 to 1.6 nm. The calculations for optical properties have been widely performed within the independent-particle approximation. The results for Si NCs embedded in SiO$_2$ are compared with the corresponding results for hydrogenated Si NCs of the same size. The electronic confinement effects are much reduced with respect to crystallites without host. The optical absorption spectra show a pronounced peak somewhat blueshifted to the bulk E_2 peak similarly to measured spectra. We extract dielectric functions of the NC material from the calculated spectra using different effective-medium theories.

O 55.11 Wed 18:30 Poster F

W$_n$S$_m$-Clusters: Possible Building Blocks for New Nano-Materials? — Wilko Westhäuser[1], •Tobias Mangler[1], Tim

Fischer[1], Sibylle Gemming[2], Gotthard Seifert[2], and Gerd Ganteför[1] — [1]University of Konstanz, Germany — [2]University of Dresden, Germany

Since bulk WS$_2$ forms layered structures similar to bulk graphite, this material might also built up stable cage-like fullerene structures. Large graphite-like structures (multiwall fullerenes, nanotubes) have been found in TEM experiments, but so far no anorganic fullerenes have been detected in the size regime of C$_{60}$. Thus, we started a search for WS$_2$ fullerenes by combining gas phase and deposition experiments. In the gas phase, we identified a variety of different structures (nanowires, nanoplatelets) in the size regime up to 30 metal atoms [1-3].

To investigate the suitability as building blocks, in a first attempt small size-selected W$_n$S$_m$-clusters were soft-landed on Ag- and Si-substrates at ultrahigh vacuum conditions. These samples were analysed via HREELS and XPS. The HREELS spectra are different for the different cluster sizes indicating that these clusters survived the soft-landing on the substrate and do not coalesce to bulk-like structures.

[1] S. Gemming, J. Tamuliene, G. Seifert, N. Bertram, Y.D. Kim and G. Ganteför, Appl. Phys. 82, 161 (2006)

[2] N. Bertram, Y.D. Kim, G. Ganteför, Q. Sun, P. Jena, J. Tamuliene and G. Seifert, Chem. Phys. Lett. 396, 341 (2004)

[3] N. Bertram, J. Cordes, Y.D. Kim, G. Ganteför, S. Gemming and G. Seifert, Chem. Phys. Lett. 418, 36 (2006)

O 55.12 Wed 18:30 Poster F

Crystal structure of transition metal oxide nano particles synthesized form ferritin — •Michael Krispin, Florian Sedlmeir, Aladin Ullrich, and Siegfried Horn — Lehrstuhl für Experimentalphysik II, Universität Augsburg, D-86135 Augsburg

We have investigated the local crystal structure of nanosized transition metal oxides by extended x-ray absorption fine structure (EXAFS). Iron and cobalt oxide nanoparticles of different diameters were produced by thermal treatment of horse spleen ferritin molecules and remineralized apo-ferritin molecules, respectively. The structure of these particles was compared to various iron oxide and ferrihydrite references as well as cobalt oxide references. The Fourier transformed (FT) EXAFS spectra of the iron oxide nanoparticles differ significantly from hematite and maghemite reference spectra and change systematically as a function of particle diameter, signalling a corresponding evolution of the structure. A possible explanation therefore is the mixture of hematite and magehmite phases in a core-shell model, in which the fraction of a γ-Fe$_2$O$_3$ like particle shell increases while the hematite core decreases with decreasing particle size. In the case of cobalt oxide nanoparticles we find good agreement of the FT EXAFS spectra to the Co$_3$O$_4$ reference.

O 55.13 Wed 18:30 Poster F

Interaction of slow highly charged ions with surfaces — •Christian Haake, Thorsten Peters, Andreas Wucher, and Marika Schleberger — Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg, Germany

A new ion beam installation has been built to investigate the mechanisms of energy dissipation in a substrate after the impact of highly charged ions. First experiments at the TU Wien made successful use of metal-insulator-metal (MIM) junctions to measure electronic excitations in the irradiated metal [1]. These MIM-junctions offer the unique possibility to detect excitations below the work function which limits the external emission of electrons. In order to separate effects induced by either the kinetic or the potential energy of the projectile, both contributions need to be controlled independently. In the Vienna experiment the ions had medium charge states of q=1 up to to q=8 and kinetic energies of 400 eV to 12 keV. The new set-up offers higher charge states and is designed for kinetic energies of less than 100 eV/q. This will enable us to produce extremely slow highly charged ions. In addition, external electron emission as well as secondary and neutral mass spectrometry (SIMS/SNMS) will be used to follow the external pathways of energy dissipation.

[1] T. Peters, C. Haake, D. Diesing, D. Kovacs, A. Golczewski, G. Kowarik, F. Aumayr, A. Wucher and M. Schleberger, Hot electrons created by (rather) cold ions, submitted to Phys. Rev. Lett.

O 55.14 Wed 18:30 Poster F

Swift Heavy Ion (SHI) modification of Ag/Au-TiO$_2$ nanocomposite thin films prepared by co-sputtering. — Venkata Sai Kiran Chakravadhanula[1], Venkata Girish Kotnur[1], Amit Kulkarni[1], Yogendra Kumar Mishra[2], Devesh Kumar Avasthi[2], Dietmar Fink[3], Thomas Strunskus[1], •Vladimir Zaporojtchenko[1], and Franz Faupel[1] — [1]Chair for Multicomponent Materials, Institute for Materials Science, Christian-Albrechts University at Kiel, Kaiserstr. 2, Kiel, Germany, 24143. — [2]Inter University Accelerator Centre, New Delhi, India, 110067. — [3]Hahn Meitner Institut, Glienicker Str. 100, Berlin, Germany, 14109.

Ag-TiO$_2$ and Au-TiO$_2$ nanocomposites with different volume fractions of metal nanoparticles were prepared by co-sputtering. The morphology of these nanocomposites was investigated by transmission electron microscopy (TEM). Metal volume fractions were determined by SEM-EDX. Optical characterization of these nanocomposites was carried out using UV/Vis/NIR spectroscopy. The nanocomposites were then irradiated by Swift Heavy Ions (SHI) with 100 MeV (Ag^{8+} ions) at different fluences ranging from 1 X 10^{12} to 1 X 10^{13} ions/cm^2. The extinction spectra of the pristine samples show plasmon resonances at wavelengths which depend on the volume fraction of metal, particle size and morphology of the composites. The influence of the SHI fluences, on the microstructure and the extinction spectra were observed. The changes in the properties of these nanocomposites are discussed in terms of ion-material interactions.

O 55.15 Wed 18:30 Poster F

X-Ray Absorption (XAS) and Magnetic Circular Dichroism (XMCD) Measurements of Mn$_6$Cr Single-Molecule-Magnets Adsorbed on Various Surfaces — •Fabian Merschjohann[1], Aaron Gryzia[1], Armin Brechling[1], Marc D. Sacher[1], Ulrich Heinzmann[1], Maik Heidemeier[2], Thorsten Glaser[2], Sönke Voss[3], Mikhail Fonin[3], Michael Burgert[3], Ulrich Rüdiger[3], and Eberhard Goering[4] — [1]Dep. of Physics, Bielefeld University — [2]Dep. of Chemistry, Bielefeld University — [3]Dep. of Physics, Konstanz University — [4]MPI für Metallforschung, Stuttgart

We report on the electronic configuration of Mn$_6$Cr-Single-Molecule Magnets (SMM) adsorbed on various surfaces. We investigated the substrate/molecule interaction, in particular the exchange of the electrons with the substrate. The manganese atoms of the Mn$_6$Cr-SMM are trivalent. X-Ray absorption measurements at the Mn-L$_2$- and L$_3$-edge indicated a certain amount of divalent Mn-atoms. This suggests a reduction of the Mn$_6$Cr molecules due to an electron transfer to the substrate. This transfer depends on the electronic configuration of the substrate material. Thus we investigated Mn$_6$Cr-SMM adsorbed on insulating (SiO$_2$), metallic (Au) and semiconducting (Highly Ordered Pyrolytic Graphite HOPG) materials. To determine the fraction of Mn$^{\mathrm{II}}$- and Mn$^{\mathrm{III}}$-ions we calculated the measured spectral shape by using di- and trivalent reference spectra. We will also show XMCD measurements of the adsorbed SMM performed at BESSY in Berlin which reflect the expected magnetic configuration of Mn and Cr.

O 55.16 Wed 18:30 Poster F

STM-Study of clean ZnO surfaces and Cu growth on ZnO — •Kroll Martin, Kuschel Thomas, Löber Thomas, and Köhler Ulrich — Ruhr Universität Bochum, Experimentalphysik IV - AG Oberflächen, Bochum, Germany

STM was used to study the polar, zinc terminated ZnO(0001)-Zn surface, the polar, oxygen terminated ZnO(000$\bar{1}$)-O surface and the nonpolar, mixed terminated ZnO(10$\bar{1}$0) surface. The influence of atomic hydrogen and water present during different annealing procedures on the large scale morphology of flat and miscut surfaces was investigated. The morphology of the clean ZnO(0001)-Zn surface with characteristic triangular islands changes dramatically when water is present during annealing and on vicinal ZnO(10$\bar{1}$0) surfaces the regularity of the step train is crucially dependent on the preparation conditions.

Additionally the deposition of Cu using MBE and CVD on the zinc terminated surface were studied. The formation of (111)-orientated Cu-clusters at room-temperature is followed by in-situ applied STM. Kink-sites at step edges and especially the apexes of triangular ZnO-substrate terraces act as preferred nucleation sites. At room temperature the decay of small Cu-islands takes place on a time scale of minutes. Larger Cu-coverages lead to an ensemble of interconnected 3D-islands of uniform height separated by trenches down to the substrate. Further annealing up to 400 °C points to a partial entrenching of the islands into the oxide support and (or) an alloy formation.

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O 55.17 Wed 18:30 Poster F

Trends in Reactivity: Gold Catalysis — •Guido Walther[1], Søren Jensen[2], and Sebastian Horch[1] — [1]CAMD, Department of Physics, DTU, 2800 Lyngby, Denmark — [2]MIC, Department of Micro and Nanotechnology, DTU, 2800 Lyngby, Denmark

Gold, as the noblest of all the metals, becomes catalytically active for several chemical reactions, when its particle size is less than 5 nm. Beside the particle size, there are many other effects, which maybe contribute to the surprisingly high activity of gold nano-particles, like support and/or electronic effects. But it is still not understood in detail yet, what accounts for these unique properties of nano-sized gold.

In a new microreactor setup, CO and H_2 oxidation were studied on TiO_2 supported Au catalysts of various well defined particle sizes. The particle size was confirmed using TEM. To analyze the reaction products, the microreactor was interfaced to a gas chromatograph.

We show a trend in reactivity in catalysis by gold for these reactions. By switching the oxidation agent from O_2 to N_2O, an investigation whether the rate-limiting step is associated with O_2 or CO, was feasible. This gives an experimental indication that CO oxidation follows an alternative pathway via a CO–O_2 intermediate.

O 55.18 Wed 18:30 Poster F

Homogeneous and front-induced surface transformations during catalytic oxidation of ammonia over Pt(1 0 0) — •Florian Lovis[1], Matias Rafti[2], Yingfeng Zeng[1], and Ronald Imbihl[1] — [1]Institut für Physikalische Chemie und Elektrochemie, Leibniz-Universitat Hannover, Callinstr. 3-3a, D-30167 Hannover, Germany — [2]INIFTA, Dto. de Química, Fac. de Cs. Exactas, Universidad Nacional de La Plata, Diag. 113 y 64, CC 16 suc. 4, (1900) B1871DCR La Plata, Argentina

The ammonia + oxygen reaction over Pt(1 0 0) single-crystal surface was studied under UHV conditions using photoemission electron microscopy (PEEM) as spatially resolving method and work function measurements via a Kelvin probe and temperature programmed reaction (TPR) experiments as integral methods. A broad hysteresis in the reaction rates occurs and one finds reaction fronts as well as spatially homogeneous transitions in the adsorbate layer.

O 55.19 Wed 18:30 Poster F

Mass selected Ag cluster based catalysis: size and shape effects — •Kristian Sell[1], Ingo Barke[1], Viola von Oeynhausen[1], Karl-Heinz Meiwes-Broer[1], Stefan Vajda[2], Sungsik Lee[2], Yu Lei[2,3], Byongdu Lee[2], Jeffrey W. Elam[2], Michael J. Pellin[2], Sönke Seifert[2], Randall E. Winans[2], Randall J. Meyer[2], and Arantxa Fraile-Rodríguez[4] — [1]Universität Rostock, Institut für Physik, Rostock, Deutschland — [2]Argonne National Laboratory, Argonne, USA — [3]University of Illinois at Chicago, USA — [4]Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland

The exceptional performance of nanocatalysts has motivated intense research as highly dispersed nanocatalysts are widely used in commercial applications. Here we study size-selected silver particles under realistic conditions in a reaction of industrial relevance.

Supported size selected Ag clusters of sub-nm to several nm size are produced by laser evaporation and an arc charge ion source (ACIS) and deposited on Al2O3 supports. These are prepared by atomic layer deposition of thin Al2O3 films on the native silicon oxide surface of Si wafers. The catalytic properties of the supported clusters are studied under atmospheric pressure reaction conditions. We use a unique approach which allows for in situ, real-time monitoring of changes in size and shape of the nanocatalysts by grazing-incidence small-angle x-ray scattering (GISAXS) with simultaneous detection of the reaction products. The relationship between cluster size/shape and its function in catalytic activity and selectivity in direct epoxidation of propylene on Ag clusters will be discussed.

O 55.20 Wed 18:30 Poster F

Inverse Au/TiO_2 model catalysts studied with in-situ high-pressure XPS — •Dumbuya Karifala, Lucasczyk Thomas, Schirmer Michael, Marbach Hubertus, Gottfried Michael, and Steinrück Hans-Peter — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg

We have prepared and investigated planar inverse TiO_2/Au model catalysts using XPS and SEM. In addition, we have studied the surface composition and the electronic structure in the presence of CO and O_2 at pressures of up to 1 mbar using high-pressure XPS. The model systems have been prepared and characterized on a polycrystalline Au foil and on an Au(111) surface. Initially, we used a recipe reported by Biener et al.[1] and prepared the TiO_2 clusters by vapor deposition of Ti on the Au surfaces at 300 K, followed by oxidation with O_2 at 300 K and annealing at 600-900 K in vacuum. We found that part of the deposited Ti forms an Au-Ti alloy during this procedure. To prevent alloying, we have developed a modified procedure in which the TiO_2 clusters are annealed in an O_2 atmosphere. SEM images of the nanoparticles on Au foil show a particle size distribution in the 10 nm range for an initial Ti coverage of 0.25 ML. At high coverages, exposure to CO and O_2 did not reveal significant changes in the oxidation states of either Au or Ti, probably because of a buried TiO_2/Au interface. In contrast, at lower TiO_2 coverages (initial Ti coverage 0.25 ML) and CO pressures above 0.1 mbar, the in-situ XP spectra show changes that are attributed to the interaction between CO and Ti. 1. Biener et al.

O 55.21 Wed 18:30 Poster F

The chemical state of iron during N_2O decomposition over iron modified zeolites ZSM-5: A high-pressure XPS study — •Karifala Dumbuya[1], Saiprasath Gopalakrishnan[2], Wilhelm Schwieger[2], J. Michael Gottfried[1], and Hans-Peter Steinrück[1] — [1]Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II — [2]Universität Erlangen-Nürnberg, Lehrstuhl für Chemische Reaktionstechnik

Iron containing ZSM-5 zeolites are employed as catalysts for the abatement of N_2O in waste gases and in partial oxidation reactions with N_2O as the oxidant. The chemical state of the active Fe centers during reaction is unknown; however, it has been speculated that an α-Fe(II) species is the active site.[1] NaOH-treatment increases the activity, which has been attributed to the alteration of the Fe centers.[2] We have studied commercial ZSM-5 (as-supplied and NaOH-treated) using XPS and in-situ XPS during N_2O exposure (pressure $\leq$ 1 mbar). No Fe was found in the surface region of the commercial ZSM-5 before or after ion-exchange with NaOH, contrary to ICP-AES results. As expected, significant amounts of Fe (mainly in the +2 and +3 oxidation states) were detectable with XPS, following Fe doping of both catalysts. The Fe content in the surface region of the NaOH-modified ZSM-5 did not change with temperature (300-650 K), while the as-supplied sample showed Fe segregation in this temperature range. Details about the electronic state of Fe in the Fe doped, NaOH-modified catalyst in the presence of N_2O ($5*10^{-8}$ - 1 mbar) will be discussed. [1] Dubkov et al., J. Catal. 207 (2002) 341. [2] Groen et al., J. Catal. 243 (2006) 212.

O 55.22 Wed 18:30 Poster F

Silver, oxygen and hydrogen deposited on the Bi terminated prestructured Si/Ge surface — •Vasily Cherepanov and Bert Voigtländer — Institute of Bio- and Nanosystems (IBN 3), and cni – Center of Nanoelectronic Systems for Information Technology, Research Centre Jülich, 52425 Jülich, Germany

Si-Ge based nanostructures like wires or dots are attractive objects since they are compatible with an existing silicon technology. The similar nature of Si and Ge allows to grow epitaxial Si/Ge nanostructures using a surfactant like Bi to suppress Si-Ge intermixing. A well ordered array of 2-3 nm wide and atomic layer in heigh Ge nanowires can be formed in a controlled way at Si(111) substrate. However to utilize the electrical properties of those structures one would need to increase the difference in the electrical properties of the wires and the substrate. The Si/Ge structures thus can be used as templates for a next step of selforganized growth of different material which selectively bonds to Si or Ge. The challenge is to find a material which at some condition would stick or interact selectively to Si or Ge. We made an attempt to explore a possible chemical selectivity for Si and Ge surface. The Bi covered surface contained Si and Ge areas was exposed to flux of silver, oxygen and atomic hydrogen at various conditions. The resulting surface structure was examined by scaning tunneling microscopy.

O 55.23 Wed 18:30 Poster F

Surface Characterisation of MOCVD Single Source Precursor Grown GaSb-films — •Andreas Seemayer[1], Alexander Hommes[1], Sascha Hümann[1], Ralf Hunger[2], Stephan Schulz[3], and Klaus Wandelt[1] — [1]University of Bonn, Institute for Physical Chemistry, Wegelerstr. 12, 53115 Bonn — [2]Hahn-Meitner-Institute Berlin GmbH c/o BESSY, Albert-Einstein-Str. 15, 12489 Berlin — [3]University of Paderborn, Department Chemie, Warburger Str. 100, 33098 Paderborn

III-V semiconductor films used for opto- and microelectronic devices have traditionally been grown by (MO)MBE and LPE processes. An alternative metal-organic CVD-process, which has been established in the last two decades for high-throughput and low-cost fabrication works for nitrides, phosphides and arsenides, but is problematic for antimonides. In particular, for GaSb films an alternative route is a CVD-process using the heterocyclic single source precursor $[tBu_2GaSbEt_2]_2$.

Subject of the present work is the investigation of the surface physical properties of the produced films as well as the gas phase behaviour of the used precursor. Therefore films were produced on a Si(100) substrate in a HV-MOCVD reactor and investigated using AES, S-XPS and AFM. In addition, growth experiments under UHV conditions were performed. The results are discussed in terms of a correlation of the electronic properties with the composition and structure of the films.

O 55.24 Wed 18:30 Poster F

Growth of large laser deposited Cu-pyramides on Si at raised temperatures — •Susanne Seyffarth and Hans-Ulrich Krebs — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Thin Cu films were prepared on Si(111) and Si(100) substrates using pulsed laser deposition (PLD) in ultra high vacuum. Especially the effect of elevated substrate temperatures on the growth of Cu on Si was investigated. While for low substrate temperatures closed films with small grains are observed, for temperatures above 200 °C epitaxial growth of three dimensional pyramides with edge lengths of a few micrometers is observed using scanning electron microscopy (SEM) and atomic force microscopy (AFM). Depending on the orientation of the substrate the base area of the islands is a triangle for Si(111) and a square for Si(100). In both cases the height of the pyramides is up to 500 nm. The epitaxial relationships with the Si substrates, the dependences of the pyramidal sizes on the number of laser pulses, the stability of the structures and possibilities for an ordering of the islands are discussed.

O 55.25 Wed 18:30 Poster F

Magnetic and structural investigations of thin iron layers on GaAs(001) and GaAs(110) surfaces with and without an MgO intermediate layer — •Carsten Godde[1], Sani Noor[1], Christian Urban[1], Igor Barsukov[2], Jürgen Lindner[2], and Ulrich Köhler[1] — [1]Institut für Experimentalphysik IV/ AG Oberflächen, Ruhr-Universität Bochum, Germany — [2]Institut für Experimentalphysik / Festkörperphysik, Universität Duisburg / Essen, Germany

The structure and the magnetic behaviour of Fe-layers on GaAs(001) and GaAs(110) were studied in a UHV system that offers the means for structural analysis by STM and LEED and magnetic characterization by MOKE during deposition. The preparation of the GaAs(001) and GaAs(110) polished wafer surfaces consisted of cycles of sputtering and annealing, in the case of the cleaved GaAs(110) surface no in situ preparation was necessary. On all samples the structure of the Fe-layer when grown at 20°C is strongly influenced by the substrate morphology. At elevated growth temperature a disrupted Fe-layer develops. Using MgO as an intermediate layer the structural quality is substantially reduced. The uniaxial anisotropy of Fe on GaAs(110) surfaces is profoundly influenced by the MgO intermediate layer. The effect of annealing up to 500°C on the structure and the magnetic behaviour were studied. Although smooth layers with large islands develop, STM shows that Ga and As from the substrate diffuse to the Fe-island top. On GaAs(001) the substrate reconstruction changes from an initially present (2x6) to a As-rich (2x4).

O 55.26 Wed 18:30 Poster F

Magnetic in situ characterization by MOKE and Kerr microscopy — •Sani Noor, Carsten Godde, Christian Urban, and Ulrich Köhler — Institut für Experimentalphysik IV, AG Oberflächen, Ruhr-Universität Bochum, Germany

A UHV system is being introduced that offers both the structural analysis by LEED and STM and the magnetic analysis by MOKE and Kerr microscopy of thin films. These can be grown by sets of MBE sources that are pointing at the sample in the STM, MOKE and Kerr microscopy positions allowing in situ measurements respectively. Our focus here shall be the magnetic characterization. The combination of a longitudinal MOKE setup and polar Kerr microscopy, which is based on a long distance microscope, enables the recording of magnetization loops for in and out of plane magnetization. The former provides angular dependent measurements by azimuthal rotation of the sample, the latter can be obtained by spatial integration of the acquired Kerr images. Test measurements have been performed including the study of the anisotropic behaviour of Fe on InAs(001)(4x2) and the Kerr microscopy of FeGd ((0.5 nm Fe/0.5 nm Gd) x 70) multilayers which feature a strong out of plane anisotropy at room temperature as confirmed by SQUID measurements.

O 55.27 Wed 18:30 Poster F

STM and STS study of atomic and electronic structure of epitaxial graphene on SiC(0001) — Peter Lauffer[1], Konstantin V. Emtsev[1], Sergey Reshanov[2], Ralf Graupner[1], •Thomas Seyller[1], Gerhard Pensl[2], Heiko B. Weber[2], and Lothar Ley[1] — [1]Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Germany — [2]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Germany

Epitaxial growth of graphene on SiC surfaces by solid state graphitization is a promising route for future development of graphene based electronics. In the present work we have studied the morphology, atomic scale structure, and electronic structure of thin films of few-layer graphene on SiC(0001) by scanning tunneling microscopy (STM) and spectroscopy (STS). We discuss the determination of layer thickness based on atomically resolved images and show that such identification can be supported by evaluation of the roughness induced by the interface. We also present and interpret thickness dependent tunneling spectra, which can serve as an additional fingerprint for the determination of the layer thickness.

O 55.28 Wed 18:30 Poster F

Morphology of epitaxial graphene films on SiC(0001) determined by LEEM — Taisuke Ohta[1,2], Farid El Gabaly[3], Aaron Bostwick[1], Jessica L. McChesney[1], Konstantin V. Emtsev[4], Andreas K. Schmid[3], •Thomas Seyller[4], Karsten Horn[3], and Eli Rotenberg[1] — [1]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California, USA — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [3]National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, California, USA — [4]Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Germany

Epitaxial films of graphene on SiC surfaces are interesting from a basic physics as well as applications-oriented point of view. In the present work we use low-energy electron microscopy (LEEM) and angle-resolved photoemission (ARPES) to study the morphology of epitaxial graphene films grown on SiC(0001) by solid state graphitization in ultrahigh vacuum (UHV). Different layer thicknesses were witnessed by characteristic electron reflectivity spectra. After relating these to the thickness dependent π-band structure determined by ARPES it is possible to unambiguously assign regions in the LEEM images to the interfacial layer and single-layer as well as bilayer graphene. This information will aid the improvement of the morphology of large scale epitaxial graphene films through optimization of preparation conditions.

O 55.29 Wed 18:30 Poster F

Interface investigations for III-V solar cells — •Ulf Seidel, Henning Döscher, and Thomas Hannappel — Hahn-Meitner-Institut, Glienicker Str. 100, 14109 Berlin, Germany

III-V multi-junction solar cells currently represent the most efficient photovoltaic devices. The device structures of the tandem solar cells, which were prepared in this work via MOVPE, contain many different layers of III-V semiconductors. For the best performance of the solar cells a sharp hetero-interface preparation via MOVPE was necessary. Here, the investigation of two interfaces is presented in detail: (1) InGaAs/GaAsSb that is needed in the tunnel junction of our low band gap multi-junction solar cell and (2) Si/GaP that is needed for the epitaxy of our III-V solar cells on silicon(100) substrates instead of InP(100). Both interfaces were characterized in-situ during the MOVPE-growth with reflectance difference spectroscopy (RDS) and after a contamination free transfer in ultra high vacuum with X-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED). Additionally AFM micrographs were recorded.

O 55.30 Wed 18:30 Poster F

Resistance of a single atom: scattering of electrons by single adatoms and small islands during homoepitaxial growth of Bi(111) films — •Hichem Hattab, Giriraj Jnawali, Boris Krenzer, and Michael Horn-von Hoegen — Fachbereich Physik, Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

Atomically smooth Bi(111) films on Si(001) were prepared following a recipe of G. Jnawali et al. (PRB 74 , 195340 (2006)) and were used as template to study the resistivity change during additional growth of Bi at 80 K by using a 4-probe technique and SPA-LEED. At very low Bi coverage of less than 0.01 bilayer (BL) a linear increase of the film resistivity was observed which suddenly changes to a square root dependence up to 0.5 BL. This behaviour is explained by a combination of Venables nucleation theory and Fuchs-Sondheimer behaviour. At very low coverage each deposited Bi adatom acts as single scatterer, which ultimately scatters the conduction electrons diffusively. The linear increase of the resistivity is proportional to the density of adatoms. With increasing Bi adatom density suddenly stable 2-dim. islands nucleate, the adatom density drops, and the islands grow in size at constant island density. Now the electrons are scattered at the step edges which density increase as square root of the coverage. At higher coverage the resistivity shows a bilayer oscillation indicating the oscillation in roughness which is followed by a 1/d behavior described by Fuchs-Sondheimer. From the slopes of the two initial regimes the effective cross-section for diffuse scattering of a single Bi adatom and of a bilayer step edge is calculated.

O 55.31 Wed 18:30 Poster F

Laser Treatment of Stainless Steel — •Christian Holzheu, Matthias Laske, and Othmar Marti — Institute of Experimental Physics, University of Ulm, 89069 Ulm, Germany

Laser treatment of stainless steel and the resulting material changes are studied. By irradiating the steel surface with short laser pulses the adhesion of polymers and especially fluorinated polymers is improved. The experiments were designed to evaluate the influence of different laser parameters on adhesion, surface morphology and composition and on surface tension. Corrosion behaviour and the durability of the material after laser treatment in comparison to untreated samples are studied in long time tests. Salt fog and mechanical pulses are used to simulate nearly realistic conditions.

O 55.32 Wed 18:30 Poster F

STM studies of surface plasmon mediated laser annealing of gold films — •Markus Schmotz, Armin Fubel, and Paul Leiderer — Universität Konstanz, Konstanz, Germany

Using a Kretschmann configuration we illuminate thin polycrystalline gold films under the surface plasmon resonance angle. Thus, a frequency doubled Nd:YAG laser locally heats the films at different intensities. The investigation of structural changes of the gold surfaces is done in situ by a homebuilt STM. To gain quantitative information we study FFT-data (fast Fourier transformation) like PSD-spectra (power-spectrum-density) and autocorrelation functions beneath typical roughness parameters like RMS (root-mean-square) and MPP-values (mean-peak-to-peak). The influence of single and multi-shot treatment is also determined at higher and lower intensities, respectively.

Preliminary results show broadening and flattening of the typical gold mounds at low intensities and thus increasing correlation lengths and grain sizes. Reproducibility checks and analysis of detailed annealing mechanisms will be reported.

O 55.33 Wed 18:30 Poster F

Interfacial layering of room temperature ionic liquids based on the tris(pentafluoroethyl)trifluorophosphate anion at the sapphire interfaces — •Markus Mezger[1], Heiko Schröder[1], Sebastian Schramm[1], Harald Reichert[1], Sebastian Schöder[1], John Okasinski[1], Moshe Deutsch[2], Benjamin Ocko[3], Emerson De Souza[1], John Ralston[4], and Helmut Dosch[1] — [1]Max-Planck-Institut für Metallforschung, Stuttgart — [2]Bar-Ilan University, Ramat-Gan, Israel — [3]Brookhaven National Laboratory, Upton, NY, USA — [4]Ian Wark Research Institute, Adelaide, Australia

A new group of room temperature ionic liquids (RTIL) based on the tris(pentafluoroethyl)trifluorophosphate (FAP) anion reveals intriguing features in comparison to conventional molten salts. Especially the improved chemical and thermal stability make them interesting candidates for a variety of technological processes. Using high energy x-ray reflectivity we get access to deeply buried solid-liquid interfaces and gain real space information with Å-resolution. In this study, we discuss reflection patterns of FAP based ionic liquids, recorded at different temperatures ranging from the highly supercooled metastable liquid state to 120 °C. By parameter refinement of a two-component distorted-crystal model we disclose pronounced layering of the anions and cations close to the solid wall. With increasing temperature, the decay length of the interfacial ordering decreases.

O 55.34 Wed 18:30 Poster F

High energy x-ray reflectivity study of the room temperature ionic liquids [bmim]$^+$ [PF$_6$]$^-$ and [bmim]$^+$ [BF$_4$]$^-$ at solid interfaces — •Sebastian Schramm[1], Markus Mezger[1], Heiko Schröder[1], Harald Reichert[1], John Okasinski[1], Moshe Deutsch[2], Benjamin Ocko[3], Emerson De Souza[1], and Helmut Dosch[1] — [1]Max-Planck-Institut für Metallforschung, Stuttgart — [2]Bar-Ilan University, Ramat-Gan, Israel — [3]Brookhaven National Laboratory, Upton, NY, USA

Room temperature ionic liquids (RTILs), being composed solely of ions, are very promising new materials. Their physical properties make them suitable for many technological processes, e.g. as solvents in catalytic reactions and electrolysis. In particular for the understanding of reactions at an interface, knowledge on the spatial arrangement of the ions at hard walls is essential. In our study, we used high energy ($\sim$ 70 keV) x-ray reflectivity to probe the structure of these liquids at the sapphire interface. The results give evidence for interfacial layering in 1-butyl-3-methylimidazolium hexafluorophosphate ([bmim]$^+$ [PF$_6$]$^-$), in contrast to 1-butyl-3-methylimidazolium tetrafluoroborate ([bmim]$^+$ [BF$_4$]$^-$) where no layering was found. In combination with the analysis of the bulk liquid structure factor, the recorded reflection patterns give both the molecular layer spacing, as well as the decay length of the spatial ordering. We compare the x-ray scattering results with optically obtained surface and interfacial tension data to gain detailed information about the nature of the chemical interaction between the sapphire substrate and the ions of the RTIL.

O 55.35 Wed 18:30 Poster F

Post annealing investigations of thin praseodymia films on Si(111) — Sebastian Gevers, •Daniel Bruns, Thomas Weisemöller, Carsten Deiter, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Due to its large oxygen capacity and oxygen mobility praseodymia is interesting for applications in modern heterogenous catalysis. For instance the selectivity of praseodymia for carbon compounds is advantageous in olefiant gas synthesis. The investigation of annealing processes leads to a better understanding of the oxygen transport in the praseodymia films. In this context thin PrO2 films were annealed at temperatures from 300°C up to 600°C under UHV conditions before they were analysed with Spot Analysis Profile Low Electron Energy Diffraction (SPALEED). The diffraction pattern indicates a phase transition to Pr2o3 at the surface. Furthermore X-Ray Diffraction experiments (XRD) show a partial subsurface phase transition from PrO2 into various oxidation states including Pr2O3.

O 55.36 Wed 18:30 Poster F

Adsorption of benzene on the Si(001)-(2×1) and the SiC(001)-(3×2) surfaces – a comparative theoretical study — •Jürgen Wieferink, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster

We have investigated the adsorption of benzene (C$_6$H$_6$) on (001) surfaces of Si and SiC employing the generalized-gradient approximation of density functional theory together with norm-conserving pseudopotentials. Using the quadratic string method [1] we have explored reaction pathways to possible final adsorption states.

At Si(001)-(2×1), we find C$_6$H$_6$ to initially adsorb via electrophilic addition in a butterfly configuration by binding two opposite (1,4) carbon atoms to the silicon atoms of one surface dimer. The energetically most favorable tight-bridge structure can then be reached by the formation of two additional bonds between the (2,3) carbon atoms and an adjacent silicon dimer [2].

At SiC(001)-(3×2), the silicon dimers are further apart from each other. As a result, this surface cannot feature bridging geometries and is thus expected to generate an ordered monolayer of butterfly benzene, where each molecule exhibits two π-bonds that are available for further reactions. An energetically more favorable dissociated adsorption structure is also discussed and shown to be kinetically unreachable. Finally, the electronic structure of the optimized geometries is examined and discussed.

[1] S. K. Burger, W. Yang, J. Chem. Phys. **124**, 054109 (2006)
[2] J.-Y. Lee, J.-H. Cho, Phys. Rev. B **72**, 235317 (2005)

O 55.37 Wed 18:30 Poster F

Insulating Ground State of Sn/Si(111)-($\sqrt(3) \times \sqrt(3)$)R30° — •Silvio Modesti[1,2,3], Luca Petaccia[1,4], Gustavo Ceballos[1,5], Ivana Vobornik[1], Giancarlo Panaccione[1], Giorgio Rossi[1], Luca Ottaviano[6], Silvano Lizzit[4], and Andrea Goldoni[4] — [1]Laboratorio Nazionale TASC-INFM, S.S. 14 Km 163.5, 34012 Trieste, Italy — [2]Dipartimento di Fisica, Universita' di Trieste, v. Valerio 2

I-34127, Trieste, Italy — [3]Institut für Angewandte Physik, Universität Hamburg, Jungiusstr. 11, D-20355 Hamburg — [4]Sincrotrone Trieste S.C.p.A., S.S. 14 Km 163.5, 34012 Trieste, Italy — [5]ICN, UAB Campus, E-08193 Bellaterra (Barcelona), Spain — [6]Universita' dell'Aquila, via Vetoio 10, 67010 Coppito-L'Aquila, Italy

The Sn/Si(111)-($\sqrt{(3)} \times \sqrt{(3)}$)R30° surface, having an odd number of electrons per surface unit cell, was so far believed to be metallic according to the electron counting argument. One third of a monolayer of tin adatoms in the T4 site forms a narrow surface state band that is half filled, and therefore prone to structural and electronic instabilities. We show, by using tunneling spectroscopy, scanning tunneling microscopy, photoemission, and photoelectron diffraction, that below 70 K this surface has a very low density of states at the Fermi level and is not appreciably distorted [1]. The experimental results are compatible with the magnetic insulating Mott-Hubbard ground state predicted by LSDA + U calculations [2]

[1] S. Modesti, et al., Phys. Rev. Lett. 98, 126401 (2007) [2] G. Profeta and E. Tosatti, Phys. Rev. Lett. 98, 086401 (2007).

O 55.38 Wed 18:30 Poster F

First-Principles Investigation of an Epitaxial Silicon Oxynitride Layer on a 6H-SiC(0001) Surface — •Peter Krüger, Björn Baumeier, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster

Recently, Shirasawa et al. [1] have experimentally shown that incorporation of nitrogen at the interface of a silicate adlayer on 6H-SiC(0001) leads to the formation of a well ordered, highly stable epitaxial silicon oxynitride (SiON) layer without dangling bond states. Scanning tunneling spectroscopy data for this system show an amazingly large band gap of about 9 eV.

We have investigated the structural and electronic properties of this novel system by employing density functional theory with self-interaction-corrected pseudopotentials. Our results support the structural model inferred from low-energy electron data [1]. In addition, our calculated filled- and empty-state scanning tunneling microscopy images are in excellent agreement with the experimental data clearly revealing that the O and Si surface states, respectively, of the silicate double-layer on top of the system give rise to the observed images. The calculated surface band structure exhibits a surface band gap of 9 eV whose physical origin is clarifed. Further investigations show that SiON overlayers on 6H-SiC(0001) and 6H-SiC(000$\bar{1}$) have qualitatively different electronic structures. While the former is free from gap states, the latter possesses two N-derived states in the fundamental band gap.

[1] Shirasawa et al., Phys. Rev. Lett. **98**, 136105 (2007)

O 55.39 Wed 18:30 Poster F

Energy barriers for dissociative adsorption of H_2 molecules on Si, SiC, and diamond (001) surfaces: A comparison — •Xiangyang Peng[1], Peter Krüger[2], and Johannes Pollmann[2] — [1]Department of Physics, Uppsala University, SE-75121 Uppsala, Sweden — [2]Institut für Festkörpertheorie, Wilhelm-Klemm-Str. 10, 48149 Münster

We report first-principles investigations of the reaction of molecular hydrogen with the Si(001)-(2×1) and C(001)-(2×1) surfaces and discuss the results in light of our previous studies of H_2 reaction with two different SiC(001) surfaces, one of which is highly reactive to H_2 uptake. The calculations reveal that the reaction of H_2 with all above surfaces depends crucially on intricate combined effects of the substrate lattice constant, the arrangement of the surface dimers as well as the orientation and spatial extent of their dangling bond orbitals. In agreement with experiment, our results confirm that Si(001) and C(001) are inert to H_2 adsorption at room temperature because all adsorption pathways considered exhibit substantial energy barriers. They are in satisfying agreement with previous density functional and quantum Monte Carlo calculations which have been carried out for two specific reaction pathways only. Guided by our earlier studies on H_2 reaction with SiC(001) surfaces, we have considered a third reaction pathway which actually turns out to have the lowest energy barrier on C(001). A comparison of the energy barriers and reaction energies for the different surfaces addressed turns out to be particularly revealing.

O 55.40 Wed 18:30 Poster F

Laser Activated Vapour Phase Processes for Silicon Substrate Cleaning — •Ulrich Abelein, Andreas Assmuth, Torsten Sulima, and Ignaz Eisele — Universität der Bundeswehr München, Institut für Physik, Werner-Heisenberg-Weg 39, 85577 Neubiberg, Germany

One of the most important issues in today's nanoelectronics fabrication is the in situ cleaning of silicon substrates, i. e. the removal of organic impurities and SiO_2, before epitaxial growth.

The currently used vapour phase methods, like the hydrogen bake, require high process temperatures above 800 °C to activate the chemical reaction which leads to the desired effect. To avoid the diffusion of dopands or the formation of SiC clusters during the cleaning process a reduction of the necessary temperature below 700 °C is desirable.

Possible solutions to achieve this aim are the activation of the gas molecules by a plasma source or by laser light. As plasma processes cause damages to insulating layers and roughen the surface the use of a laser to provide the energy is more suitable.

We have integrated a process chamber, equipped with a 193 nm ArF Excimer Laser and up to four gases, in an UHV cluster tool. The laser beam is guided parallel to the substrate to ensure that only the gas molecules are affected and not the silicon. An RTP lamp heater can be used to adjust the substrate temperature independent from the laser energy. The efficiency of this approach will by demonstrated by the results achieved with a cleaning process using laser activated GeH_4 to remove carbon and SiO_2.

O 55.41 Wed 18:30 Poster F

The interface between diamond and aqueous electrolyte — •Markus Dankerl, Moritz Hauf, Ulrich Stützel, Andreas Reitinger, Jose Garrido, and Martin Stutzmann — Walter Schottky Institut, Technische Universität Müunchen, Am Coulombwall 3, 85748 Garching

Diamond, which is terminated with hydrogen at the surface, shows the intriguing property of being p-type surface conductive with a two-dimensional hole gas forming beneath the surface. If brought into electrolyte solutions, this surface conductivity shows a dependence on the diamond electrode potential. This allows for the fabrication of in-plane FETs with the electrolyte functioning as gate, therefore called EGFETs. We report on the characterization of the surface conductivity of single crystalline hydrogen terminated diamond in contact with electrolyte. The focus is put on the effect coulombic screening of charge at the interface by salts with different valency has on the surface conductivity. Experimental results are compared to simulations based on the screening effect. In this context the mechanism of the pH sensitivity is discussed, where the effect of ionic strength on pH sensitivity suggests, that pH-dependent surface charges have an equivalent effect on the surface conductivity as a change of the electrode potential.

O 55.42 Wed 18:30 Poster F

Scanning tunneling microscope study of Fe, Co, and Cu- Phthalocyanine growth on metal surfaces — •Shih-Hsin Chang[1], Alessandro Scarfato[1,2], Germar Hoffmann[1], and Roland Wiesendanger[1] — [1]Institut für Angewandte Physik, Universität Hamburg, Germany — [2]Dipartimento di Fisica, University of Salerno, Italy

The growth behaviour of Fe-, Co-, and Cu- Phthalocyanine (Pc) molecules on Cu(111) surfaces has been studied by a variable-temperature scanning tunneling microscope. For all three kinds of Pcs, we find perfect alignment of one molecular axis relative to one of the equivalent crystallographic axis of Cu(111) at submonolayer coverage. At about 1 ML short-range ordered domains appear and molecular configurations are found to have a mismatch angle from the crystallographic axis of Cu(111) due to molecule-molecule interaction. Above 1 ML, well-ordered domains of second layer molecules are formed. Based on STM images molecules were found to be tilted out-of-plane. Still, a substantial variation of the growth behaviour for the different Pc is observable. We will discuss these variations in terms of molecule-molecule and molecule-substrate interactions.

O 55.43 Wed 18:30 Poster F

Design and construction of a 300 mKelvin / 17 Tesla ultra-high vacuum scanning tunneling microscope for molecular studies — •Jörg Schwöbel, Matthias Nohme, Robert Ravlić, Jan Wienhausen, Germar Hoffmann, and Roland Wiesendanger — Institut für Angewandte Physik, Universität Hamburg, Germany

The detailed investigation of molecular excitations and molecular magnetism is a prerequisite to establish molecules as building blocks for tailor made materials. Here, we present the design of a new ultra-high vacuum system for the local study of molecular magnetism with scanning tunneling microscopy (STM) and spectroscopy (STS).

To resolve magnetic molecular levels this system operates at ultra-low temperatures (300 mK), thereby increasing energy resolution, and is equipped with a 17 Tesla magnetic field to achieve splitting of magnetic states. Organic magnetic molecules will be prepared on metal substrates as well as on substrates covered by insulating layers for electronic decoupling. For the preparation of heterogeneous layers from different materials and of single molecules we developed new vacuum components for a flexible growth at temperatures between 1 and 500 K. Metal and molecule evaporators are mounted on individual sample holders. Therefore, evaporators can be easily exchanged and operated in the preparation chamber as well as within the 300 mK cryostat.

We will discuss the design concept of the STM system and the vacuum components we developed on portable evaporators, as well as for the preparation of crystals with high melting temperatures. First results on the in-situ preparation of molecular systems will be presented.

O 55.44 Wed 18:30 Poster F

STM / STS investigation of porphyrin and corrole molecules on surfaces — •Germar Hoffmann, Stefan Kuck, Jens Brede, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg

Porphyrins and corroles are metallo-organic compounds with a single metal ion in their central positions. Previous studies of porphyrin systems revealed unique electronic and magnetic features[1] making this class an interesting material for future spintronic devices. These spectroscopic features are influenced by the structural adsorption of the molecule on the surface. We employ scanning tunneling microscopy to compare the adsorption of tetra-phenyl-porphyrin and tri-phenyl-corrole revealing a saddle deformation of the molecule's aromatic core. The influence of the deformed molecular macrocycle on the molecular states near the Fermi energy is studied in detail by means of scanning tunnelling spectroscopy (STS). To investigate the metal-molecule interaction, molecules with different ligands and thin isolating layers of NaCl are employed to electronically decouple the molecules from the metallic substrate.

[1] H.Wende et al., Nature Materials, 6:516-519 (2007).

O 55.45 Wed 18:30 Poster F

Water adsorption on stepped and flat Pt(111) surfaces – combined TDS and STM measurements — •Alexander Picolin[1], Alex Redinger[1], Carsten Busse[1], Markus Morgenstern[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]II. Physikalisches Institut B, RWTH Aachen, Germany

An extensive insight into the water-metal-bonds and a deeper understanding of corrosion and catalytic reactions require knowledge about the behaviour of water molecules on metallic surfaces. Therefore, adsorption mechanism, resulting phases, and preferred bonds of the ice double layer on Pt(111) are investigated with thermal desorption spectroscopy (TDS) and scanning tunneling microscopy (STM).

After adsorption of water at 120 K on a flat Pt(111) surface, TDS measurements only show the well-known multilayer (at 150-160 K) and monolayer desorption peaks (∼168 K). When the sample is prepared by 5 keV Ar^+ ions (fluence 10^{17} ions/cm^2) under grazing incidence (83° against surface normal) a rippled morphology with a high step density (∼5% of adsorption sites) results. Subsequent TDS on this surface shows a shift in temperature of the monolayer peak as well as two further desorption peaks at 180 K and 195 K. These two additional peaks are absent, if a small amount of CO is adsorbed at 400 K prior to H_2O adsorption. As CO binds preferentially to steps, the two additional H_2O desorption peaks from the clean surface are attributed to molecules bound to {100} and {111}-microfacetted steps. Binding energies and the order of desorption for step edges are determined. The preference of step edge occupation is also observed in STM images.

O 55.46 Wed 18:30 Poster F

STM observation of antiphase boundaries in Fe_3O_4(001)/MgO thin epitaxial films — •David Serrate[1], Julia M. Orna[2], Luis Morellón[2], Andre Kubetzka[1], Kirsten von Bergman[1], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, University of Hamburg, Hamburg, Germany — [2]Instituto de Nanociencia de Aragón, University of Zaragoza, Zaragoza, Spain

Due to its high Curie temperature and half-metallic nature, Fe_3O_4 thin films are archetypal candidates as electrodes for spin-valve type devices. However, the spin filtering effects achieved at room temperature up to date are modest[1]. The reason is that the properties of the Fe_3O_4 surface play a mayor role on the TMR of magnetic tunnel junctions, and therefore a better understanding of the surface termination is mandatory. Several STM experiments have been published on the (001) surface of bulk single crystals, but the surface of artificial thin films remains unexplored. The most likely defects occurring in Fe_3O_4 epitaxial films are the so-called antiphase boundaries (APB)[2], which arise from the coalescence of two crystallographic domains. We report the direct observation of APB in thin epitaxial Fe_3O_4 (40 nm) by means of STM topography showing atomic resolution. Fe3O4(001) was grown on MgO(001) by pulsed laser deposition. Surface preparation for STM measurements consisted of cycles of Ar^+ etching and O_2 annealing at 5×10^{-7} mbar. The results provide a structural model for the APB and confirm the origin of the in-plane MR characteristic of ultrathin Fe_3O_4 films[2]. [1] H. Matsuda et al., Jpn. J. Appl. Phys. 41, L387 (2002) [2] W. Eerestein et al., Phys. Rev. Lett. 88, 247204 (2002)

O 55.47 Wed 18:30 Poster F

Metal coatings prepared by organometallic chemical vapour deposition (OMCVD) — •Jörn Wochnowski[1], Thimo Göllnitz[1,2], Germar Hoffmann[2], Roland Wiesendanger[2], and Jürgen Heck[1] — [1]Institute of Inorganic and Applied Chemistry — [2]Institute of Applied Physics; University of Hamburg

In microtechnology, the coating of temperature-sensitive substrates with high melting-point materials is challenging. The use of volatile organometallic compounds can be an answer to solve this ambitious task. We developed an experimental set-up for the deposition of elements, oxides, and functional composites in glass hollowware by means of OMCVD. With the first experimental set-up [1], the thermally induced decomposition of numerous elementorganic and metallorganic precursors has been tested for the deposition of catalytic or optic materials.

Here, we will present experimental data of the thermal deposition of different metals as tungsten [2] on a glass surface. We used Atomic Force Microscopy as one standard analytical surface method to obtain structural and morphological information of the deposited metal layers. We will discuss the preparation and the analytics of the prepared surfaces. With the objective to bring the deposition temperature of $W(CO)_6$ further down to room temperature, we developed a new photolytic OMCVD set-up. We will demonstrate and discuss the realization of our experimental setup.

[1] J. Heck et al., DE 198,52,722, 2000, EP 1,001,050 A2, 2000.

[2] J.Wochnowski, doctoral thesis Hamburg 2007.

O 55.48 Wed 18:30 Poster F

Study of formation and thermal stability of Fe layers on ZnO surfaces — Alexander Demund, Daniel Wett, Sylvia Reiche, Rüdiger Szargan, and •Reinhard Denecke — Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnéstr. 2, 04103 Leipzig

Formation and thermal stability of Fe layers on ZnO surfaces have been studied by means of X-ray Photoelectron Spectroscopy and Low Energy Electron Diffraction. Experiments were performed on the polar surfaces ZnO(0001) and ZnO(000-1) and on the non-polar (1120) surface. The results indicated a pseudo 2D growth mode for iron on ZnO at room temperature, which was less pronounced on the Zn-terminated (0001) surface. Under ultra high vacuum conditions low coverages of deposited Fe^0 on all ZnO single crystal surfaces were partially oxidized by a small fraction of residual -OH-groups and ZnO to FeO. A strong temperature dependence of the interface reactivity was found upon annealing. Starting from 200 - 300°C iron was first oxidized to bivalent iron oxide. After complete oxidation of Fe^0 to Fe^{2+} at around 400°C, Fe^{2+} reacted to Fe^{3+}. Above temperatures of 500°C the deposited metallic iron was completely oxidized to trivalent iron. Differences observed for the different surface orientations will be discussed.
Work has been supported by DFG (FG 404 Sz58/15).

O 55.49 Wed 18:30 Poster F

Investigation of MgO thin films on Mo(100) by scanning tunneling microscopy and spectroscopy — •Mike Pezzotta, Dinesh Subramaniam, Marco Pratzer, and Markus Morgenstern — II. Physikalisches Institut B, Otto-Blumenthal-Straße, RWTH Aachen and JARA-FIT, 52074 Aachen

Oxide thin films on metallic substrates offer the possibility of investigating the electronic structure of metallic or ferromagnetic atoms at low electronic coupling to the substrate. Magnesium oxide films on a molybdenum substrate are favored because of their flat and nearly defect-free epitaxial growth [1].

We studied the growth of MgO islands on Mo(100) by scanning tunneling microscopy and spectroscopy on the clean Mo surface as well as on the Mo-carbide reconstruction. MgO thin films were prepared by molecular beam epitaxy of magnesium in oxygen athmosphere ($p=1*10^{-7}$ mbar). The oxidation process has been controlled by Auger spectroscopy. Annealing temperatures in the range of 900 K to 1100 K result in MgO island sizes up to 50 nm in width and up to 1 nm in height. First spectroscopic dI/dU and dz/dU measurements are presented.

[1] S. Benedetti et. al., Chemical Physics Letters 430 (2006) 330-335.

O 55.50 Wed 18:30 Poster F

Direct metalation of phthalocyanine and tetraphenylporphyrin on Ag(111) with co-adsorbed iron atoms — •Yun Bai, Florian Buchner, Matthew Wendahl, Robert Staehle, Ina Kellner, Andreas Bayer, Hubertus Marbach, Jörg Michael Gottfried, and Hans-Peter Steinrück — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen, Germany

Metalloporphyrins and metallophthalocyanines are promising candidates for the functionalization of surfaces on the nanoscale because they combine a reactive metal ion with a planar organic ligand, which serves as a structure-forming element. Potential applications of such functionalized surfaces include heterogeneous catalysts with well-defined active sites and sensor systems. In this contribution, we report the in-situ preparation of related model systems, in particular Fe(II)-phthalocyanine and Fe(II)-tetraphenylporphyrin monolayers on Ag(111). Both complexes are sensitive toward oxidation and react readily with molecular oxygen, which makes the preparation of the adsorbates by ex-situ metalation of the ligands in solution and subsequent deposition difficult. Instead, we deposited monolayers of the less reactive metal-free ligands and metalated them with the stoichiometric amounts of vapour-deposited Fe atoms in an ultra-high vacuum environment. This surface-mediated redox reaction was studied with XPS and STM and was found to proceed with high yield (up to 95%). Supported by the DFG through SFB 583.

O 55.51 Wed 18:30 Poster F

Enhancement of photodesorption by vibrational excitation — •Tijo Vazhappilly[1], Stephanie Beyvers[1], Tillmann Klamroth[1], Rigoberto Hernandez[2], and Peter Saalfrank[1] — [1]Institut für Chemie, Universität Potsdam, D-14476 Potsdam, Germany — [2]School of Chemistry and Biochemistry, Georgia Institute of Technology,Atlanta, GA 30332-0400

The effect of selective excitation of adsorbate vibrations by tailored IR laser pulses, on the photodesorption of H_2 and D_2 from a Ru(0001) surface has been investigated theoretically. A two-dimensional model is used for the Desorption Induced by Electronic Transitions (DIET) limit. A jumping wavepacket algorithm is employed with different initial states, starting from ground vibrational state to vibrationally excited states and vibrational wavepackets[1]. This model is extended to Desorption Induced by Multiple Electronic Transitions (DIMET) by incorporating electronic temperatures from femtosecond UV/vis laser excitation of metal electrons. In this regime, the IR+UV/vis strategy to control the photodesorption is realized by the Monte Carlo Wave Packet (MCWP) method [2], and Molecular Dynamics (MD) with electronic friction. Vibrational preexcitation appears to be successful in both DIET and DIMET.

References: [1] T. Vazhappilly, S. Beyvers, T. Klamroth, M. Luppi, and P. Saalfrank, Chem. Phys. **338**, 299 (2007). [2] P. Saalfrank, T. Vazhappilly, S. Beyvers, G.K. Paramonov, and T. Klamroth, Surf. Sci. (submitted).

O 55.52 Wed 18:30 Poster F

Adsorption, Dissociation and Desorption of Acetylene on Steel — •Andreas Bayer[1], Jürgen Rossa[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

One way to improve the hardness and wear resistance of crude steel is low-pressure carburisation. In this process, the surface near region of steel is enriched with carbon, produced in-situ by dissociative adsorption of hydrocarbons followed by diffusion of carbon atoms into the bulk. In order to gain a detailed understanding of this process, adsorption, dissociation and desorption of acetylene (C_2H_2) on steel at temperatures between 500 and 1200 K were studied by mass spectrometry and Auger electron spectroscopy utilising molecular beam techniques. At low temperatures (T<700 K), the sticking probability for C_2H_2, measured by the technique of King and Wells, is very small. Nevertheless, an increase in surface carbon coverage can be seen at 500 K, indicating a slow diffusion rate at this temperature. Upon raising temperature, the sticking coefficient reaches a maximum of 0.3 at 1000-1050 K. For even higher temperatures, the sticking probability decreases again due to nitrogen, segregating to the surface and blocking the adsorption of C_2H_2. Increasing the kinetic energy of C_2H_2 molecules by seeding with helium leads to smaller sticking coefficients at all temperatures, proposing a non-activated adsorption process.

This work was supported by BMBF (03X2506C).

O 55.53 Wed 18:30 Poster F

Chemical reactivity of the polar O-ZnO(000-1) surface investigated by vibrational spectroscopy — •Hengshan Qiu, Yuemin Wang, and Christof Wöll — Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, 44780 Bochum, Germany

Zinc oxide is an important material with a wide range of technological applications in catalysis, solar cells, as gas sensor and in semiconductor devices [1]. In catalysis, the heterogeneous catalyst system Cu/ZnO has been widely applied for the industrial methanol synthesis. Recently, the oxygen terminated polar (000-1) surface has been demonstrated to be the most active surface for methanol synthesis from syngas ($CO/CO_2/H_2$) on ZnO powders [2]. It is found that the clean, H-free O-ZnO(000-1) surface is (1x3) reconstructed and exposes 0.33 ML O vacancies. In this contribution, the interaction of different molecules (CO, CO_2 CH_2O and HCOOH) with the clean O-ZnO(000-1) surface was studied by high-resolution electron energy loss spectroscopy (HREELS), thermal desorption spectroscopy (TDS) and low-energy electron diffraction (LEED). The present results provide detailed information about the chemical reactivity of defect sites (in particular O vacancies) towards different adsorbates. The corresponding reactions can be monitored by vibrational spectroscopy.

[1] Ch. Wöll, Prog. Surf. Sci. 82 (2007) 55. [2] M. Kurtz, J. Strunk, O. Hinrichsen, M. Muhler, K. Fink, B. Meyer and Ch. Wöll, Angew. Chem. Int. Ed. 2005, 44, 2790

O 55.54 Wed 18:30 Poster F

SPA-LEED investigations on the growth of NiO films on MgO passivated Ag(001) — •Lars Boewer[1], Bernd Zimmermann[2], and Joachim Wollschlaeger[2] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, D-44221 Dortmund — [2]Fachbereich Physik, Universität Osnabrück, D-49076 Osnabrück

Thin oxide films are important for nanoelectronic devices. For instance, they serve as tunneling barriers for tunneling magneto resistors (TMR). NiO is used for TMR devices due to its antiferromagnetic properties.

In this work we studied the growth of NiO on Ag(001) as model for lattice matched oxide films on metals. In addition, we deposited MgO films, which are also lattice matched, prior to the deposition of NiO to passivate the Ag substrate and to avoid alloying of Ni and Ag.

Oxide films were prepared by MBE of metals (Ni or Mg) in oxygen atmosphere at room temperature. The stoichiometry was investigated by AES. SPA-LEED was used to study the morphology of the oxide films at different growth stages. The NiO film initially nucleates with islands of two monolayer height. After completion of 2ML the growth continues in the layer-by-layer growth mode. Finally, we observe the formation of mosaics due to misfit dislocations.

O 55.55 Wed 18:30 Poster F

Properties of ultrathin In layers on the Ni(111) face — •Wojciech Linhart, Tomasz Tokarz, Agnieszka Gorzelska, Zbigniew Jankowski, and Aleksander Krupski — Institute of Experimental Physics, University of Wroclaw, pl. Maxa Borna 9, 50-204 Wroclaw, Poland

The atomic structure and morphology of ultrathin In layers on the Ni(111) face deposited in ultrahigh vacuum at the substrate temperature ranging from 150 K to 700 K were investigated with the use of Auger electron spectroscopy (AES), low-energy electron diffraction (LEED) including I-V LEED and directional elastic peak electron spectroscopy (DEPES).

O 55.56 Wed 18:30 Poster F

Phases with long-range order observed in the interaction of silver with the Re$(10\bar{1}0)$ surface. — •Viktor Scherf[1], Christian Pauls[1], Lyria Messahel[1,2], and Klaus Christmann[1] — [1]Institut für Chemie und Biochemie der FU Berlin, D-14195 Berlin — [2]University of Sciences and Technology H. Boumediène, U.S.T.H.B., Faculty of

Chemistry, B.P.32, El-Alia 16111, Bab Ezzouar, Algiers, Algeria.

We have studied the interaction of silver with the Re(10$\bar{1}$0) surface in UHV in the temperature range between 300 and 800 K by means of low-energy and medium-energy electron diffraction (LEED and MEED) as well as with temperature-programmed thermal desorption (TPD). Deposition of Ag from submonolayer to multilayer coverages was accomplished in small coverage increments; the monolayer concentration was calibrated using MEED and examined using LEED-(I,V) calculations. Short annealing at 800 K ensured thermodynamic equilibrium of the Ag phases formed, since it is not until 950 K that Ag desorbs in noticeable amounts. Within the submonolayer coverage regime the following ordered LEED phases could be observed with increasing Ag coverage: c(2x2); p(1x4); p(1x5), and (1x1), whereby all phases turn out to be uniquely correlated with temperature and surface coverage. We develop structure models of the Ag phases and discuss and compare our data with recent studies of Au on Re(10$\bar{1}$0) and Ag on Ru(10$\bar{1}$0) surfaces.

O 55.57 Wed 18:30 Poster F

A Monte Carlo study of surface diffusion driven growth of a single droplet — •Robert Heimburger — Institute for Crystal Growth, Berlin, Germany

The Vapour-Liquid-Solid-Mechanism (VLS) is proven to be a promising way to grow spatially arranged seed crystals for the growth of polycrystalline silicon layers on amourphous substrates. The study of coalescence and growth of liquid metal droplets on partially wetted surfaces is of great interest as the process is an important partial step of the Vapour-Liquid-Solid-Mechanism.

We present a detailed study of the diffusion driven evolution of droplet size in dependence of growth temperature, surface roughness and deposition rate neglecting coalescences of droplets using the Monte Carlo method. Additionally spatial concentration profiles of the growing matter are discussed. The estimates will be compared with experimental results of droplet formation on a molybdenum surface by evaporation of indium.

O 55.58 Wed 18:30 Poster F

Vibrational features of copper adatoms on Cu(111) — •Diana Vogel, Olaf Skibbe, and Annemarie Pucci — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, D-69120 Heidelberg

It is known that some stepped copper surfaces show vibrational features that are introduced by the steps [1]. The energies of some of these vibrations are higher than those of the bulk phonons. We found with high-resolution electron energy loss spectroscopy (HREELS) similar features by looking at the Cu(111) surface on which we evaporated copper at liquid nitrogen temperature. The behavior of these vibrational features will be shown as a function of the amount of added copper and the annealing temperature, respectively.

The aim of this study is to characterize the roughened surface which can serve as a nano-structured template for the adsorption of molecules. The interaction of adsorbates with the surface is known to be influenced strongly by the presence of defect sites [2].

[1] A. Kara, P. Staikov, and T. S. Rahman, Phys. Rev. B **61**, 5714 (2000).

[2] O. Skibbe, M. Binder, A. Otto, and A. Pucci, in preparation.

O 55.59 Wed 18:30 Poster F

The growth and structure of titania films on a rhenium(0001) surface — •Susanne Schubert and Klaus Christmann — Institut für Chemie und Biochemie der FU Berlin, Germany

In view of the significance of titanium dioxide as a catalyst support for low-temperature CO oxidation we have studied the epitaxy and chemical properties of titanium dioxide films grown on a clean and oxygen-covered Re(0001) surface. Titania films were prepared by codeposition of Ti vapor in an oxygen atmosphere at elevated temperatures (T≥830K). The structure and chemical (surface) composition of these films were analyzed by means of low-energy electron diffraction (LEED), low-energy ion scattering (LEIS) and X-ray photoelectron spectroscopy (XPS) as a function of deposition rate and film thickness starting from the monolayer regime up to concentrations of 10 to 40 monolayers. While the overall film stoichiometry is close to TiO_2 (rutile) independent of film thickness we find a moiré LEED pattern at low surface concentrations, faceting with hexagonal phases in three domains of rutile(110) rotated by 120° against each other in the medium coverage regime, and well-ordered unfaceted rutile films for thicknesses beyond ≈ 40 monolayers. The respective growth behavior can be described by a Stranski-Krastanov mechanism.

O 55.60 Wed 18:30 Poster F

The Pt_xRu_{1-x}/Ru(0001) surface alloy formation process studied by STM — •Andreas Bergbreiter, Harry E. Hoster, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

Pt_xRu_{1-x}/Ru(0001) surface alloys were prepared by vapor deposition of Pt on a Ru(0001) single crystal, followed by annealing to 1350 K. According to high resolution STM analyses with chemical contrast, the composition of the Pt_xRu_{1-x}/Ru(0001) surface is homogeneous on both nanometer and micrometer length scale. For x<0.8, the amount of Pt exactly matches the initial coverage by pseudomorphic Pt islands. Even after alloy formation we find islands on the surface. These islands are more compact in shape and larger in size than the initial Pt islands, but have the same Pt:Ru ratio as the surrounding terraces. Together with the homogeneous composition, the conserved amount of Pt surface atoms means, that virtually no Pt is buried below these alloy islands. Pt deposition at high temperatures and Ru overgrowth of Pt islands show that the absence of Pt in the subsurface layer (below the islands) can be rationalized by a preference of both Pt and Ru to occupy Ru 3-fold sites. High exchange rates between Pt (Ru) adatoms and atoms in the underlying layer allow equilibration of the topmost layers. The site preferences fit well to effective pair interaction energies derived from lateral atomic distribution within the Pt_xRu_{1-x}/Ru(0001) surface alloys.

O 55.61 Wed 18:30 Poster F

Temperature effects in the growth of Ru on Pt(111) — András Berkó[1,2], •Andreas Bergbreiter[1], Petra M. Erne[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 Adress: Institute of Surface Chemistry and Catalysis, University of Szeged, H-6701 Szeged, Dóm tér 7, Hungary

The growth of Ru on Pt(111) at substrate temperatures in the range of 50-500°C was studied by high resolution STM and Auger electron spectroscopy (AES). Ru deposition at temperatures up to 250°C leads to the formation of triangular bilayer islands [1]. The lateral dimensions of these bilayer islands become more uniform with increasing substrate temperature, but show little dependence on evaporation rate and Ru coverage. At deposition temperatures of 300°C or higher, in contrast the islands are only of monoatomic height. Based on STM-imaging with chemical contrast and AES analyses, this is associated with the onset of surface alloy formation. The influence of the different strengths of Pt-Pt, Pt-Ru, and Ru-Ru interactions as well as the role of lattice mismatch effects are discussed.

[1] H. Hoster, T. Iwasita, H. Baumgärtner, W. Vielstich; Phys. Chem. Chem. Phys. 3; 2001; 337.

O 55.62 Wed 18:30 Poster F

Atomic-scale self-organization of Fe nanostripes on stepped Cu(111) surfaces — •Nikolay N. Negulyaev[1], Valeri S. Stepanyuk[2], Wolfram Hergert[1], Patrick Bruno[2], and Jurgen Kirschner[2] — [1]Physics Department, Martin-Luther-University, Halle-Wittenberg, 06099 Halle, Germany — [2]Max Planck Institute of Microstructure Physics, 06120 Halle, Germany

Growth of Fe nanostripes on a vicinal Cu(111) surface is investigated on the atomic scale performing molecular dynamics and kinetic Monte Carlo simulations [1]. We involve in our study the kinetic mechanisms of incorporation of Fe atoms into the stepped Cu(111) surface. The atomic processes responsible for the interlayer mass transport and the self-assembly of 1 ML high Fe stripes are identified. The role of temperature is revealed. We demonstrate that strain relaxations at steps have a strong impact on the self-assembly of one-dimensional Fe atomic structures on vicinal Cu(111).

1. N.N. Negulyaev et al., Phys. Rev. B, submitted.

O 55.63 Wed 18:30 Poster F

Influence of sputtering effects during homoepitaxial growth of Cu(100) using electron-beam evaporation — •Henning Prüser, Martin Wenderoth, Alexander Weismann, and Rainer G. Ulbrich — IV. Physikalisches Institut der Georg-August-Universität Göttingen

It is well known that ion assisted deposition influences the growth processes in thin film formation. Electron beam evaporators which apply high voltage to the crucible produces a significant fraction of ionized atoms that are accelerated to the sample. We have investigated the impact of this effect on the homoepitaxial growth of copper films using Scanning Tunneling Microscopy. During growth different electrical fields were applied to suppress ion bombardment at varied substrate temperatures. At room temperature without ion suppression a nanostructured surface is found. Rectangular shaped vacancy islands are created quite similar to those obtained by [1]. If an electric field is applied, a multilayer growth mode can be observed. Ion-free deposition at higher substrate temperatures results in a layer by layer growth. This work was supported by DFG SFB 602 TPA3.

[1] M. Ritter et al, Surface Science **348** (1996) 243-252

O 55.64 Wed 18:30 Poster F

The growth of Co on Fe/W(110)investigated by STM and STS — •Torsten Methfessel and Hans-Joachim Elmers — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudingerweg 7, D-55099 Mainz

Highly spinpolarised metals are of great interest e.g. for the application in spin-valves. Recently observed large tunneling magnetoresistance (TMR) effect values of 410 % at room temperature for Co/Fe(100) electrodes indicate a high spin-polarisation at the Fermi energy of bcc Co [1]. Instead of a (100) oriented substrate, we grow bcc Co on Fe(110), where the symmetry change from hcp to bcc becomes obvious in the (110) surface plane, in contrast to the (100) orientation. In order to prepare a Fe(110) substrate, we deposited a 8 ML Fe film on W(110) that was annealed to 500 K. The annealing results in large separated islands with an ideal Fe(110) surface, that serves as a substrate for the deposition of Co. Using scanning tunneling microscopy and spectroscopy (STM and STS) we investigated the local structural and electronic properties of the bcc Co films. The first monolayers of Co grow as pseudomorphic bcc layers, which shows periodic lattice distortions similar to the growth of Co on Cr(110) [2]. Single point spectroscopy reveals a peak of the LDOS at +1 eV in contrast to the peak at +0.6 eV observed for the second monolayer bcc Co/Cr(110), which might be explained by the differences in the lattice constants of Fe and Cr.

[1] S. Yuasa et al., Appl.Phys.Lett. 89 (2006) 042505.

[2] T. Methfessel et al., Suf.Sci. 601 (2007) 5026.

O 55.65 Wed 18:30 Poster F

Adsorption of CO, O_2 and ethene on $Pt_xCe/Pt(111)$ surface alloys. A HREELS-, TPD-study. — Jan Markus Essen, •Conrad Becker, and Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstrasse 12, 53115 Bonn, Germany

It is well known that alloying can change the adsorption and reaction properties of surfaces significantly. In this study we investigated the Pt-Ce system. Evaporating Ce onto Pt(111) followed by annealing to 1000 K forms ordered alloys. Depending on the cerium fraction a (2x2) and a (1,96x1,96)+(1,96x1,96)R30° LEED pattern is observed. Our TPD and HREELS study of CO, O_2 and ethene adsorption shows a very low reactivity of these surface alloys. Concerning CO adsorption we find a significantly decreased desorption temperature of about 280 K compared to 400 K for a CO saturation coverage on pure Pt(111). Likewise oxygen adsorbed at 90 K, followed by annealing, cannot oxidize these surface alloys. In comparison with Pt(111) neither is molecularly bonded oxygen observed at 90 K nor can desorption of oxygen caused by recombination of atomic oxygen at 750 K be detected as on Pt(111). Our results support the model for the $Pt_xCe/Pt(111)$ surface alloy consisting of a Pt Kagomé net as the top layer. Because of the low reactivity we conclude that the top layer of the surface alloy contains no Cerium-atoms.

O 55.66 Wed 18:30 Poster F

Preparation and investigation of galvinoxyl on potassium bromide — •Miriam Klusmann and Marika Schleberger — Universität Duisburg-Essen, Fachbereich Physik, Lotharstraße 1, D-47048 Duisburg, Germany

Molecular magnets are supposed to offer storage densities up to some tera bits per square inch. But before any technical application can be realized a suitable preparative method to produce well-ordered structures of such molecular assemblies is required. Most of the molecular magnets cannot be deposited on surfaces by conventional techniques like organic molecular beam epitaxy (OMBE) due to thermal decomposition of the molecules below the operating temperature of the evaporator. To avoid this problem we use a pulsed valve to spray a solution that contains molecular magnets onto the bare substrat. Preparation takes place under ultra-high vacuum (UHV) conditions. The idea is that the solvent evaporates while the molecules adsorb (ideally intact) onto the surface. We report on results obtained with the stable radical galvinoxyl ($C_{29}H_{41}O_2$) dissolved in ethanol p. a. and injected onto a freshly cleaved (100)-surface of the insulator potassium bromide (KBr). Investigation of the surface before and after injection is done by atomic force microscopy in the nondestructive dynamic mode (FM-AFM) under ultra-high vacuum conditions.

O 55.67 Wed 18:30 Poster F

Contact charging between insulators by organic molecule adsorption — •Wei Chen, Christoph Tegenkamp, and Herbert Pfnuer — Leibniz-Universität Hannover, Institut für Festkörperphysik, Appelstr. 2, 30167 Hannover, Germany

It has been shown that adsorption of simple organic acids on wide band gap insulators can introduce unoccupied electronic states in the band gap. These unoccupied states of adsorbates can lower electron excitation energy significantly, which makes it possible for charge exchanges between insulators. The adsorbates are thus decisive for contact charging problems as the electronic states of the surfaces are well defined by the them.

In this paper, the electronic states of benzoic acids attached to various functional groups are investigated by density functional theory calculations. The results show that salicylic acid (SA) and anthranilic acid (AA) are ideal for contact charging between insulators because of their higher binding energy of the uppermost π_z orbital of the COOH group. The corresponding anti-bonding state (i.e. the LUMO) is thus located closer to the VB edge of the insulators, resulting a smaller effective band gap. Moreover, the HOMO-LUMO separation of AA is 0.12 eV smaller compared to SA. Further, we represent first results of atomic force microscopy measurements which are performed on organic molecule adsorbed NaCl surface using KCl coated cantilevers in order to study contact charging between the alkali chlorides.

O 55.68 Wed 18:30 Poster F

The structure of the first layer of acetylene adsorbed on NaCl(100) — Aldo Cartagena, •Jochen Vogt, and Helmut Weiss — Chemisches Institut der Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

Acetylene adsorbed on NaCl(100) is considered as a model system of physisorption under the conditions of a moderate lattice mismatch and, moreover, the formation of hydrogen bonds between neighboring molecules. Hydrogen bonds are known to cause red-shifts of the IR-active C–H stretch modes of the molecules. In low-energy electron diffraction experiments, a $(3\sqrt{2} \times \sqrt{2})$R45° symmetry of the first layer of acetylene is observed at 75 K, in agreement with a previous study [1]. Under the same conditions, polarization infrared spectroscopy reveals a splitting of the asymmetric stretch mode in three absorptions at 3227.3, 3230.5, and 3248.7 cm^{-1}, respectively, also in agreement with a previous study [2]. We use potential calculations to determine the structure of the adlayer and vibrational exciton theory guided by ab initio calculations to give a new assignment of the observed IR transitions to molecules on inequivalent sites, the latter being interlinked by different numbers of hydrogen bonds.

[1] A. Glebov et al., Phys. Rev. B 106 (1997) 6499

[2] S. K. Dunn et al., J. Phys. Chem. 96 (1992) 5284

O 55.69 Wed 18:30 Poster F

Oxygen incorporation from CO2 and H2O in Fe-doped SrTiO3 single crystals — •Florian Voigts[1], Dominik Schwendt[1], Sebastian Dahle[1], Pradyot Datta[2], Jana Grosse-Brauckmann[2], Lars Dörrer[2], Christos Argirusis[2], and Wolfgang Maus-Friedrichs[1] — [1]Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstrasse 4, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Metallurgie, TU Clausthal, Robert-Koch-Strasse 42, 38678 Clausthal-Zellerfeld, Germany

Strontium titanate is a promising candidate for the development of a new generation of resistive high temperature oxygen sensors. The analysis of automobile exhaust is regarded as a possible main application. An interpretation of the sensors signal in such an environment will only be possible with an understanding of the cross-sensitivity of the strontium titanate for other present gases like water or carbon dioxide.

Our results for the interaction of donor-doped strontium titanate single crystals with these species are presented in this poster. Metastable Induced Electron Spectroscopy and Ultraviolet Photoelectron Spectroscopy are used to study adsorption and dissociation processes under ultra high vacuum conditions. Oxygen tracer diffusion experiments performed under realistic conditions using Secondary Ion Mass Spectroscopy as well as investigations with X-ray Photoelectron Spectroscopy and Temperature Programmed Desorption give evidence to the oxygen incorporation into the strontium titanate. Furthermore, diffusion processes can be investigated. We try to correlate the results to develop a model for the occurring interaction processes.

O 55.70 Wed 18:30 Poster F

Interaction of $SrTiO_3$ nanoparticles with reactive gases — •Dominik Schwendt[1], Florian Voigts[2], Wolfgang Maus-Friedrichs[2], Christos Argirusis[3], and Jana Grosse-Brauckmann[3] — [1]Institut für Materialien und Bauelemente der Elektronik, Leibniz Universität Hannover, Appelstr. 11A, 30167 Hannover, Germany — [2]Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [3]Institut für Metallurgie, TU Clausthal, Robert-Koch-Straße 42, 38678 Clausthal-Zellerfeld, Germany

$SrTiO_3$ is known for its capability as high temperature oxygen sensor. The most interesting application of this sensor would be the analysis of automobile exhaust, allowing the optimisation of fuel injection and catalytic oxidation of toxic exhaust.

Metastable Impact Electron Spectroscopy as wells as Ultraviolet Photoelectron Spectroscopy are used to analyse the valence band structure of $SrTiO_3$ and its adsorbates, while we use X-ray Photoelectron Spectroscopy to check the stoichiometry of the samples. In this poster we present the results of the interaction of $SrTiO_3$, produced via a sol-gel-route, with different reactive gases, such as H_2O, CO_2, CO, and NO. The results are being compared to the interaction of these gases with $SrTiO_3(100)$ single crystalls.

O 55.71 Wed 18:30 Poster F

Growth Study of Salene Molecules on NaCl(001) — •Knud Lämmle, Alexander Schwarz, and Roland Wiesendanger — Institut für Angewandte Physik, Jungiusstrasse 11a, 20355 Hamburg

Combining magnetism with the properties of organic molecules opens new options to develop unique materials. An example would be a transparent magnet. For our investigation we choose Salenes which exhibit a metallic centre and a planar structure. By exchanging the centre atoms, it is possible to tune the magnetic properties. Moreover, several molecules can be attached to each other to study the intramolecular magnetic coupling between the metallic centres via chemical bonds in such molecules. As a first step we study the growth of Co-Salene molecules using atomic force microscopy. To investigate these molecules without hybridisation effects we use the large bandgap insulator NaCl(001) as substrate. The molecules were evaporated with a homebuilt Knudsen cell at temperatures around 220 °C, while the evaporation rate was monitored by a quartz crystal microbalance. At low coverages the molecules decorate step edges only. At increased coverages the molecules form wires which also grow across large terraces. Increasing the amount of evaporated material further leads to network formation. We observed that the wires grow primarily oblique to the crystallographic axes.

O 55.72 Wed 18:30 Poster F

Spin-dependent Electron Transmission through Organized Organic thin Films — •Benjamin Göhler[1], Arne Rosenfeldt[1], Volker Hamelbeck[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, Rehovot, Israel

Electron dichroism has been reported for vapours of chiral molecules [1]. The interaction of longitudinally spin-polarized electrons with chiral molecules can be different for two enantiomers or stated the other way around for one enantiomer and electrons of opposite helicities. The attenuation of polarized electron beams shows a dependence upon the spin of the electrons.

Here photoelectrons are detected that are emitted from a gold surface covered by an organized organic thin film (OOTF). Photoelectrons excited from gold by circularly polarized light have a longitudinal spin polarization of up to 15% [2]. The photoelectron yield of gold covered with OOTF also varies with the circular polarization of the incident laser light [3]. When the photon energy applied (5.9 eV) is not sufficient to ionize the adsorbed molecules but emit electrons from the gold substrate, those results suggest that the electron transmission through the organic layer is spin dependent. To analyze this spin filter effect a new set-up is built with a small-size conventional electron polarimeter (Mini Mott) to determine the spin polarization of the transmitted electrons through the OOTF. [1] PRL 74, 4803, 1995. [2] PRL 47, 374, 1981. [3] Science 283, 814, 1999.

O 55.73 Wed 18:30 Poster F

Self-assembled monolayers on gold containing azobenzene ligands — •F. Vogel[1], M. Borg[1], F. Bretthauer[2], U. Siemeling[2], and F. Träger[1] — [1]Institut für Physik and Center for Interdisciplinary Nanostructure Science and Technology - CINSaT, Universität Kassel, Kassel — [2]Institut für Chemie and Center for Interdisciplinary Nanostructure Science and Technology - CINSaT, Universität Kassel, Kassel

Two azobenzene-derivatized 1,2-dithiolanes were synthesized and used for the preparation of self-assembled monolayers (SAM) on gold. Azobenzene derivatives can be switched between their "cis" and "trans" isomers by irradiation with light and represent the most widely studied system for photoresponsive SAMs. However, in SAMs based on thiols and symmetric disulfids on gold, the chromophores are densly packed and show little free volume to allow photoisomerisation. The binding unit of the investigated molecules with their two attachment points and increasing size should lead to considerable void spaces between the individual photoresponsive azo units. Photoswitching was confirmed by ellisometric measurements. The kinetics of film formation of the two molecules have been compared by in situ optical second harmonic generation (SHG). It has been shown that the absorption of the molecules on the gold substrate is best described by second order Langmuir kinetics for the investigated concentration of 100 μmol/l.

O 55.74 Wed 18:30 Poster F

Vapour phase deposition of biphenylthiol self-assembled monolayers — •Laxman Kankate, Andrey Turchanin, and Armin Gölzhäuser — Department of Physics, Physics of Supramolecular Systems, University of Bielefeld, D-33615 Bielefeld

Self-assembled monolayers (SAMs) with aromatic moieties caused recently a particular interest due to their applications in molecular electronics, nanolithography and biotechnology. To achieve high reproducibility of the SAM-based devices and nanostructures the utilization of high quality, well defined monolayers is necessary. The traditional *wet chemistry* preparation of SAMs suffers from solvent, ambient and substrate contaminations resulting often in poor quality of the molecular assemblies. On the contrary, the preparation of SAMs in UHV provides a high degree of control over the experimental parameters. We have studied the formation of 1,1*-biphenyl-4-thiol (BPT) and 4*-nitro-1,1*-biphenyl-4-thiol (NBPT) SAMs on Au surfaces by vapour deposition in UHV. The deposition parameters and the quality of monolayers were optimized and characterized by mass spectrometry and X-ray photoelectron spectroscopy (XPS). The formation of both SAMs was tuned from the sub-monolayer to the monolayer regimes.

O 55.75 Wed 18:30 Poster F

Vapour phase deposition of biphenylthiol self-assembled monolayers — •Laxman Kantake, Andrey Turchanin, and Armin Gölzhäuser — Department of Physics, Physics of Supramolecular Systems, University of Bielefeld, D-33615 Bielefeld

Self-assembled monolayers (SAMs) with aromatic moieties caused recently a particular interest due to their applications in molecular electronics, nanolithography and biotechnology. To achieve high reproducibility of the SAM-based devices and nanostructures the utilization of high quality, well defined monolayers is necessary. The traditional *wet chemistry* preparation of SAMs suffers from solvent, ambient and substrate contaminations resulting often in poor quality of the molecular assemblies. On the contrary, the preparation of SAMs in UHV provides a high degree of control over the experimental parameters. We have studied the formation of 1,1*-biphenyl-4-thiol (BPT) and 4*-nitro-1,1*-biphenyl-4-thiol (NBPT) SAMs on Au surfaces by vapour deposition in UHV. The deposition parameters and the quality of monolayers were optimized and characterized by mass spectrometry and X-ray photoelectron spectroscopy (XPS). The formation of both SAMs was tuned from the sub-monolayer to the monolayer regimes.

O 55.76 Wed 18:30 Poster F

Valence band spectroscopy on functionalized cellulose surfaces — •Lothar Klarhöfer[1], Kai Volgmann[1], Wolfgang Maus-Friedrichs[1], Volker Kempter[1], and Wolfgang Viöl[2] — [1]TU-Clausthal, Institut für Physik und Physikalische Technologien, Leibnizstraße 4, D-38678 Clausthal-Zellerfeld — [2]HAWK FH Hildesheim/Holzminden/Göttingen, Fakultät Naturwissenschaften

und Technik, Von-Ossietzky-Straße 99, 37085 Göttingen

XPS (X–Ray Photo–Electron Spectroscopy) has become a popular technique in pulp and paper science. Nevertheless, neither XPS valence band spectra nor UPS spectra (Ultra Violet Photo Electron Spectroscopy) were reported so far, although valence band spectra is well–known to provide detailed information of the chemical state at the surfaces enabling the analysis of different treatments.

We use XPS core level and valence band spectra in combination with UPS (HeI/HeII) and MIES (Metastable Impact Electron Spectroscopy). In order to understand the recorded spectra of cellulose several spectra of so–called "fingerprint" molecules were prepared and compared with the origin cellulose spectra.

Both the Cellulose and the model surfaces, were plasma treated by a dielectric barrier discharge in order to enhance the wetting behavior of the surface. Untreated and synthetic–air–plasma treated model surfaces were compared with respect to the surface composition of functional groups. Functionalities containing oxygen were significantly increased on plasma–treated samples, shown both with core level XPS and UPS and MIES.

O 55.77 Wed 18:30 Poster F

Surface investigations of wood constituents and wood-based compounds — •Thomas Haensel[1], Andreas Comouth[1], Nicolas Zydziak[2], Pierre Lorenz[1], Syed Imad-Uddin Ahmed[1], Stefan Krischok[1], Axel Kauffmann[2], and Juergen A. Schaefer[1] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565,Germany — [2]Fraunhofer Institut für Chemische Technologie (ICT), Joseph-von-Fraunhofer-Straße 7, 76327 Pfinztal, Germany

Graphite is a common bipolar plate material in direct methanol fuel cells. However, the graphite used is synthetically manufactured in an energy intensive and costly process. Efforts are underway to replace synthetic graphite with pyrolyzed compounds that consist largely of natural wood-based components. In this study, the surface characteristics of unpyrolyzed and pyrolyzed cellulose and lignin were investigated using contact angle measurements and X-ray photoelectron spectroscopy. Since an important consideration for any replacement material is its reactivity to methanol, the adsorption process on these surfaces was also examined by offering methanol. All results were compared with highly oriented pyrolytic graphite. The results indicate that methanol does not react in any significant manner with the pyrolyzed surfaces. The charging and X-ray degradation problems associated with the study of native compounds are also discussed.

O 56: Evening Talk Peter Grünberg

Time: Wednesday 20:00–21:00 Location: Urania

Vom Riesenmagnetowiderstand zur Computerfestplatte

O 57: Plenary Talk Helmut Grubmüller

Time: Thursday 8:30–9:15 Location: H 0105

Forces and Conformational Dynamics in Biomolecular Nanomachines

O 58: Symposium: Beyond Optical Wavelengths: Time-Resolved Spectroscopy of Surface Dynamics with EUV and XUV Radiation I (Invited Speakers: Reinhard Kienberger, Martin Aeschlimann)

Time: Thursday 9:30–11:00 Location: HE 101

Invited Talk O 58.1 Thu 9:30 HE 101

First steps of attosecond spectroscopy in condensed matter — •Reinhard Kienberger — Max-Planck-Institut für Quantenoptik, Hans Kopfermann Str. 1, 85748 Garching, Deutschland

The generation of ever shorter pulses is a key to exploring the dynamic behavior of matter on ever shorter time scales. Electronic dynamics inside atoms often evolve on an attosecond (1 as = 10-18 s) timescale and require sub-femtosecond pulses for capturing them. Atoms exposed to a few oscillation cycles of intense visible or near-infrared light are able to emit a single electron and XUV photon wavepacket of sub-femtosecond duration. Precise control of these sub-femtosecond wavepackets have been achieved by full control of the electromagnetic field in few-cycle light pulses. These XUV pulses together with the few-cycle (few-femtosecond) laser pulses used for their generation have opened the way to the development of a technique for attosecond sampling of electrons ejected from atoms or molecules. First experiments have been carried out to measure sub-femtosecond behavior of matter like the dynamics of the photoionization process on solids. Not only that attosecond metrology now enables clocking on surface dynamics, but also the individual behaviour of electrons of different type (core electrons vs. conduction band electrons) can be resolved. Here, we measured a time delay of about 100 as on the emission of the aforemention two types of electrons.

Invited Talk O 58.2 Thu 10:00 HE 101

Time- and angle-resolved photoemission spectroscopy using a femtosecond high-harmonic light-source — •Martin Aeschlimann — Department of Physics, TU Kaiserslautern, 67663 Kaiserslautern

To date, femtosecond high-harmonic (HHG) light sources have been used successfully in a number of IR-pump XUV-probe photoemission experiments to study the ultrafast dynamics of surface processes. Examples include electron relaxation in materials, surface adsorbate dynamics, photoacoustic dynamics, and molecular dissociation. All these IR-XUV geometries are accompanied by incident laser fields of $> 10^{11} W/cm^2$ leading to additional interesting laser-assisted strong-field dynamic processes on solid surfaces. For instance, just recently the laser assisted photoelectric effect (LAPE) could be demonstrated for IR-XUV excitation of a Pt(111) surface [1] as well as laser assisted auger decay (LAAD). Recent experimental results in this field will be presented. Furthermore, time resolved IR-XUV photoemission can be extended to the momentum space by the use of state-of-the-art 2D photoelectron spectrometers [2]. First ARPES spectra recorded with HHG light pulses will be presented, showing the potential of this technique for future investigations of surface dynamics.

[1] L. Miaja-Avila et al., Phys. Rev. Lett. 97, 113604 (2006)
[2] S. Mathias et al., Rev. Sci. Instr. 78, 083105 (2007)

O 58.3 Thu 10:30 HE 101

Core-level shifts induced by femtosecond laser excitation — Andrea Melzer, Daniel Kampa, Jinxiong Wang, and •Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen

The Si(001)(2x2)-Ga surface was used to investigate time-dependent Ga(3d) core-level shifts by pumping electrons from the valence to the conduction band by femtosecond laser pulses with 1.59 eV photon energy. The Ga(3d) core level was probed with higher harmonics generated in argon from the same laser source (1.4 mJ pulse energy, 30 fs pulse length, 779 nm wavelength, 1 kHz repetition rate). The time resolution for the 25th harmonic (40 eV photon energy) was ∼400 fs after a grating monochromator. The band bending of about 110 meV of the p-doped Si(001)(2x2)-Ga surface is completely lifted by illumination of the surface with 1.59 eV laser pulses. The Ga(3d) core level shows a slow time-dependent shift attributed to the build-up (~1 ns) and decay (~100 ns) of the photovoltage. The upper limits for the Ga(3d) core-level shift and broadening on the subpicosecond timescale was determined to be less than 12 meV at the used pump pulse intensity of 20 mJ/cm^2. Experiments with pump pulses of 3.18 eV photon energy showed similar results. Possible reasons for the small core-level shift will be discussed.

O 58.4 Thu 10:45 HE 101

Surface spectroscopy of CO/Pt(111) with High Harmonics in the XUV — •Thorben Haarlammert[1], Sebastian Wegner[1], Grigorius Tsilimis[1], Helmut Zacharias[1], and Alexander Golovin[2] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Münster — [2]Institute of Physics, St. Petersburg State University

We report on the generation of High Harmonic radiation in the photon energy range up to 100 eV with up to 10 kHz repetition rate, based on the conversion of femtosecond Ti:sapphire radiation in rare gases. The fundamental laser is based on a single stage, multiple pass amplification of a cavity-dumped oscillator. Output pulse energies of 1 mJ and pulse durations of les than 30 fs at adjustable repetition rates up to 10 kHz are achieved. The generated High Harmonics are separated by a toroidal grating and directed to the surface. A time-of-flight detector with multiple anodes registers the kinetic energies of emitted photoelectrons. The angular distributions of photoelectrons emitted form CO/Pt(111) under s-polarized excitations have been measured for a variety of initial photon energies. Different from gas phase results a significant intensity of photoelectrons are emitted also in the normal direction, i.e., in the direction of the C - O chemical bond. A first theoretical investigation supports qualitatively the observed angular distributions.

O 59: Molecular Nanostructures

Time: Thursday 9:30–12:00 Location: MA 041

O 59.1 Thu 9:30 MA 041

Organic Molecular Nanowires: N,N'-dimethylperylene-3,4,9,10-bis(dicarboximide) on KBr(001) and NaCl(001) — •Markus Fendrich, Christian Weiss, Manfred Lange, Tobias Kunstmann, and Rolf Möller — Fachbereich Physik, Universität Duisburg-Essen, D-47048 Duisburg

The growth of N,N'-dimethylperylene-3,4,9,10-bis(dicarboximide) (DiMe-PTCDI) on KBr(001) [1] and NaCl(001) has been studied by frequency modulation atomic force microscopy. On both substrates, DiMe-PTCDI forms molecular wires with a length of up to 600 nm at low coverages. The height of the wires is two or more molecular layers; all wires grow along the [110] and [$\bar{1}$10] direction of the alkali halide (001) substrates. There is no wetting layer of molecules: Atomic resolution of the substrates can be achieved between the wires. Due to their size and shape, the molecular nanowires might act as a model system for organic electronics research on insulating substrates. Calculations using empirical potentials reveal possible growth mechanisms for both substrates.

[1] M. Fendrich and T. Kunstmann, Appl. Phys. Lett. 91, 023101 (2007)

O 59.2 Thu 9:45 MA 041

Structural coherency of graphene on Ir(111) — •Coraux Johann, N'Diaye Alpha, Busse Carsten, and Michely Thomas — University of Cologne - Institute of Physics 2, Zuelpicher Str. 77, 50937 Cologne, Germany

We investigate the high structural quality of monolayers of graphene prepared on Ir(111). Using scanning tunneling microscopy, we show that graphene prepared this way exhibits remarkably large-scale continuity of its carbon rows over terraces and step edges. The graphene layer contains only a very low density of defects. These are zero-dimensional defects, edge dislocation cores consisting of heptagon-pentagon pairs of carbon atom rings, which we relate to small-angle in-plane tilt boundaries in the graphene. We quantitatively examined the bending of graphene across Ir step edges. The corresponding radius of curvature compares to those of thin single-wall carbon nanotubes. *J. Coraux, A. T. N'Diaye, C. Busse, T. Michely, submitted.*

O 59.3 Thu 10:00 MA 041

Orientationally ordered (7×7) superstructure of C_{60} on Au(111) — Guillaume Schull and •Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Long range orientational order within C_{60} monolayers on Au(111) is observed with low-temperature scanning tunneling microscopy. A unit cell comprised of 49 molecules which adopt 11 different orientations is found. It can be divided in a faulted and an unfaulted half similar to the (7×7) reconstruction of Si(111). A model is proposed, which shows how through a Moiré-like effect, the substrate induces minute changes in the orientation of the C_{60} molecules. Intermolecular interactions are shown to play a major role in stabilizing the superlattice

O 59.4 Thu 10:15 MA 041

Morphology of C58 layers deposited on HOPG — •Stefan-Sven Jester, Daniel Löffler, Patrick Weis, Artur Böttcher, and Manfred M. Kappes — Institut für Physikalische Chemie, Universität Karlsruhe, 76131 Karlsruhe, Germany

The low energy cluster beam deposition technique, LECBD, has been applied to grow monodisperse layers comprising of mass-selected carbon clusters, so called non-IPR fullerenes, Cn, 50<n<60 /1/. The morphology of the Cn layers deposited on HOPG has been studied by applying atomic force microscopy. The deposition has been performed at hyperthermal kinetic energies, E0, ranging from 1 - 49 eV. The initial capability of the Cn cages to adhere to the surface is governed by the lateral density of step edges which act as pinning and nucleation centers for migrating cages. Consequently the surface exhibits large areas of empty terraces and decorated step edges. The flat terraces become decorated by dendritic Cn islands only in later deposition stages. Both, the mean size of the 2D islands and the mean distance between nearest islands, d, scale with the size of the terraces. The topography of the islands depends sensitively on the primary kinetic energy, E0, and the surface temperature, TS. We explain these findings by considering the loss of the primary kinetic energy induced by molecular friction experienced by the Cn cages during their ballistic sliding/slipping path across the surface /2/.

[1] A. Böttcher, P. Weis, A. Bihlmeier, M.M. Kappes, PCCP 6 (2004) 5213 [2] a) W.D. Luedtke and U. Landman, Phys. Rev. Lett. 82 (1999) 3835, b) E. Molinari, M. Tomellini, Surf. Sci., 601 (2007) 1

O 59.5 Thu 10:30 MA 041

A scalable open-pore network: melamine and fatty acids on graphite — •Hermann Walch, Anne-Kathrin Maier, Wolfgang M. Heckl, and Markus Lackinger — LMU München, Sektion Kristallographie, Theresienstr. 41, 80333 München

Scanning tunneling microscopy (STM) at the liquid-solid interface was utilized to investigate bimolecular open pore networks comprised of melamine and the homologous series of fatty acids extending from pentanoic through dodecanoic acid. Since at room temperature longer fatty acids (from decanoic acid on) are solid a novel heatable sample holder for measuring at slightly elevated temperatures was designed. Structural properties of the self-assembled mononlayers (SAMs) were deduced from the STM data and modelled by force field calculations. Melamine is a heterocyclic aromatic molecule consisting of a triazine ring functionalized with three amine-groups at the 2-, 4-, and 6-positions. In this study, the fatty acids serve as a solvent for melamine but are also incorporated into the SAMs. For all solvents hexagonal honeycomb structures were observed, where the lattice parameter increases linearly from 2.8 nm to 3.8 nm with the chain length of the solvent. All networks exhibited a similar architecture: melamine molecules are located at the corner of hexagons and two adjacent melamins are interconnected by fatty acid molecules in head to tail configuration. Each of the connecting fatty acid molecules forms two H-bonds with one of the melamine molecules. Hence, melamine accounts for the symmetry of the structures, whereas the fatty acid molecules act as a spacer, thus giving rise to the remarkable scalability of these bimolecular networks.

O 59.6 Thu 10:45 MA 041

Aromatic vs. Hydrogen Bonds in Self-Assembled Monolayers of Organic Molecules, a STM-Study — •Rico Gutzler, Sophie Lappe, Wolfgang M. Heckl, and Markus Lackinger — LMU München, Sektion Kristallographie, Theresienstr. 41, 80333 München

The monolayer structure of two distinct organic molecules is investigated by STM. We demonstrate how a small modification of a polyaromatic molecule, which does not affect the functional groups, can have dramatic impact on the structure of the self-assembled monolayer. Both molecules exhibit C3 symmetry, have a central benzene ring in common and three carboxylic groups at the 1,3,5 positions, each separated by a rigid spacer. One compound exhibits methyl groups at the 2,4,6 positions of the central benzene ring, the other remains unsubstituted. This change in molecular structure was found to result in completely different self-assembly behaviour at the liquid-graphite interface. The unsubstituted molecule adsorbs in a row structure, where the molecules are stacked with their planes almost perpendicular to the substrate. The methylated molecule self-assembles into a sixfold chickenwire network where the molecules are adsorbed planar. Based on our experimental finding and supported by force field calculations, we propose that in the first case the intermolecular binding is dominated by aromatic interaction between the extended pi-electron systems, whereas in the latter case the chickenwire structure is driven by twofold intermolecular hydrogen bonds between the peripheral carboxylic groups. This finding is explained by weakening of the pi-pi stacking due to steric hindrance imposed by the methyl groups.

O 59.7 Thu 11:00 MA 041

Template Readout of Hierarchical Coordination Networks at Surfaces — •Alexander Langner[1], Steven L. Tait[1], Nian Lin[1], Chandrasekar Rajadurai[2], Mario Ruben[2], and Klaus Kern[1,3] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart — [2]Forschungszentrum Karlsruhe GmbH — [3]Ecole Polytechnique Fédérale de Lausanne, Switzerland

Self-assembly of organic molecules into supramolecular networks is an efficient strategy to pattern surfaces with functional nanostructures. Highly ordered architectures can be achieved if the spontaneous self-organization process is steered by selective and directional non-covalent interactions. Here we demonstrate that from a mixture of organic ligands, several unique structures can be "read out" by adjusting the external environment of the mixture. We report on the self-organization of mixtures of multiple ligands with metal atoms at the Cu(100) surface under ultra high vacuum (UHV) conditions. The generated architectures exhibit a hierarchy of supramolecular interactions: highly stable metal-organic coordination bonding and somewhat weaker hydrogen bonding. With scanning tunneling microscopy (STM) we demonstrate that modification of external parameters, e.g. commensurability with substrate or introduction of guest molecules, causes distinct structural configurations for identical ligand binding units, even leading in some cases to complete ligand segregation. Due to the hierarchy of bonding strengths, it is possible to modify only the lower level of structural organization resulting in new metal-organic architectures with identical primary structural units.

O 59.8 Thu 11:15 MA 041

Structure and Charge Transfer in Metal-TCNQ Complexes on Cu (100) — •Tzu-Chun Tseng[1], Steven L. Tait[1], Xiong Liu[1], Nian Lin[1], and Klaus Kern[1,2] — [1]Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]Institut de Physique des Nanostructures, Ecole Polytechnique Fédéral de Lausanne (EPFL), 1015 Lausanne, Switzerland

Organic-based alternatives to conventional magnets offer the possibility to form self-organized nanometer-scale structures at surfaces with specific magnetic properties. For example, coordination compounds of metal ions (M) with the organic molecule 7,7,8,8-tetracyanoquinodimethane (TCNQ) in solution have been shown recently to have a high magnetic ordering temperature for large M:TCNQ ratios (R. Jain et al., Nature 445 (2007) 291-294). A critical issue for the development of metal-organic structures in magnetic or electronic applications is the relationship of electronic configuration to physical structure. Here we correlate structural information of 2D M-TCNQ (M = Mn, Fe, Co, Ni, Cu) networks from scanning tunneling microscopy and low energy electron diffraction with charge transfer information obtained by X-ray photoemission spectroscopy. M-TCNQ mixtures at Cu(100) self-organize into ordered structures, whose coordination ratio and domain size depend strongly on the choice of metal. XPS results identify distinct core level shifts in N 1s spectra of M-TCNQ for 2D coordination to different metal centers compared to neutral TCNQ.

O 59.9 Thu 11:30 MA 041

Video-STM investigation of the dynamic behavior of bis-terpyridine submonolayers on Ag(111)-oriented films — •Thomas Waldmann, Harry E. Hoster, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

We present a quantitative analysis of the dynamic exchange of single molecules between two phases [1] of a bis-terpyridine derivative (2,4'-BTP) [2] adlayer adsorbed on Ag(111)-oriented thin films on Ru(0001). The analysis is based on video-STM measurements in ultra high vacuum at room temperature. The adlayer was produced by evaporation on a highly ordered (111)-oriented Ag film, which leads to the formation of a quasi-quadratic network (QQN) [2, 3]. Via thermal desorption it is possible to create defects in the QQN, which leads to a new disordered phases with a quasi-hexagonal short-range order (QHP). Depending on the BTP coverage 70-90% of the molecules in the QHP are rotating, while the rest exhibits preferred orientations in steps of 30°. At the QQN/QHP phase boundary, we observed molecules jumping back and forth between both phases. From the different probabilities to find the molecules in either phase we estimated the corresponding energy difference via a Boltzmann-approach.

[1] Poster O 18.58

[2] C.Meier et al., J.Phys.Chem.B 109, 21015 (2005)

[3] H.E.Hoster et al., Langmuir 23, 11570 (2007)

O 59.10 Thu 11:45 MA 041

Bottom-up construction of covalently bound molecular nanostructures — •Leonhard Grill[1], Matthew Dyer[2], Leif Lafferentz[1], Mats Persson[2], Maike Peters[3], and Stefan Hecht[3] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, Berlin — [2]Department of Chemistry, University of Liverpool, Liverpool L69 3BX, UK — [3]Institut für Chemie, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 2, Berlin

The ultimate goal of molecular electronics consists in the use of single functionalized molecules for circuits at the atomic scale. In possible future applications, such molecular arrays need to be highly stable and allow charge transport between the molecular building blocks. Hence, covalent bonds are desired for the intermolecular connections. However, up to now only rather weak interactions have been reported for supramolecular networks on surfaces.

We report on the controlled formation of covalently bound networks of porphyrin molecules on a gold surface upon deposition of thermally activated molecular building blocks and their subsequent chemical reaction at predefined connection points [1]. Scanning tunneling spectroscopy measurements, lateral manipulation, and density functional theory calculations unambiguously reveal the covalent character of the intermolecular bonds. Furthermore, we show that the dimensions and shape of these nanostructures can be precisely engineered by controlling the number of bromine substituents of the molecular building block, leading to the formation of dimers, chains and networks.

[1] L. Grill et al., Nature Nanotech. 2, 687 (2007).

O 60: Symposium: Bimetallic Nanosystems: Tuning Physical and Chemical Properties I (Invited Speakers: Harald Brune, Michael Hilgendorff, Konstantin Neyman)

Time: Thursday 9:30–12:15 Location: MA 005

Invited Talk O 60.1 Thu 9:30 MA 005
Interface *vs.* Alloy Contribution to Magnetic Anisotropy in Bi-Metallic Nanostructures — •Harald Brune — Swiss Federal Institute of Technology (EPFL), Lausanne, Switzerland

We investigate the magnetic anisotropy of atoms located at atomically sharp interfaces between two metals and of those situated in a homogeneous alloy. The numbers we derive enable to estimate whether homogeneous alloys or onion type alternations of two metals lead to higher anisotropies for a given size. The model systems are two-dimensional bi-metallic islands on Pt(111). The magnetic properties are determined by means of magneto-optical Kerr effect for island ensembles for which the morphology is derived from STM.

The blocking temperature of $\mathrm{Fe}_x\mathrm{Co}_{1-x}$ alloy islands is highest for $x = 0.5$ and with $T_\mathrm{b} = 160$ K two times higher than the one of pure Co ($T_\mathrm{b} = 90$ K) or pure Fe islands ($T_\mathrm{b} = 80$ K) of identical size and shape. This yields to an alloy contribution to the barrier for thermally induced magnetization reversal of $E_\mathrm{alloy} = 0.14$ meV/atom. Co-core–Fe-shell islands reveal a steep increase of T_b, starting with minute amounts of Fe and ending at a shell being only 2 atomic rows wide. Further addition of Fe leads to a much more shallow increase of T_b, similar to the one of pure Fe or Co. From this behavior we infer that the interface between Co and Fe contributes by $E_\mathrm{int} = 0.9$ meV/pair. These values suggests that abrupt 1D interfaces between two metals have significantly higher anisotropies than homogeneous alloys. For Co islands decorated by Pd we find very different anisotropies for lateral compared with vertical interfaces.

Invited Talk O 60.2 Thu 10:00 MA 005
Magnetic-Noble Metal Nanocomposites with Size-Dependent Magnetic Properties and Morphology-Dependent Optical Response — •Michael Hilgendorff — caesar research center, Bonn, Germany

This talk aims at presenting the preparation and the properties of bimetallic magnetic AgCo, PtCo, and PdCo core/shell nanocrystals and Au-CoPt3, Ag-CoPt3, and Au-FePt heterodimers.

Stable bimetallic AgCo, PtCo, and PdCo core/shell colloids with a narrow particle size distribution and a controlled shell-thickness have been obtained in organic solvents (toluene, diethylether or dioctylether) by means of wet chemistry. All three bimetallic particle systems are ferromagnetic at low temperatures and superparamagnetic at room temperature. Coercivity, blocking temperature, and oxidation stability depend on the thickness of the Co-shell.

The bimetallic heterodimers have been prepared by a seeded-growth approach in the presence of a cationic surfactant (cetyltrimethylammonium bromide, CTAB). Hydrophobic CoPt3 and FePt nanoparticles were transferred into water using CTAB as a phase-transfer agent and were subsequently used as seeding materials for the reduction of gold and silver precursors to produce the nanocomposites. Through the modification of the growth conditions, Au-CoPt3 nanocomposites with various morphologies (spheres, cubes, rods) were prepared, providing an opportunity to tailor the optical response of these composite nanoparticles while maintaining the magnetic properties of the original seeds, even upon phase transfer into water.

Invited Talk O 60.3 Thu 10:30 MA 005
Density functional studies of bimetallic nanosystems — •Konstantin Neyman — ICREA, Dept. de Química Física & IQTCUB, Universitat de Barcelona, Barcelona, Spain

Impressive progress in the computer performance together with drastically increased software efficiency has been recently achieved. This enabled computational studies of building blocks of metallic nanostructures that contain ˜100 (and more) atoms, thus approaching dimensions of the species dealt with experimentally, to be performed almost routinely using accurate density functional methods. In this way, even more complex nanosystems consisting of more than one metal also became treatable at this high computational level.

Opportunities for density functional calculations of bimetallic nanosystems will be discussed and the present status of the theoretical research in the field will be overviewed in the talk. Examples will be provided to illustrate effects of the second metal M in bimetallic nanoparticles and thin films Pd(1-x)M(x), (M = Zn, Ag, Au) on the adsorption properties and surface reactivity. Adsorbate-induced restructuring of bimetallic surfaces will also be addressed.

O 60.4 Thu 11:00 MA 005
Irradiation effects in FePt nanoparticles — Michael Müller and •Karsten Albe — Institut f. Materialwissenschaft, TU Darmstadt, Petersenstr. 23, D-64287 Darmstadt

FePt nanoparticles are a promising candidate material for ultra high density data storage because of their huge magnetic anisotropy energy in the chemically ordered L1_o phase (fct). Particles can be prepared in ordered arrays, but are mostly disordered and also occur in multiply twinned configurations. Since thermal annealing leads to a destruction of the patterned arrays, alternative methods are needed to transform the particles into the thermodynamically stable single crystalline ordered phase. In this contribution we use atomic scale computer simulations in order to study the possibility of structural modification and enhanced ordering of L1_o nanoparticles by ion irradiation. Molecular dynamics simulations are used to investigate defect production and sputtering as well as phase transformation processes in twinned and single-crystalline nanoparticles. Lattice-based Kinetic Monte Carlo simulations are employed in order to study the influence of athermal vacancies on the ordering kinetics. We compare the case of He-irradation at low and elevated temperatures while taking into account defect production and sputtering yields as obtained from our MD-simulations.

O 60.5 Thu 11:15 MA 005
Non-Intensive Phase Diagrams of Pt-Rd Nanoalloys — Johann Pohl, •Karsten Albe, and Mathias Nalepa — Institut f. Materialwissenschaft, TU Darmstadt, Petersenstr. 23, D-64287 Darmstadt

We present computer simulation studies on size dependent phase diagrams of Pt-Rh nanoparticles, which exhibit ordered low temperature phases. We will first give a short review of a refined BOS mixing model, which is used in lattice Monte-Carlo simulations. These simulations serve as input for the thermodynamic integration of free energies as function of size and composition. The resulting phase diagrams will be discussed for different particle sizes. We specifically address the question of how to interpet a two-phase regions in the phase diagram and explore the role of surface segregation. Finally, the kinetics of alloying processes is studied for free and supported particles by dynamic Monte-Carlo simulations.

O 60.6 Thu 11:30 MA 005
Doping of monoatomic Cu chains with single Co atoms — •Christophe Nacci, Jérôme Lagoute, and Stefan Fölsch — Paul Drude Institute for Solid-State Electronics, Hausvogteiplatz 5-7, 10117 Berlin, Germany

Close-packed Co-Cu chains (interatomic spacing 255 pm) of various length and composition were assembled from single Co and Cu atoms on Cu(111) by atom manipulation in a low-temperature scanning tunneling microscope [1]. Co atoms can be attached to monoatomic Cu chains to terminate the structure but also incorporated into the chain to occupy a predefined site. Local spectroscopy reveals significant electronic Co-Cu coupling leading to confined quantum states delocalized along the heteroatomic chain. The quantum state densities of composite Co-Cu chains are modified compared to those of pure Cu chains [2]. The modifications are well reproduced by a simple tight-binding analysis. Co-Cu chains provide an interesting model case in which the quantum state of an atomic-scale host structure can be tuned by the controlled incorporation of foreign atoms.

[1] J. Lagoute, C. Nacci, S. Fölsch, Phys. Rev. Lett. **98**, 146804 (2007)

[2] S. Fölsch, P. Hyldgaard, R. Koch, K. H. Ploog, Phys. Rev. Lett. **92**, 56803 (2004)

O 60.7 Thu 11:45 MA 005
Optical properties of supported core-shell and alloy silver/gold nanoparticles — •Frank Hubenthal and Frank Träger — Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

For many applications like surface enhanced Raman scattering in which the optical field enhancement associated with surface plasmon excitation is exploited, tunability of this collective resonance over a wide range is required. For this purpose we have prepared core-shell and alloy nanoparticles consisting of Ag and Au. The core-shell nanoparticles were made by subsequent deposition of Ag and Au atoms and vice versa on dielectric substrates followed by diffusion and nucleation. One of the most interesting among the numerous results is that the plasmon frequency can be tuned from 2.8 eV (442 nm) to 2.1 eV (590 nm) depending on the Au shell thickness. Subsequent annealing of the core-shell nanoparticles causes a shift of the resonance frequency to 2.6 eV. Theoretical modelling allows us to attribute this observation to the formation of alloy nanoparticles. Finally, we have measured the dephasing time T2 of the alloy nanoparticles by means of spectral hole burning. T2 amounts to 8.1 +/- 1.6 fs, in good agreement with the dephasing time T2 = 8.9 fs that is included in the dielectric function of the bulk.

O 60.8 Thu 12:00 MA 005

Tuning of the particle plasmon resonance in 2D and 3D polymer nanocomposites with bimetallic alloy particles prepared by vapor phase co-deposition — •Vladimir Zaporojtchenko, Venkata Sai Kiran Chakravadhanula, Haile Takele, Carolin Schulz, Thomas Strunskus, and Franz Faupel — Chair for Multicomponent Materials, Institute for Materials Science, Christian-Albrechts University at Kiel, Kaiserstr. 2, Kiel, Germany, 24143.

2D- and 3D- nanocomposite films consisting of bimetallic Ag-Cu or Ag-Au nanoparticles embedded in a nylon matrix were prepared by co-deposition of the components from three different evaporators in high vacuum. The microstructure of the nanocomposites and of the nanoparticles were investigated by TEM, XPS, XAFS, Electron Loss Spectroscopy and UV-Visible spectroscopy, with a focus on alloy formation, and the changes of the plasmon resonance bands. Shifts of the plasmon resonance of bimetallic alloy nanocomposites in a large spectral range (between 300 and 1000 nm) were observed by varying the ratio of the involved metals at a constant metal filling factor in the composites. The influence of substrate temperature on alloy formation in the core-shell nanoparticles was also studied. Shifting of the particle plasmon resonance either excited by light absorption or low energy electron scattering opens a new possibility to study the alloy formation in bimetallic nanoparticles.

O 61: SYEC: Exact-Exchange and Hybrid Functionals Meet Quasiparticle Energy Calculations I (Invited Speakers: Gustavo Scuseria, Andreas Görling, Georg Kresse, Angel Rubio, Mark van Schilfgaarde, Michael Rohlfing; FV: O+HL+DF+TT)

Time: Thursday 9:30–12:30 Location: A 151

See SYEC for details about the program.

O 62: Metal Substrates: Adsorption of Inorganic Molecules

Time: Thursday 9:30–12:30 Location: MA 042

O 62.1 Thu 9:30 MA 042

Tuning Surface Energy Landscapes in Metallic Quantum Films using Alkali Adsorbates — •Alexander Khajetoorians[1], Shengyong Qin[1], Wenguang Zhu[2], Holger Eisele[1], Zhenyu Zhang[2], and Chih-Kang Shih[1] — [1]Department of Physics, University of Texas at Austin, Austin, Texas, USA — [2]Solid State Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

Quantum confinement shows a strong interplay with growth and kinetics in thin metal systems where the Fermi wavelength has a special relationship to the surface normal lattice constant. In the case of Pb/Si(111) systems, this relationship reveals an interesting thickness-dependent bilayer oscillation in the density of states up to a phase. In the limit where surface energy oscillations are strong, this interplay can result in the formation of magic quantum stable islands and film thicknesses. In this paper, we report on a novel effect: tuning of the energy landscape of a flat-top quantum Pb mesa using Cs adsorbates. Using STM/STS, we show that depositing Cs adsorbates on a thin Pb mesa promotes quantum stable Pb nanoislands on preferentially unstable thicknesses. Thickness-dependent nanoisland densities show a strong bilayer oscillation correlating with quantum stability. By modifying the Cs coverage on the mesa surface, we can tune the lateral size distribution of the nanoislands and the overall amplitude of the island density oscillation. Nanoisland formation seems intricately linked to a step decoration of Cs adatoms along the step edge of the nanoisland. The role of surface reactivity on these properties will also be discussed. Support: NSF-IGERT DGE-0549417; NSF-FRG 26-1126-8750

O 62.2 Thu 9:45 MA 042

Quantum size effects on the adsorption of rare gases on Ag monolayer covered noble metal surfaces — •Frank Forster, Andreas Nuber, Hendrik Bentmann, Johannes Ziroff, and Friedrich Reinert — Universtät Würzburg, Experimentelle Physik II, 97074 Würzburg, Germany

In the recent past it has been demonstrated that Shockley states on (111) surfaces of Cu, Ag, and Au are a sensitive probe for interactions between surfaces and adsorbates. Their significant change in binding energy, band mass and spin-orbit coupling allows an access to the comprehension of adsorption mechanisms like physisorption. On the example of Xe monolayers on noble metal surfaces we show vice versa that the Shockley states influence the adsorption dynamics of rare gas atoms. For that purpose we present real-time and high resolution ARPES investigations on Xe adsorption on Cu(111) and Au(111) substrates with Shockley states modified by a pre-adsorption of layer-by-layer grown Ag-films of various thickness. In the case of Xe on Ag/Cu(111) we found that the rare gas prefers the adsorption on the thickest Ag film to the disadvantage of thinner layers or the clean substrate. A similar behaviour could be observed for Ag/Au(111) with the exception of a single Ag layer, which is always unfavoured for Xe coverage. Within a simplified model, the local DOS of the Shockley state at the modified surfaces are compared to the obtained ARPES results.

O 62.3 Thu 10:00 MA 042

Insight into water molecules bonding on 4*d* metal surfaces — •Javier Carrasco[1], Angelos Michaelides[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]London Centre for Nanotechnology and Department of Chemistry, University College London, London WC1E 6BT, United Kingdom

H_2O-metal interactions are of capital importance to a wide variety of phenomena in materials science, catalysis, corrosion, electrochemistry, etc. Here we address the nature of the bond between water molecules and metal surfaces through a careful systematic study. Specifically, the bonding of isolated H_2O molecules to a series of close-packed transition metal surfaces—Ru(0001), Rh(111), Pd(111) and Ag(111)—has been examined in detail with density functional theory (DFT). Aiming to understand the origin behind energetic and structural trends along the 4*d* series we employ a range of analysis tools, such as decomposition of the density of states, electron density differences, and inspection of individual Kohn-Sham orbitals. The results obtained allow us to rationalize the bonding between water and transition metal surfaces as a balance of covalent and electrostatic interactions. A frontier orbital scheme based on so-called two-center four-electron interactions between molecular orbitals of H_2O— mainly $3a_1$ and $1b_1$—and d band states of the surface proves incisive in understanding these systems.

O 62.4 Thu 10:15 MA 042

Adsorption and thermal decomposition of NO_2 on two

stepped platinum surfaces — •Michael Peter Andreas Lorenz[1], Regine Streber[1], Christian Papp[1], Andreas Bayer[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

The adsorption of NO_2 on stepped Pt surfaces, namely Pt(322) and Pt(355), and its behaviour during heating to elevated temperatures was studied by in-situ high resolution XPS using synchrotron radiation at BESSY II. The motivation for our study was to obtain high oxygen precoverages, in order to study CO oxidation on stepped surfaces in this coverage regime. For the flat Pt(111) surface, Dahlberg et al. [1] showed that by dosing NO_2 oxygen coverages can be obtained, which are three times higher than those obtained by conventional exposure to O_2; for the more reactive stepped surfaces one could expect even higher coverages. Our study shows that at low temperatures, up to 250 K, NO_2 molecularly adsorbs on both surfaces as could be observed in the O 1s and N 1s regions. During heating, NO_2 starts to decompose to NO and O above 270 K. Thereby, NO desorbs completely up to 400 K. Significantly higher oxygen coverages than those formed by dissociation of O_2 can only be reached by adsorption of NO_2 at 400 K, resulting in the formation of clean oxygen layers without any nitrogen impurities. Supported by BMBF (05 ES3XBAI5).

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O 62.5 Thu 10:30 MA 042

Kinetic passivation of steps with sulfur and CO/S site exchange processes on stepped Pt surfaces

— •Regine Streber[1], Christian Papp[1], Michael Peter Alexander Lorenz[1], Andreas Bayer[1], Reinhard Denecke[2], and Hans-Peter Steinrück[1] — [1]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstrasse 3, 91058 Erlangen — [2]Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnéstrasse 2, 04103 Leipzig

We studied the influence of sulfur on the adsorption and thermal evolution of CO on the stepped Pt(355) and Pt(322) surfaces by in-situ XPS. At low temperatures, we observe a passivation of the step sites for both surfaces, along with a decrease of the total CO coverage. Upon heating the CO covered surfaces a repopulation of the step sites with CO occurs at 185 K for Pt(355) and 240 K for Pt(322). For Pt(355), finally the same step coverage as for the clean surface is obtained, whereas for Pt(322) only half the value of the clean surface is found. This behavior is attributed to the S induced formation of double steps on Pt(322), which are stable in the investigated temperature range. From the lifting of the step passivation by sulfur upon heating for both surfaces we conclude that, under the experimental conditions applied, an occupation of steps sites by CO is energetically favored over occupation with S, with the CO-S site exchange process being kinetically hindered at low temperatures. The differences found for the two different step orientations are attributed to differences in the electronic structure and local adsorption sites. Supported by BMBF (05 ES3XBA/5).

O 62.6 Thu 10:45 MA 042

Adsorption of CO on Ni decorated Rh(553)

— Priyanka Singnurkar, Hans Peter Koch, and •Robert Schennach — Instiute of Solid State Physics, Graz University of Technology, Austria

Carbon monoxide is a widely used probe molecule in surface science. In addition, it is an important reactant and intermediate in several catalytic reactions (e.g. oxidation of carbon monoxide to carbon dioxide in automotive catalysts), making the adsorption and reaction of carbon monoxide a thoroughly investigated system on many different metal surfaces. In the work presented here, the adsorption and desorption of carbon monoxide on Ni decorated steps on Rh(553) has been studied using reflection absorption infra red spectroscopy (RAIRS) and thermal desorption spectrometry (TDS). Previous scanning tunneling microscopy (STM) experiments have shown, that the Rh(553) surface has rather stable mono atomic steps. The steps are (111) oriented and the (111) terraces are 4 atomic rows wide, as can be predicted from the crystal structure. The steps of the Rh(553) surface can be decorated by evaporating about 0.2 mono layer Ni under ultra high vacuum conditions and at a substrate temperature of 150°C, leading to one to two atoms wide Ni wires running along the steps of the Rh(553) substrate, according to STM data. No carbon monoxide dissociation is found when the steps are decorated with Ni. TDS results and RAIRS results on the Ni decorated surface are discussed with respect to the results obtained with the clean Rh(553) surface.

O 62.7 Thu 11:00 MA 042

Towards a full undertanding of the “CO Adsorption”puzzle: advanced many-body electronic structure calculations of CO-adsorbed Cu custers

— •Xinguo Ren[1], Patrick Rinke[2], and Matthias Scheffler[1,2] — [1]Fritz-Haber-Institut der MPG, 14195 Berlin, Germany — [2]Materials Reserach Lab, University of California at Santa Babara, CA 93106

Density functional theory, within its present-day local/semi-local approximations (LDA/GGA), has known difficulties for describing certain surface chemical processes. For instance, for a CO molecule adsorbed at the Cu(111) surface, both LDA and GGA predict the wrong adsorption site, favoring the threefold-coordinated hollow site rather than the onefold-coordinated top one [1]. The energetic order of these two adsorption sites can be correctly reversed by applying a “local XC correction”scheme [2], in which an exchange-correlation (XC) energy correction can be obtained by using an improved XC treatment for relatively small clusters. However, such single-point total energy calculations do not reveal the underlying mechanism behind the improved description. To shed new light on the “CO adsorption puzzle”we have performed quasiparticle energy calculations for CO adsorbed on selected Cu clusters in second-order Møller-Plesset perturbation theory and the *GW* approach. The resultant energy spectra are analyzed in terms of charge transfer and energy level shifts with respect to LDA/GGA. [1] Feibelman *et al.*, J. Phys. Chem **105**, 4018 (2001). [2] Q.-M. Hu, K. Reuter, and M. Scheffler, Phys. Rev. Lett **98**, 176103 (2007); **99**, 169903(E) (2007).

O 62.8 Thu 11:15 MA 042

New adsorption states of carbon monoxide on Cu(110)

— •Erkan Demirci and Adolf Winkler — Graz University of Technology, Institute of Solid State Physics, Graz, Austria

The adsorption of carbon monoxide on a Cu(110) surface has been investigated by Auger electron spectroscopy (AES), thermal desorption spectroscopy (TDS) and low energy electron diffraction (LEED). The carbon monoxide desorption spectra as known from literature exhibit only a peak at 210K (α state) when adsorption takes place at T = 100 K -150 K, correlated with a (2x1) superstructure [1,2]. When CO is adsorbed at 180 K and using high enough exposure the TDS clearly shows additional peaks at 245 K, 290 K and 355 K (β_1, β_2, β_3 states). The population of these peaks is adsorption temperature dependent. The peak maxima of β_1 and β_2 shift to higher temperature with increasing coverage, in contrast to the α and β_3 peaks, which show coverage independent peak maxima. LEED shows a (1x2) superstructure when CO is adsorbed at 300 K. From these results we conclude that a missing row reconstruction is induced by CO, which leads to the new adsorption states. Additional quantitative TDS and angle resolved TDS measurements were performed to support this idea. *Financial support by the Austrian Science fund (FWF), Proj. No. P 20026 is gladly acknowledged.*

[1] C. Harendt, J. Goschnick and W. Hirschwald, Surf. Sci. 152/153 (1985) 453

[2] K. Horn, M. Hussain and J. Pritchard, Surf. Sci. 63 (1977) 244

O 62.9 Thu 11:30 MA 042

Monte-Carlo lattice gas simulation of the thermal desorption behavior of CO from Pt_xAu_{1-x}/Pt(111) surface alloys

— •Harry E. Hoster[1], Yoshihiro Gohda[2], Andreas Bergbreiter[1], Menhild Eyrich[1], Joachim Bansmann[1], Axel Gross[2], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, 89069 Ulm, Germany — [2]Institute of Theoretical Chemistry, Ulm University, 89069 Ulm, Germany

The thermal desorption behavior of CO adsorbed on Pt_xAu_{1-x}/Pt(111) surface alloys was studied by Monte Carlo simulations in a lattice gas approximation [1,2], comparing different Pt:Au ratios and initial CO_{ad} coverages. Based on thermal desorption data and DFT calculations, the CO molecules preferentially occupy Pt on-top sites of Pt_xAu_{1-x}/Pt(111) surface alloys, and the adsorption energies are approximately constant for different numbers of neighboring Au atoms (ligands). Au sites are not occupied at room temperature. The atomic distribution in the surface layer used in the simulations was derived from STM data with chemical contrast, and the adsorption energies stem from DFT calculations. At higher CO_{ad}-coverages, the CO-CO repulsions are considered via a pair interaction parameter determined by fitting to the experimental data. The accuracy of the lattice gas approach for inhomogeneous surfaces is discussed by comparing with the experimental thermal desorption data.

[1] J.L.Sales, G.Zgrablich, V.P.Zhdanov, Surf.Sci 209(1989)208

[2] V.P.Zhdanov, J.L.Sales, R.O.Unac, Surf.Sci.Lett.381(1997)L599

O 62.10 Thu 11:45 MA 042

CO adsorption on bimetallic Au$_x$Pt$_{1-x}$ surface alloys studied by TPD and IRAS — •Menhild Eyrich, Heinrich Hartmann, Thomas Diemant, Andreas Bergbreiter, Harry Hoster, Joachim Bansmann, and Rolf Juergen Behm — Institute of Surface Chemisty and Catalysis, Ulm University, D-89069 Ulm, Germany

The interaction of CO with bimetallic Au$_x$Pt$_{1-x}$ surface alloys supported on Pt(111) is investigated by temperature programmed desorption and infrared reflection absorption spectroscopy to study the influence of the Au content on the chemical properties of the surface alloys. The surface composition and the distribution of surface atoms were determined by scanning tunnelling microscopy, showing a tendency for the segregation of both metals on the surface. Due to the preference for the formation of homo-atomic domains, the adsorption of CO on the Pt part of the surface alloys is only weakly affected up to very high Au concentrations and very similar to the pristine Pt(111). This behaviour is manifested in an almost constant initial CO desorption energy and the successive occupation of on-top and bridged adsorption sites with increasing CO coverage. Since the adsorption of CO is not possible on the Au part of the surface alloys under the conditions of this study, a decrease of the CO saturation coverage and of the initial sticking coefficient are observed with increasing Au content.

O 62.11 Thu 12:00 MA 042

CO adsorption on Ag/Pd(111) surface alloy — •Yunsheng Ma, Joachim Bansmann, and Rolf Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

The growth of Ag on Pd(111), Ag/Pd surface alloy formation and the chemical properties of these surfaces using CO probe molecules were studied by X-ray Photoemission Spectroscopy (XPS), CO Temperature Programmed Desorption (TPD) and High Resolution Electron Energy Loss Spectroscopy (HREELS). At room temperature, thermal evaporation of Ag leads to a layer-by-layer growth mode on Pd(111) [1]. Annealing the Ag film induces a down-shift of the binding energy of the Ag 3d peak by 0.6 eV, indicating surface alloy formation. CO desorption peaks in the temperature range between 350 K and 500 K are observed upon varying the Ag/Pd ratio of the surface alloy. The different CO TPD peaks obtained on Ag/Pd surface alloys can be attributed to CO desorption from different Pd/Ag or Pd ensemble. The results are discussed in comparison with previous experimental and theoretical results on Au/Pd(111) [2].

[1] B. Eisenhut, J. Stober, G. Rangelov, Th. Fauster, Phys. Rev. B 47 (1993) 12980

[2] M. Ruff, N. Tahehiro, P. Liu, J.K. Norskov, R.J. Behm, Chem. Phys. Chem. 8 (2207) 2068

O 62.12 Thu 12:15 MA 042

Interaction of CO and H$_2$ with Zn/ZnO modified Pd(111) surfaces — •Markus Kratzer[1], Anton Tamtögl[1], Jörg Killmann[1], Robert Schennach[1], Adolf Winkler[1], Gunter Weirum[1], and Svetlozar Surnev[2] — [1]Institute of Solid State Physics, Graz University of Technology — [2]Department of Physics, Karl-Franzens University Graz

Due to its increased use in methanol reforming the Zn/Pd and ZnO/Pd system came to the fore of surface science. Especially, the interaction with CO and hydrogen with these surfaces is of specific importance. In this work the adsorption/desorption kinetics of CO and H$_2$ on Zn and ZnO thin film covered Pd(111) was studied using TPD, LEED, AES and STM. TPD, LEED and AES results show that the ZnO modified palladium surfaces undergo a change in the surface configuration during CO and H$_2$ desorption due to reduction of the ZnO layer. In case of CO-TPD temperatures up to 650 K are required, which additionally lead to the formation of a ZnPd alloy. In the literature one can find UPS measurements as well as DFT based calculations that point out that ZnPd alloys should have similar electronic properties as the Cu(111) surface [1]. Indeed, CO desorption on Zn covered Pd(111) shows a similar low temperature desorption peak at 220 K as measured on Cu-surfaces [2].

This work was supported by the Austrian Science Fund: Project Nr. P20016 and P19198.

[1] A. Bayer et.al. Surface Science, 600 (2006) 78

[2] S. Vollmer et.al. Catalysis Letters 77 (2001) 97

O 63: Symposium: Frontiers of Surface Sensitive Electron Microscopy II (Invited Speakers: Jürgen Kirschner, Liviu Chelaru, Michael Bauer, Claus Schneider)

Time: Thursday 9:30–12:30 Location: MA 043

Invited Talk O 63.1 Thu 9:30 MA 043

Development of a "momentum microscope" for imaging of valence band electron states — •Juergen Kirschner[1], Burkhard Kroemker[2], and Matthias Escher[3] — [1]MPI fuer Mikrostrukturphysik, Weinberg 2, 06120 Halle — [2]Omicron Nanotechnology GmbH, Taunusstein — [3]Focus GmbH, Hünstetten-Hesselsbach

Our aim is to image the momentum distribution of photoexcited valence band electron states in an energy plane through the Brillouin Zone. Our design is based on a modified NanoESCA comprising a Photoelectron Emission Microscope (PEEM) with an imaging energy filter. The basic idea is not to use the real space image from the objective lens but to transfer the momentum image in the focal plane into a hemispherical analyzer by an additional transfer lens. The aberrations of the analyzer are compensated by a second hemisphere such that the inner electron trajectories in the first sphere become the outer trajectories in the second sphere. Thus, an aberration corrected image of the angular distribution of the electrons leaving the sample within a certain area (˜ 70 μm diameter) appears at the exit of the second analyzer. The projected image displays the dispersion of the valence electrons within a plane of constant energy. The full valence band can be observed by a sequence of parallel cuts through the Brillouin zone. Because of the parallel detection of all electrons within a given energy window the process is very fast. We demonstrate with a Cu(111) surface and a standard discharge laboratory source (HeI) that complete dispersion planes can be obtained within a couple of minutes.

Invited Talk O 63.2 Thu 10:00 MA 043

Imaging Surface Plasmon Polaritons: Time-resolved Two-Photon Photoelectron Emission Microscopy — •Liviu I. Chelaru — Institut für Festkörperforschung, Elektronische Eigenschaften, Forschungszentrum Jülich, Germany

Routing and manipulation of light on nanoscale metallic circuits as surface plasmon polaritons (SPPs) is seen today as a way of integrating microscale photonics and nanoscale electronics on the same chip. A fundamental understanding of the interaction between light and metallic nanostructures is an essential prerequisite for the realisation of functional devices based on SPPs. In this presentation I will focus on the excitation and propagation of SPPs in single-crystalline Ag nanostructures of different shapes and sizes that are formed in-situ by self-assembly during deposition on Si surfaces. Imaging of the SPPs is accomplished by time-resolved two-photon photoelectron emission microscopy (TR-2PPEEM). Here the excited SPP wave is visualised as a result of the interference (beat pattern) between the laser pulses and the travelling SPP wave at the sample surface. I will present time-resolved high-resolution images of the propagating SPP waves recorded using a pump-probe setup. The problem of guiding the SPP waves, and the coupling of light into and out of the nanostructures is discussed by comparing nanostructures of different geometry.

O 63.3 Thu 10:30 MA 043

A PEEM Study of the Substrate Dependence of Pentacene Thin Film Growth on Silicon — •Simone Möllenbeck[1], Dagmar Thien[1], Peter Kury[1], Kelly R. Roos[1,2], Dirk Wall[1], Michael Horn-von Hoegen[1], and Frank-J. Meyer zu Heringdorf[1] — [1]Department of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE) Universität Duisburg-Essen, D-47057 Duisburg, Germany — [2]Department of Physics, Bradley University, Peoria, IL 61625, USA

We used Photoemission Electron Microscopy (PEEM) to compare the well known behavior of Pentacene on Si(001) with the growth of Pentacene on different silicon surfaces with orientations between Si(111) and Si(001). The growth mode and morphology of Pentacene films are neither changed by an increase of the surface step density nor by the transition from a threefold to a twofold symmetry of the surface. An explanation for the observed behavior is the covalently bonded, disordered wetting layer, that acts as an interfactant layer and isolates the film from substrate defects and the substrate's structure. Furthermore, we have studied the electronic properties of thin Pentacene films on Si(001) with time-resolved PEEM. As result we get spatially resolved pump-probe traces whereby a "lifetime map"can be generated. The observed lifetime $\tau = 200fs$ for electronic excitation in the Pentacene wetting layer is by a factor two smaller than the lifetime for the first layer. We attribute this to the difference in electronic coupling of the monolayers to the substrate, that is also apparent in the different work-function of these layers.

Invited Talk O 63.4 Thu 10:45 MA 043

Subwavelength control of nano-optical fields probed by non-linear PEEM — Martin Aeschlimann[1], •Michael Bauer[2], Daniela Bayer[1], Tobias Brixner[3], F. Javier Garcia de Abajo[4], Walter Pfeiffer[5], Martin Rohmer[1], Christian Spindler[6], and Felix Steeb[1] — [1]FB Physik, TU Kaiserslautern — [2]IEAP, Universität Kiel — [3]Inst. für Phys. Chemie, Universität Würzburg — [4]CSIC, Madrid — [5]Fakultät für Physik, Universität Bielefeld — [6]FZ Jülich

Theoretically it has been demonstrated that the interaction of polarization-shaped laser pulses with a nanostructure allows the control of the spatial and temporal evolution of an optical near-field [1]. Recently we succeeded in demonstrating this scheme experimentally [2]. Silver nano-particles are illuminated with polarization shaped femtosecond laser pulses. The near-field in the vicinity of these nanostructures is mapped by the two-photon photoemission pattern as recorded using a photoemission electron microscope. We show that the emission pattern depends on the time-dependent polarization state of the laser pulse. Furthermore, the adaptive polarization pulse shaping technique allows optimizing a particular emission pattern with sub-diffraction resolution. The experiments show that the local interference of the optical near-fields generated by the two orthogonal incident polarization components can be utilized to manipulate the local field distribution in space and time.

[1] T. Brixner et al., Phys. Rev. Lett. 95, 093901 (2005). [2] M. Aeschlimann et al., Nature 446, 301 (2007).

O 63.5 Thu 11:15 MA 043

Energy and time resolved photoelectron emission microscopy (PEEM) measurements of nanostructured surfaces — •Christian Schneider[1], Martin Rohmer[1], Daniela Bayer[1], Michael Bauer[2], and Martin Aeschlimann[1] — [1]Department of Physics, TU Kaiserslautern, Erwin Schrödinger Str. 46, 67663 Kaiserslautern — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24908 Kiel

The combination of two photon photoemission and photoelectron emission microscopy is a versatile tool to study electron dynamics at nanostructured surfaces with high spatial and temporal resolution. The fast parallel image acquisition allows to obtain "lifetime maps" with a temporal accuracy of a few femtoseconds, however, in general without any spectral selectivity. In the past year, our setup was upgraded with an interchangeable delayline-detector allowing simultaneously energy resolved measurements. The performance and the high energy resolution provided with this detector will be demonstrated at the example of the Shockley surface state of Cu (111). The simultaneous access to space, time and energy by the combination of PEEM, time-resolved 2PPE and delayline-detector provides thus the potential to study coupling effects between nanoparticles as well as plasmon decay in realtime. We will show first results of specially shaped silver nanoparticles measured with high spatial, temporal and spectral resolution, including lifetime-maps created for different electron energies.

Invited Talk O 63.6 Thu 11:30 MA 043

Probing thin film magnetism by photoemission microscopy — •Claus M. Schneider — Institut f. Festkörperforschung IFF-9, Forschungszentrum Jülich, D-52425 Jülich, Germany

X-ray photoemission microscopy (X-PEEM) has matured into a versatile tool for high-resolution studies of thin film and surface magnetism. Exploiting the intrinsic time structure of the synchrotron radiation even time-resolved investigations on the sub-nanosecond time scale have become possible. This contribution will address the opportunities and perspectives of photoemission microscopy in the field of magnetism. In this course we will give examples for the information that can be obtained from static XPEEM experiments on the magnetic domain structures and coupling phenomena in heteromagnetic film systems. Time-resolved experiments reveal a wealth of micromagnetic processes governing the dynamics of magnetic microstructures on the nanosecond and sub-nanosecond regime [1].

[1] G. Schönhense, H.-J. Elmers, S.A. Nepijko, and C. M. Schneider, in: Advances in Imaging and Electron Physics Vol. 142, ed. P. Hawkes. (Academic Press, London, 2006).

O 63.7 Thu 12:00 MA 043

Microscopic investigation of exchange bias in Ni/FeMn bilayers — •Florian Kronast, Joachim Schlichting, Ruslan Ovsyannikov, Florin Radu, Shrawan Mishra, Hermann Dürr, and Wolfgang Eberhardt — BESSY GmbH , Berlin, Germany

The exchange interaction at the interface between an antiferromagnet (AF) and a ferromagnet (FM) is responsible for exchange bias, i.e. an unidirectional anisotropy seen by a shift of the FM hysteresis loop. Element specific magnetic imaging by photoelectron emission microscopy (PEEM) is a powerful tool to investigate the arrangement of magnetic moments near the interface. Recent PEEM studies of Co/FeMn bilayers demonstrated the presence of uncompensated Fe and Mn spins at the AF interface [1]. But their influence on the exchange bias could not be revealed so far.

Here we report on the first attempt to investigate the magnetic interface coupling in Ni/FeMn bilayers by PEEM using applied magnetic fields during imaging. A magnetic yoke was especially designed to minimize the deflection of photoelectrons by the Lorentz force. We studied the domain structure in the FM layer and the arrangement of magnetic moments at the interface of the AF as a function of magnetic field. Our main objective was to obtain a nano-scale image of the exchange bias strength in Ni/FeMn bilayers and correlate this with the magnetic arrangement of uncompensated spins at the AF interface. Saturating the FM layer by the applied magnetic field we can separate pinned and unpinned spins at the interface of the AF which are expected to be essential for the exchange bias. [1] PRB 75, 224406 (2007)

O 63.8 Thu 12:15 MA 043

Imaging ferroelectric domains with reflected low energy electrons — •Salia Cherifi — CNRS-Institut Neel, BP166, F-38042 Grenoble, France

In the very-low electron energy regime, reflected electrons from a specimen mirror are highly sensitive to topography and to electric surface potential. The sensitivity of the so-called mirror electron microscopy have been exploited in this study for imaging periodic -up and down- ferroelectric nano-strips designed on thin ferroelectric films and multiferroics. The ferroelectric domains have been written with a conducting tip of an atomic force microscope (AFM) and imaged initially using piezoelectric force microscopy (PFM). The images obtained in mirror electron microscopy (MEM) show periodic bright and dark microstripes that can be clearly matched to the ferroelectric domains imaged with PFM. AFM measurements performed prior and after the mirror electron microscopy experiment exclude the contribution of topography in the MEM contrast and confirm the possibility of imaging ferroelectric domains using MEM. This direct imaging mode will open new possibilities -especially when combined with PEEM- for the study of dynamical processes in ferroelectric systems and multiferroics.

O 64: Metal Substrates: Adsorption of Organic/Bio Molecules IV

Time: Thursday 11:15–12:45 Location: HE 101

O 64.1 Thu 11:15 HE 101

Molecular Recognition on Surfaces: Controlling Dimensionality and Periodicity of Supramolecular Tetraarylporphyrin Assemblies by the Interplay of Cyano and Alkoxy Substituents — •Nikolai Wintjes[1], Jens Hornung[2], Jorge Lobo-Checa[1], Tobias Voigt[2], Tomáš Samuely[1], Carlo Thilgen[2], Meike Stöhr[1], François Diederich[2], and Thomas Jung[3] — [1]Department of Physics, University of Basel, CH-4056 Basel — [2]Laboratorium für Organische Chemie, ETH-Zürich, Hönggerberg, HCI, CH-8093 Zürich — [3]Laboratory for Micro- and Nanotechnology, Paul Scherrer Institute, CH-5232 Villigen PSI

The self-assembly of three porphyrin derivatives was studied in detail on a Cu(111) substrate by means of Scanning Tunneling Microscopy (STM). All derivatives bear two 4-cyanophenyl substituents in opposing meso-positions of the porphyrin core but differ in the nature of the other two meso-alkoxyphenyl substituents. At coverages below 0.8 monolayers, two derivatives form molecular chains which evolve into nanoporous networks at higher coverages. The third derivative self-assembles directly into a nanoporous network without showing a one-dimensional phase. The pore-to-pore distances for the three networks depend on the size and shape of the alkoxy substituents. All observed effects are explained by (i) an interplay between the steric demand of the alkoxy residues, (ii) polar bonding involving both cyanophenyl and alkoxyphenyl substituents, and (iii) the entropy/enthalpy balance of the network formation.

O 64.2 Thu 11:30 HE 101

A structural study of porphyrins interacting with a metallic surface — •Jens Brede, Germar Hoffmann, and Roland Wiesendanger — Institut of Applied, University of Hamburg

A Porphyrin is a heterocyclic macrocycle derived from pyrrolic subunits interconnected via methine bridges. Porphyrins are an ubiquitous class of naturally occurring compounds with important biological representatives including hemes and chlorophylls. We prepared various tetra phenyl prophyrins (TPP) with different central metal (M) ions on metallic substrates. The molecular systems were investigated by scanning tunnelling microscopy and spectroscopy. The experiments were performed in a home-built low temperature STM working at 6 K in ultra-high vacuum conditions. Upon deposition of porphyrins on metal substrates the aromatic core of the molecule may undergo a structural deformation depending on the details of the molecule-substrate interaction. We will discuss the structural conformation of TPPs and their electronic properties.

O 64.3 Thu 11:45 HE 101

Ordering Aspects of Porphyrin Derivates on Ag(111) — •Hubertus Marbach, Florian Buchner, Karmen Comanici, and Hans-Peter Steinrück — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, D-91058 Erlangen

Porphyrins appear to be ideal candidates to generate functional molecular devices, due to their self assembly properties and their versatile functionality. In the present contribution, we focus on general aspects of ordered phases of different porphyrin derivates in the monolayer regime on Ag(111) investigated by STM. Tetraphenylporphyrins (TPP) always appear to arrange themselves in a square configuration, with a lattice constant of 1.4 nm at RT, independent of the central metal ion. Micrographs with submolecular resolution reveal the details of the molecular arrangement and allow to identify a "T-type" intermolecular interaction in between the phenyl substituents as the main reason for the observed ordering. Interestingly, the TPP molecules tend to rearrange upon exposure to large doses of small molecules (e.g., NO), which is interpreted as due to coadsorption of the dosed molecules. In contrast to TPP, the more bulky Tetrakis-(3,5-di-tert-butyl)-phenyl porphyrins (TTBPP) exhibit different coexisting phases. An specific route to prepare a monolayer, namley the thermal desorption of exess multilayers, leads to an extremley stable CoTTBPP layer, due to a highly interwoven structure. The role of intermolecular and intramolecular interactions and adsorbate/substrate interactions in respect to the observed phases and 2D-chirality aspects will be dicussed. This work has been funded by Sonderforschungsbereich 583.

O 64.4 Thu 12:00 HE 101

Formation, electronic structure, and reactivity of adsorbed metalloporphyrin complexes — •J. Michael Gottfried, Ken Flechtner, Yun Bai, Andreas Kretschmann, Marie-Madeleine Walz, Andreas Bayer, and Hans-Peter Steinrück — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II

Supported metal complexes are promising candidates for novel, regularly nanostructured catalysts. The coordinated metal centers represent well-defined active sites, which are immobilized by anchoring the ligands to a solid surface. Thus, these systems combine the advantages of homogeneous and heterogeneous catalysts. To develop a fundamental understanding of their functional principles, we have studied the formation, the electronic structure, and the reactivity of various porphyrin-based metal complexes on Ag(111) using photoelectron spectroscopy and complementary techniques. Specifically, we will discuss the axial coordination of NO on adsorbed Co(II)-tetraphenylporphyrin (CoTPP) and the influence of this ligand on the electronic interaction between the Co ion and the underlying Ag surface.[1] In addition, the formation of the complex H_3N-ZnTPP (by reaction between tetraphenylporphyrin, Zn, and NH_3 on an Ag(111) surface) will be used to illustrate a novel two-step route for the in-situ synthesis of adsorbed metalloporphyrin complexes.[2] — Supported by the DFG through SFB 583. — [1] K. Flechtner, A. Kretschmann, H.-P. Steinrück, J.M. Gottfried, J. Am. Chem. Soc. 129 (2007) 12110. — [2] K. Flechtner, A. Kretschmann, L.R. Bradshaw, M.M. Walz, H.-P. Steinrück, J.M. Gottfried, J. Phys. Chem. C 111 (2007) 5821.

O 64.5 Thu 12:15 HE 101

Voltage-dependent contrast of Co-Tetraphenylporphyrin Molecules on Ag(111) — •Florian Buchner, Karmen Comanici, Ken Flechtner, Thomas Lukasczyk, J. Michael Gottfried, Hubertus Marbach, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

The self-assembly of molecules on single-crystal surfaces is an approach towards the creation of novel materials with outstanding properties. Porphyrins represent a group of molecules which are of great interest for applications as well as for fundamental research. In this contribution, it will be shown that the appearance of tetraphenylporphyrins (TPP) in scanning tunneling microscopy (STM) topographs strongly depends on the applied bias voltage. Here we report the observation and identification of certain features in STM images of CoTPP layers on Ag(111). A significant portion of an ordered monolayer of CoTPP appears as depression at bias voltages around -1 V. At reduced negative bias voltages, the contrast of the depressions fade and at bias voltages around +1 V, the contrast is inverted. Investigating the electronic structure of CoTPP and 2HTPP layers by means of ultraviolet photoelectron spectroscopy (UPS) and scanning tunneling spectroscopy (STS), the contrast mechanism could be clarified, enabling us to interpret the depressions as 2HTPP. Additional evidence could be provided by imaging layers of different mixtures and by high-resolution STM images of the features in CoTPP. This work has been funded by the DFG through Sonderforschungsbereich 583.

O 64.6 Thu 12:30 HE 101

Conformational study of FeTPC molecules on Cu(111) with STM — •Stefan Kuck, Germar Hoffmann, and Roland Wiesendanger — Institute of Applied Physics, Jungiusstr. 9a, 20355 Hamburg

When porphyrin molecules are studied on surfaces, an important issue is the conformation of the molecule. So far, it was not possible to determine with STM whether the molecules are in a saddle or in a planar geometry. To answer this question, we introduce corroles as a new class of molecules in the field of STM studies, which are related to porphyrins but with reduced symmetry. Here, we address Iron-Tri-Phenyl Corrole (FeTPC) molecules deposited on the Cu(111) surface with scanning tunneling microscopy. We will discuss the bending of the corrole core into the saddle conformation and the configuration of the phenyl legs in contact with the metallic substrate.

O 65: Methods: Theory and Experiment

Time: Thursday 12:00–14:45 Location: MA 141

O 65.1 Thu 12:00 MA 141

Quantum well states and Rashba-type spin-orbit splitting in ultrathin Bi films — •Gustav Bihlmayer[1], Yury M. Koroteev[2,3], Eugene V. Chulkov[3,4], and Stefan Blügel[1] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institute of Strength Physics and Materials Science, RAS, 634021, Tomsk, Russia — [3]Donostia International Physics Center (DIPC), 20018 San Sebastiàn, Spain — [4]Departamento de Física de Materiales, UPV/EHU, 20080 San Sebastiàn, Spain

In this contribution a systematic study of the electronic properties of thin ($1-6$ bilayers) films of the semimetal bismuth in (111) and (110) orientation is presented, employing calculations based on density functional theory. Due to the different coordination of the atoms in these two different surfaces, a large variation of the conducting properties of the films is found, ranging from small-bandgap semiconducting to semimetallic and metallic. The evolution of the Bi(111) and Bi(110) surface states is studied as a function of the film thickness and by comparison to thicker films and simulations of the semiinfinite crystals. Interesting features arise from the strong spin-orbit effects in Bi and the resulting Rashba-type spin-splitting of the surface states. The spin-polarization of these states can be seen to change as these states transform into quantum well states at the Brillouin zone boundary. These results will be compared with recent experimental results on thin Bi films on Si substrates.

[1] T. Hirahara *et al.*, Phys. Rev. B **76**, 153305 (2007)
[2] T. Hirahara *et al.*, Phys. Rev. Lett. **97**, 146803 (2006)

O 65.2 Thu 12:15 MA 141

Efficient calculation of electronic band structure and the application to angular resolved photoemission spectroscopy experiments — •Victor Joco[1], Nikolai Mikuszeit[2], Jesús Martínez Blanco[3], and Enrique García Michel[3] — [1]Centro de Microanalisis de Materiales, Univ. Autónoma de Madrid, Spain — [2]Institute of Applied Physics, Univ. of Hamburg, Germany — [3]Dpto. Física de la Materia Condensada, Univ. Autónoma de Madrid, Spain

Angular resolved photoemission spectroscopy (ARPES) is an experiment to directly probe the valence band electronic structure of solids. Theoretical band structure calculations are of great help in understanding the ARPES data. A tight binding (TB) model interpolates the results from first-principles calculations or even experiments. This approach correctly shows all symmetry properties of the energy bands. The precision of the results are of comparable accuracy to first-principles calculations but three orders of magnitude faster.

A simulation program for comprehensive energy band and constant energy surfaces calculations has been developed. Based on the TB model the program allows precise calculation of constant energy surfaces, band structure in arbitrary surface directions and projected bulk band plots. An optimized general isosurface calculation for accurate energy surfaces as well as broadening of initial and final states have been implemented to simulate data close to ARPES experiments. The speed on a standard personal computer enables almost instant simulation during experiment. The calculations are compared to ARPES measurements on Cu(111).

O 65.3 Thu 12:30 MA 141

Anisotropic electron-phonon coupling strength at the Be(0001) surface — M. Fuglsang Jensen[1], •E. D. L. Rienks[1], T.-Y. Chien[2], I. Yu. Sklyadneva[3], A. Eiguren[3], P. M. Echenique[3], E. V. Chulkov[3], E. W. Plummer[2], and Ph. Hofmann[1] — [1]Institute for Storage Ring Facilities, University of Aarhus, Århus, Denmark — [2]Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee, USA — [3]Donostia International Physics Center, San Sebastian, Basque Country, Spain

Electronic surface states are useful model systems for understanding many-body effects in solids, such as electron-phonon coupling (EPC). Advances in angle-resolved photoemission spectroscopy not only allow one to assess the strength of the EPC, but also enable experimental determination of the Eliashberg function, that fully characterizes the electron phonon coupling in a given system.

Although the electronic structure of the Be(0001) surface is well studied, there is no agreement on the strength of the EPC at this surface. This strength is described by the mass enhancement parameter λ. An anisotropic coupling might account for this discrepancy, as these results are obtained along different crystal directions.

This study is aimed at obtaining a full description of EPC at this surface. Experimentally, the Eliashberg function (and λ) can be determined from the renomalized dispersion of the $\overline{\Gamma}$ surface state at the Fermi energy crossing. Preliminary results show that there is indeed a substantial variation of λ between the $\overline{\Gamma M}$ and the $\overline{\Gamma K}$ directions. The same trend is observed in a first principles study of this system.

O 65.4 Thu 12:45 MA 141

Electronic transport over single atoms — •Martyna Polok, Dmitry V. Fedorov, Peter Zahn, and Ingrid Mertig — Department of Physics, Martin Luther University Halle-Wittenberg, 06099 Halle (Saale), Germany

Scanning Tunneling Microscope (STM) experiments are important examples of the tunneling through single atoms. We try to develop a general understanding of the transport phenomena in complex structures through a case study of the STM setup.

The density functional theory (DFT) in the Korringa-Kohn-Rostoker (KKR) Green's function formulation is implemented to obtain the ground state electronic structure of the system. The transport properties are calculated in the linear response limit using the Baranger and Stone formalism.

In our ab initio investigation we consider a Cu and Co STM tip approaching a Cu (001) surface decorated with a single Cu or Co adatom. Depending on the chemical and geometrical structure of the constriction different transport channels contribute to the total conductance. Based on the spatial current distribution we can classify the open eigenchannels according to the symmetry of different angular momentum contributions i.e. the type of valence orbitals available at the Fermi energy.

The aim of this work is to demonstrate the interplay between the structure of the constriction and the electronic transport properties.

O 65.5 Thu 13:00 MA 141

Spin-orbit split two-dimensional electron gas with tunable Rashba and Fermi energy — •Christian R. Ast[1], Daniela Pacile[2], Luca Moreschini[2], Mihaela Falub[2], Marco Papagno[2], Klaus Kern[1,2], Marco Grioni[2], Jürgen Henk[3], Arthur Ernst[3], Sergey Ostanin[3], and Patrick Bruno[3] — [1]MPI für Festkörperforschung, Stuttgart, Germany — [2]EPFL, Lausanne, Switzerland — [3]MPI für Mikrostrukturphysik, Halle, Germany

In the Rashba-Bychkov-Model the strength of the spin-orbit splitting — the Rashba energy E_R — introduces a new energy scale influencing the electronic structure and competing against other energy scales, such as the Fermi energy E_F. However, in most of the known systems up to now the Rashba energy is a perturbative correction. We demonstrate that it is possible to tune the Rashba energy and the Fermi energy in a two-dimensional electron gas by a controlled change of the stoichiometry of an artificial surface alloy. In the $\mathrm{Bi}_x\mathrm{Pb}_{1-x}/\mathrm{Ag}(111)$ surface alloy the spin-orbit interaction maintains a strong influence on the band dispersion for arbitrary Bi concentration x, as is shown by angle-resolved photoelectron spectroscopy. The Rashba energy E_R and the Fermi energy E_F can be tuned to achieve values larger than one for the ratio E_R/E_F, which opens up the possibility for observing new phenomena, such as corrections to the Fermi liquid or a superconducting state. Relativistic first-principles calculations explain the experimental findings.

O 65.6 Thu 13:15 MA 141

Temperature dependence of stick-slip friction on graphite — •Lars Jansen[1,2], Harald Fuchs[1,2], and André Schirmeisen[1,2] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Wilhlem-Klemm-Strasse 10, 48149 Münster — [2]CeNTech, Center for NanoTechnology, Heisenbergstrasse 11, 48149 Münster

The so called stick-slip phenomenon, where the tip of an atomic force microscope performs a saw-tooth like motion over a surface, is believed to be a fundamental process in atomic friction, whose investigation has become a huge challenge over the past years [1,2].

We measured atomic scale stick-slip friction on a graphite surface with an atomic force microscope under ultrahigh vacuum conditions in a temperature range from 100 K to 300 K.

In this talk, we show the results of our experiments concerning friction vs. scan-speed curves for different temperatures. Furthermore we compare our experimental results to the thermally activated Prandtl-Tomlinson-model as described by Sang et al. [3]. This allows us the direct evaluation of crucial parameters like the energy barrier and the microscopic damping coefficient, which is often assumed to be in the lower limit of aperiodic damping.

[1] Schirmeisen, Jansen, Fuchs, PRB 71, p. 245403 (2005)
[2] Evstigneev, Schirmeisen, Jansen, Fuchs, Reimann, PRL 97, p. 240601 (2006)
[3] Sang, Dubé, Grant, PRL 87, p. 174301 (2001)

O 65.7 Thu 13:30 MA 141

Temperature dependence of the energy dissipation in dynamic force microscopy — •Tino Roll, Tobias Kunstmann, Markus Fendrich, Rolf Möller, and Marika Schleberger — Universität Duisburg-Essen, Fachbereich Physik, Lotharstraße 1, D-47048, Germany

Operating an atomic force microscope under UHV conditions can be used to study energy loss processes. This can be achieved by measuring the energy necessary to maintain the amplitude of the cantilever (damping) at a given frequency shift. The dissipation of energy is usually described in terms of an adhesion hysteresis mechanism. This mechanism should become less efficient with increasing temperature. To verify this prediction we have measured topography and dissipation data with dynamic force microscopy in the temperature range from 100 K up to 300 K. We used 3,4,9,10-perylenetetracarboxylic-dianhydride (PTCDA) grown on KBr(001). At room temperature, the energy dissipated into the sample (or tip) is 2.5 eV/cycle for PTCDA and 1.5 eV/cycle for KBr, respectively, and is in good agreement with an adhesion hysteresis mechanism. The energy dissipation over the PTCDA surface decreases with increasing temperature yielding a negative temperature coefficient. For the KBr substrate, we find the opposite behaviour: anincrease of dissipated energy with increasing temperature. While the negative temperature coefficient in case of PTCDA agrees rather well with the adhesion hysteresis model, the positive slope found for KBr points to a hitherto unknown dissipation mechanism.

O 65.8 Thu 13:45 MA 141

The Surface state of Au(111) and characterization of the tunneling tip in STM — •Berndt Koslowski, Anna Tschetschetkin, Stefania C. Bobaru, and Paul Ziemann — Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm, Germany

Based on a recently developed method for recovering the electronic density of states (DOS) from Scanning Tunneling Spectroscopy (STS) data [1], we re-examine the well-known Shockley-like surface state (SS) of Au(111) at 6.2K. To do so, we employ the 3D WKB approximation for the special case of a 2-dimensional SS leading to an analytical solution for the DOS recovery. The goal of this contribution is threefold: firstly, we show why the SS does not show up as a step function in STS. Secondly it will be demonstrated, how the SS can be exploited to extract information about the tip DOS resulting in a *calibrated* tunneling sensor. Thirdly, we discuss details of the tunneling spectra such as the cross-over from 2D to 3D tunneling below the band edge of the SS.

[1] B. Koslowski, Ch. Dietrich, A. Tschetschetkin, P. Ziemann, Phys.Rev. B 75, 035421 (2007).

O 65.9 Thu 14:00 MA 141

Dynamic superlubricity on insulating and conductive surfaces — Enrico Gnecco[1], •Pascal Steiner[1], Anisoara Socoliuc[2], Sabine Maier[3], Thilo Glatzel[1], Jonas Gessler[1], Alexis Baratoff[1], and Ernst Meyer[1] — [1]Department of Physics, Klingelbergstr. 82, 4056 Basel, Switzerland — [2]Nanonis GmbH, Technoparkstr. 1, 8005 Zürich, Switzerland — [3]Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

Friction between a sharp silicon tip and various atomically flat surfaces (NaCl, KBr, graphite, mica) is minimised by piezo-induced oscillations at well-defined resonance frequencies. This procedure extends an electro-capacitive way to achieve the same effect, which was recently introduced by our group and tested on insulating alkali halide crystals in ultra-high vacuum [1]. A controlled reduction of friction is observed now also on conductive surfaces like graphite, and in ambient conditions, which is quite promising for technological applications to micro-electromechanical devices. The theory previously used to interpret 'dynamic superlubricity' under general conditions is supported by new experimental observations showing that the contact between tip and sample is well maintained when the oscillations are applied.

[1] A. Socoliuc et al., Science, Vol. 313, 207 (2006).

O 65.10 Thu 14:15 MA 141

Space–Charge Effects in Photoelectron Spectroscopy at FLASH — •Martin Marczynski-Bühlow, Matthias Kalläne, Stefan Hellmann, Sabrina Lang, Claas Thede, Tim Riedel, Sönke Harm, Kai Rossnagel, and Lutz Kipp — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098

With its brilliant, ultrashort, and coherent photon pulses ranging from the VUV to the soft X–ray regime FLASH (Free–Electron Laser in Hamburg) offers the possibility to study a variety of "new physics" with novel as well as with traditional synchrotron radiation techniques. We have determined general limits for photoelectron spectroscopy experiments with these highly intense photon pulses with regard to radiation damage, space–charge effects, and FLASH machine parameters. Here we present angle–resolved as well as core–level photoelectron spectra of the transition–metal dichalcogenide $1T$–TaS_2 in the Mott insulating phase (T = 140 K). The photoelectron spectra were investigated particularly with respect to the occurrence of space–charge effects as a function of pulse intensity and compared with self-consistent N-body simulations based on the Barnes & Hut Treecode Algorithm. The measurements were carried out at the monochromator beamline PG2 of FLASH using the 3rd FEL harmonic ($h\nu = 115.5$ eV).

This work is supported by the Innovationsfond des Landes Schleswig-Holstein.

O 65.11 Thu 14:30 MA 141

Commissioning of a dedicated Soft X-Ray energy dispersive beamline for NEXAFS and other CFS/CIS studies — •D. Batchelor[1], Th. Schmidt[1], R. Follath[2], C. Jung[2], R. Fink[3], A Schöll[1], M. Knupfer[4], B. Büchner[4], and E. Umbach[1,5] — [1]Universität Würzburg, Experimentelle Physik II, Würzburg — [2]BESSY GmbH, Berlin — [3]Physikalische Chemie II, Universität Erlangen-Nürnberg — [4]IFW Dresden — [5]Forschungszentrum, Karlsruhe

We have recently published a design for a dedicated Soft X-Ray dispersive beamline (NIMA 575 (2007) 470-475) using photoelectron spectroscopy. The new dispersive technique allows not only NEXAFS without the time-consuming scanning of the photon energy but also high resolution CFS/CIS spectroscopic studies such as Auger/autoionization spectroscopy. The technique provides data with much more accuracy and detail hitherto achieved by simply stepping the photon energy. The method was originally tested using a "Pilot"setup which exploited extending the depth of focus of the monochromator by limiting the beamline angular aperture. Although very successful the decrease in angular beamline aperture obviously had drawbacks in terms of signal and also mode of operation of the monochromator (low Cff values). We will present commissioning results from the upgraded monochromator demonstrating that the new design overcomes most of these difficulties.

O 66: Metallic Nanostructures I (on Metals)

Time: Thursday 12:45–15:15 Location: MA 041

O 66.1 Thu 12:45 MA 041

Photochemical tuning of plasmon resonances in gold nanostructures — •Thomas Härtling[1], Yury Alaverdyan[2], Marc Tobias Wenzel[1], René Kullock[1], Mikael Käll[2], and Lukas M. Eng[1] — [1]Insitut für Angewandte Photophysik, TU Dresden, 01062 Dresden, Germany — [2]Department of Applied Physics, Chalmers University of Technology, SE-41296 Göteborg, Sweden

A photochemical method for the in-situ controlled tuning of size and shape of individual gold nanostructures is presented. This novel nano-optical fabrication technique combines the top-down approach of electron beam lithography with the genuine bottom-up strategy of autocatalytic nanoparticle growth to reach highest precision in nanoscale structure manufacturing on the sub-10-nm length scale. The technique is preeminently suitable for the fabrication of spectrally optimized nano-optical antennas used for instance as SERS substrates or surface-plasmon-based biosensors. The fabrication method is demonstrated by syntonizing the localized surface plasmon resonances of sub-wavelength nanoparticles, i.e., single spheres, single and paired nanodiscs, as well as ellipsoids. We show how a distinct red- or blueshifted surface plasmon resonance can be achieved due to photochemical tuning of size and shape of the particles.

O 66.2 Thu 13:00 MA 041

Tunable Quantum Wires: New Horizons in Plasmonics — •Dominic Zerulla[1], Michael Berndt[2], Stephanie Rehwald[3], Stephan Schwieger[4], and Erich Runge[4] — [1]UCD Dublin, School of Physics, Dublin 4, Ireland — [2]MPI of Molecular Cell Biology and Genetics, Dresden, Germany — [3]Heinrich-Heine-University Duesseldorf, Germany — [4]TU Ilmenau, Theor. Physik I, Germany

Here we report on the excitation of surface plasmon polaritons (SPP's) on a periodical arrangement of quantum wires with tunable periodicity. The ability to vary its two-dimensional lattice constant results in an additional degree of freedom, permitting excitation of SPP's for any combination of wavelength and angle of incidence within the tuning range of the system. Moreover it allows crucial questions on a fundamental level to be answered by shedding light on the characteristic localization properties of SPP's. Planar waveguides and photonic crystal structures are being intensively investigated as primary solutions for integrated photonic devices. However, there may be an alternative approach to the manufacturing of highly integrated optical devices with structural elements smaller than the wavelength, which nevertheless enables strong guidance and manipulation of light - the use of metallic and metallodielectric nanostructures in conjunction with Surface Plasmon Polaritons (SPP's). Our novel design opens new vistas regarding the tuneability of SPP localisation, propagation and coupling efficiencies.

[1] S. Rehwald, M. Berndt, F. Katzenberg, S. Schwieger, E. Runge, K. Schierbaum, D. Zerulla, Phys. Rev. B 76, 085420 (2007)

O 66.3 Thu 13:15 MA 041

Tailoring Surface Plasmon Polariton Propagation via Specific Symmetry Properties of Nanostructures — •Brian Ashall[1], Michael Berndt[2], and Dominic Zerulla[1] — [1]UCD Dublin, School of Physics, Dublin 4, Ireland — [2]MPI of Molecular Cell Biology and Genetics, Dresden, Germany

SPs are electromagnetic surface waves propagating along the interface of two materials with dielectric functions of opposite sign. They are essentially light waves that are trapped on the surface as a result of interactions between the illuminating wave and the free electrons of the conductor, and are called Surface Plasmon Polaritons (SPPs) to reflect this hybrid nature. Recent advances in fabrication technologies have created new opportunities to control SPP properties to reveal new aspects of their underlying science, and to tailor them for specific applications. We report on an experimental investigation on SPP propagation and interaction on 2D arrays of differing symmetry properties. Providing the required symmetry variations, and forming the basis of the arrays, are tailor designed nanostructures. The symmetry properties of the nanostructures have a definite impact on the SPP propagation direction on the surface. In particular, it is demonstrated how in certain orientations our rotor nanostructures have interesting wave-guiding interactions with propagating SPPs, and polarization twisting effect on the SPP re-radiated light.

[2] B. Ashall, M. Berndt, D. Zerulla; Appl. Phys. Lett. 91, 203109 (2007)

O 66.4 Thu 13:30 MA 041

Influence of arrays of nanodiscs on surface plasmon propagation — •Stefan Griesing, Andreas Englisch, and Uwe Hartmann — Saarland University, Experimental Physics Department, P.O.Box 151150, D-66041 Saarbruecken

Arrays of discs were produced by means of electron-beam lithography (EBL) on top of a 40nm thick silver layer. The discs with a diameter of 250nm were realized in two different ways: On the one hand as 30nm thick gold structures produced by a lift-off process, on the other hand as polymer structures with a thickness of 130nm by using a direct-writing process. The distance between the discs varies between 1.5 microns and 300nm. A plasmon beam was excited by a focused laser beam of 673nm wavelength passing through the Kretschmann configuration. The plasmon beam with a half-width of 5 microns propagates from the excitation spot to the nanostructures. The influence on the propagation behavior in dependence on the period is studied by scanning near-field microscopy for normal and oblique incidence. The results are compared with finite elements calculations.

O 66.5 Thu 13:45 MA 041

Optical Properties of Metal Nanorod Arrays — •René Kullock[1], Paul R. Evans[2], Robert J. Pollard[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, TU Dresden, 01062 Dresden, Germany — [2]Centre for Nanostructured Media, IRCEP, The Queens University of Belfast, Belfast BT7 1NN, UK

Single gold or silver nanorods strongly interact with visible light due to surface plasmon resonances (SPRs) [1]. By periodically arranging multiple nanorods, these SPRs can be easily tuned [2], hence allowing such structures to be used either for manipulating optical light transmission or generating high optical near-field strengths.

Here, we report on the optical near- and far-field properties of such gold and silver nanorod arrays with individual rods of 300 nm length and 20 nm width beeing arranged with a 60 nm periodicity. Using the semi-analytical method of multiple-multipoles, we study the electromagnetic near-field distribution of the SPRs, which are completely changed compared to the single nanorod case, and strongly depend on the geometry of our structures. Hence, we are able to identify various modes having different energies and shapes [3]. Furthermore, we are also interested on the far-field properties of the structure, and therefore investigate the influence of the structure on light transmission both theoretically and expmerimentally. Finally, applications of these near- and far-field effects in such structures are discussed.

[1] S. Link et al., J. Phys. Chem. B 103, 3073 (1999).

[2] R. Atkinson et al., Phys. Rev. B 73, 235402 (2006).

[3] P. Evans et al., *submitted.*

O 66.6 Thu 14:00 MA 041

fabrication of ordered cluster arrays on pre-structured surfaces — •Jian Zhang[1], Violetta Sessi[1], Jan Honolka[1], Axel Enders[1,2], and Klaus Kern[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Dept. of Physics and Astronomy, University of Nebraska, Lincoln NE 68588, USA

We will present results on the fabrication of ordered cluster arrays on structured surfaces. Fe and Co clusters of less than 3 nanometer diameter were prepared by buffer layer assisted growth1 (BLAG). The advantage of this method is that the clusters are formed before they make contact with the substrate. Thus, their initial structure is not affected by the substrate. While the resulting clusters are randomly distributed on flat crystalline surfaces, we find that cluster ordering can be promoted with pre-structured surfaces. Two examples will be discussed. On stepped a Pt(997) surface the clusters are arranged along the steps after landing, resulting in linear chains of clusters. Hexagonally arrays of isolated clusters can be achieved on a periodically corrugated boron-nitride nanomesh template. Here, the clusters preferentially occupy the pores in the BN layer. High nanomesh filling is achieved by repeated cluster deposition cycles. However, the maximum nanomesh filling is still limited by the cluster diffusion on the nanomesh, as will be discussed.

O 66.7 Thu 14:15 MA 041

Role of surface roughness in superhydrophobicity — •Chunyan Yang, Ugo Tartaglino, and Bo Persson — IFF, FZ-Juelich, 52425, Germany

Superhydrophobic surfaces, with liquid contact angle theta greater than 150 degree, have important practical applications ranging from self-cleaning window glasses, paints, and fabrics to low-friction surfaces. Many biological surfaces, such as the lotus leaf, have hierarchically structured surface roughness which is optimized for superhydrophobicity through natural selection. Here we present a molecular dynamics study of liquid nanodroplets in contact with self-affine fractal surfaces. Our results indicate that the contact angle for nanodroplets depends strongly on the root-mean-square surface roughness amplitude but is nearly independent of the fractal dimension of the surface[1,2].

References: [1] C. Yang, U. Tartaglino and B.N.J. Persson, Phys. Rev. Lett. 97, 116103 (2006) [2] C. Yang, U. Tartaglino and B.N.J. Persson, arXiv:0710.3264

O 66.8 Thu 14:30 MA 041

Strain induced micro-island formation on Ni/Ru(0001) monolayers — Kai Anhut and •Peter Jakob — Fachbereich Physik und Wissenschaftliches Zentrum für Materialwissenschaften, Philipps-Universität Marburg, D-35032 Marburg, Germany

Morphological changes of Ni monolayers on Ru(0001) induced by oxygen adsorption have been investigated using scanning tunneling microscopy. Specifically, the creation of well defined and uniform Ni micro-islands consisting of 3, 6 or 9 Ni atoms is reported and their geometrical structure, as well as their coordination with respect to the substrate lattice determined. The island formation is directly linked to a phase transition of the pseudomorphic Ni layer (lattice constant $\Delta d = d_{Ru-Ru} = 2.706$ Å) into a densified, moiré-distorted phase (lattice constant $\Delta d = d_{Ni-Ni}= 2.492$ Å) as Ni areas grow to lateral sizes beyond about 200 Å. An increasing lateral stress within such densified Ni monolayers induced by the adsorption of oxygen is held responsible for the expulsion of Ni clusters from the monolayer film. The micro-islands represent unusually stable units (with respect to recombination of neighboring islands) which is tentatively attributed to oxygen atoms attached to the trimers and hexagons.

O 66.9 Thu 14:45 MA 041

Adsorbate-Induced Faceting of Ir and Re Surfaces — •Payam Kaghazchi, Timo Jacob, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Faradayweg 4-6, D-14195 Berlin

Since high-index clean metal surfaces typically have lower surface atom densities and higher surface free energies compared to the close-packed surfaces of the same metal they can be used as the basis for surface reconstruction and facet formation experiments. In this context the group of T.E. Madey at Rutgers University found recently that on Ir(210) and Re($11\bar{2}1$) surfaces strongly interacting adsorbates are able to induce the formation of well defined nanostructures after annealing the system at elevated temperatures.

Using density functional theory calculations with the PBE functional and *ab initio* atomistic thermodynamics we studied the adsorption of oxygen and nitrogen on the different surface orientations, which are involved in the nanostructures on Ir(210) and Re($11\bar{2}1$). Constructing the corresponding (p, T)-surface phase diagrams, we find that at experimental pressure conditions ($p_{O_2} = 5 \cdot 10^{-10}$ atm) above 1100 K for Ir and above 1200 K for Re the planar surfaces are stable, while lowering the temperature stabilizes the nanofacets found experimentally. While on Ir(210) most nanoscale pyramids consist of smooth and unreconstructed planes, some (110) faces show a stepped double-missing row superstructure, which is only stable at higher temperatures ($1000\,\mathrm{K} < T < 1100\,\mathrm{K}$). Interestingly, we find that this superstructure only appears at the faceted surface, but turns out to be unstable on a Ir(110) substrate.

O 66.10 Thu 15:00 MA 041

Fabrication and metallic filling of sub30nm-nanoholes by PLD — Marc Saitner, •Christian Pfahler, Achim Manzke, Alfred Plettl, and Paul Ziemann — Solid State Physics, University of Ulm, D-89069 Ulm, Germany

Gold or platinum nanoparticles with diameters between 6 and 14nm were produced using a micellar technique and H_2 plasma ashing. Preparing such particles on e.g. silicon substrates, they act as a mask in subsequent anisotropic reactive ion etching with a CF_4/CHF_3 gas mixture. Direct processing results in nanopillars, whereas nanoholes can be created by inversion of this mask. Diameter and height of the holes are typically in the range of 10-40nm and 10-250nm, respectively. Aside from crystalline silicon it is possible to transfer the whole process directly to amorphous silicon, silicon oxide or nitride and thus to corresponding multilayer systems.

By using Pulsed Laser Deposition (PLD) these nanoholes can be filled with different metals. The influence of the substrate, the shape of the holes and the energy density of the laser will be discussed, and applications will be presented.

O 67: Prize Talk Fedor Jelezko (Walter Schottky Prize)

Time: Thursday 13:00–13:45 Location: H 0105

Quantum information processing with single spins in diamond

O 68: Metal Substrates: Solid-Liquid Interfaces

Time: Thursday 13:15–14:45 Location: MA 043

O 68.1 Thu 13:15 MA 043

In situ STM characterisation of electrochemically prepared ultrathin copper sulfide films on Au(1 0 0) — •Christian Schlaup, Peter Broekmann, and Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, D-53115 Bonn

An ultrathin copper sulfide compound film was prepared on a Au(1 0 0) electrode using the technique of electrochemical atomic layer epitaxy (ECALE). In a first step, a copper monolayer was deposited on a Au(1 0 0) electrode by Cu underpotential deposition from a sulfuric acid solution. By subsequential electrolyte exchanges this copper film was subjected to a sulfide containing sodium hydroxide solution. In situ STM measurements revealed a close packed commensurate c(2 × 2) adlayer structure indicating a sulfur layer with a significantly increased coverage ($\Theta_S = 0.5$ ML) with respect to a sulfur adlayer on a blank Au(1 0 0) surface at the same potential. The relative copper to sulfur ratio of 2:1 within the assumed Cu-S bilayer structure supports an interpretation of this structure as a Cu_2S species, which was already supposed for similar Cu-S compound films on a Au(1 1 1) electrode. These compound films are rather stable in a wide potential range, neither sulfur desorption at lower potentials nor a structural transition pointing to the formation of CuS at higher potentials can be observed. Instead the film dissolves completely at anodic potentials, probably due to the formation of soluble copper-thio-oxo species.

O 68.2 Thu 13:30 MA 043

Electrochemical oxygen reduction at pseudomorphic Pt thin films on Ru(0001) — •Otávio B. Alves, Harry E. Hoster, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

We report on the electrochemical properties of model surfaces consisting of 1-5 pseudomorphic Pt layers on Ru(0001), which are fabricated by vapor deposition under ultrahigh vacuum conditions. Due to electronic ligand and strain effects, the interaction of these surfaces with H_{ad}, OH_{ad}, and O_{ad} is weakened compared to Pt(111). According to theoretical predictions,[1,2] this can lead to a higher activity for the electrochemical reduction of oxygen, similar to the behavior previously reported for Pt_3Ni model electrodes.[3] By changing the layer thickness, it is possible to tune the adsorption properties within a certain range.[4] We investigated the oxygen reduction current as a function of potential under well-defined mass transport conditions for all model surfaces in an electrochemical flow cell coupled to a UHV system. The electrochemical behaviour of the pseudomorphic Pt films was found to be clearly different from that of Pt(111). The results are discussed in comparison to the behavior of other model electrodes and to theoretical predictions.

[1] M. Mavrikakis *et al.*, Phys. Rev. Lett. 1998, 81, 2819.
[2] J. R. Kitchin *et al.*, J. Chem. Phys. 2004, 120, 10240.
[3] V. R. Stamenkovic *et al.*, Science 2007, 315, 493.
[4] A. Schlapka *et al.*, Phys. Rev. Lett. 2003, 91, 016101.

O 68.3 Thu 13:45 MA 043

Additives for the copper damascene process - in-situ EC-STM and XPS studies — •Knud Gentz[1], Sascha Hümann[1], Stefan Breuer[1], Ralf Hunger[2], Klaus Wandelt[1], and Peter Broekmann[1] — [1]Institute of Physical and Theoretical Chemistry, Bonn University — [2]Institute of Material Research, Technical University of Darmstadt

Copper has become a focus of research activities over the last two decades due to its use as interconnect material in microchip design. Presently the dimensions of circuit layout is dependent on the wavelength of the applied light. To continue the ongoing process of miniaturization, cationic organic molecules have been studied as additives in the copper damascene process. In the present investigation the influence of various halides on structure and reactivity of a Diphenylviologen (DPV) layer adsorbed on a Cu(100) surface have been studied by in-situ electrochemical STM and high-resolution XPS, conducted at the synchrotron source BESSY2.

N,N'-diphenyl-4,4'-bipyridinium (Diphenylviologen, DPV) spontaneously adsorbs on a halide-modified Cu(100)-surface, forming a striped pattern , which has been characterized by in-situ Scanning Tunneling Microscopy. Cyclic Voltammetry indicates that the building block is the radical cation of the viologen. These result have been confirmed by ex-situ high resolution XPS after transfer into UHV in a process allowing conservation of the surface redox-states upon emersion. A careful analysis of the N1s and C1s core level shifts then allows the determination of the redox-state of the adsorbed viologens.

O 68.4 Thu 14:00 MA 043

Electrochemical Faceting of Ir(210) — Payam Kaghazchi[1], Khaled A. Soliman[2], Felice C. Simeone[2], Ludwig A. Kibler[2], and •Timo Jacob[1,2] — [1]Fritz-Haber-Institut der MPG, D-14195 Berlin — [2]Institut für Elektrochemie, Universität Ulm, D-89081 Ulm

Highly-disperse nanoparticles are often used to catalyze (electro)-chemical reactions. Unfortunately not all nanoparticles have the same size and shape, but rather show a relatively large distribution, limiting our understanding of the ongoing processes.

Focusing on Ir(210), which experimentally was found to form pyramidal-like nano-facets in presence of oxygen [1], we used density functional theory and the extended *ab initio* atomistic thermodynamics approach [2] to study the adsorption of oxygen on these surfaces being involved in the nanostructures on Ir(210). Constructing the corresponding (p,T,ϕ)-phase diagram for Ir(210) in contact with an aqueous electrolyte, we found that the same nano-facets should be stable under electrochemical conditions. Recently we were able to confirm this theoretical prediction by cyclic voltammetry and *in-situ* scanning tunneling microscopy. The presence of nanofacets for Ir(210) gives rise to a characteristic current-peak in the hydrogen adsorption region for sulfuric acid solution. Regarding the electrocatalytic behavior of the nano-facets we found a considerably lower activity compared to planar Ir(210).

[1] I. Ermanoski, C. Kim, S. P. Kelty, T. E. Madey, Surf. Sci. 2005, 596, 89.

[2] T. Jacob, J. Electroanal. Chem., **607**, 158–166 (2007).

O 68.5 Thu 14:15 MA 043

A new approach to obtain electrochemical E/pH diagrams derived from the viewpoint of semiconductor defects — •Mira Todorova and Jörg Neugebauer — Max-Planck Institut für Eisenforshung, Düsseldorf

We present a novel approach for obtaining Pourbaix diagrams, which depict possible thermodynamically stable phases of an aqueous electrochemical system under given environmental conditions as a function of potential and pH. Such diagrams play a crucial role in corrosion science and various areas of chemistry.

Being similar to the approach used in defect chemistry [1] the new method is safely based on the formation energy of ions in the host matrix. Within the new approach the electrode potential and the pH-scale can be easily understood. We obtain an astonishingly good agreement with the standard electrochemical potential series. The construction of E/pH diagrams for any given environmental conditions and without *a priory* assumptions about ion concentrations is possible and will be demonstrated by the example of zinc and iron.

[1] C.G. Van de Walle and J. Neugebauer, J. Appl. Phys. **95**, 3851 (2004).

O 68.6 Thu 14:30 MA 043

A Quantum Chemistry Roadmap Towards Highly Accurate Adsorption Energies at Ionic Surfaces — •Bo Li[1], Angelos Michaelides[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Materials Simulation Laboratory, London Centre for Nanotechnology and Department of Chemistry, University College London, London WC1E 6BT, U.K.

A roadmap is established to compute adsorption energies of molecules at ionic surfaces with an accuracy approaching chemical accuracy (a precision of 1 kcal/mol or ∼43 meV). The approach relies on established quantum chemistry methodologies and involves a separation of the total adsorption energy into contributions from Hartree-Fock and electron correlation, the use of embedded cluster models of the substrate, and extrapolations to the complete basis set limit. Application of the procedure to the example of water on salt, with electron correlation treated at the CCSD(T) level, yields an adsorption energy for a water monomer on NaCl(001) of 480 ± 20 meV.

O 69: Symposium: Size-Selected Clusters at Surfaces III

Time: Thursday 14:00–15:00 Location: MA 042

O 69.1 Thu 14:00 MA 042

Size-dependent structure and bonding of Ir clusters on Graphene / Ir(111) — •Carsten Busse[1], Alpha T. N'Diaye[1], Johann Coraux[1], Peter J. Feibelman[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Sandia National Laboratories, Albuquerque, USA

Small Ir clusters are grown by deposition of Ir onto a graphene moiré on Ir(111) and analyzed using scanning tunneling microscopy (STM). The clusters are arranged in a hexagonal lattice with perfect ordering and exhibit a narrow, tunable size distribution.

The apparent cluster height for monolayer clusters shows a pronounced increase with cluster size from 1.8 Å for trimers to 2.5 Å for 11-clusters. Density functional theory (DFT) calculations rule out a geometric explanation of this effect, so we attribute it to differences in electronic structure. The majority of clusters are stable and immobile at room temperature, but for certain cluster sizes we observe a jiggling motion (trimer to heptamer) or rapid shape changes (tetramer).

For the experimentally observed binding sites of the clusters within the moiré unit cell, DFT reveals that the bonding of the clusters to the substrate induces a rehybridization of the C directly underneath the particles. The bonding changes from a graphene-like (sp^2) into a diamond-like (sp^3) arrangement, thus explaining the strong binding of the clusters to the substrate.

Work supported in part by the DOE Office of Basic Energy Sciences, Div. of Mat. Sci. and Eng. Sandia is operated by the Lockheed Martin Co. for the U.S. DOE's NNSA, under contract DE-AC04-94AL85000.

O 69.2 Thu 14:15 MA 042

Density functional modeling of supported clusters: on the road to an understanding of nanoscale catalysis — •Michael Moseler[1,2] and Bernd Huber[2] — [1]Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstr. 11, 79108 Freiburg — [2]Freiburg Materials Research Center, Stefan-Meier-Str. 21, 79104 Freiburg

Understanding and predicting heterogeneous catalysis remains one of the main motivations underlying the science of supported nanocluster. Surface science experiments provide important insights into nano-particles catalysed reactions [1]. Often however, this progress is only achieved in combination with quantum-chemical atomistic simulations. Here we show how density functional theory can be used to understand experimental size evolutionary patterns in the activity of metal-oxide supported Pd clusters [2,3]. We provide theoretical as well as experimental evidence that the reaction of supported Pd clusters with molecular oxygen results in the formation of nano-oxides which are in epitaxy with the ceramic support. These oxides serve as a Mars-van-Krevelen oxygen reservoir and therefore play an important role in the catalyzed combustion of carbon monoxide.

[1] U.Heiz, E.L.Bullock, Mater. Chem. 14, 564 (2004)

[2] B.Huber, P.Koskinen, H.Häkkinen, M.Moseler, Nature Materials 5, 44 (2006)

[3] B.Huber, M.Moseler, Eur. Phys. J. D online-First (2007)

O 69.3 Thu 14:30 MA 042

X-ray photoelectron spectroscopy on deposited nobel metal clusters — •Matthias Neeb, Baris Balkaya, Nicoletta Ferretti, and Wolfgang Eberhardt — BESSY, Albert-Einstein Str. 15, 12489 Berlin

Noble metal clusters (Cu, Ag, Au) were produced in a magnetron sputter source and mass-selected by a magnetic sector field prior to soft-landing on a p-doped Si-wafer. XPS, XANES, UPS and Auger spectra of the supported metal clusters at a surface coverage of ~ 1 % have been measured with soft X-ray synchrotron radiation. The cluster spectra are compared with the respective bulk spectra of an evaporated metal film. In general, the core binding energies of the clusters vary with size and are blue shifted with respect to the bulk value. Similarly, the L_3 absorption edge of Cu-clusters up to 70 atoms is blue shifted with respect to Cu-bulk. For larger Cu-clusters (≥ 13) a multiple-scattering NEXAFS-feature is detected behind the L_3 absorption edge, indicating an icosahedral structure. The Auger energy of the clusters shows a red shift with respect to the bulk value. Moreover, the kinetic energy of the Auger electron is influenced by post-collison interaction (PCI) and varies with cluster size.

O 69.4 Thu 14:45 MA 042

Electrospray Ion Beam Deposition of Nonvolatile Molecules and Nanoparticles in High- and Ultrahigh Vacuum — •Stephan Rauschenbach, Thomas Weitz, Alicia Forment, Jens Boettcher, Giovanni Costantini, Nicola Malinowski, and Klaus Kern — Max-Planck-Institute for Solid State Research, Stuttgart, Germany

Electrospray Ionization is a soft ionization technique with which nonvolatile molecules or nanoparticles from a solution can be transferred into the gas phase. Based on this technique we developed a novel vacuum deposition apparatus, which is capable to transfer these ions into high- or ultrahigh vacuum, mass select them and deposited them on a surface [S.Rauschenbach et. al., Small 4 (2006)]. Destruction free deposition (soft landing) can be achieved, since the kinetic energy of the ions can be controlled. An UHV-STM/AFM is connected to the system for in-situ analysis.

The capability to deposit the large organic molecules, clusters and nanoparticles is demonstrated with a variety of systems. Soft landing of molecules is proven by fluorescence spectroscopy and TOF-SIMS identification of deposited dye molecules. Au-nanoparticles (5 - 20 nm) and carbon nanotubes deposited from ion beams were found intact on the surface identified by atomic force microscopy (AFM). CdS nanorods (30 nm diameter) and V_2O_5 nanowires (5 nm diameter) observed in AFM after deposition are identified by TOF-SIMS. Estimations of the charge state and the mass-to-charge-ratio show that the nanoparticle ion beams mainly consist of very highly charged particles.

O 70: SYMS: Modern Developments in Multiphysics Materials Simulations I (Invited Speakers: David Pettifor, Alessandro De Vita, Chris Wolverton, Ingo Steinbach, Walter Thiel, Karsten Reuter; FV: O+HL+MM)

Time: Thursday 14:00–17:00 Location: A 151

See SYMS for details about the program.

O 71: SYEC: Exact-Exchange and Hybrid Functionals Meet Quasiparticle Energy Calculations II (FV: O+HL+DF+TT)

Time: Thursday 14:00–17:00 Location: A 053

See SYEC for details about the program.

O 72: Symposium: Beyond Optical Wavelengths: Time-Resolved Spectroscopy of Surface Dynamics with EUV and XUV Radiation II (Invited Speakers: Wilfried Wurth, Hermann Dürr, Shik Shin)

Time: Thursday 14:00–17:00 Location: HE 101

Invited Talk O 72.1 Thu 14:00 HE 101

First Experiments at FLASH and the Core-Hole Clock — •Wilfried Wurth — Institut für Experimentalphysik, Universität Hamburg, Luruper Chaussee 149

Time-resolved soft x-ray spectroscopy has the potential to provide unique element specific and chemical state selective information on the complex wave packet evolution at surfaces and interfaces.

With the core-hole-clock method this potential has been utilized to determine ultrafast electron delocalization at specific atomic sites. However, here, dynamic information is only accessible in the time range given by the fixed decay time of core-excited states. In order to really follow the temporal evolution at selected atomic sites, we have to develop atom specific and chemically selective X-ray spectroscopy further towards a femtosecond time resolving technique.

With the Free-Electron Laser in Hamburg (FLASH) at DESY a unique source for femtosecond XUV-pulses with unprecedented brillance is operational since 2005. In the talk I will present some ideas how femtosecond X-ray pulses from Free Electron Lasers can be used to study surface and interface dynamics. First time-resolved experiments from FLASH will be presented and implications for future experiments will be discussed.

This work is supported by the BMBF in the framework of the Forschungschwerpunkt 301 FLASH: Matter in the light of ultrafast and extremely intense X-ray pulses.

O 72.2 Thu 14:30 HE 101

Excitation of electrons in Silicon with an ultrashort XUV free electron laser pulse: a Monte-Carlo study — •Nikita Medvedev and Baerbel Rethfeld — Technische Universitaet Kaiserslautern, 67653, Germany

The new light source FLASH at DESY in Hamburg provides ultrashort high intensity XUV pulses. We study the interaction of this new kind of irradiation with condensed matter theoretically. In this contribution we present first simulations, applying Classical Trajectory Monte Carlo simulation (CTMC) to describe the dynamics of electronic excitation and ionization within a solid silicon target, irradiated with femtosecond XUV laser pulse (25 fs, $\hbar\omega = 38$ eV). The CTMC-method was extended to take into account the electronic band structure and Pauli's principle for electrons excited into the conduction band. Secondary excitation and ionization processes were included as well. We calculate the temporal distribution of the density of exited and ionized electrons, the energy of these electrons and the energy distribution function. The influence of the band structure on the redistribution of free electrons on subpicosecond time-scale is studied. It is demonstrated that the final kinetic energy of free electrons is much less than the total energy provided by the laser pulse, because some part of energy is spended to overcome ionization potentials and is kept by holes. It was found that the total number of free electrons is significantly less than estimated by $n_e = \hbar\omega/E_{\text{gap}}$. We introduce the concept of an "effective band gap", which can be applied to estimate the free electron density for collective electronic excitation with a high-intensity XUV laser pulse.

O 72.3 Thu 14:45 HE 101

Single-shot femtosecond EUV-pump/visible-probe cross-correlation on GaAs — •Theophilos Maltezopoulos[1], Stefan Cunovic[2], Marek Wieland[3], Martin Beye[3], Armin Azima[1], Harald Redlin[1], Maria Krikunova[3], Roland Kalms[3], Ulrike Fruehling[1], Filip Budzyn[3], Wilfried Wurth[3], Alexander Foehlisch[3], and Markus Drescher[3] — [1]HASYLAB at DESY, Notkestrasse 85, 22607 Hamburg, Germany — [2]Department of Physics, Bielefeld University, Universitaetsstrasse 25, 33615 Bielefeld, Germany — [3]Institut fuer Experimentalphysik, University of Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

The Free Electron Laser in Hamburg (FLASH) is currently the most intense femtosecond light source in the extreme-ultraviolet (EUV) range, which facilitates efficient pumping of inner shells in solid targets. For pump-probe experiments, a synchronized optical fs laser system is available at the facility. In our set-up, the EUV pulse (wavelength 28 nm, pulse length 20-30 fs) and the visible pulse (400 nm, 130 fs) are non-collinearly overlapped in space and time on the surface of a GaAs crystal. Along its path, the EUV pump pulse changes the reflectivity of the GaAs sample for the visible probe pulse, the latter being imaged onto a CCD array. The spatial position of the reflectivity change captures the dynamics of the process in a single exposure. The technique can be utilized to determine individual EUV-visible delays with a precision of about 40 fs.

15 min. break

Invited Talk O 72.4 Thu 15:15 HE 101

Ultrafast Magnetization Dynamics Probed by Femtosecond X-Ray Spectroscopy — •Hermann A. Dürr — BESSY GmbH, Albert-Einstein-Str. 15, 12489 Berlin, Germany.

When the electronic system of a solid is rapidly heated by absorbing a femtosecond optical laser pulse it takes time to re-establish thermal equilibrium. This timescale is ultimately determined by energy transfer from the electronic system to the lattice. For ferromagnets this process can also lead to an ultrafast quenching of the ferromagnetic order. Angular momentum conservation dictates that an exchange of spin angular momentum with a reservoir such as the lattice should occur. So far real time studies of these processes were limited to the use of femtosecond laser pump-probe spectroscopy [1]. We show that an efficient novel channel for angular momentum dissipation to the lattice can be opened by fs laser excitation of a ferromagnet [2]. The quenching of spin angular momentum and its transfer to the lattice with a time constant of 120 fs is determined unambiguously with x-ray magnetic circular dichroism by separating spin and orbital contributions to the magnetization. Fs time-resolved x-ray absorption spectroscopy shows an unexpected increase in valence electron localization during the first 120 fs possibly providing the driving force behind fs spin-lattice relaxation.

[1] E. Beaurepaire, et al., Phys. Rev. Lett. 76, 4250 (1996).

[2] C. Stamm, et al., Nature Materials 6, 740 (2007).

O 72.5 Thu 15:45 HE 101

Non-equilibrium spin-dynamics of Gd(0001) studied by magnetic linear dichroism in 4f core-level photoemission — •Alexey Melnikov[1], Helena Prima-Garcia[2], Martin Lisowski[1], Tanja Giessel[2], Ramona Weber[2], Roland Schmidt[2], Cornelius Gahl[2], Nadezhda Bulgakova[3], Uwe Bovensiepen[1], and Martin Weinelt[1,2] — [1]Freie Universität Berlin, Fachb. Physik, Arnimallee 14, 14195 Berlin, Germany — [2]Max-Born-Institut, Max-Born-Straße 2 A, 12489 Berlin, Germany — [3]Institute of Thermophysics SB RAS, pr. Lavrentiev 1, 630090 Novosibirsk, Russia

The magnetic linear dichroism of the Gd 4f core-level is studied in a time-resolved photoemission (PE) experiment at BESSY II employing 1.55eV, 100fs laser pump and 60eV, 50ps synchrotron-radiation probe-pulses. We define the dichroic contrast $\Delta M(T)$ at temperature T averaging the difference of PE spectra for opposite magnetization direction. $\Delta M(T)$ follows the spontaneous magnetization, vanishes at the Curie temperature T_C, and can therefore be used to map the order of the 4f spin-system. The latter is reduced upon optical excitation of the 5d6s valence electrons. Remarkably, $\Delta M(T)$ remains at 80% of the equilibrium value while the lattice temperature increases up to T_C. A simulation of $\Delta M(T(\tau))$ by a quasi-equilibrium model predicts an at least two times larger reduction of $\Delta M(T)$ for delays τ below 100 ps. We conclude that at these early times equilibration between lattice and 4f spin subsystems has not been established. This reveals principal differences to the spin dynamics in itinerant ferromagnets, where the valence electrons excited by the laser also carry the magnetic moment.

Invited Talk O 72.6 Thu 16:00 HE 101

Sub-meV-resolution photoemission spectrocopy on solids using VUV laser — •shik shin — Institute for Solid State Physics, Chiba277-8581, Japan

We developed the ultrahigh-resolution photoemission system using quasi-CW VUV laser. VUV laser, photoemission analyzer, and cooling system were newly developed for ultrahigh resolution photoemission. The total resolution of the Laser-PES system is estimated to be about 0.15 eV by using the gold Fermi edge at 1.8 K at present. This is the highest resolution of the world. We will present the angle-integrated and angle-resolved photoemission results on several superconducting materials as well as the heavy Fermion materials. We will also shows the high resolution PES on surface states of Ag.

O 72.7 Thu 16:30 HE 101

Femtosecond time- and angle-resolved photoelectron spectroscopy: A tool to study non-equilibrium states of electronic structure — •Uwe Bovensiepen — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

During the last 20 years angle-resolved photoemission spectroscopy has turned from an established surface science technique to a powerful experimental system that maps the electronic structure of valence bands in solids. Intense optical excitation by femtosecond laser pulses drives this electronic subsystem in condensed matter into a non-equilibrium state and its energy content is characterized by electronic temperatures of several thousand Kelvin. The ion-ion interaction is determined by the screened electron-ion potential and the intense optical excitation can be expected to modify the screening contribution. We excite metallic structures by 1.5 eV laser pulse at absorbed fluences of 0.1 – 1 mJ/cm^2 and probe the transient state of the electronic structure by 6 eV UV laser pulses in time- and angle-resolved photoemission. For the 5d$_{z^2}$ surface state of Gd(0001) and for the highest occupied quantum well state originating from the 6p$_z$ band in epitaxial Pb films on Si(111) we observe a transient binding energy increase by 50 – 100 meV before electron-phonon scattering has lowered the excess energy in the electronic subsystem. Thus, we conclude that the optical excitation leads to a stabilization of both these systems. First experiments on RTe3 charge density wave materials show that under comparable conditions even a transition from an insulating to a metallic state can be induced optically.

O 72.8 Thu 16:45 HE 101

Ultrafast charge transfer at silicon surfaces investigated by the core hole clock method: Band structure influences — Silvano Lizzit[1], Guillermo Zampieri[1,2], Luca Petaccia[1], Rosanna Larciprete[1,3], Krassimir L. Kostov[4], Georgi Tyuliev[5], and •Dietrich Menzel[6,7] — [1]Sincrotrone Trieste, Area Science Park, 34012 Trieste, Italy — [2]Centro Atómico Bariloche, 8400 S.C. de Bariloche, Argentina — [3]CNR-Istituto dei Sistemi Complessi, 00016 Monterotondo (RM), Italy — [4]Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria — [5]Institute of Catalysis, Bulgarian Academy of Sciences, Sofia, Bulgaria — [6]Physik-Dept.E20, TU Muenchen, 85748 Garching, Germany — [7]Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany

With the well-known core hole clock method to measure charge transfer (CT) at surfaces by resonant core excitation and decay under resonant Auger Raman conditions (bandwidth of exciting photons below the lifetime width) the lifetimes of 4s electrons on core-excited Ar adsorbed on clean and H-covered n- and p-Si(100) have been determined. CT times are in the range of 1 to 4 fs. They do not depend on doping and are about twice larger on H-covered than on clean Si. Distinct structure is found as a function of excitation energy, similarly on both surfaces. It is explained by the influence of the empty band structure of Si(100), into which the excited 4s electron is transferred. The concepts and mechanisms will be discussed. Time allowing, the relation of this method to laser pump-probe techniques will be discussed.

O 73: Symposium: Bimetallic Nanosystems: Tuning Physical and Chemical Properties II (Invited Speakers: André Fielicke, Thomas Risse, Jürgen Behm)

Time: Thursday 14:00–17:30 Location: MA 005

Invited Talk O 73.1 Thu 14:00 MA 005

Doped clusters in light of an IR-FEL — •André Fielicke[1], Philipp Gruene[1], Gerard Meijer[1], Ewald Janssens[2], Vu Thi Ngan[2], Minh Tho Nguyen[2], and Peter Lievens[2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Leuven, Belgium

Changing the composition of a metal cluster naturally will alter its physical and chemical properties; however, often these changes are not gradual but lead to very different and unexpected behavior. In the last years several of such mixed cluster systems have been predicted by theory and also identified in experiments to exhibit unusual stabilities. In many cases this stabilization is supposed to be related to the formation of structures that are stabilized by both, electronic and geometrical effects. We focus on the determination of the geometrical structure of such isolated clusters in the gas-phase via vibrational spectroscopy. Cluster complexed with weakly bound ligands, i.e. rare gas atoms, are irradiated with intense and tunable far-IR radiation from the Free Electron Laser for Infrared eXperiments FELIX. Absorption leads to a heating of the cluster and subsequent evaporation of the ligand. This process is observed via mass spectrometry that allows determining the clusters far-IR spectra size and composition selectively. The influence of doping on the structural properties will be exemplified for silicon and gold clusters doped with transition metal atoms.

Invited Talk O 73.2 Thu 14:30 MA 005

Molecular adsorption on bimetallic particles supported on well defined oxide surfaces — •Thomas Risse — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany

The admixture of a second metal has proven to be a suitable method to tune the desired properties of solid-supported metal particles. This presentation will focus on the adsorption properties of molecules on nanometer-sized bimetallic particles deposited on single crystalline oxide films. Such systems can serve as model systems for heterogeneous catalysts, which allow investigations with the rigor of modern surface science while grasping essential aspects of the complexity of real catalytic systems. The adsorption properties of molecules on bimetallic particles depend on a variety of parameters such as elemental and surface composition, particle size, or metal substrate interaction. Co/Pd and Fe/Pd particles grown by physical vapor deposition on a well defined alumina film will be used as model systems to explore the dependence of the adsorption properties on the abovementioned parameters. The experiments take advantage of the nucleation properties of the different metals which allow -by appropriate deposition conditions- to tune the particle's surface composition, shape, or degree of crystallinity. To allow for a microscopic analysis of the observed effects, investigations of the adsorption properties will be amended by structural characterization of the systems. Furthermore experiments on simple reactions such as reaction of the systems with oxygen or methanol decomposition will be discussed with respect to their susceptibility to the admixture of a second metal component.

Invited Talk O 73.3 Thu 15:00 MA 005

Bimetallic Catalysis - Fundamental effects studied on well defined model systems — •R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

Bimetallic catalysts are well known to often exhibit a significantly better performance, in activity and/or selectivity, than the respective components [1]. Based on catalytic measurements using catalysts with varying composition, different electronic and geometric effects were introduced to explain there observations [2]. Direct proof, however, was hardly possible because of the mostly unknown surface composition of the catalyst particles. Adsorption and reaction studies on bimetallic surfaces with well-defined, varied distribution of surface atoms, as identified, e.g., by high resolution scanning tunneling microscopy with chemical contrast, allow for the first time to directly identify and separate these effects [3]. Furthermore, they provide a solid basis for comparison with theory [3]. The potential of combined experimental and theoretical studies is demonstrated using different adsorption/reaction systems as example.

1. J.H. Sinfelt, Surf. Sci. 500 (2002) 923.
2. W.M.H. Sachtler, in Handbook of Heterogeneous Catalysis, G. Ertl, H. Knözinger, and J. Weitkamp, Eds. (VCH-Wiley, Weinheim, 1997), Vol. 3.
3. M. Ruff, N. Takehiro, P. Liu, J.K. Norskov, R.J. Behm, Chem. Phys. Chem. 8 (2007) 2068.

O 73.4 Thu 15:30 MA 005

Specific Synthesis of Pt Nanowires for Catalytic Applications — •Daniela Fenske[1,4], Holger Borchert[2,4], Jan Kehres[1,4], Joanna Kolny-Olesiak[2,4], Marcus Bäumer[3,4], and Katharina Al-Shamery[1,4] — [1]IRAC, University of Oldenburg, Germany — [2]EHF, University of Oldenburg, Germany — [3]IAPC, University of Bremen, Germany — [4]Center of Interface Science (CIS), Germany

Metallic nanomaterials are of great interest in the last years due to their interesting properties as new materials for optical, electronic, magnetic or catalytic applications. Particularly size and morphology of such nanoparticulate systems offer also high potential for material improvement. A promising issue is the preparation of platinum nanowires by means of colloidal chemistry which allows obtaining particles with well-defined size and shape by use of stabilizing ligands.

Recent efforts have been focused on the development of synthesis based on Jana and Peng et.al. [1] to obtain these nanowires. Therefore we were able to prepare dodecylamine-capped Pt nanowires with 2 nm in diameter and several multiple in length in varying the synthesis conditions. The influence of temperature, stabilisers and reducing agents on the morphology has been investigated. The catalytic activity of such nanowires immobilized at different oxidic supports could also be demonstrated on the example of CO oxidation and will be compared to spherical Pt and bimetallic colloidal nanoparticles [2]. [1]: N. R. Jana, X. Peng, J. Am. Chem. Soc. 2003, 125, p.14280-14281 [2]: H. Borchert, D. Fenske, J. Kolny-Olesiak, J. Parisi, K. Al-Shamery, M. Bäumer, Angew. Chem. Int. Ed. 2007, 46, p.2923-2926

O 73.5 Thu 15:45 MA 005

Structural fluxionality in the CO adsorption on pure and binary silver-gold clusters $Ag_nAu_m^+$ — •Denisia M. Popolan and Thorsten M. Bernhardt — Institut für Oberflächenchemie und Katalyse, Albert-Einstein-Allee 47, Universität Ulm, 89069 Ulm, Germany

Temperature dependent reactivity measurements performed in a low energy ion beam apparatus, consisting of a sputter cluster ion source and a temperature variable octopole ion trap combined with an tandem mass spectrometers arrangement, shed new light on the reactive behaviour of pure and binary silver-gold cluster cations with CO. Several trends in the size and composition dependent reactivity were observed. While all investigated clusters form carbonyl products, the formation kinetics and maximum number of adsorbed CO strongly vary for the different cluster ions. In the case of the trimers, the largest saturation coverage is observed for Au_3^+. In contrast, for the pentamer clusters the maximum number of adsorbed CO molecules, at low temperatures, increases with increasing number of silver atoms n in $Ag_nAu_m^+$, correlated with a decrease in the CO binding energy. The results are discussed in terms of enhanced structural fluxionality due to the larger silver content in combination with a gradual change in the bonding type of CO to the metal clusters.

15 min. break

O 73.6 Thu 16:15 MA 005

Ligand versus ensemble effects in the adsorption on nanostructured bimetallic surfaces — Sung Sakong[1], Yoshihiro Gohda[2], and •Axel Gross[3] — [1]Fachbereich Physik, Universität Duisburg-Essen, Duisburg, Germany — [2]Department of Applied Physics, The University of Tokyo, Japan — [3]Institut für Theoretische Chemie, Universität Ulm, Germany

We have performed total energy calculations based on density functional theory addressing the reactivity of nanostructured bimetallic surface alloys. The catalytic activity of alloys is determined by electronic, geometric and structural factors which are often summarized employing the terms *ligand* and *ensemble* effects. Using the systems PdCu [1] and PtAu [2] as examples, we show that bimetallic systems can exhibit properties that do not correspond to an intermediate behavior in between those of the pure components but that are rather beyond those of both components [3]. Furthermore, whereas single atoms of the surface alloys can show a decreasing interaction strength with adsorbates (ligand effect), the binding at the most favorable adsorption sites can still become stronger when the concentration of the more reactive metal is increased (ensemble effect). The electronic and geometric effects underlying these phenomena will be addressed.

[1] S. Sakong, C. Mosch, and A. Groß, PCCP **9**, 2216 (2007).
[2] Y. Gohda and A. Groß, Surf. Sci. **601**, 3702 (2007).
[3] A. Groß, Topics Catal. **37**, 29 (2006).

O 73.7 Thu 16:30 MA 005

From adlayer to surface alloy - Change in chemical properties of bimetallic PtRu/Ru(0001) surfaces — •Thomas Diemant, Andreas Bergbreiter, Joachim Bansmann, Harry Hoster, and Rolf Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

The chemical and catalytic properties of bimetallic surfaces are of high interest as model systems for bimetallic catalysts. We studied the influence of the structural properties of PtRu/Ru(0001) model systems on their chemical properties. STM measurements show a change of the surface morphology in dependence of the deposition/annealing temperature. Deposition of Pt at room temperature (300 K) leads to dendritic Pt islands, while heating to 700 K results in rounded Pt islands. Annealing to even higher temperatures leads to the gradual formation of a surface alloy, which is completed at 1300 K. This surface alloy is characterised by a statistical distribution of the constituents in the surface layer. The change of the structural properties induces changes in the chemical surface properties, which were tested by the interaction of CO and D_2 with the model surfaces. The CO and D_2 TPD spectra show a redistribution of the intensity in the desorption peaks due to the modification of the surface structure. The influence of the surface structure is also evidenced in IR spectra of CO adsorbed on the model surfaces. We will correlate the change of the chemical properties of the bimetallic PtRu/Ru(0001) model systems to the modification of the structural properties and explain the variation of the chemical properties in terms of ligand, ensemble, and strain effect.

O 73.8 Thu 16:45 MA 005

Adsorption of CO on PdRu surfaces alloys studied by infrared reflection absorption spectroscopy — •Heinrich Hartmann, Thomas Diemant, Joachim Bansmann, and Rolf Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

The adsorption of CO on PdRu surface alloys on Ru(0001) has been studied by IRAS. The surface alloys were created by evaporating Pd on a Ru(0001) substrate and subsequent annealing to 1100 K. STM imaging shows a tendency toward island formation (phase separation) of the two constituents. IRAS experiments were performed to determine the CO adsorption sites on these bimetallic alloys. CO shows the same tendency for occupation of adsorption sites on the mixed PdRu surface as on the pure Ru(0001) and Pd(111) surfaces. On the Ru parts of the alloys CO adsorbs in a linear on-top configuration, on the Pd parts the adsorption of CO takes place on threefold-hollow sites (at small CO coverages) and on linear and bridge sites at (higher CO coverages). For all absorption bands the C-O vibration shifts to lower frequencies compared to the pure Ru(0001) and Pd(111) surfaces. These shifts are attributed to a modification of the electronic properties of the system.

O 73.9 Thu 17:00 MA 005

Decomposition of methanol by Pd, Co and bimetallic Co-Pd catalysts: model studies bridging the pressure gap — Tobias Nowitzki[1], Holger Borchert[1], Birte Jürgens[1], Peter Behrend[2], Yulia Borchert[1], Thomas Risse[3], •Volkmar Zielasek[1], Suzanne Giorgio[4], Claude R. Henry[4], and Marcus Bäumer[1] — [1]Institut für Angewandte und Physikalische Chemie, Universität Bremen — [2]UFT, Universität Bremen — [3]Fritz-Haber-Institut der Max-Plack-Gesellschaft, Berlin — [4]CRMCN-CNRS, Campus de Luminy, Marseille

Bimetallic particles may exhibit catalytic activities which reach far beyond those of the monometallic components. For the Co/Pd combination which is, e.g., of technological relevance for the hydrogenation of CO on the route from natural gas to liquid fuel, we have studied the interaction of model catalysts with methanol in order to obtain mechanistic information on decomposition reactions. In UHV studies, STM, TPD and XPS were performed at mono- and bimetallic nanoparticles prepared by PVD on thin epitaxial alumina films on NiAl(110). In comparison, the performance of Co/Pd nanoparticles, wet-chemically prepared on MgO, was studied in continuous flow reactors using DRIFTS and gas phase analysis at ambient pressure. This dual approach provides a consistent picture: The decomposition of methanol proceeds in two reaction pathways, the relative importance of which varies with the particle compositions. CO desorption is the limiting factor for activity at lower temperatures. Although electronic effects in the bimetallic system facilitate CO desorption, they do not compensate the lower intrinsic activity of Co sites compared to Pd sites.

O 73.10 Thu 17:15 MA 005

UPS investigations of ultrathin Au films deposited on Pd(110) — •Marco Moors[1], Tomasz Kobiela[1], Marko Kralj[2], Tobias Pertram[1], Conrad Becker[1], and Klaus Wandelt[1] — [1]Institute of Physical and Theoretical Chemistry, University of Bonn, Germany — [2]Institute of Physics, University of Zagreb, Croatia

The surface morphology and the local electronic properties of ultrathin Au films deposited on Pd(110) under UHV conditions have been studied by ultraviolet photoelectron spectroscopy and related methods. Investigations of bimetallic systems concerning morphology and adsorption properties are of great interest for the development of new catalysts with higher efficiency and durability. Our UPS and PAX experiments verified former STM studies [1] which showed a strong temperature dependence of the surface morphology. The Au-Pt surface prepared at 150 K is already quite flat and undergoes only a weak smoothening by annealing to 250 K. At a surface temperature of * 600 K gold starts to diffuse into the bulk forming a well ordered Au-Pd surface alloy with a maximal alloy concentration on the surface reached at 850 K. At an annealing temperature of 1050 K the surface gold depletion is completed. Besides the characterization of the Au-Pt system several adsorption experiments with various catalytic relevant molecules like CO and methanol have been performed.

[1] M. Kralj, A. Bailly, M.-C. Saint-Lager, S. Degen, A. Krupski, C. Becker, P. Dolle, M. De Santis, K. Wandelt; Surf. Sci. 600 (2006) 2614.

O 74: Metal Substrates: Adsorption of O and/or H

Time: Thursday 15:00–17:15 Location: MA 141

O 74.1 Thu 15:00 MA 141

Structure determination for the W(100)-(2×2)-O surface phase — •Wolfgang Meyer, Kerstin Biedermann, Lutz Hammer, and Klaus Heinz — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

For oxygen adsorbed on the W(100) surface and annealed at a temperature of 1000°C a (2×2) reconstruction is observed for which an O coverage larger than 1.0 ML has been reported [1]. Although the existence of this surface phase has been known for long, its structure is still unknown. We investigated this W(100)-(2×2)-O phase by means of quantitative LEED. The analysis reveals that the surface comprises two coexisting domains with p(2×2) and p(2×1) order, respectively. The p(2×1) structure is the already known missing row reconstruction with 1 ML oxygen atoms residing in the three-fold sites along the tungsten chains [2]. The p(2×2) domain consists of a single W atom per (2×2) unit cell decorated by four O atoms. Another oxygen atom is located on top of the 3^{rd} layer tungsten atoms, resulting in a total oxygen coverage of 1.25 ML for this domain. The surface is covered with the two domains at a fraction of 60 % for the (2×2) order and 40 % for the (2×1) order. The W(100)-(2×2)-O surface phase can be considered as a precursor for the (2×1) missing row structure which is fully developed for higher annealing temperatures.

[1] E. Bauer et al., Surf. Sci. **58** (1976) 517
[2] H. Yamazaki et al., Surf. Sci. **477** (2001) 174

O 74.2 Thu 15:15 MA 141

Oxidation of Fe$_3$Al followed by surface X-ray diffraction — •Claus Ellinger, Vedran Vonk, Navid Khorshidi, Andreas Stierle, and Helmut Dosch — Max-Planck-Institut für Metallforschung,

The interaction between oxygen and alloy surfaces plays a key role in many processes, such as thin film growth, corrosion and catalysis. Due to preferential surface segregation in binary alloys, one of the constituents will react with oxygen to form a thin oxide layer. These oxide layers are used as templates for model catalysts, tunneling barriers in electronic devices, or corrosion-resistant devices. To study the structural composition of the alloy surfaces at realistic conditions and to follow their oxidation process, surface sensitive x-ray diffraction (SXRD) provides a non-destructive in-situ technique. In this talk, the oxidation of Fe$_3$Al(110) will be discussed and compared to NiAl(110). Using AES, LEED and SXRD, we find a chemically well ordered surface of a clean Fe$_3$Al crystal. After exposure to a small amount of oxygen this ordering of the substrate completely disappears in the near surface region and a smooth thin Al$_2$O$_3$ layer is formed. While the fundamental, disordered A2 phase of Fe$_3$Al still exists in the surface region after the oxidation, the two ordered phases of the alloy are only found in the bulk. We therefore conclude that the substrate-oxide interface is still sharp and well-defined, while there is an oxygen induced shift of the stoichiometry within the surface towards the A2 phase.

O 74.3 Thu 15:30 MA 141

Oxidation of palladium surfaces and nanoparticles — •Nicola Seriani[1], Florian Mittendorfer[1], Georg Kresse[1], Jan Klikovits[2], Evelyn Napetschnig[2], Michael Schmid[2], Peter Varga[2], Rasmus Westerstrom[3], and Edvin Lundgren[3] — [1]University of Vienna, Austria — [2]TU Vienna, Austria — [3]Lund University, Sweden

Palladium finds wide application as oxidation catalyst, where a fundamental role is played by the interaction of its surfaces with oxygen. We have investigated formation of adsorption structures and surface oxides on selected Pd surfaces at atomistic level by density functional theory and first-principles thermodynamics as complement to experimental investigations. Surface oxide monolayers with stoichiometry close to that of bulk PdO have been observed and characterized and conditions for their thermodynamic stability have been predicted. Surface free energies of formation are then used in a Wulff construction to predict the shape of nanoscopic particles of palladium in dependence of temperature and oxygen pressure.

O 74.4 Thu 15:45 MA 141

Hot adatom motion tackled from first-principles — •Jörg Meyer and Karsten Reuter — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin (Germany)

The initial stages of the oxidation of metal surfaces are still far from being understood - despite their essential importance for example in the field of oxidation catalysis. In view of the exothermicity of the dissociative adsorption of O$_2$ at most metal surfaces, one fundamental question concerns the energy dissipation into the substrate, which, if sufficiently slow, could give rise to a transient mobility of the adsorbed, but not yet equilibrated oxygen atoms. In order to address this issue by first-principles theory we separate the molecular encounter with the surface into two stages: At large distances from the surface, substrate mobility can still be neglected and we focus our density-functional theory calculations on the six-dimensional potential-energy surface (PES) representing the molecular degrees of freedom. Performing extensive molecular dynamics (MD) runs on this suitably interpolated PES we evaluate the steering of thermal molecules into specific entrance channels. The corresponding molecular orientations and positions at intermediate heights above the surface form then statistically relevant starting geometries for first-principles MD trajectories of the remaining dissociation path that consider a full substrate mobility in large surface unit-cells. Applying this scheme to the O$_2$ dissociation over Pd(100), we will critically discuss a possible transient mobility especially in view of the restrictions on phononic dissipation inside the employed supercell geometry.

O 74.5 Thu 16:00 MA 141

Step decoration studied with first-principles statistical mechanics — •Yongsheng Zhang and Karsten Reuter — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin (Germany)

With respect to oxidation catalysis or oxide formation, surface defects like steps, kinks, or vacancies are widely believed to play a decisive role, e.g. in form of active sites or as nucleation centers. Despite this suggested importance, first-principles investigations qualifying this role for gas-phase conditions that are representative of these applications are scarce. This is mostly due to the limitations of electronic-structure calculations in tackling the large system sizes and huge configuration spaces involved. We overcome these limitations with a first-principles statistical mechanics approach coupling density-functional theory (DFT) calculations with grand-canonical Monte Carlo simulations, and apply it to obtain the phase diagram of on-surface O adsorption at a (111) step on a Pd(100) surface. The link between the electronic and mesoscopic techniques is achieved by a lattice-gas Hamiltonian expansion, in which we parameterize the lateral interactions affected by the step from DFT calculations at a Pd(117) vicinal surface, and all remaining lateral interactions from calculations at Pd(100). For a wide range of O gas-phase conditions we find the (111) step to be decorated by a characteristic zig-zag structure. Intriguingly, this structure prevails even up to the elevated temperatures characteristic for catalytic combustion reactions, where only small amounts of disordered oxygen remain at the Pd(100) surface.

O 74.6 Thu 16:15 MA 141

Hindered Spin-Transitions in the Dissociative Adsorption of O$_2$ on Al(111) — •Christian Carbogno[1], Jörg Behler[2], Axel Gross[1], and Karsten Reuter[3] — [1]Institut für Theoretische Chemie, Universität Ulm, Germany — [2]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Germany — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The low sticking probability for thermal O$_2$ molecules at Al(111) has recently been related to spin selection rules, which hinder transitions from the initial O$_2$ gas-phase triplet state to the singlet state of the adsorbed O atoms [1]. A constrained DFT approach was employed to compute potential energy surfaces (PESs) of O$_2$ in different spin-configurations from the surface, and the experimental sticking probability was qualitatively reproduced when restricting the O$_2$ molecule to motion on the spin-triplet PES only. Here, we extend these studies by considering the dissociation dynamics on multiple spin PESs, allowing transitions between them within Tully's fewest-switches algorithm as recently implemented [2]. The required non-adiabatic coupling elements have been derived in an *ab initio* fashion from the comparison between adiabatic and constrained-DFT PESs. Within this framework we obtain both good agreement with experiment for the fundamental features of the system as well as deeper insight into more peculiar characteristics of the dynamics. Based on our results, we propose experiments which can be used for the validation of our approach.

[1] J. Behler *et al.*, Phys. Rev. Lett. **94**, 036104 (2005).
[2] C. Bach *et al.*, Israel J. Chem. **45**, 46 (2005).

O 74.7 Thu 16:30 MA 141

Wechselwirkung von Wasserstoff mit einer Rhodium(210)-Oberfläche — •Henan Li, Christian Pauls und Klaus Christmann — Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany

In Fortsetzung unserer Studien zur Wechselwirkung von Wasserstoff mit fcc(210)-Oberflächen haben wir die Adsorption von Wasserstoff auf Rh(210) im Bereich zwischen 70 und 700 K mittels LEED, Thermodesorption, H2-D2-Isotopenaustausch- und Austrittsarbeits-($\Delta\varphi$)-Messungen untersucht. Bei 70 K adsorbiert Wasserstoff in mindestens vier Bindungszuständen (β_3, β_2, β_1 und α), die sequentiell bevölkert werden. β_3 (T$_{des}$ = 300...360 K) und β_2 (200...250 K) desorbieren mit (leicht bedeckungsgradabhängigen) Energien von ca. 80 bzw. 63 kJ/Mol nach 2. Ordnung und zeigen eine Erhöhung der Austrittsarbeit um ca. 120 meV, während der β_1-Zustand (T_{des} = 150 K mit E_{des} = 35 kJ/Mol) ebenso wie der α-Zustand (T_{des} = 93 K mit E_{des} = 23 kJ/Mol) eine Desorptionsordnung von 1 aufweist und zudem mit einer deutlichen $\Delta\varphi$-Erniedrigung verknüpft ist ($\Delta\varphi_{\beta 1} \approx -80$ meV; $\Delta\varphi_{\alpha} \approx -300$ meV). Ähnlich wie bei Pd(210) und Ni(210) bildet keiner der Zustände eine LEED-Überstruktur. H2-D2-Isotopenaustausch weist die β-Zustände klar als atomare H-Zustände aus, während die reduzierte HD-Intensität des α-Zustandes sowie dessen starke Austrittsarbeitsabnahme - ähnlich wie bei Pd(210) - zumindest Anteile von *molekular chemisorbiertem* Wasserstoff nahelegen. Im Unterschied zu Pd(210) erhalten wir jedoch keine Hinweise auf Subsurface-Wasserstoff.

O 74.8 Thu 16:45 MA 141

Strain effects in the adsorption on early transition metals — •Sebastian Schnur and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, Germany

Strain effects in the adsorption on transition metal surfaces have recently attracted a lot of attention. Strain can significantly change the electronic structure and thus the reactivity and catalytic properties of these metals. These effects occur, e.g., if a metal grows pseudomorphically on another metals. In this context, only late transition metals have been investigated so far [1] because they are the common catalytically active metals. However, early transition metals such as titanium or manganese represent promissing candidate materials in light intermetallic compounds for hydrogen storage.

Compressive strain leads to a reduced overlap of the wave functions and thus to a narrowing of the d-band. Charge conservation leads either to a downshift of the d-band in early transition metals or to an upshift in late transition metals because of the different degree of filling. According to the d-band model, a downshift of the d-band should cause weaker interactions with adsorbates [1]. We performed density functional theory calculations to study for the first time strain effects in several early transition metals using hydrogen and CO adsorption energies as a probe for their reactivity. The DFT results confirmed the predictions of the d-band model, thus providing guidance for a rational modification of the chemical properties of early transition metals. [1] M. Mavrikakis, B. Hammer, and J.K. Nørskov, Phys. Rev. Lett. **81**, 2819 (1998).

O 74.9 Thu 17:00 MA 141

Femtosecond laser desorption of atomic hydrogen from graphite in the visible and in the XUV using FLASH — •Robert Frigge[1], Tim Hoger[1], Björn Siemer[1], Carsten Thewes[1], Marcus Rutkowski[1], Helmut Zacharias[1], Stefan Düsterer[2], and Rolf Treusch[2] — [1]Physikalisches Institut, Münster, Germany — [2]Hasylab, Hamburg, Germany

The desoption of hydrogen from HOPG is of great interest in astrophysics. In so called H-I-clouds particles form areas of higher density in which protostars develop. The rise of protostars out of H clouds is not yet fully understood. This talk presents the laser desorption of hydrogen from HOPG. The velocity distribution of atomic hydrogen from HOPG is examined after surface excitation with fs pulses of 800 nm and 400 nm from a Ti:Sa laser system and 32 nm from a free electron laser(FLASH).
The atomic hydrogen is ionised via the 1s → 2s transition using a 2+1 REMPI detection scheme. Ionised H atoms are detected by a time-of-flight mass spectrometer. The arrival time distribution of H atoms at the ionised volume is measured by varying the delay between the pump and the probe laser. The transformation into a velocity distribution yields extremely slow velocities. The results are discussed more generally with the two temperature model and also in light of a recent DFT calculation. [Hornekaer et al., Phys. Rew. Lett.**97**, 186102 (2006)]

O 75: Oxides and Insulators: Epitaxy and Growth

Time: Thursday 15:15–17:15 Location: MA 042

O 75.1 Thu 15:15 MA 042

Preparation of High-Quality Ultrathin Free-Standing Bismuth Films — •Thomas Payer, Manuel Ligges, Ivan Rajković, Ping Zhou, Dietrich von der Linde, Michael Horn-von Hoegen, and Frank Meyer zu Heringdorf — Universität Duisburg-Essen, FB Physik, Duisburg, Germany

High-quality ultrathin free-standing metal films are used in many applications like X-ray filters or TEM/TED sample preparation. Deposition on top of sodium chloride templates is a well-known method to grow such films. Typically the crystals are either cleaved in UHV and material is deposited immediately afterwards yielding textured films. Alternatively crystals are cleaved in air making the preparation easier but yielding only lower-quality films. Due to step bunches from the cleaving only small area films can be grown. Our new preparation technique yields high-quality films on a millimeter scale.

We start from large (25mm and above) commercially sold sodium chloride single crystals. As sold, the sodium chloride disks are polished for optical applications in the infrared. The surface exhibits a large roughness and 100nm particle contaminations. Using a water rinse on a spin coater, the contaminations are completely removed. After an additional propanol rinse, AFM shows the presence of atomically flat terraces and regularly spaced atomic steps on the surface. Transfer into UHV yields the clean NaCl LEED pattern. Bismuth films of 20nm thickness are deposited in UHV at room temperature. Ex-situ AFM showed a roughness of only 1.5nm and crystallite sizes of 200nm. Additionally the crystallinity was studied with TED and TEM

O 75.2 Thu 15:30 MA 042

EBSD measurements and optimization of MBE-growth of Aluminum — •rudolf nüssl, torsten sulima, and ignaz eisele — Universität der Bundeswehr, Institut für Physik, Werner-Heisenberg-Weg 39, 85577 Neubiberg

The analysis of microstructure has become an important link between the science and the technology of materials. Since a few years the microstructure-analysis has been revolutionized by a new technique called Electron-Backscatter-Diffraction (EBSD). In this lecture it is shown, how EBSD can be used to optimize metallization systems of microelectronic devices by determining the epitaxial properties of the metallization layers. The metal especially treated in this report is Aluminum, which is deposited on substrates of LiTaO3 using MBE. When Aluminum is deposited directly on the substrate the metal will grow polycristalline. In contrast, if a thin matching-layer of Titanium is added on the crystalline substrate, Aluminum shows highly textured or even epitaxial growth. Additionally the texture quality depends on substrate-heating during deposition. The minimum thickness of the Aluminum film to obtain accurate EBSD-measuring-results was determined to be 200nm.

O 75.3 Thu 15:45 MA 042

Thin film growth of Fe$_2$O$_3$ on Ag(111) and Al$_2$O$_3$(0001) — •Maike Lübbe, Alexander M. Gigler, and Wolfgang Moritz — LMU, Department für Geo- und Umweltwissenschaften, Theresienstr. 41, D-80333 München

Hematite, α-Fe$_2$O$_3$, is an interesting and important iron oxide, most notably due to its magnetic and catalytic properties. However, the bulk material is a semiconductor with a wide band gap, $E_g = 2.1\,\mathrm{eV}$, which renders electron spectroscopic measurements very difficult.

We therefore grew Fe$_2$O$_3$ thin films on Ag(111), a system similar to Fe$_2$O$_3$ on Pt(111) (see e. g. [1]), which has not been reported up to now. The thin films were grown by MBE at low substrate temperatures, $T_{\mathrm{sub}} \leq 100°\mathrm{C}$, in an $\mathrm{O} + \mathrm{O}_2$ atmosphere, $p \approx 10^{-7}$ mbar, using an atomic oxygen source. The samples were characterised by different methods including Auger spectroscopy, XRD, AFM and Raman spectroscopy.

For comparison, we also grew Fe$_2$O$_3$ thin films on Al$_2$O$_3$(0001), a more commonly known system (see e. g. [2]). We had to choose higher substrate temperatures, $T_{\mathrm{sub}} \approx 500°\mathrm{C}$, to get reasonable results. Analysis revealed that thin films grown on Al$_2$O$_3$ are much smoother than those grown on Ag.

XRD measurements that will help to figure out structural differences between Fe$_2$O$_3$ thin films grown on Ag(111) or Al$_2$O$_3$(0001) are still in progress.

[1] A. Barbier *et al.*, Phys.Rev. B **72**, 245423 (2005)
[2] I. J. Lee *et al.*, J. Vac. Sci. Technol. A **23**, 1450 (2005)

O 75.4 Thu 16:00 MA 042

Growth and characterization of ultrathin CeO$_x$ films on Pt(111) — Jan Markus Essen, Tobias Pertram, •Conrad Becker, and Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstrasse 12, 53115 Bonn, Germany

The use of cerium oxides in catalysis is mainly motivated by its good redox properties and oxygen storage capability. The reproducible preparation of well characterized thin films of CeO$_x$ on a conducting material is important for using these films as model catalyst for the investigation of simple reactions with surface sensitive techniques. In this study we investigated CeO$_x$ films grown on Pt(111) with CO-TPD and HREELS.In order to produce CeO$_x$ thin films we followed three different routes: 1) Oxidation of Pt-Ce surface alloys at different temperatures; 2) oxidation of pure vapor deposited Ce films on Pt(111); and 3) evaporation of Ce in an oxygen atmosphere followed by annealing in oxygen. For Pt-Ce surface alloys oxidized at 900 K HREELS shows a pure CeO_2 film composition. Oxidation at 700 K and 1000 K however, does not lead to full oxidation of Ce, but a mixed oxide is suggested by the phonon spectra. CO-TPD measurements show that the pure CeO_2 films on Pt(111) are not closed. In contrast, exposing the Ce-covered Pt(111) surface to oxygen at 90 K followed by annealing to 1000 K does generate a fully covered surface, but again with a mixed oxide. Evaporating Ce in oxygen atmosphere also produces fully oxidized CeO_2 films but they show no good long-range order.

O 75.5 Thu 16:15 MA 042

Growth of well-ordered Mn_xO_y films on Pt(111): An in-vivo STM/STS study at elevated temperatures — •Benjamin Bochmann, Christian Hagendorf, Steffen Sachert, and Wolf Widdra — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle

Growth behavior as well as atomic and electronic structure of ultra thin epitaxial manganese oxide films on Pt(111) have been studied using STM/STS and LEED. The films have been prepared by reactive deposition of manganese in an oxygen atmosphere of 10^{-8} to 10^{-6} mbar. STM measurements performed during growth (in vivo) at elevated temperatures (400-600 K) reveal three different well-ordered monolayer structures depending on the preparation conditions: At lowest oxygen pressure a (19×1) uniaxially reconstructed MnO(100)-like layer is formed. STM data which resolve all atoms within one sublattice reveal details of the reconstruction. At higher oxygen pressure, an intermediate Mn_xO_y monolayer grows. It is complex, but characterized by sharp LEED pattern which corresponds with atomically resolved STM images of the periodic 1,5 nm × 1,5 nm unit cell structure. Under highly oxidizing conditions a quasi-hexagonal monolayer with MnO_2 stoichiometry is formed. LEED shows sharp satellite peaks which can be understood as a Moiré structure with 7% misfit to the Pt(111) substrate. STM images indicate a wagon wheel like reconstruction. The characterization of thicker Mn_xO_y films up to 6 ML is performed by STM and by noncontact-AFM. The latter allows also imaging of insulating films.

O 75.6 Thu 16:30 MA 042

Vibrational and electronic properties of ultrathin MnO(100) films — •Sebastian Polzin[1], Steffen Sachert[1], Krassimir Kostov[2], and Wolf Widdra[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Institute of Physics, Halle — [2]Bulgarian Academy of Science, Sofia, Bulgaria

The vibrational properties of ultrathin MnO(100) films on Pt(111) have been studied using high-resolution electron energy loss spectroscopy (HREELS). It was found that the strong optical phonon of the 1st monolayer at 368 cm^{-1} shifts to 382 cm^{-1} with increasing coverage up to 2 ML. At coverages above 1 ML a new phonon at 547 cm^{-1} is observed and identified as Fuchs-Kliewer phonon. Isotopic $^{16}O/^{18}O$ substitution reveales that a collective vibration of the oxygen against the manganese sublattice causes both phonons. For film thickness' up to 13 ML the Fuchs-Kliewer phonon shifts down to 539 cm^{-1}.

Electronic excitations in the energy range of 0-7.5 eV show well defined and narrow d-d band excitations for MnO(100) films from 1 to 10 ML. They converge nicely with increasing thickness towards MnO(100) single crystal data [1].

[1] B. Fromme et al., Phys. Rev. B 58, 9783 (1998).

O 75.7 Thu 16:45 MA 042

Structure of epitaxial cobalt oxide films on Ir(100)-(1×1) — •Daniela Hock, Wolfgang Meyer, Kerstin Biedermann, Matthias Gubo, Lutz Hammer, Stefan Müller, and Klaus Heinz — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Epitaxial cobalt oxide films were prepared on unreconstructed Ir(100). Visual LEED shows the resulting films to be of (111) orientation with, dependent on preparation details, either a distorted or ideal hexagonal unit mesh. In the distorted case there is, above 320 K, a (1×1) phase. The ideally hexagonal phase is accompanied by a (2×2) superstructure. In both cases the film thickness prohibits scattering contributions from the iridium substrate.

LEED intensities were taken for both the distorted (1×1) and the undistorted (2×2) phase. They were analysed by TensorLEED using phaseshifts alternatively for ions and neutral atoms. The distorted (1×1) phase turns out to be of the CoO(111) rocksalt structure with, however, substantial layer relaxations. Also, a stacking fault near the surface appears to be essential to get a good fit quality. In contrast to the distorted (1×1) phase, the undistorted (2×2) structure is due to a spinel-type $Co_3O_4(111)$ surface terminated by an oxygen layer with 1/4 ML Co on top. For both phases convincing comparison between experimental and model intensities is achieved (Pendry R-factor 0.19 and 0.13, respectively). The replacement of ionic by atomic phase shifts results in the same structural parameters within the limits of errors and similar best-fit R-factors.

O 75.8 Thu 17:00 MA 042

Phases of epitaxial cobalt oxide films on Ir(100)-(1×1) — •Kerstin Biedermann, Matthias Gubo, Daniela Hock, Wolfgang Meyer, Lutz Hammer, and Klaus Heinz — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

The unreconstructed (metastable) Ir(100)-(1×1) surface was used as support for the formation of thin epitaxial films of cobalt oxide. They were prepared by deposition of different amounts of cobalt and simultaneous exposure to an oxygen atmosphere at 320 K followed by annealing at higher temperatures. Dependent on exposure and annealing various structures can be observed. LEED shows that all of them own a hexagonal unit mesh which, however, can be slightly distorted. As a consequence, the oxides formed must consist of polar bilayers.

Ultrathin films (1-2 bilayers) form a c(10×2) superstructure which, according to its appearance in the STM, can be interpreted as rocksalt-type CoO(111) bilayers. Thicker films (≥4 bilayers), when oxygen rich and annealed at up to about 720 K, exhibit an ideal hexagonal unit mesh with a (2×2) superstructure. By further annealing at higher temperatures this transforms (irreversibly) to a $(\sqrt{3} \times \sqrt{3})$R30° phase with the basic hexagonal unit mesh slightly distorted. As monitored by TDS the transformation is accompanied by the loss of about a quarter of the oxygen content. This suggests that structurally this is a transition from spinel-type Co_3O_4 to rocksalt-type CoO as in fact corroborated by independent quantitative LEED analyses. At about 340 K the $(\sqrt{3} \times \sqrt{3})$R30° structure undergoes a reversible transition to a (1×1) phase.

O 76: Organic, Polymeric, Biomolecular Films - also with Adsorbates

Time: Thursday 15:15–17:30 Location: MA 043

O 76.1 Thu 15:15 MA 043

The Adsorption of Calcium on Regioregular Poly(3-Hexylthiophene) Studied by Microcalorimetry and X-Ray Photoemission Spectroscopy — •Fabian Bebensee[1], Wanda Lew[2], Junfa Zhu[3], Jack Hess Baricuatro[2], Hans-Peter Steinrück[1], J. Michael Gottfried[1], and Charles T. Campbell[2] — [1]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, D-91058 Erlangen, Germany — [2]Department of Chemistry, University of Washington, Seattle, WA 98195, USA — [3]National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, Anhui 230029, China

Regioregular poly(3-hexylthiophene) (rr-P3HT) is a semiconducting polymer used in organic electronics (OLED, OFET). In such applications, the interface structure and the interaction strength between the polymer and the electrode (e.g. Ca) play a crucial role in the performance of the device. The energetics of the interface, which directly reflects the interactions strength between the polymer and the metal film, is not accessible with conventional surface science techniques, but can be studied using adsorption microcalorimetry. We present a microcalorimetric study of the adsorption of Ca onto freshly prepared and, via electron irradiation, predamaged rr-P3HT films. Calorimetric measurements are supplemented by high-resolution XPS. The unusual combination of these complementary techniques leads to a new level of understanding of this technologically relevant interface. Financial

support by the DAAD and the NSF is gratefully acknowledged.

O 76.2 Thu 15:30 MA 043

Mercaptopyridine and 4-aminothiophenol self-assembled layers in metal-molecule-metal contacts: a computational DFT study — •Jan Kucera and Axel Gross — Institute für Theoretische Chemie, Universität Ulm, Germany

Recently it has become possible to deposit two-dimensional Pd layers on top of a 4-mercaptopyridine (Mpy) or a 4-aminothiophenol (4-ATP) self-assembled monolayer (SAM) on Au(111) leading to metal-molecule-metal contacts [1]. We performed periodic density functional theory (DFT) calculations in order to contribute to the interpretation of the experimentally observed geometric and electronic structures.

The calculations show that the adsorption structures of Mpy and 4-ATP on Au(111) are very similar. Both molecules prefer to bind to bridge-hollow sites at low as well as at high coverages. At low coverages, the molecules are significantly tilted from the Au(111) surface normal, whereas a denser packing leads to more upright configurations. The Pd/SAM interfaces correspond to metastable configurations in spite of the relatively strong Pd-Au interaction. The Pd-SAM contact is made through one-fold coordinated Pd-N bonds. In agreement with the experiment, the density of states (DOS) of Pd layer shows a significant reduction close to the Fermi level with respect to bulk Pd due to the Pd-N interaction. Also in agreement with experiment, the calculations confirm that 4-ATP is able to form bilayer structures connected through hydrogen bonds between the sulfur head group and up to to three hydrogen atoms of the amino group.

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

O 76.3 Thu 15:45 MA 043

Self-assembled monolayers of aromatic tellurides on gold and silver substrates — Tobias Weidner[1], Andrey Shaporenko[1], Jan Müller[2], Michael Höltig[2], Andreas Terfort[2], and •Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany — [2]Faculty of Chemistry, University of Marburg, 35032 Marburg, Germany

Self-assembled monolayers (SAMs) formed from bis(4'-methylbiphenyl-4-yl) ditelluride (BBPDTe) precursors on Au(111) and Ag(111) substrates were characterized by high-resolution X-ray photoelectron spectroscopy and near-edge X-ray absorption fine structure spectroscopy. BBPDTe was found to adsorb dissociative on both substrates, resulting in the formation of well-defined, densely packed, and ordered BPTe SAMs, with a larger molecular inclination, a lower packing density, and inferior crystallinity on Au than on Ag. However, both BPTe/Au and BPTe/Ag were not stable under ambient conditions, but underwent a rapid autooxidation, which affected exclusively the tellurolate headgroups. The BPTe molecules in the oxidized films remained, however, bound to the substrate by the terminal O atoms coordinated to the Te moieties, and the quality of the films, given by parameters such as packing density, degree of the orientational order, and average tilt angle of the SAM constituents was not noticeably affected by the autooxidation. In addition, the BPTe SAMs were compared with the analogous thiol- and selenol-based systems, and common tendencies for the different chalcogen headgroups, ranging from Te to O, were derived.

O 76.4 Thu 16:00 MA 043

Fabrication of multifunctional surface structures via laser patterning of silicon bound organic monolayers — •Benjamin Klingebiel[1], Luc Scheres[2], Steffen Franzka[1], Nils Hartmann[1], and Han Zuilhof[2] — [1]Fachbereich Chemie and Center for Nanointegration Duisburg-Essen (CeNIDE), Universität Duisburg-Essen (UDE), 45141 Essen, Germany — [2]Laboratory of Organic Chemistry, Wageningen University, Dreijenplein 8, 6703 HB Wageningen, The Netherlands

Silicon substrates are widely used as platforms in many micro- and nanofabrication schemes, e. g. in order to build up functional organic templates. For this purpose suitable patterning and functionalization techniques are needed [1-2]. Here we present a facile routine which allows to fabricate multifunctional organic surface structures. H-terminated Si(111) samples were functionalized with 1-hexadecene and 1-hexadecyne, respectively. Laser patterning of the primary monolayer then was carried out following a photothermal routine creating structures down to 100 nm and below [2]. For secondary functionalization of the depleted lines the samples were etched in ammonium fluoride solution and coated with hexadecynoic acid. Using N-hydroxysuccinimide (NHS) coupling chemistry this provides a means to bind biochemical compounds with primary amine groups. In order to test this functionality the samples were treated with NHS and dodecylamine.

1. L. Scheres, A. Arafat, H. Zuilhof, Langmuir 23 (2007) 8343.
2. D. Dahlhaus, S. Franzka, E. Hasselbrink, N. Hartmann, Nano Letters 6 (2006) 2358.

O 76.5 Thu 16:15 MA 043

Selective polymerization on laser patterned organic templates: Towards switchable surface structures — Mareike Mathieu, Alexander Friebe, Steffen Franzka, Mathias Ulbricht, and •Nils Hartmann — Fachbereich Chemie and Center for Nanointegration Duisburg-Essen (CeNIDE), Universität Duisburg-Essen (UDE), 45141 Essen, Germany

Stimuli responsive polymeric hydrogels provide a means to build up membranes with switchable pore structures [1]. Here we present results from experiments which aim at the fabrication of hydrogel nanostructures on planar surfaces. Native silicon wafers were coated with octadecylsiloxane monolayers and patterned following a photothermal procedure. In conjunction with postfunctionalization routines hydroxyl-terminated organic surface structures with a lateral dimension down to 100 nm and below have been prepared [2], and those were used to introduce initiator sites for heterogeneous graft copolymerization. Temperature-responsive poly(N-isopropylacrylamide) (PNIPAAm) was then grafted onto these structures via surface-initiated atom transfer radical polymerization (ATRP). The thickness and structure of the polymer coating were characterized using atomic force microscopy (AFM). Work in progress also addresses the temperature responsive properties of these polymer structures.

1. A. Friebe, M. Ulbricht, Langmuir 23 (2007) 10316.
2. D. Dahlhaus, S. Franzka, E. Hasselbrink, N. Hartmann, Nano Letters 6 (2006) 2358.

O 76.6 Thu 16:30 MA 043

Discrete laser patterning of phospholipid multilayers — •Mareike Mathieu, Daniel Schunk, Steffen Franzka, Christian Mayer, Eckart Hasselbrink, and Nils Hartmann — Fachbereich Chemie and Center for Nanointegration Duisburg-Essen (CeNIDE), Universität Duisburg-Essen (UDE), 45141 Essen, Germany

Phospholipid bilayers are widely recognized as model systems for biological membranes. Phospholipid multilayers also have been used as a matrix to arrange metallic nanoparticles into 2D structures [1]. Here we report on a photothermal procedure to pattern such phospholipid bilayer stacks. For patterning dioleyl-phosphatidic acid (DOPA) films were deposited on native silicon samples using the spin coating technique. Irradiation with a focused beam from an argon ion laser operated at a wavelength of 514 nm allows to locally remove the coating [2]. At a spot diameter of about 2.5 microns structures with lateral dimensions down to 400 nm were prepared. Most remarkably, however, partial removal can be carried out at incremental steps leaving a distinct number of bilayers behind. This offers an opportunity to build up discrete topographies, which could be used as 3D templates for the fabrication of multilevel architectures of nanoscopic components.

1. A. Terheiden, C. Mayer, K. Moh, B. Stahlmecke, S. Stappert, M. Acet, B. Rellinghaus, Appl. Phys. Lett. 84 (2004) 3891.
2. T. Balgar, S. Franzka, N. Hartmann, Appl. Phys. A 82 (2006) 689.

O 76.7 Thu 16:45 MA 043

Growth of phospholipid membrane systems on self-organized semiconductor templates — Gerald Trummer, Gregor Hlawacek, Daniel Pressl, and •Christian Teichert — Montanuniversität Leoben, Austria

Here, we use atomic force microscopy (AFM) to study the formation of solid-supported lipid bilayers on a variety of nanofaceted self-organized SiGe films on Si(001)[1] and ion eroded semiconductor surfaces [2] in comparison to smooth Si(001) wafers. 1-Palmitoyl-2-Oleoyl-sn-Glycero-3-Phosphoethanolamine (POPE) and 1,2-Dipalmitoyl-sn-Glycero-3-Phosphocholine (DPPC) were used as model systems. The resulting film morphology and the change of surface roughness have been investigated as a function of initial roughness and morphology of the substrate. Phase imaging is used to distinguish between the soft lipid layers and the hard semiconductor substrate. On SiGe templates showing a dislocation network it was found that the ridge trench structures appearing at the surface guide the terrace edges of DPPC layers. When the lipid coverage is very low, 100 nm x 100 nm pits of {105} faceted SiGe film act as preferential deposition sites for lipid bilayers resulting in ordered arrays of small POPE islands.

[1] C. Teichert, Phys. Rep. 365 (2002) 335. [2] S. Facsko, et. al., Science 285 (1999) 1551; T. Bobek, et al., Phys. Rev. B 68 (2003) 085324.

O 76.8 Thu 17:00 MA 043

High Frequency QCM Flow Cell with Enhanced Accuracy for Liquid and Biochemical Sensing — •Brigitte Paula Sagmeister[1], Hermann Gruber[2], and Reinhard Schwödiauer[1] — [1]Soft Matter Physics, Johannes Kepler University, Altenbergerstrasse 69, 4040 Linz, Austria — [2]Institute for Biophysics, Johannes Kepler University, Altenbergerstrasse 69, 4040 Linz, Austria

Throughout the last twenty years, acoustic wave sensors have been proven to be an extremely sensitive and accurate device for a wide variety of physical, chemical and biochemical sensing applications. Systems based on thickness sheer mode (TSM) quartz resonators, working in a liquid environment with resonance frequencies between 5 and 15 MHz, are already established for real-time measuremets of biochemical interactions and commercially available on the market. The utilisation of high frequency fundamental (HFF) quartz resonators, with resonance frequencies up to 150 MHz (and beyond), could further improve the sensitivity of such systems by orders of magnitude. We present a fully biocompatible flow cell, designed for HFF quartz resonators which, in spite of their small size, can be removed and exchanged quickly and with ease . The system performance is evaluated and quantified by a number of experiments including various viscosity measurement of sugar based solutions, the detection of a BSA proteine monolayer and other biochemical reactions. We further address some specific problems especially related to reusability and cleaning procedures.

O 76.9 Thu 17:15 MA 043

Preparation and Surface Characterisation of Thermally Deposited Ultrathin Ionic Liquid Films — •Till Cremer[1], Manuela Killian[1], Claudia Kolbeck[1], J. Michael Gottfried[1], Peter Wasserscheid[2], Florian Maier[1], and Hans-Peter Steinrück[1] — [1]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstrasse 3, 91058 Erlangen — [2]Lehrstuhl für Chemische Reaktionstechnik, Universität Erlangen

Due to their unique physico-chemical properties, ionic liquids (ILs) are promising candidates for many applications in electrochemistry, analysis, synthesis, separation and lubrication technology, and in catalysis.

In surface science, ILs open up interesting new possibilities: Since most ILs exhibit negligible vapour pressures at room temperature, various surface science techniques that employ ultra-high vacuum can be applied, enabling detailed investigations of their surface chemical composition and electronic structure. Furthermore, at elevated temperatures, thermal evaporation of ILs takes place, providing a new way for the in-situ preparation of ultrathin IL films on planar substrates.

In an angular dependent photoelectron spectroscopy (XPS) study we investigated imidazolium-based IL films of nanometer thickness, deposited on glass. For 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ($[EMIM]^+$ $[Tf_2N]^-$), we were able to demonstrate that the initial film growth occurs via a bilayer structure, with the $[Tf_2N]^-$ anions pointing away from the surface while the $[EMIM]^+$ cations are oriented towards the surface.

This work is supported by the DFG through SPP1191.

O 77: Methods: Scanning Probe Techniques I

Time: Thursday 15:30–17:30 Location: MA 041

O 77.1 Thu 15:30 MA 041

Advanced Spherical Probes for Atomic Force Microscopy — •Jan-Erik Schmutz, Marcus M. Schäfer, and Hendrik Hölscher — CeNTech, Universität Münster, Heisenbergstr. 11, 48149 Münster, Germany

In some areas of scanning probe microscopy it is highly important to use tips with a well defined radius [1]. This problem is commonly solved by glueing a microsphere onto the end of a tipless cantilever [2]. Though this technique is widely used we found some drawbacks especially for spheres with a radius smaller than 5 μm. Both in friction force microscopy (FFM) and in dynamic force microscopy (DFM) the effective tip height is an important parameter. In FFM the torsional spring constant is inversely propotional to the square of the tip height. Therefore, increasing the tip height decreases the torsional spring constant which leads to an enhanced sensitivity. Moreover with an increased tip height the risk of the cantilever edge touching a rough surface is being reduced. The main problem in DFM with a small tip height is the increased damping due to the compressed air in the gap between the cantilever and the surface [3]. Here we present a new cantilever design which avoids these disadvantages.

[1] W. A. Ducker et al., Nature **353**, 239 (1991)
[2] L. H. Mak et al., Rev. Sci. Instrum. **77**, 046104 (2006)
[3] O. I. Vinogradova et al., Rev. Sci. Instrum. **72**, 2330 (2001)

O 77.2 Thu 15:45 MA 041

Detection of Ferroelectric Domain Boundaries with Lateral Force Microscopy — Tobias Jungk, Akos Hoffmann, and •Elisabeth Soergel — Institute of Physics, University of Bonn, Wegelerstrasse 8, 53115 Bonn, Germany

The contrast mechanism for the visualization of ferroelectric domain boundaries with lateral force microscopy is generally assumed to be caused by mechanical deformation of the sample due to the converse piezoelectric effect. We show, however, that electrostatic interactions between the charged tip and the electric fields arising from the surface polarization charges dominate the contrast mechanism. A quantitative estimate of the expected electrostatic forces as well as comparative measurements on LiNbO3 and KTP crystals sustain this explanation.

O 77.3 Thu 16:00 MA 041

Evaluating Electrostatic Force Microscopies for the Investigation of Near-Surface Dopant Distribution in Silicon — •Markus Ratzke[1], Mario Birkholz[2], Joachim Bauer[2], Detlef Bolze[2], and Juergen Reif[1] — [1]LS Experimentalphysik II, BTU Cottbus und IHP/BTU JointLab, Konrad-Wachsmann-Allee 1, D-03046 Cottbus — [2]IHP, lm Technologiepark 25, D-15236 Frankfurt (Oder)

The still ongoing decrease in semiconductor device dimensions, both laterally and in depth, requires a sub-micron-scale mapping of surface potential, surface capacitance and near surface dopant distribution. Corresponding methods should operate non-invasively, leaving the specimen intact. Scanning-probe based techniques like Scanning Kelvin Probe Microscopy (SKM) and non-contact Scanning Capacitance Microscopy (SCM) represent promising tools.

To evaluate these techniques doping patterns produced by standard CMOS technology on silicon were investigated experimentally. Lattices of alternating p- and n-type doping in the 10^{17} to 10^{19} cm^{-3} range and a pitch of 360 nm were prepared by As^+ ion implantation. The results are compared to FEM calculations for a correlation with the expected carrier distributions. It turns out that SCM, mapping electrostatic forces at the second or third harmonic frequency of the AC driving voltage, yields higher resolution and contrast compared to SKM. In addition this technique appears to be less influenced by the actual surface conditions like roughness and surface charge. The physical significance of the higher harmonics will be considered.

O 77.4 Thu 16:15 MA 041

Fe/W(001) - a structurally, electronically and magnetically inhomogeneous system studied by force microscopy — •Rene Schmidt, Ung Hwan Pi, Alexander Schwarz, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, 20355 Hamburg

Since force microscopy detects all kinds of electromagnetic forces simultaneously, imaging of inhomogeneous samples is particularly challenging. We studied Fe films of around 1.3 atomic layers epitaxially grown on W(001), which are in this respect a prototypical sample system, as the structural, electronic and magnetic properties differ between first and second layer. Iron grows pseudomorphically on W(001) whereby the layers are highly strained. When imaging the surface, an electrostatic contrast with bias dependent apparent step heights can be observed, which is related to different work functions of first and second layer. Kelvin Probe Force Microscopy allows to map the work function and to measure the correct topography. Interestingly, we found that even on the same layer, different work functions are observed. Moreover, the first and second layer are magnetically different. The first layer is antiferromagnetically ordered, while double layers are ferromagnetic. As a result, a magnetostatic contrast from double layer islands is visible at relatively large tip-sample distances with ferromagnetic tips, while no magnetic signal is obtained on monolayer areas. However, at small separations the antiferromagnetic c(2x2) structure of the iron monolayer can be resolved by detecting the short-ranged magnetic exchange force between tip and sample.

O 77.5 Thu 16:30 MA 041

Resolution improvement for mid infrared nearfield optical microscopy through gold nanoparticle scatterers — •Marc Tobias Wenzel[1], Susanne C. Schneider[1], Lukas M. Eng[1], Stephan Winnerl[2], and Manfred Helm[2] — [1]Institute of Applied Photophysics, Technische Universität Dresden, 01062 Dresden — [2]Institute of Ion Beam Physics and Materials Research, Forschungszentrum Dresden-Rossendorf, 01314 Dresden

We present the implementation of 80 nm sized gold nanoparticles as tips for scattering nearfield optical investigations in the mid IR using a tunable free electron laser source (available frequency range 4 - 200 μm). At IR frequencies an efficient electric field confinement is advantageous for deducing the local dielectric and optical properties such as phonon vibration modes and local refractive indices of nm-sized implants. Our approach is based on confining the scattering volume by using gold-nanoparticles of different diameters. First, every single nanoparticle is characterized optically and then attached to an ordinary AFM cantilever tip. The cantilever is used as a spatial manipulator for the metal-nanoparticle scatterer in an AFM based scattering scanning nearfield optical microscope set-up (s-SNOM). Using these enhanced tips, we optically inspected anisotropic dielectrics at mid IR frequencies. As a result, we obtain a considerably improved confinement of the optical signal as demonstrated by tip/sample approach curves and theoretical modelling. Our experimental findings are in good agreement with our dipolar scattering theory.

O 77.6 Thu 16:45 MA 041

Frequency Modulation Atomic Force Microscopy and Spectroscopy on DPPC in Liquid — •Daniel Ebeling[1,2], Hendrik Hölscher[1,2], and Boris Anczykowski[3] — [1]Center for Nanotechnology (CeNTech), Heisenbergstr. 11, 48149 Münster — [2]Physikalisches Institut, Wilhelm-Klemm-Str. 10, 48149 Münster — [3]nanoAnalytics GmbH, Heisenbergstr. 11, 48149 Münster

The application of dynamic force spectroscopy in vacuum allows the mapping of tip-sample forces down to the atomic-scale. However, it has been shown that dynamic force spectroscopy works also in ambient conditions [1] and liquids [2] enabling the precise measurement of tip-sample forces. By adding a Q-Control electronics to the set-up of the constant-excitation mode of the frequency-modulation atomic force microscope we are able to increase the effective Q-factor of a self-oscillated cantilever in liquid to values comparable to ambient conditions [3]. During imaging of a DPPC bilayer on a mica substrate we observed an increased corrugation of the topography with increased Q-factors. This effect is caused by the reduction of tip-sample indentation forces [4]. Furthermore, dynamic force spectroscopy allows to measure the tip-sample forces and can be used as a powerful tool to determine the mechanical properties of the DPPC bilayer.

[1] H. Hölscher and B. Anczykowski. Surf. Sci. **579**, 21 (2005).
[2] T. Uchihashi et al., Appl. Phys. Lett. **85**, 3575 (2004).
[3] D. Ebeling, H. Hölscher, B. Anczykowski, Appl. Phys. Lett. **89**, 203511 (2006).
[4] D. Ebeling and H. Hölscher, J. Appl. Phys (accepted).

O 77.7 Thu 17:00 MA 041

Metal cross–substitution in the misfit layer compound $(\mathbf{PbS})_{1.13}\mathbf{TaS}_2$ — •Matthias Kalläne[1], Hans Starnberg[2], Kai Rossnagel[1], Martin Marczynski-Bühlow[1], Sven Stoltz[2], and Lutz Kipp[1] — [1]Institute for Experimental and Applied Physics, University of Kiel, D-24098 Kiel, Germany — [2]Department of Physics, Göteborg University, SE-412 96 Göteborg, Sweden

Bonding in layered materials is a challenging problem because it includes various types of interactions ranging from strong local covalent bonds over electrostatic interactions to rather weak nonlocal van der Waals forces. Consisting of alternatingly stacked slabs of hexagonally ordered transition metal dichalcogenides (TMDCs) and cubic monochalcogenides, the layered TMDC misfit compounds are hetero–structures with a complex layer–to–layer interface due to the different symmetries of the subsystems. Their incommensurability, the alternation of different layers, and the occurrence of monochalcogen bilayers all act against a low total energy. It is thus surprising that they show such a remarkable stability. To investigate the nature of the interlayer bonding, angle– as well as spatially–resolved photoelectron spectroscopy measurements were performed on the layered misfit compound $(PbS)_{1.13}TaS_2$. The results provide direct evidence for metal cross–substitution between the layers which alters the charge balance between alternating layers and can explain the remarkable stability of misfit compounds.

Photoemission experiments were carried out at HASYLAB, MAXLAB, and the ALS. Work supported by DFG FOR 353.

O 77.8 Thu 17:15 MA 041

Plan view and UHV-cross-sectional STM of GaN structures — •David Krüger, Thomas Schmidt, Stephan Figge, Detlef Hommel, and Jens Falta — Institute of Solid State Physics, University of Bremen, Germany

GaN-growth technology, though still mainly on sapphire substrates today, will be more and more directed towards homoepitaxial growth. Here, not only the polar c-plane of GaN is of interest, especially the non-polar perpendicular planes (e.g. m-plane) may be of even greater importance. XSTM investigations of GaN substrates cleaved under UHV conditions have been untertaken to reveal structural properties of their cross-sections. Moreover, STM-investigations of InGaN grown on sapphire based c-plane GaN-templates will be presented.

O 78: SYSA: Tayloring Organic Interfaces: Molecular Structures and Applications VIII (Invited Speaker: Tomasz Kowalewski; FV: DS+CPP+HL+O)

Time: Thursday 17:00–18:30 Location: H 2032

See SYSA for details about the program.

O 79: Invited Talk Stefan Tautz

Time: Thursday 17:45–18:30 Location: HE 101

Invited Talk O 79.1 Thu 17:45 HE 101

Bonding, Structure and Function of Highly Ordered Molecular Adsorbate Layers on Metal Surfaces — •Stefan Tautz — Institut für Bio- und Nanosysteme 3, Forschungszentrum Jülich, 52425 Jülich

The adsorption of large π-conjugated organic molecules on solid surfaces is attracting increasing interest, because it presents some fundamentally new aspects compared to small molecule adsorption. Moreover, molecular semiconductors have been developed to a point where devices such as OLEDs and OFETs are feasible. In these devices, interfaces between molecular phases and inorganic materials are important functional elements, and hence an additional, technological interest to study the adsorption of π-conjugated molecules has arisen.

In the present contribution, we focus on highly ordered organic adsorbate layers as model systems and discuss selected aspects of their bonding, structure and functional properties. The following issues are addressed: (1) The *bonding* of π-conjugated molecules often involves chemical contributions from different functional groups of the molecule.

Using a well-studied example molecule, the particular properties of such bonds and their interplay are discussed. (2) Intermolecular interactions have an important influence on the *structure formation* at the interface, leading to complex phase behaviour, for which examples are discussed. (3) Charge transport is the most relevant *function* of organic semiconductors. Transport experiments through a single-molecular wire, contacted covalently with an STM tip and gated mechanically by tip manipulation, demonstrate the strong influence of the metal-molecule bond on the transport characteristics.

O 80: Invited Talk Hari Manoharan

Time: Thursday 18:30–19:15 Location: HE 101

Invited Talk O 80.1 Thu 18:30 HE 101

Imaging Quantum Phase Information Using Isospectral Electronic Nanostructures — •Hari Manoharan — Department of Physics, Stanford University, Stanford, CA 94305, USA

At the juncture of geometry and wave mechanics lurks a subtle yet far-reaching spectral ambiguity. There exist drum-like manifolds that resonate at identical frequencies but possess different shapes, making it impossible to invert a measured spectrum of excitations into a unique physical reality. An ongoing mathematical quest has recently compacted this conundrum from higher dimensions to planar geometries. Inspired by these isospectral domains, we introduce a class of quantum nanostructures characterized by matching electronic structure but divergent physical structure. We perform quantum measurements (scanning tunneling spectroscopy) on these “quantum drums” (degenerate two-dimensional electrons confined by individually positioned molecules) to reveal that isospectrality provides an extra topological degree of freedom enabling the reconstruction of complete electron wavefunctions—including internal quantum phase information—from measured single-eigenmode probability densities. These methods are general and extensible to other nanostructures and fabrication techniques.

In these experiments we utilize the exciting technology of atomic and molecular manipulation: a custom-built scanning tunneling microscope, operating at low temperature in ultrahigh vacuum, is used to assemble nanostructures atom-by-atom to generate versatile quantum laboratories at the spatial limit of condensed matter.

O 81: Poster Session IV - MA 141/144: SYMS II and SYEC III (Modern Developments in Multiphysics Materials Simulations; Exact-Exchange and Hybrid Functionals Meet Quasiparticle Energy Calculations)

Time: Thursday 18:30–19:30 Location: Poster F

See SYMS and SYEC for details about the program.

O 82: General Meeting of the Surface Science Division

Time: Thursday 19:30–20:00 Location: HE 101

Report of the Chairman of the DPG Surface Science Division

O 83: Post Deadline Session (followed by Surface Science Symposion)

Time: Thursday 20:00–21:00 Location: HE 101

4 contributed talks to be determined

O 84: Plenary Talk Wolfgang Kleemann

Time: Friday 8:30–9:15 Location: H 0105

Multiferroic and Magnetoelectric Materials

O 85: Prize Talk Hagen Kleinert (Max Born Prize)

Time: Friday 9:15–10:00 Location: H 0105

Multivalued Fields in Condensed Matter, Electrodynamics, and Gravitation

O 86: Oxides and Insulators: Adsorption

Time: Friday 9:30–11:15 Location: MA 141

O 86.1 Fri 9:30 MA 141

Water Adsorption on Fe_3O_4(001): A First Principles Study — •Narasimham Mulakaluri[1], 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

The mode of adsorption of water (dissociative versus molecular) as well as its effect on the structural and electronic properties of the Fe_3O_4(001) surface is studied using density functional theory (DFT) calculations with the FP-LAPW method in the WIENK2k implementation. We vary the concentration of water and hydroxyl groups starting from a single water molecule per $(\sqrt{2}\times\sqrt{2})R45^\circ$ unit cell and compare the surface stability of the different terminations as a function of the O_2 and H_2O partial pressure within the framework of *ab-initio*

thermodynamics. Over a substantial range above the oxygen and water poor conditions, a clean Jahn-Teller distorted bulk termination is most favorable (*modified* B-layer) [1]. With increasing water pressure a water monomer, parallel to the surface, and finally a fully hydroxylated B-layer is stabilized. The calculations give indications of a lifting of the $(\sqrt{2} \times \sqrt{2})R45°$-reconstruction upon hydroxylation, consistent with low energy electron diffraction (LEED) measurements.
[1] R. Pentcheva et al., Phys. Rev. Lett. 94,126101 (2005).

O 86.2 Fri 9:45 MA 141

Water adsorption at low-indices (001) and (100) V2O5 surfaces. Cluster DFT studies. — Pawel Hejduk and •Malgorzata Witko — Institute of Catalysis and Surface Chemistry, PAS, Krakow, Poland

Vanadia-based materials are well known as the catalysts for numerous number of different chemical processes, as a consequence of an existence of non-equivalent active centers, both O and V types, localized on various faces of the catalyst crystal. Dependently on the preparation technique the V2O5 crystals can expose different surfaces, where the low-indices faces like (010), (001) and (100) are the most common. The (010) face is built of fully saturated V and O sites, whereas both (001) and (100) surfaces of unsaturated V and O surface atoms. Thus, the faces built of unsaturated character should behave differently in catalytic reactions compared to the (010) surface and an adsorption of small molecules should be enhanced.

In the present study water adsorption at the unsaturated surfaces is examined using cluster DFT approach. In addition a comparison with respect to saturated (010) surface is done. Results of calculations show that water molecule stabilizes at unsaturated surfaces due to the interaction of lone electron pair from O (from water) and unoccupied 3d states of vanadium. Upon adsorption, with low dissociation energy, water can dissociate and two hydroxyl groups are formed V(surface)-OH and O(surface)-H. It is in contrast to the (010) surface where water molecule undergo stabilization but only due to weak hydrogen bonding and its dissociation does not occur.

O 86.3 Fri 10:00 MA 141

Electronic properties of the active sites present at the (011)MoO2 surface. Periodic and cluster DFT quantum chemical studies. — •Renata Tokarz-Sobieraj[1], Malgorzata Witko[1], and Robert Grybos[2] — [1]Institute of Catalysis and Surface Chemistry PAS, Niezapominajek 8, 30-239 Krakow, Poland — [2]Faculty of Physics and Center for Computational Materials Science, Universitaet Wien, Sensengasse 8, A-1090 Wien, Austria

DFT method is applied to describe electronic structure of catalytically important (011) surface of molybdenum dioxide. MoO2 exists in literature mainly as a product of MoO3 reduction; however the problem of its role in catalytic process is still unsolved. In present paper attention is focused on the properties of surface active sites, both Mo and O, which are present at the selected (011) surface. In addition, comparison of (011)MoO2 and (100)MoO3 surfaces is carried out due to a fact that both surfaces contain not only the differently coordinated O sites but also the bare Mo centers. The electronic structure of studied systems is calculated using both periodic (VASP code) and cluster (StoBe code) approaches with gradient corrected functional. Local properties of different surface sites that are exposed at both surfaces are examined by means of charge densities, bond orders indices and molecular orbital diagrams whereas the global properties of both surfaces are discussed by density of states. The differences (existence of pairs of metallic sites on (011)MoO2 surface) and similarities (electronic states of bare Mo ions in both surfaces) in electronic properties of active sites are investigated taking adsorption of hydrogen and oxygen as examples.

O 86.4 Fri 10:15 MA 141

Wavefunction-based ab-initio results for the adsorption of CO on Ceria (110) surface — Carsten Müller[1], Björn Herschend[1], •Beate Paulus[2], and Kersti Hermansson[1] — [1]Department of Materials Chemistry, Uppsala University, Lägerhyddsvägen 1, 75121 Uppsala, Sweden — [2]Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin

For the ab-initio description of the adsorption process on surfaces it is necessary to model all interactions on the same theoretical footing. The standard density functional methods have their difficulties with describing dispersion forces. But especially for the physisorption, where no covalent bonds are formed between the adsorbant and the surface these interactions are essential. They can only well described with wavefunction based correlation methods. With the method of increments [1] it is possible to apply these methods to extended systems. Here we want to present the first application to an adsorption process. As example we have chosen CO on ceria 110 surface. The idea is to partition the correlation part of the adsorption energy according to localized orbital groups of the adsorbant and the individual atoms in the surface. The main part of the binding are the correlation energies of the absorbant with the different atoms of the surface. Therefore, with the method of increments it is not only possible to yield highly accurate results for the adsorption energy, but also gain information about the individual contributions to the adsorption.

[1] B. Paulus, Phys. Rep. 428, 1 (2006).

O 86.5 Fri 10:30 MA 141

The thermal behavior of H in O-ZnO(000-1) subsurface: a HREELS study — •Hengshan Qiu, Yuemin Wang, and Christof Wöll — Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, 44780 Bochum, Germany

The presence of H adatoms has pronounced effects on the structure and chemical properties of metal oxide surfaces [1]. The structure and stabilization mechanisms of the polar O-terminated ZnO(000-1) surface are still under discussion [2]. In this work, the interaction of atomic hydrogen with the O-ZnO(000-1) surface was studied using high-resolution electron energy loss spectroscopy (HREELS), thermal desorption spectroscopy (TDS) and low-energy electron diffraction (LEED). It is found that the clean, H-free O-ZnO surface exhibits a (1*3) reconstruction with one third of the surface O atoms missing, in good agreement with the results obtained by He-atom scattering (HAS)[2]. Adsorption of atomic H (or H_2O) at room temperature converts the (1*3) reconstruction to (1*1) with formation of OH species. In addition, The HREELS data reveal that exposing the clean O-ZnO surface to atomic hydrogen leads to a significant broadening of the incoherent elastic peak, indicating a surface metallization as determined on the ZnO(10-10) surface [3]. The metallization is induced by hydrogen adsorbed in subsurface. Upon heating these H atoms -instead of recombinative desorption- undergo migration into the bulk.

[1] Ch. Wöll, J. Phys. Condens. Matter. 16 (2004) 2981. [2] Ch.Wöll, Prog. Surf. Sci. 82 (2007) 55. [3] Y. Wang, et al., Phys. Rev. Lett. 95 (2005) 266104.

O 86.6 Fri 10:45 MA 141

Single adatom adsorption on SiO2 thin films — •Stefan Ulrich, Niklas Nilius, and Hans-Joachim Freund — Fritz-Haber-Institut, Berlin, Germany

The contribution discusses the unusual adsorption characteristic of a thin SiO2 film grown on Mo(112), which strongly depends on the geometric size of the adsorbates. The SiO2 layer consists of a network of -Si-O- hexagons exposing nano-pores with 3-4 Angstrom diameter. As revealed from low-temperature STM measurements, Pd adatoms penetrate this opening with nearly no barrier and bind strongly to the Mo-SiO2 interface. Au atoms on the other hand are too big and adsorb only at line defects in the oxide surface, where larger pores are exposed. The electronic properties of the adatoms and their interaction with the SiO2 support are deduced from tunneling spectroscopy.

O 86.7 Fri 11:00 MA 141

Self-Organization of MgPc Molecules on FeO Thin Films — •Xiao Lin and Niklas Nilius — Fritz-Haber-Institut, Berlin, Germany

The spatial arrangement of Magnesium Phthalocyanine (MgPc) has been investigated on FeO films grown on Pt(111) with low-temperature STM and STS. The polar oxide film forms a coincidence lattice with the Pt support and exhibits a surface dipole between the Fe(+) / O(-) layers that varies within the Moiré unit cell. The MgPc molecules preferentially adsorb on regions with large dipole strength. The rotational orientation of the molecules, on the other hand, is determined by their interaction with the atomic Fe-O lattice. The influence of the different binding configurations on the electronic structure of MgPc is revealed from spectroscopic investigations.

O 87: Symposium: Beyond Optical Wavelengths: Time-Resolved Spectroscopy of Surface Dynamics with EUV and XUV Radiation III (Invited Speakers: Christian Spielmann, Matias Bargheer, Philippe Wernet)

Time: Friday 9:30–12:00 Location: HE 101

Invited Talk O 87.1 Fri 9:30 HE 101

Time-resolved x-ray absorption spectroscopy with sub-20fs resolution — •Christian Spielmann — Physikalisches Institut EP1 Universität Würzburg, Würzburg, Germany

The development of reliable femtosecond solid-state laser brought new possibilities into time-resolved spectroscopy. For the first time it became possible monitoring the nuclear motion of molecules, crystal lattices and other out-of-equilibrium structures. However, usually it is very difficult to map the experimental observations to the structural dynamics. Therefore, experimental approaches are needed that can overcome the limitation of optical studies for structural determination, while the high temporal resolution of femtosecond lasers is maintained. Structural techniques such as x-ray diffraction (XRD) or x-ray absorption spectroscopy (XAS) deliver much more direct information about the structure. In this contribution we report on the optimized generation of sub-20fs x-ray pulses via high harmonic generation (HHG) resulting in an extension of the cut-off to nearly 3 keV. The x-ray radiation is intense enough over a broad energy range opening the way to time-resolved EXAFS (extended x-ray absorption fine structure). In a first proof-of principle experiment we followed structural changes in Silicon after excitation with an intense laser pulses. From the subsequent temporal evolution of the absorption spectrum far above the L and K-absorption edge, we gained direct information about the atomic motion. The observed dynamic is in good agreement with previous all-optical measurements.

Invited Talk O 87.2 Fri 10:00 HE 101

Direct observation of lattice dynamics by femtosecond x-ray diffraction — •Matias Bargheer — Institut für Physik, Uni Potsdam, Am Neuen Palais 10, 14469 Potsdam — Max-Born-Institut, Max-Born-Str. 2a, 14489 Berlin

The ultrafast photoinduced lattice dynamics of hybrid nanolayers composed of oxides with perovskite crystal structure is investigated by femtosecond x-ray diffraction, using a laser-based table-top hard-x-ray plasma source. The coupling of the optically excited electrons in metallic layers to optical phonon modes and the directed phonon-phonon coupling to particular modes is unravelled by directly observing the lattice motion in real time with sub-picosecond time resolution and sub-picometer accuracy of the structural information. In particular, the photoassisted ultrafast manipulation of ferroelectric polarization by switching giant strain in the GPa range is demonstrated.

O 87.3 Fri 10:30 HE 101

Toward Imaging Ultrafast Evolution on the Nanoscale — •William Schlotter[1,2], Ramon Rick[2], Andreas Scherz[2], Stefan Eisebitt[3], Christian Günther[3], Wolfgang Eberhardt[3], Olav Hellwig[4], Jan Lüning[5], and Joachim Stöhr[2] — [1]Institut für Experimentalphysik Universität Hamburg, Hamburg, Germany — [2]Stanford Synchrotron Radiation Laboratory, SLAC, Menlo Park, California, USA. — [3]BESSY m.b.H., Berlin, Germany — [4]San Jose Research Center, Hitachi Global Storage Technologies, San Jose, California, USA — [5]LCP-MR Université Pierre et Marie Curie, Paris, France.

Panoramic full field imaging with nanoscale resolution is demonstrated with soft x-ray Fourier transform holography. To extend the effective field of view, multiple regions of interest distributed about the sample are strategically paired with a holographic reference wave. In this way, images of each local region are simultaneously reconstructed without compromising spatial resolution. Using a nanoscale test structure fabricated by focused ion beam lithography we image four local regions on the sample spanning 180 μm with sub 100 nm spatial resolution.

Applying this holographic method to a cross-beam pump probe geometry, a technique is proposed for capturing multiple ultrafast images of a sample with a single x-ray pulse. In a cross-beam experimental geometry temporal phenomena are captured with respect to spatial position, and thus higher spatial resolution translates to faster dynamics. In this way the high spatial resolution and full field capabilities of holography are exploited to encode temporal information in a hologram, which could be recorded with a single pulse.

O 87.4 Fri 10:45 HE 101

Surface High Harmonic Generation: A route to ultra-intense attosecond pulses — •Rainer Hörlein[1,2], Yutaka Nomura[1], Brendan Dromey[3], Paraskevas Tzallas[4], Jens Osterhoff[1], Zsuzsanna Major[1,2], Stefan Karsch[1], Dimitris Charalambidis[4], Matthew Zepf[3], Ferenc Krausz[1,2], and George D. Tsakiris[1] — [1]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching, Germany — [2]Fakultät für Physik, Ludwig-Maximilians-Universität München, Am Coulombwall 1, 85748 Garching, Germany — [3]Department of Physics and Astronomy, Queen's University Belfast BT7 1NN, UK — [4]Foundation for Research and Technology Hellas, Institute of Electronic Structure and Laser, Heraklion Crete

High harmonic generation from solid surfaces (SHHG) constitutes a route towards generating very high harmonics (HH) and ultra intense attosecond pulses. In contrast to the generation of high harmonics from gases the SHHG mechanism is not limited in the laser intensity that can be used. On the contrary, the conversion efficiency and harmonic cutoff scale very favorably with driving laser intensity.

We present recent experimental results on the generation and characterization of HH radiation from solid targets. We present, amongst others, the generation of diffraction limited harmonic beams at 40nm and show our progress towards the temporal characterization of HHs from surfaces.

We also present an outlook towards possible applications of surface HHs as ultra-intense attosecond XUV probe beams for experiments.

Invited Talk O 87.5 Fri 11:00 HE 101

Femtosecond photoelectron spectroscopy with high-order laser harmonics at photon energies of above 20 eV — •Philippe Wernet, Kai Godehusen, Jerome Gaudin, Olaf Schwarzkopf, and Wolfgang Eberhardt — BESSY, Albert-Einstein-Strasse 15, D-12489 Berlin, Germany

Both bonding and structure of matter change at the atomic level and on ultrafast time scales during chemical reactions. The combination of x-ray spectroscopy, linking electronic and geometric structures, with the recently available short-pulse x-ray sources promises unprecedented access to the ultrafast dynamics in matter. We use high-order harmonics of a femtosecond (fs) laser as a source of fs vacuum ultra violet (VUV) pulses for time-resolved photoelectron spectroscopy. With a stable, reliable source for spectroscopy in mind different ways of generation, monochromatization and focussing of fs VUV pulses will be discussed. Our recent results on the electronic structure of gas phase Br_2 during dissociation will be used as a benchmark test. Laser pulses (400 nm) were used to excite the molecules to a dissociative state and the delayed VUV (53 nm wavelength) probe pulses ionized the molecules (overall temporal resolution 140 fs). Changes of the valence band spectrum indicate ultrafast breaking of the chemical bonds and rearrangements of the valence electronic structure are monitored all the way from the excited molecules into separate atoms.

O 87.6 Fri 11:30 HE 101

Structure and Dynamics of Free Nanoparticles studied by XUV Radiation — •Eckart Rühl — Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany

Recent progress on experiments using free nanoparticles is reviewed, where the perspectives on ultrafast processes are focus of the presentation. The targets come preferentially from colloidal chemistry approaches that allow one the preparation of structured nanoscopic objects of well-defined size-dependent properties. These nanoparticles are transferred from the liquid phase via an aerodynamically focused nanoparticle beam into a high vacuum surroundings, where the structural and dynamical properties of single nanoparticles are probed. This approach is complementary to studies on single, trapped nanoparticles. Results and perspectives involving XUV sources, such as synchrotron radiation, free electron laser radiation, as well as short pulse lasers in combination with higher harmonics and laser-produced plasma radiation are discussed along with proper detection techniques, including velocity map imaging of photoelectrons and elastic light scattering. Perspectives on attosecond dynamics involving free nanoparticles are briefly discussed.

O 87.7 Fri 11:45 HE 101

Ultrafast Phase Transitions in Metastable Water Near Liquid Interfaces — •Bernd Abel — Institut fuer Physikalische Chemie, Universitaet Goettingen, Tammannstr. 6, 37077 Goettingen, Germany

Liquid-gas phase transitions in water are an everyday occurrence, however, phase transitions of metastable superheated water are hardly understood so far despite their importance in many technical processes. By using short laser pulses to deposit heat at a rate faster than the thermal expansion rate, it is possible to prepare extreme states of matter at temperatures well above the normal boiling point. Electron spectroscopy for chemical analysis (ESCA) is a powerful tool for the quantitative analysis of the composition and the chemical environment of molecular systems. Employing high harmonics soft X-ray (50 eV) and near infrared femtosecond pulses and liquid water microbeams in vacuum we were able to add the dimension of time to the liquid interface ESCA technique. Tracing time dependent chemical shifts, electron orbitals and *energies of valence electrons in liquid water in time, we have investigated the timescale and molecular signature of laser induced phase transitions of metastable water on a femto- and picosecond timescale. The time-resolved data have been compared and analyzed with quantum chemistry and molecular dynamics calculations.

O 88: Metallic Nanostructures II (on Semiconductors)

Time: Friday 9:30–12:30 Location: MA 005

O 88.1 Fri 9:30 MA 005

Interactions Between Ag Nanoclusters on Carburized W(110) — •Magdalena Bachmann, Martin Gabl, Norbert Memmel, and Erminald Bertel — Institute of Physical Chemistry, University of Innbruck, A-6020 Innsbruck, Austria

Silver nanoclusters arranged in quasi-one dimensional chains were prepared on the R(15x12)-C/W(110) surface. Evidence is presented that these silver cluster chains form thermodynamic equilibrium structures. We address the question of possible interactions between neighbouring clusters by studying the length distributions of silver cluster chains with scanning tunnelling microscopy. Data are compared with theoretical expectations for various cluster-cluster interaction strengths. Best agreement between theory and experiment is obtained for a non-vanishing, slightly repulsive interaction energy of 14 +- 10 meV, despite the rather large cluster distance of 1.4 nm.

O 88.2 Fri 9:45 MA 005

Faceted silver clusters on HOPG and their stability — •Niklas Grönhagen, Farhad Ghaleh, and Heinz Hövel — Technische Universität Dortmund, Experimentelle Physik I, 44221 Dortmund

Silver clusters are interesting objects due to their optical and electronic properties. Close to the Fermi level silver is a nearly free electron metal where the electron delocalization leads to strongly cluster size dependent states [1]. However, the influence of the d-electrons is not negligible, e.g. for the optical properties of the clusters [2]. This interesting electronic structure is combined with a moderate chemical reactivity, which may be the reason why silver is used in many of the experiments for clusters on surfaces.

In the present study we produce faceted silver clusters by depositing silver atoms on HOPG samples, prestructured with nanometer sized pits [3,4]. Subsequently the clusters are investigated with STM. In these experiments we observe different shapes of the cluster facets as well as discrete cluster heights. Furthermore we investigate the clusters in terms of stability in different environments, e.g. air, bad vacuum or after STM-tip interaction.

[1] H. Hövel, B.Grimm, M. Bödecker, K. Fieger, B. Reihl: Surf. Sci. 463, L603 (2000)

[2] U. Kreibig, M. Vollmer, Optical properties of Metal Clusters: Springer Tracts in Materials Science 25 (Springer-Verlag, 1995)

[3] H. Hövel, Appl. Phys. A 72, 295 (2001)

[4] F. Ghaleh, R. Köster, H. Hövel, L. Bruchhaus, S. Bauerdick, J. Thiel, R. Jede: J. Appl. Phys. 101, 044301 (2007)

O 88.3 Fri 10:00 MA 005

Anisotropic Photoemission from Faceted Au Clusters on Graphite — •Ingo Barke[1], Heinz Hövel[2], Farhad Ghaleh[2], Richard C. Hatch[3], and Hartmut Höchst[3] — [1]Universität Rostock, Universitätsplatz 3, D-18051 Rostock — [2]Technische Universität Dortmund, Otto-Hahn-Str. 4, D-44221 Dortmund — [3]Synchrotron Radiation Center, 3731 Schneider Dr., Stoughton, WI 53589, USA

Quantized Shockley surface states have been observed on hexagonal facets of large Au clusters by means of scanning tunneling spectroscopy [1] and photoelectron spectroscopy [2]. Here we report on recent results obtained by angle resolved photoelectron spectroscopy (ARPES) with synchrotron radiation at the Synchrotron Radiation Center in Stoughton, WI (USA). Optimized preparation parameters resulted in narrow size distributions which allow for the direct observation of the size-dependent peak distance of quantized states. Angle resolved spectra reveal another striking difference between cluster facets and the bulk surface: we observe an unexpected asymmetry of emission intensity with respect to the emission angle which is very sensitive to the photon energy. With a suppression of almost 100% for one of the two branches of the parabolic dispersion this effect is much stronger and of opposite sign compared to the bulk Au(111) surface state.

[1] I. Barke, H. Hövel, Phys. Rev. Lett. 90, 166801 (2003).

[2] H. Hövel, I. Barke, Prog. Surf. Sci. 81, 53 (2006).

O 88.4 Fri 10:15 MA 005

Enhanced Bonding of Gold Nanoparticles on Oxidized TiO2(110) — •Stefan Wendt, Daniel Matthey, Jianguo Wang, Jesper Matthiesen, Renald Schaub, Erik Laegsgaard, Bjørk Hammer, and Flemming Besenbacher — Interdisciplinary Nanoscience Center (iNANO), and Department of Physics and Astronomy, University of Aarhus, DK-8000 Aarhus C, Denmark

We studied the nucleation of gold clusters on TiO2(110) surfaces in three different oxidation states by high-resolution scanning tunneling microscopy (STM). The three TiO2(110) supports chosen were (i) reduced having bridging oxygen vacancies, (ii) hydrated having bridging hydroxyl groups, and (iii) oxidized having oxygen ad-atoms. At room temperature gold clusters nucleate homogeneously on the terraces of the reduced and oxidized supports, whereas on the hydrated TiO2(110) surface clusters form preferentially at the step edges [1]. From interplay with density functional theory (DFT) calculations, we identified two different gold-TiO2(110) adhesion mechanisms for the reduced and oxidized supports. The adhesion of gold clusters is strongest on the oxidized support, and the implications of this finding for catalytic applications are discussed.

[1] Matthey, D.; Wang, J. G.; Wendt, S.; Matthiesen, J.; Schaub, R.; Laegsgaard, E.; Hammer, B.; Besenbacher, F., Science, 315, 1692 (2007).

O 88.5 Fri 10:30 MA 005

Aluminum oxide on Ni$_3$Al(111). A Template for Ordered Fe and Co Cluster Growth — •Andreas Buchsbaum[1], Micheal Schmid[1], Georg Kresse[2], and Peter Varga[1] — [1]Inst. f. Allg. Physik, TU Wien, Austria — [2]Faculty of Physics, CMS, University of Vienna, Austria

The structure of the aluminum oxide on Ni$_3$Al(111), which has been solved recently, exhibits holes at the corner of the $(\sqrt{67}\times\sqrt{67})$ R12.2° unit cell, reaching down to the metal substrate [1]. These holes are large enough to trap atoms of any kind of metal. Therefore, the ultrathin oxide film, forming a nanomesh, should be a perfect template for growing highly regular arranged metal clusters. Several metals have been deposited on the aluminum oxide and the clusters grown have been studied by scanning tunneling microscopy. The unmodified oxide, however, is not a good template for most metals. While Pd atoms nucleate in the corner holes and, hence, show a perfect hexagonal arrangement, Fe and Co clusters grow on other local defects, indicating a barrier to jump into the hole. By predeposition of a Pd seed layer, however, we can create a metallic nucleation site on each corner hole and Fe as well as Co clusters form a well-ordered hexagonal arrangement, making the oxide to a versatile template for growing highly regular arranged metal clusters [1]. We have also studied the morphology of the clusters and applied different methods to determine the orientation of the clusters. We have found different types of clusters, where only few of them show flat close-packed facets on top.

[1] M.Schmid et al., Phys. Rev. Lett. 99, 196104 (2007).

O 88.6 Fri 10:45 MA 005

Boron nitride nanomesh: an ultrathin insulating template — •Ivan Brihuega, Christian H Michaelis, Jiang Zhang, Sangita Bose, Violetta Sessi, Jan Honolka, Alexander M Schneider, Axel Enders, and Klaus Kern — Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

A key challenge in nanotechnology is the search of new materials suitable to act as nanoscale templates and also the growth of ultrathin insulating layers on metal surfaces which can be used to electronically decouple adsorbates from the substrate. Great success has been obtained in the formation of materials with templating or insulating capabilities, however, the combination of both abilities in the same system has not been yet achieved. In this work we show that the recently discovered BN nanomesh [1] combines both properties: templating at the nanoscale and electronic decoupling from the substrate. By covering the Rh(111) surface only partially with the Boron Nitride (BN) nanomesh, we have been able to directly compare the electronic properties of the BN nanomesh with the ones of the bare metal. Our low temperature scanning tunneling microscopy and spectroscopy experiments show that the BN nanomesh acts both as a nanotemplate, laterally ordering Co clusters deposited on it with a nearest neighbor distance of 3.2 nm, and as an insulator, electronically decoupling the clusters from the metal substrate.

[1] Corso, M. et al. Science 303, 217 (2004).

O 88.7 Fri 11:00 MA 005

Optical properties of single Mg particles on MgO thin films — •Philipp Myrach, Hadj Mohamed Benia, Niklas Nilius, and Hans-Joachim Freund — Fritz-Haber-Institut, Berlin, Germany

Light emission spectroscopy with an STM is employed to study the optical properties of single Mg particles grown on 5-10 ML thick MgO films on Mo(001). The particles exhibit distinct rectangular shapes with edges that align with the close-packed O rows of the oxide support. Luminescence spectra taken in the field emission regime (U>40 V) reveal a photon peak at 550 nm in addition to the well-known exciton emission of bare MgO at 400 nm. A similar emission peak is detected in the tunneling mode (U<10 V) for individual particles. The emission is assigned to a plasmon excitation in the Mg deposits. The high spatial resolution of the method allows also mapping of the emission intensity within one particle, thus providing information on the symmetry of the underlying optical mode.

O 88.8 Fri 11:15 MA 005

Two metal nano-particle enhanced Raman spectroscopy and microscopy — •Phillip Olk[1], Jan Renger[2], Marc Tobias Wenzel[1], Thomas Härtling[1], and Lukas M. Eng[1] — [1]Institut für angewandte Photophysik, TU Dresden — [2]ICFO-Institut de Ciencies Fotoniques, Barcelona

The distance and polarization dependent near-field enhancement of two coupling metal nanoparticles (MNPs) is analyzed by means of the novel Scanning Particle-enhanced Raman Spectroscopy (SPRM) technique [1]. In contrast to single MNP Raman experiments, the near-field coupling between two dissimilar MNPs leads to a Raman hot spot yielding an extra enhancement factor, as proven here both in experiment and theory.

The Au80 MNP is attached to the apex of an optical fiber manipulator and exposed to the exctitation light. A monolayer of 1-octanethiol molecules covering the Au80 MNP serves as the electric field prober when scanning the substrate carrying the Au30 MNP through the optical focus.

This constellation allows recording the Raman signatures from a very low number of well confined molecules. Moreover, also the spectral and spatial dependence could be explored with a superb sensitivity and very low integration time.

[1] P. Olk, J. Renger, T. Härtling, M. T. Wenzel, and L. M. Eng. *Nano Lett.* 6(7), 1736–1740, 2007.

O 88.9 Fri 11:30 MA 005

Evaluation of near field enhanced Raman spectroscopy on industrial Silicon structures — •Benjamin Uhlig[1], Jens-Hendrik Zollondz[2,3], Marc Tobias Wenzel[4], Martin Haberjahn[2,3], Peter Kücher[3], and Lukas M. Eng[4] — [1]Fraunhofer -Institut für Keramische Technologien und Systeme, Winterbergstrasse 28, 01277 Dresden, Germany — [2]Qimonda Dresden GmbH & Co. OHG, Königsbrücker Strasse 180, D-01099 Dresden, Germany — [3]Center of Competence CoC Metrology/Analytic, Fraunhofer-Center Nanoelektronische Technologien CNT, Königsbrücker Straße 180, D-01099 Dresden, Germany — [4]Institut für Angewandte Photophysik, TU Dresden, George-Bähr-Straße 1, D-01069 Dresden, Germany

Following Moores Law, semiconductor structures become smaller and smaller. The understanding of stress intentionally implemented in devices or stress in multi layer components due to thermal mismatch is a major challenge for metrology. A promising technique to obtain highly localized stress information is Tip Enhanced Raman Spectroscopy (TERS). This paper discusses under which conditions TERS can be applied to industrial semiconductor structures and which effects can be expected. In order to obtain an idea of the enhancement effects on Silicon, we show several Surface Enhanced Raman Spectroscopy (SERS) experiments using Au nanoparticles. By varying particle diameter, incident laser wavelength, aperture angle, aswell as incoming and scattered polarization orientation we achieve up to 100% enhancement on bulk Silicon (100 nm Au nanoparticles, 633 nm laser excitation).

O 88.10 Fri 11:45 MA 005

Design of SERS-active metallo-dielectric nanostructures — •André Siegel, Manuel Rodrigues Gonçalves, and Othmar Marti — Institute of Experimental Physics, Ulm University, Albert-Einstein-Allee 11, D-89069 Ulm, Germany

Since its discovery in the 1970‘s surface enhanced Raman scattering (SERS) has been an active field of research. Its attraction stems from the possibility to detect very tiny concentrations of certain molecules. These high sensitivities are correlated to strong local electric fields, which are usually generated by exploiting the plasmonic properties of metallic nanostructures at optical frequencies. However, many approaches ranging from irregularly shaped nanoparticles, dimers and clusters of nanoparticles to nanoporous metallic films can show very strong SERS spectra, though their reproducibility is mostly not satisfactory.

Therefore we have concentrated on the design and fabrication of periodic metallo-dielectric nanostructures using colloidal crystals as templates, as well as on FEM calculations to predict the associated local field enhancements. The used techniques and our results will be presented.

O 88.11 Fri 12:00 MA 005

Fabrication of metallic cones for optical near-field investigations — •Monika Fleischer[1], Florian Stade[1], Kai Braun[2], Johannes Stadler[2], Andreas Heeren[1], Michael Häffner[1], Marcus Sackrow[2], Catrinel Stanciu[2], Alfred J. Meixner[2], and Dieter P. Kern[1] — [1]Institute of Applied Physics, Auf der Morgenstelle 10, 72076 Tübingen, Germany — [2]Institute of Physical and Theoretical Chemistry, Auf der Morgenstelle 8, 72076 Tübingen, Germany

Metallic cones with dimensions of the order of 100 nm are highly favourable objects for optical near-field investigations using visible light. Upon illumination, strong electric field enhancement can be observed up to a few nanometers above the cone tip. However, fabricating well-defined metallic cones with a sharp tip on the nanoscale is nontrivial. We present a process flow in which arrays of cones are shaped from a continuous metal sandwich layer on silicon by subtractive ion milling. In the process, patterned hydrogen silsesquioxane resist (HSQ) is used as an etch mask. The resulting cones have tunable base diameters around 150 nm and tip radii down to less than 10 nm. Their optical characteristics are investigated by means of apertureless optical near-field microscopy. Field enhancement at the cone tip has been demonstrated both by simulation and by experiment. In combination, the metallic scanning probe of the microscope and the cone form a vertical antenna configuration. This antenna features a small tunable gap and strong variable field enhancement within the gap region.

O 88.12 Fri 12:15 MA 005

Analysis of damascene-fabricated Cu lines by electron backscatter diffraction and X-ray diffraction — •Anastasia Moskvinova, Steffen Schulze, Michael Hietschold, Ramona Ecke, Ina Schubert, and Stefan E. Schulz — Solid Surface Analysis Group and Center for Microtechnologies, Chemnitz University of Technology, 09107 Chemnitz, Germany

Electroplated copper has become the method of choice for filling narrow interconnect features for microelectronics applications in one processing step. However, as the trench width decreases, the influence of the physical-vapour deposited (PVD) seed layer becomes more important. Due to changes in the growth dynamics the volume fraction of the PVD copper rises significantly compared with the ECD copper. Therefore we focused our interest on understanding the grain growth mechanism in thin PVD copper films and its differences from the growth dynamics in ECD copper structures and films. For that reason we analyzed the grain size and crystallographic orientation by electron backscatter diffraction (EBSD) and X-ray diffraction. Both techniques indicate a strong (111) texture. The grain structure of the Cu line in the trenches may differ considerably from that of blanket films. Grain size of copper within the trenches is affected by size constraints Cu. In narrow lines we find more small grains than in wider lines, suggesting that the grain structure depends on the line geometry.

O 89: Metal Substrates: Epitaxy and Growth

Time: Friday 9:30–12:30 Location: MA 041

O 89.1 Fri 9:30 MA 041

Real time observation of multiphoton photoemission and surface second harmonic generation during the growth of Fe on Cu(001) — •Cheng-Tien Chiang, Aimo Winkelmann, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle(Saale), Germany

We observed simultaneously the multiphoton photoemission and second harmonic generation (SHG) at 3.1 eV incident photon energy during the growth of Fe on Cu(001). The well-known intensity variations observable in medium energy electron diffraction measurements of Fe/Cu(001) were correlated with the variations of the SHG signal. Using SHG as a reference, we assign the different phases of the Fe growth to the observed photoemission spectra. With this approach, we obtain the work function variations as a function of film thickness from the photoemission spectra. For the first 4 monolayers (ML) of Fe deposited on Cu(001), a non-monotonic variation of the work function is observed, with a decrease of 0.14 eV for 1 ML Fe. This value is consistent with theoretical calculations [1]. In correspondence to the work function variations, a resonant three-photon photoemission (3PP) feature oscillates in intensity as a result of the fixed relationship between the vacuum level and an intermediate image potential state. From the exponentially decaying part of 3PP signal we can estimate the inelastic mean free path of electrons with kinetic energy of 4 eV above the Fermi level to be about 10Å.

[1] S. Achilli *et al.*, J. Phys.:Condens. Matter **19**, 305021 (2007)

O 89.2 Fri 9:45 MA 041

The buried Ni/Cu(001) interface at the atomic scale — •Holger L. Meyerheim[1], Dirk Sander[1], Nikolay Negulyaev[1], Valeri S. Stepanyuk[1], Radian Popescu[1], Iona Popa[2], and Jürgen Kirschner[1] — [1]MPI-Halle, Weinberg 2, D-06120 Halle (Germany) — [2]ESRF, BP 220, F-38043 Grenoble (France)

We present a combined surface x-ray diffraction and theoretical analysis of the buried Ni/Cu(001) interface structure after deposition of 3 and 5 monolayers of Ni at room temperature. Highly accurate reflection intensities along the integer order crystal truncation rods were collected at the beamline ID3 of the ESRF in Grenoble (France). The analysis reveals interface mixing where 27±10% of top layer Cu-atoms are exchanged by Ni. In addition, a 0.13 Å inward relaxation of top layer Ni-atoms is determined. Atomic scale simulations reveal a kinetic pathway for the Ni/Cu-exchange process and explain the observed limited degree of intermixing. A disperse distribution of Ni within the Cu surface with a preferential Ni-Ni separation of 3-4 nearest neighbor distances is found [activation energy for exchange (E_b) equal to 0.65 eV]. Intermixing is spatially confined to two atomic layers adjacent to the interface in agreement with experiment. The calculations also provide an explanation for the markedly different behavior of intermixing reported for Fe-Cu(001)interface, where Fe forms embedded clusters in the Cu surface [1].

[1] D.D. Chambliss and K.E. Johnson, Phys, Rev. B 50, 5012 (1993)

O 89.3 Fri 10:00 MA 041

SXRD study at both sides of a temperature induced surface phase transition on Sn/Cu(001) — •jesus martinez-blanco[1], victor joco[2], carlos quiros[3], pilar segovia[2], and enrique g michel[2] — [1]Fritz Haber Institut, Berlin, Germany — [2]Universidad Autonoma de Madrid, Spain — [3]Universidad de Oviedo, Spain

The crystalline structure of 0.5 monolayer of Sn atoms adsorbed on Cu(001) has been studied by surface X-ray diffraction (SXRD) measurements. This surface undergoes a temperature-induced phase transition at 360 K from a single domain $(\sqrt{2} \times \sqrt{2})$R45° phase at high temperature to a two rotated domains $(3\sqrt{2} \times \sqrt{2})$R45° phase at low temperature. A full data set including in-plane reflections, superstructure rods and crystal truncation rods was measured for each phase. The optimization method employed for fitting the experimental data for both the high and low temperature phases is a type of genetic algorithm called Differential Evolution, used in this work for the first time to extract crystallographic information from SXRD data. For the low temperature phase, our results confirm the removing of every third row of copper in the alloyed top layer. For the high temperature phase, the overall dependence of the measured structure factors with the perpendicular momentum transfer is similar to the values extracted from the low temperature phase, suggesting a disordered nature for the high temperature phase. We propose a detailed model for this phase and for the nature of the thermal induced disorder. We discuss possible mechanisms to keep the local structure across the phase transition and the nature of the high temperature disordered phase.

O 89.4 Fri 10:15 MA 041

Ripple growth and - orientation during grazing incidence deposition of Cu/Cu(001) — •Herbert Wormeester, Frits Rabbering, Georgiana Stoian, Raoul van Gastel, and Bene Poelsema — Solid State Physics, MESA+ Institute for Nanotechnology, University of Twente, The Netherlands

We have studied the consequences of oblique incidence deposition for the morphology of the growth-front for a "prototypical"system Cu/Cu(001). Previous electron diffraction measurements showed that deposition at grazing incidence leads to the evolution of ripples, oriented perpendicular to the plane of incidence of the atom beam. New experimental results with high resolution low energy electron diffraction and STM will be presented. The ripple formation has also been studied with kMC simulations, which support and predicted experimentally observed changes in ripple orientation at later stages in growth. The relevant activation barriers for intra- and interlayer diffusion processes in these simulations have been tuned to describe quantitatively(!) experimentally observed morphologies in a wide range of temperatures (150-300 K) and coverages (up to 40 ML). A change in ripple orientation from perpendicular to parallel to the plane of incidence has been detected around a coverage of 40 ML at a temperature of 250K and a polar deposition angle of 80°. At 230K and at more grazing incidence this orientation transition has been found to occur at a much earlier stages in growth. This change in ripple orientation is related to the Super Poisson roughening of the growth front.

O 89.5 Fri 10:30 MA 041

Initial growth of Cu on Cu(001) by in-situ pulsed laser deposition at low temperatures — •Andreas Dobler and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

In previous studies we have characterized the initial growth of Cu on Cu(001) by pulsed-laser deposition (PLD) near room temperature by scanning tunneling microscopy (STM). In order to extend the temperature range to lower temperatures, we designed a setup which permits direct deposition onto the sample in the STM at pressures of 1.5×10^{-10} mbar. The distance between the ablation target and the sample is 270 mm and the incidence angle is 60° relative to the sample normal. The deposition rate is 2.5×10^{-5} atomic layers per pulse at a fluence of 3.5 J/cm^2.

We present first results on the initial growth of Cu on Cu(001) using the in-situ PLD setup. At the large incidence angle, sputtering holes appear on the surface due to the high kinetic energies of the deposited particles. We analyzed the densities of monolayer and vacancy islands at different temperatures and laser fluences and compared the results to thermal deposition measurements at identical conditions. Self-sputtering can be reduced by lowering the fluence and applying a magnetic field which eliminates ions of the ablation plume.

O 89.6 Fri 10:45 MA 041

What causes the high island densities in pulsed laser deposition? — Georg Rauchbauer, Florian Wimmer, Andreas Buchsbaum, Gerhard Betz, Peter Varga, and •Michael Schmid — Inst. f. Allg. Physik, TU Wien, Österreich

Pulsed laser deposition (PLD) is a method for growing thin films that combines nonthermal particle energies (typically 30 to 200 eV) with ultrahigh-vacuum compatibility. Compared to thermal deposition, PLD-grown films show a significantly higher island density and improved layer-by-layer growth. These features were attributed to either the high instantaneous particle flux or the high particle energies. Using scanning tunneling microscopy (STM), we have studied the nucleation and growth of Pt and Co on Pt(111) by PLD and we show that the high particle flux is not sufficient to explain the island densities observed. Experiments at low temperature, where adatom motion is frozen, and molecular dynamics simulations show that particle energies of $\approx$ 100 eV are sufficient to create small adatom clusters by “failed sputtering”. These clusters serve as nucleation centers and explain the differences between thermal deposition and PLD. We propose that the same mechanism is effective in sputter deposition.

O 89.7 Fri 11:00 MA 041

Double layer growth of Ru on Pt(111) - the contributions of strain and metal-metal bonds — •Petra M. Erne[1], András Berkó[1,2], Andreas Bergbreiter[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 Adress: Institute of Surface Chemistry and Catalysis, University of Szeged, H-6701-Szeged, Dóm tér 7, Hungary

As found in previous STM-studies, vapor deposition of Ru onto Pt(111) leads to the formation of double layer islands of rather small lateral dimensions [1,2], similar to the behavior reported for Co/Cu(111) [3]. In order to clarify wether this behavior is mainly due to the lattice mismatch between Pt(111) and the hexagonally packed Ru(0001) surface, or wether the main reason is a much stronger local Ru-Ru interaction as compared to the Ru-Pt intermetallic bond, we carried out Ru growth experiments on pseudomorphic Pt/Ru(0001) monolayer islands and films, where lattice mismatch effects should play no role. The results indicate that the differences between the Ru-Pt bond and the Ru-Ru bond are the dominating effects.

[1] Poster O 55.61

[2] H. Hoster, T. Iwasita, H. Baumgärtner, W. Vielstich; Phys. Chem. Chem. Phys. 3; 2001, 337.

[3] J. de la Figuera, J.E. Prieto, C. Ocal, R. Miranda; Surf. Sci. 307-309; 1994; 538.

O 89.8 Fri 11:15 MA 041

Atomic ensembles in Au_xPt_{1-x}/Pt(111) surface alloys - linking a quantitative STM study with DFT calculations — •Andreas Bergbreiter[1], Harry E. Hoster[1], Yoshihiro Gohda[2], Axel Gross[2], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — [2]Institute for Theoretical Chemistry, Ulm University; D-89069 Ulm, Germany

The knowledge of the available adsorption sites on catalyst surfaces is essential for the understanding of their adsorption and catalytic properties. 2D alloys, in which intermixing is confined to the surface, are excellent model systems to study correlations between the atomic distribution and the adsorption or reaction behavior. Based on high-resolution STM imaging with chemical contrast, the atomic distribution in Au_xPt_{1-x}/Pt(111) surface alloys is characterized by a segregation into homoatomic aggregates. This can be rationalized by an effective repulsion between unlike atoms in the outermost layer, which is supported also by DFT calculations. Using a 2D lattice gas Hamiltonian, we are able to simulate the atomic distribution via a Metropolis Monte-Carlo (MC) algorithm [1]. The effective interaction parameters for the Hamiltonian were derived from DFT-calculated energies for different ordered Au_xPt_{1-x}/Pt(111) slabs. The measured surface densities of different atomic ensembles, as counted in the STM data, and the MC generated distribution agree well, even though only pairwise interactions are considered in the Hamiltonian.

[1] A. Bergbreiter et al.; Phys. Chem. Chem. Phys. 9, 2007; 5127.

O 89.9 Fri 11:30 MA 041

Zn/Pd(111) - Adlayer versus Alloy Formation: An Investigation by Low-Energy Ion Scattering — •Werner Stadlmayr and Norbert Memmel — Institute of Physical Chemistry, University of Innsbruck, A-6020 Innsbruck, Austria

The system Zn/Pd(111) has recently attracted attention due to its relevance for methanol steam reforming. However, conflicting growth modes were reported in XPS studies [1] and TPD/CO-titration investigations [2], respectively. While the former work postulates the onset of alloy formation already slightly above room temperature, the latter work excludes alloy formation below 600 K. We apply low-energy ion scattering spectroscopy with monolayer sensitivity to clarify this issue. [1] A. Bayer, K. Flechtner, R. Denecke, H.P. Steinrueck, K.M. Neyman, N. Roesch, Surf. Sci. 600, 78 (2006). [2] H. Gabasch, A. Knop-Gericke, R. Schloegl, S. Penner, B. Jenewein, K. Hayek, B. Kloetzer, J. Phys. Chem B 110, 11391 (2006).

O 89.10 Fri 11:45 MA 041

Anomalous scaling of Cu-island dynamics on Ag(100) — •Christopher Zaum and Karina Morgenstern — Institut für Festkörperphysik, Gottfried Wilhelm Leibniz Universität, Appelstr. 2, D-30167 Hannover, Germany

We deposited Cu-islands containing 10 to 500 atoms on a clean Ag(100) surface at room temperature and investigated diffusion and decay of these islands with a fast scanning tunneling microscope. Islands at sizes above 80 atoms per island are adsorbed in hollow-sites. Islands at sizes below 80 atoms per island are adsorbed in bridge-sites. Diffusion and decay behavior of the hollow-site islands is similar to the behavior of both Ag-islands on Ag(100) and Cu-islands on Cu(100). In contrast, the diffusivity and the decay time of the bridge-site islands are significantly higher than any previously measured values. This indicates a novel mechanism of diffusion.

O 89.11 Fri 12:00 MA 041

DFT study of epitaxial graphene on Ru(0001) — •bin wang[1], marie-laure bocquet[1], stefano marchini[2], sebastian günther[2], and joost wintterlin[2] — [1]Laboratoire de Chimie, Ecole Normale Supérieure de Lyon, Lyon, France — [2]Department Chemie, Ludwig-Maximilians-Universität München, München, Germany

Graphene is a flat monolayer of carbon atoms with a honeycomb lattice, which has been a rising star in materials science for its unique electronic structure. It can also grow on surfaces if the lattice constants of the surface and of graphene match. In case of lattice mismatch, as in the case of metal surfaces like Ru(0001) [1] or Ir(111) [2], epitaxial growth leads to a moiré structure. We have investigated epitaxial graphene on a Ru(0001) substrate by means of large-scale density functional theory (DFT) calculations. We show that, contrary to other substrates, the graphene electronic structure displays massive local changes, alternatingly varying between a zero gap and a band gap of 2 eV. This result is caused by alternating weak and strong contact areas of the graphene on the Ru surface, correlated with a large geometric buckling of 1.5 Å over the 30 Å periodic moiré superstructure. The mismatching lattice between graphene and the substrate thus leads to a changing symmetry and electronic structure that both vary regularly on the nanometer scale. The results are in good agreement with recent STM experiments [1].

[1] Marchini S., Günther S. & Wintterlin J., Phys. Rev. B. 76, 075429 (2007) [2] N'Diaye A.T., Bleikamp S., Feibelman P. J. & Michely T., Phys. Rev. Lett. 97, 216501 (2006)

O 89.12 Fri 12:15 MA 041

Incommensurate epitaxy of graphene on Ir(111) — •Alpha N'Diaye, Johann Coraux, Carsten Busse, and Thomas Michely — II. Physikalisches Institut, Universität zu Köln

Graphene can epitaxially be grown on Ir(111) by thermal decomposition of hydrocarbons. Due to the incommensurate lattices of graphene and the underlying Ir(111) surface, a large supercell moiré with a periodicity of 25 Å emerges. Despite the incommensurability of the two lattices, graphene grows well ordered on Ir(111) with the dense packed iridium $[1\bar{1}0]$ direction parallel to the $[11\bar{2}0]$ of graphene.

We present two ways of preparing graphene on Ir(111). One method employs preadsorption of ethylene (C_2H_4) and subsequent thermal decomposition. This yields a high graphene island. The average island size can be controlled by temperature, while the coverage is fixed to about 20 % of the surface area. Based on the analysis of the evolution of graphene flake size distribution with time and temperature, we propose the coalescence of graphene flakes as a coarsening mechanism.

The second method is based on continuous exposure of the hot Ir(111) surface to ethylene. At the chosen temperatures (between 970 K and 1320 K) ethylene decomposes on iridium, but not on graphene. This process is suited to covering the whole surface with one layer of graphene. Nucleation of graphene flakes takes place exclusively at step edges.

Epitaxial perfection increases with the domain size. The domain size is crucially dependent on the preparation temperature. At 1320 K this size exceeds the micrometer scale.

O 90: Methods: Scanning Probe Techniques II

Time: Friday 10:15–12:00 Location: MA 042

O 90.1 Fri 10:15 MA 042

Multiple distance scanning tunneling spectroscopy of organic layers

— •Christian Wagner and Torsten Fritz — Institut für Angewandte Photophysik, TU-Dresden, George Bähr Str. 1, 01069 Dresden

Scanning tunneling spectroscopy (STS) has been proven to be a powerful tool to investigate the energetic position of electronic states of organic molecules adsorbed on conductive surfaces. Since already the front orbitals are typically situated 1 to 2 eV below and above the substrate's Fermi energy, one inherent problem is the need to apply equivalently high voltages, which might in turn damage the rather sensitive organic layer. One technique which is able to limit the electric field strength is the multiple distance STS, where several I- V spectra are recorded subsequently at a fixed lateral position while increasing the tip sample distance and voltage range from one spectrum to the next [1]. In our contribution we want to discuss the applicability of this method to organic adsorbates on the example of unsubstituted quaterrylene on Au, a molecule which has a large π-system and a comparably small HOMO-LUMO gap. We answer the question whether the multiple distance STS can be combined with a DOS calculation via the 1D WKB model [2]. As this method allows including the tip sample distance directly into the evaluation process, one could calculate an unambiguous sample DOS from the multiple I- V curves.

[1] R. M. Feenstra and J. A. Stroscio, J. Vac. Sci. Technol. B **5**, 923 (1987)

[2] C. Wagner et al., Phys. Rev. B **75**, 235432 (2007)

O 90.2 Fri 10:30 MA 042

Novel design for luminescence detection in the low temperature STM

— •Klaus Kuhnke, Alexander Kabakchiev, and Klaus Kern — Max-Planck Institut für Festkörperforschung, Stuttgart

We present a novel design for the detection of luminescence from the STM tunnel junction. Three optical paths are introduced into an existing low temperature STM. We employ free optical light propagation using lenses and mirrors which fully preserve essential information carried by the light like angular distribution, polarization, and emission time. Care has been taken to minimize the thermal input through the light paths into the liquid He cryostat. Possible operation modes are discussed and demonstrated by preliminary measurements.

O 90.3 Fri 10:45 MA 042

Alignment of molecular energy levels between two biased metal electrodes

— •Nikolai Severin[1], Hua Liang[1], Stefan Hecht[2], Ragnar Stoll[2], Klaus Müllen[3], Igor M. Sokolov[1], and Jürgen P. Rabe[1] — [1]Department of Physics, Humboldt University Berlin, Newtonstr 15, D-12489, Germany — [2]Department of Chemistry, Humboldt University Berlin, Brook-Taylor-Str. 2, D-12489, Germany — [3]Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany

Understanding the alignment of molecular energy levels in a monolayer of molecules located between two biased metal electrodes in a tunneling contact is of paramount importance in the fast developing field of molecular electronics. Current rectification in such systems has been described taking into account a strong dependence of the energy levels on the relative position of the molecules between the electrodes. However, to our knowledge such dependence has not been experimentally examined yet; it is also not self-evident, since also different simple pictures of energy level alignment may be rationalized. Here we report on the dependence of the current rectification ratio on the relative position of different molecules between a highly ordered pyrolytic graphite substrate and a Pt/Ir scanning tunneling microscope tip immersed in 1-phenyloctane. The variation of the relative position of the molecules within the gap is achieved by the variation of the tip-surface distance. We find that the variation of current rectification ratio is substantially different for different molecules. We propose a simple model which rationalizes the experimental observations.

O 90.4 Fri 11:00 MA 042

Spectroscopic THz near-field microscope

— •Hans-Georg von Ribbeck[4,1], Markus Brehm[1], Daniel van der Weide[2], Manfred Helm[3], Oleksy Drachenko[3], Stephan Winnerl[3], and Fritz Keilmann[1] — [1]Max-Planck-Institut für Biochemie and Center of Nanoscience, 82152 Martinsried*Max-Planck-Institut für Biochemie and Center of Nanoscience, Martinsried, Germany — [2]Dept. of Electrical and Computer Engineering, University of Wisconsin, Madison, WI 53706-1691, USA — [3]Forschungszentrum Dresden-Rossendorf, 01314 Dresden, Germany — [4]Institut für Angewandte Photophysik, TU Dresden, Germany

We demonstrate operating a scanning near-field opticalmicroscope of scattering type (s-SNOM) with broadband THz illumination. A homemade cantilevered W tip is used in a tapping-mode AFM. The direct scattering spectrum is obtained and optimized by asynchronous optical sampling (ASOPS), while near-field scattering is observed by using a space-domain delay stage and harmonic demodulation of the detector signal. True near-field interaction is manifested from the distance-dependence of gold samples. Furthermore scattering spectra of differently doped silicon are presented.

O 90.5 Fri 11:15 MA 042

Studying the spatial distribution of reactant gases above catalytically active microstructures by means of scanning mass spectrometry

— •Matthias Roos, Stefan Kielbassa, Joachim Bansmann, and Rolf Juergen Behm — Institute of Surface Chemisty and Catalysis, Ulm University, D-89069 Ulm, Germany

We present an apparatus for spatially resolving scanning mass spectrometry for measuring the 3D gas composition above planar catalytically active surfaces, which enables us to quantitatively determine local reaction rates, e.g., on individual fields of microstructured model catalysts. A piezo-electrically driven positioning substage allows control of the lateral and vertical positioning of the sample under a stationary capillary probe with micrometer-scale resolution. The diameter of the capillary orifice, connecting the reaction chamber with a differentially pumped quadrupole mass spectrometer, varies from 50 to 150 μm, depending on the used capillary. Measurements can be performed at pressures in the range of $10^{-3} - 10\,mbar$ and temperatures between room temperature and 450°C. The CO oxidation reaction on planar Pt microstructures was used as a test reaction for determining the lateral resolution of the setup and the spatial distribution of reactant gases. The CO_2 formation and CO consumption above the microstructures was evaluated as function of lateral displacement and distance between sample and probe to study the effects of gas transport in the regime between sample and probe. Furthermore, the feasibility of determining absolute reaction rates on individual microstructures is demonstrated.

O 90.6 Fri 11:30 MA 042

Smoothing of surfaces by deposition of amorphous PSZ

— •Johanna Röder and Hans-Ulrich Krebs — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany

Nowadays the investigation of growth characteristics is of great interest, as for many thin film technologies the surface morphology plays an important role. Especially for optical, electrical or mechanical properties it is important to control features like surface and interface roughnesses during the deposition of thin films. Up to now a lot of experimental and theoretical work has been done to investigate the roughness evolution during film growth on a smooth substrate. In this contribution another approach is chosen and the growth of films deposited on an already rough surface is investigated. Here smoothing phenomena may occur depending on the materials used. As rough substrates thin Ag-films on Si were used, which show distinct island growth and thus exhibit statistic roughness (rms of 0.9 nm). Smoothing is done by deposition of an additional amorphous layer of partially stabilized zirconium oxide (PSZ) with an rms-roughness of 0.1 nm on Si and the results were discussed with respect to the dominating smoothing mechanisms that occur during deposition. Therefore stochastic differential equations were consulted and the scaling behaviour of the roughness evolution was investigated. All samples were deposited by pulsed laser deposition and investigated via atomic force microscopy. Power spectral densities as well as autocorrelation functions were calculated.

O 90.7 Fri 11:45 MA 042

Experimental Observation of Amontonian und Superlubric Sliding in Extended Nanocontacts — •Dirk Dietzel[1,2], Tristan Mönninghoff[1], U. D. Schwarz[3], Claudia Ritter[3], Harald Fuchs[1,2], and Andre Schirmeisen[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]INT, Forschungszentrum Karlsruhe (FZK), Karlsruhe, Germany — [3]Department of Mechanical Engineering, Yale University, New Haven, CT, USA

One of the most fundamental questions in nanotribology is the contact area dependence of frictional forces on the nanometer scale. Unfortunately, conventional friction force microscopy techniques are limited for analyzing this problem due to the unknown and ill-defined tip-sample contact. This limitation can be circumvented by measuring the lateral force signal during the manipulation of nanoscale particles with a well-defined, clean contact to the substrate. In our study, the samples under investigation were metallic islands with diameters between 50-500 nm grown by thermal evaporation of antimony on highly oriented pyrolytic graphite (HOPG). Experiments that included the controlled manipulation of a large number of nanoparticles in ultrahigh vacuum show two distinct frictional states during particle sliding: While some particles show finite friction increasing linearly with interface area, thus reinforcing Amonton's law at the nanoscale, other particles assume a state of frictionless or 'superlubric' sliding. This unexpected duality of friction states can be explained by contamination effects of the interface that alter the frictional properties.

O 91: SYEC: Exact-Exchange and Hybrid Functionals Meet Quasiparticle Energy Calculations IV (FV: O+HL+DF+TT)

Time: Friday 10:15–12:30 Location: A 151

See SYEC for details about the program.

O 92: SYMS: Modern Developments in Multiphysics Materials Simulations III (FV: O+HL+MM)

Time: Friday 10:15–13:00 Location: A 053

See SYMS for details about the program.

O 93: Surface Chemical Reactions

Time: Friday 10:15–13:00 Location: MA 043

O 93.1 Fri 10:15 MA 043

A two-step mechanism for the oxidation of vacancies in graphene — •Johan M. Carlsson, Felix Hanke, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin

Complete oxidation of graphitic carbon materials leads to combustion and the formation of CO_2, but it has been suggested that partial oxidation of vacancies on the basal plane can yield catalytically interesting materials. The characterization of such oxidized graphite in temperature-programmed desorption (TPD) experiments detected a surprising amount of CO and significantly less CO_2 [1]. This work aims to clarify the oxidation mechanisms and surface structures under different experimental conditions. We use density functional calculations with PBE exchange-correlation to obtain the structural and energetic properties of oxidized graphene vacancies. To understand the TPD spectra, reaction barriers and rates for CO and CO_2 desorption are calculated from transition state theory and the nudged elastic band method. An *ab-initio* thermodynamics analysis shows a significant partial pressure-dependence of the oxygen content in vacancies. This indicates a two step mechanism for the initial oxidation, by which strongly bound CO-releasing C-O-C and C=O groups saturate the vacancies under the ultra-high vacuum conditions of TPD experiments. Atmospheric partial pressures lead to additional oxygen adsorption into extended groups such as C-O-C=O and O=C-O-C=O, which in return can desorb as CO_2. [1] B. Marchon *et al.*, Carbon **26**, 507 (1988).

O 93.2 Fri 10:30 MA 043

Structure and Composition of the TiO_2(110) Surface: From UHV to Realistic Reaction Conditions — •Piotr Kowalski, Bernd Meyer, and Dominik Marx — Lehrstuhl fuer Theoretische Chemie, Ruhr-Universitaet, D-44780 Bochum, Germany

Using DFT-based ab-initio calculations in combination with a thermodynamic formalism we have calculated the relative stability of various structural models of the nonpolar, mixed-terminated TiO_2(110) surface in contact with a surrounding gas phase at finite temperature and pressure. Adsorption and desorption of hydrogen atoms and water molecules, as well as the formation of O vacancies were considered. Assuming thermodynamic equilibrium between the TiO_2 surface and an oxygen, hydrogen and water containing atmosphere, we constructed a phase diagram of the lowest free energy surface structures.

For a wide range of temperatures and pressures we find that water will be adsorbed at the surface. At full monolayer coverage, a molecular adsorption of water is preferential. The most stable adsorption site for hydrogen atoms is on-top of the bridging O atoms. Surprisingly, we find that in thermodynamic equilibrium the bridging O atoms can not be fully saturated which hydrogen, but only a maximum coverage of about 0.6 monolayer can be reached. The formation energy for O vacancies is found to be rather high so that O defects should only form at extreme oxygen poor conditions.

O 93.3 Fri 10:45 MA 043

Dissociation of oxygen on Ag(100) by electron induced manipulation — •Carsten Sprodowski, Michael Mehlhorn, and Karina Morgenstern — Institut für Festkörperphysik, Abteilung Oberflächen, Leibniz Universität Hannover, Appelstr. 2, 30167 Hannover, Germany

Low-temperature scanning tunneling microscopy is used to study oxygen dissociation on Ag(100). Deposition of oxygen on Ag(100) at 80K leads to small clusters of 1 to 10 molecules. Inelastic electron tunnelling manipulation is used for the manipulation of these molecules. Thereby the STM tip is set above them, the feedback loop of the STM is switched off and a voltage is applied between tip and sample for exciting the electronical states of the molecules. For small energies (1500meV with 0.3 nA) the cluster reorders, while above a distinct energy threshold the electron induced manipulation leads to a dissociation of the single molecules within the cluster. After manipulation in some cases dissociated pairs at different distances are found. However mostly only one atom of the dissociated molecule is observed.

During the dissociation the tunnelling current rises until a plateau of 5nA (3500mV) and remains there for some milliseconds. One possible explanation is a vertical orientation of the molecules as a metastable state before dissociating. In addition atomic resolution and a dissociated cluster during the same scan let us identify the adsorbate places of the dissociated atoms.

O 93.4 Fri 11:00 MA 043

Modeling NO_x Storage Materials: Adsorption and interaction of NO_2 with BaO nanoparticles — •Thorsten Staudt[1], Aine Desikusumastuti[1], Sandra Gardonio[2], Silvano Lizzit[2], Erik Vesselli[3], Alessandro Baraldi[3], and Jörg Libuda[1] — [1]Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen, Germany — [2]Sincrotrone Trieste, Italy — [3]Physics Department, University of Trieste, Italy

In order to obtain a fundamental understanding of the underlying processes of NO_x storage and reduction (NSR) catalysts we have studied the reaction of NO_2 with BaO nanoparticles supported on an ordered Al_2O_3 thin film on NiAl(110). We use a combination of high-resolution XPS obtained at the synchrotron radiation facility ELETTRA in Triest, vibrational spectroscopy (IRAS) and molecular beam (MB) techniques. Various nitrogen-oxo surface intermediates are identified by XPS and IRAS and the reaction behaviour shows a strong temperature dependence. At 300 K surface nitrites are formed and the conversion into surface nitrates occurs only at a very low rate. These reactions are only limited to the surface of the BaO particles. At 500 K the conversion into nitrates is more facile and nitrate formation proceeds beyond the particle surface, which yields to the formation of ionic nitrates.

Decomposition experiments exhibit that the stability of the barium nitrate nanoparticles is strongly depended on the particle size [1]. The larger particles are stable up to a temperature of 650 K, whereas the surface related species on small particles decompose at a temperature of 350-450 K. [1] A. Desikusumastuti et al., Catal. Lett., in press

O 93.5 Fri 11:15 MA 043

Internal exoemission in K/p-Si(001) Schottky diodes — •Kornelia Huba, David Krix, and Hermann Nienhaus — Fachbereich Physik, Universität Duisburg-Essen, Duisburg

Ultrathin potassium films of typically 1 nm thickness were deposited on hydrogen terminated p-Si(001) surfaces at low temperatures. Using a softly approached gold ball, an electric contact to the thin film was formed and current/voltage characteristics were recorded as a function of the substrate temperature. The K/p-Si contacts are Schottky diodes with low reverse currents of below 10 pA. Applying thermionic emission theory a homogeneous Schottky barrier height of 0.56 eV was determined. Oxidation of the K films by exposures to molecular oxygen leads to chemically induced electronic excitations. They were studied by measuring the internal exoemission currents, i.e. chemicurrents, in the diodes. The chemicurrent transients exhibit a maximum and less significant additional features after longer exposures. In addition to the current measurements, the oxygen uptake as well as the K film thickness and morphology were characterized by Auger electron spectroscopy and Kelvin probe measurements.

O 93.6 Fri 11:30 MA 043

Non-adiabatic Phenomena during Oxidation of K/Pd-Thin-Films on Silicon — •David Krix, Kornelia Huba, and Hermann Nienhaus — Fachbereich Physik, Universität Duisburg-Essen, Duisburg

Large area, nanometer thick Pd films were grown on silicon substrates. On H-terminated, Boron doped H:p-Si(001) surfaces a Schottky barrier height of $\Phi_p = 0.38\,\mathrm{eV}$ could be extracted from I-V-measurements using thermionic emission theory. With nearly ideal behavior the diodes show reverse currents of below 1 nA at low temperatures of 120 K. Applying small amounts of K to the surface makes it highly sensitive to oxidizing gases. Similar to exoemission experiments, hot charge carriers are produced during oxygen exposure which can be measured as a chemicurrent, i.e. internal exoemission, flowing in a circuit involving the Schottky diode as a sensor.

Sensor parameters like K coverage and Pd film thickness were modified to study their influence on the time resolved chemicurrent transients. The total chemicurrent yield, i.e. the total amount of charge detected, was found to be exponentially attenuated with increasing Pd thickness at a constant value of $\lambda \approx 1.1\,\mathrm{nm}$. Auger emission spectroscopy and Kelvin probe measurements were used to compare the evolution of the chemicurrents to the oxygen uptake of the samples.

O 93.7 Fri 11:45 MA 043

Particle size dependence of adsorption state and photodesorption of NO on AgNPs on thin alumina film — •Daniel Mulugeta[1], Ki Hyun Kim[1], Kazuo Watanabe[1], Dietrich Menzel[1,2], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institute der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin — [2]Physik-Department E20, Technische Universität München, 85747 Garching

We report on the particle size dependence of adsorption state and photodesorption (PD) of NO adsorbed on Ag nanoparticles (AgNPs) with average diameter (d) between 2.5 and 12 nm, by using temperature programmed desorption (TPD) and mass selected time-of-flight (MS-TOF) measurements. NO adsorbed at 75 K forms dimers which partly desorb and partly dissociate to form 2NO and N_2O+O when heated. In TPD of NO shifts to higher peak temperature are found with increasing d. The PD cross section of NO at 2.3 and 4.7 eV in p-polarization increases monotonously when the particle size is reduced (∼2 times for d=2.5 nm). At 3.5 eV in p-polarization, the PD cross section of NO increases rapidly as d decreases up to d=5 nm (∼9 times) and then decreases as d is further reduced. At 2.3 and 3.5 eV the translational temperature of photodesorbing NO (T_t=∼700 K) does not change significantly with varying d. This indicates that the plasmon does not change the desorption dynamics of NO. However, at 4.7 eV a dramatic increase of T_t (up to ∼1250 K) is observed for very small d ($\leq$ 5 nm). We interpret these changes in terms of the size dependences of adsorption energy, plasmon strength, decay paths, and confinement.

O 93.8 Fri 12:00 MA 043

Chemicurrent studies on bimetallic surfaces — •Beate Schindler, Eckart Hasselbrink, and Detlef Diesing — Fachbereich Chemie and Centre for Nanointegration (CeNIDE), Universität Duisburg-Essen, D-45117 Essen, Germany

Chemical reactions on metal surfaces like adsorption and desorption reactions may dissipate their excess energy to substrate and adsorbate vibrations or to electronic degrees of freedom. This means excitation of e-h pairs directly at the surface. If the energy of the excited electrons is larger than the metal work function, the excess energy could be measured by light emission. Electronic surface excitations with smaller energies can be detected as internal currents in thin film tunnel or Schottky devices. We use tantalum–tantalum oxide–top metal tunnel junctions. As top metal 5 nm thick Pt films or 12 nm thick Au films were used. Both enable a ballistic transport of excited electrons (holes) with excess energies up to 1 eV from the surface to the oxide interface. The excited carriers are then detected in the tantalum backelectrode as a tunnel current. We compare the tunnel current traces induced by bunches of hydrogen atoms ($5 \cdot 10^{15}$ atoms in 20 sec) on the Au and Pt surfaces. For weak chemisorption systems constant chemicurrents are typical, which scale linearly with the atom flux j_H. For strong chemisorption systems like Pt-H exponentially decaying chemicurrent traces ($e^{-j_H \cdot t}$) are typical. Evaporating Au on top of Pt one can monitor the change of the chemicurrent trace from an exponentially decreasing type to a constant current type. This clearly shows that the adsorbate-surface chemistry determines the e-h pair excitation.

O 93.9 Fri 12:15 MA 043

Investigating the binding sites of solvated electrons in polar layers adsorbed on Cu(111) — •Michael Meyer, Julia Stähler, Uwe Bovensiepen, and Martin Wolf — Freie Universität Berlin, Arnimallee 14, 14195 Berlin

Electron solvation is a well known phenomena in polar environments like NH_3 and D_2O, i.e., the localization and energetic stabilization of an excess electron due to the reorientation of the surrounding molecules. The properties and dynamics of solvated electrons constitute an active field of research. Here we present a surface science approach to determine the solvation site of excess electrons at the interface between polar molecular layers and a metallic substrate. We investigate the localization of excess electrons in amorphous D_2O clusters and layers as well as amorphous ammonia layers, which are condensed on a Cu(111) substrate. Using two-photon photoemission spectroscopy(2PPE) we excite and probe excess electrons by UV and VIS laser pulses, respectively. For surface bound electrons adsorption of Xe leads to a change in binding energy due to a change of the dielectric environment which is directly measured by 2PPE. A transition from bulk bound solvated electrons to surface bound ones is found to occur at coverages of $\approx$ 3 molecular layers where the continuous ice layers break up into laterally separated ice clusters. Remarkably the excess electrons in NH_3-layers are always bound on the surface for the investigated thickness range of 2 to 22 layers. Possible scenarios regarding injection and detection probabilities as well as site configurations will be discussed.

O 93.10 Fri 12:30 MA 043

Electronic valence band structure of V_2O_5 — •Torsten Stemmler, Maximilian Kauert, Helmut Dwelk, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin

We will present high-resolution ARPES measurements of V_2O_5 single crystals carried out with He I resonance lamp and synchrotron radiation. The obtained experimentally band structure will be compared with calculations, e.g.[1] and [2]. By varying the excitation energy we have utilized the ARPES techniques to study also the time and photon flux dependence of valence band changes. This problem of degradation of the surface due to the high reactivity will be discussed referring to the previous 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 93.11 Fri 12:45 MA 043

STM-induced Switching of Hydrogen on a Silicon(100) Surface: An Open-System Density Matrix Study — •Karl Zenichowski, Tillmann Klamroth, and Peter Saalfrank — Theoretical Chemistry, Institute of Chemistry, University of Potsdam, Germany

STM (scanning tunneling microscope) techniques offer the possibility to reversibly switch a hydrogen atom between two stable conformations on a silicon(100) surface dimer at room temperature [1].

We study the switching dynamics of a hydrogen atom, using an open-system density matrix formalism. The Liouville-von Neumann equation in Lindblad form [2] is solved. Vibrational upward rates are calculated within the framework of first order perturbation theory, including expressions for resonant scattering and dipole coupling with tunneling electrons [3,4]. Vibrational deexcitation is treated by applying harmonic selection rules and scaling laws. Temperature is included via the principle of detailed balance.

The switching process in the high current regime is found to be governed by vibrational "ladder climbing" and subsequent tunneling in the electronic ground state. The influence of current, bias voltage, isotope mass, electric field, and dissipation strength is examined [5].

[1] U.J. Quaade et al., Surf. Sci. **415**, L1037 (1998). [2] G. Lindblad, Commun. Math. Phys. **48**, 119 (1976). [3] B.N.J. Persson, J.E. Demuth, Solid State Commun. **57**, 769 (1986). [4] B.N.J. Persson, A. Baratoff, Phys. Rev. Lett. **59**, 339 (1987). [5] K. Zenichowski, T. Klamroth, P. Saalfrank, in preparation.

O 94: Methods: Other Experimental Techniques II

Time: Friday 12:00–13:15 Location: MA 141

O 94.1 Fri 12:00 MA 141

***In situ* Präparation von kristallographisch orientierten Spitzen in der Rasterkraftmikroskopie** — •Thorsten Wutscher, Sebastian Gritschneder und Franz J. Giessibl — Universität Regensburg, Institut für Experimentelle und Angewandte Physik, 93 040 Regensburg

Die atomare Konfiguration und die chemische Identität der Spitze eines Kraftmikroskops ist von zentraler Bedeutung für die Abstands- und Winkelabhängigkeit der Kraft zwischen Spitze und Probe [1, 2]. Bisher wurden die Spitzen mittels eines elektrischen Feldes, einer Kollision mit der Probenoberfläche oder durch Ionenbeschuss präpariert. Hier wird versucht *in situ* eine saubere und kristallographisch wohldefinierte Spitze aus leicht spaltbaren Materialien herzustellen. Für Nickeloxid, ein Material mit Kochsalzstruktur, wurden drei unterschiedliche Spaltgeometrien entwickelt. Die mit einer Wafersäge bearbeiteten Nickeloxidstücke werden als Balken und Würfel auf einem stabilen Quarzfederbalken (qPlus Sensor) kristallographisch orientiert fixiert. Eine auf gesägte Sollbruchstellen wirkende Kraft leitet das Spalten in einer oder mehrerer Ebenen ein. Die Eignung der dadurch entstehenden Spitzen für hochauflösende Kraftmikroskopie wird durch erste Resultate atomarer Auflösung auf NiO (0 0 1) demonstriert.

[1] Yoshiaki Sugimoto, Pablo Pou, Masayuki Abe, Pavel Jelinek, Rubén Pérez, Seizo Morita and Óscar Custance, Nature, Vol. 446, 64 - 67 (2007)
[2] Stefan Hembacher, Franz J. Giessibl, Jochen Mannhart, Science, Vol. 305, 380 - 383 (2004)

O 94.2 Fri 12:15 MA 141

Scanning of the near-field thermal heat transfer — •Robert Berganski, Uli Wischnath, and Achim Kittel — Energy and Semiconductor Research Laboratory - University of Oldenburg

The heat transfer is measured by means of a scanning near-field thermal microscope based on a commercial scanning tunnelling microscope (STM). Hereby a miniaturized coaxial thermocouple is kept at a constant distance above the surface by using the constant current mode of the STM while the change of the temperature at the tip is recorded. Thereby the heat transfer and the sample topography are measured at the same time and, thus, the heat transfer can be correlated to the surface morphology. The investigated heat transfer relies on evanescent modes of the thermal transfer between the tip at room temperature and the sample at about 110K. All other interfering heat transfer mechanisms are excluded by using ultra high vacuum conditions. In the present contribution the focus lies on the material dependence of these evanescent modes which are reaching a few nano-meter into the vacuum. By varying the material of the sample surface the influence of the dielectric properties of the material and the morphology of the surface are studied.

O 94.3 Fri 12:30 MA 141

The mono-cantilever method of performing multi-contact measurements of surface conductivity — •Justin Wells[1], Karsten Hardrup[1], Fei Song[1,2], Jesper Kallehauge[1], Lauge Gammelgaard[3], Shi ning Bao[2], and Philip Hofmann[1] — [1]ISA and iNano, University of Aarhus, 8000 Aarhus C, Denmark — [2]Department of Physics, Zhejiang University, P.R. China — [3]MIC, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark

Despite the paramount importance of conductance measurements to bulk solid state physics, surface conductance is very poorly understood. A prominent example for the sorry state of the field is the Si(111)(7×7) reconstruction. Several claims to measure the surface conductance have been made but these span 5 orders of magnitude.

In this work, we present a multi-contact mono-cantilever probe, which differs from earlier monolithic 4-point probes by that fact that all contacts are mounted on a single cantilever. In this approach, the minimum spacing can be reduced to the order of 250 nm, whilst keeping the cantilever size in the micrometer range (and thus it is strong and easily visible).

As an example, we will present measurements made on Bi(111). In contrast to the semimetallic bulk, this surfaces support metallic surface states, forming a quasi two-dimensional metal. Using measurements with different probe spacings, we are able to estimate an upper limit of the conductance through these surface states.

O 94.4 Fri 12:45 MA 141

XRR investigations of II-VI and III-nitrid based DBR-structures, multilayers and superlattices. — •Radowan Hildebrand, Thomas Schmidt, Ardalan Zargham, Moritz Speckmann, Carsten Kruse, Detlef Hommel, and Jens Falta — Institute of Solid State Physics, University of Bremen, Germany

Thin layers, especially distributed bragg reflectors (DBR), are important components in vertical cavity surface emitting laser (VCSEL)-structures. The investigation of AlN/InGaN and MgS/ZnCdSe DBR structures with the method of x-ray reflection (XRR) enables the determination of electron density, multilayer thickness and roughness of the interfaces. Reducing the roughness is of peculiar interest to achieve high reflective DBRs.

O 94.5 Fri 13:00 MA 141

Stereographic intensity maps of elastically backscattered electrons in directional elastic peak electron spectroscopy — •Irek Morawski and Marek Nowicki — Institute of Experimental Physics, University of Wrocław, pl. M. Borna 9, PL 50-204 Wrocław, Poland

The full hemispherical intensities of elastically backscattered electrons from Au(111) were measured using directional elastic peak electron spectroscopy (DEPES) [1] at primary electron beam energies in the range from 0.5 till 2.0 keV. The enhancement of recorded intensities is observed when the primary electrons strike the crystalline sample along the close packed rows of atoms. Experimental stereographic intensity maps reveal a three-fold symmetry of the substrate, which gives straightforward identification of the sample crystalline structure. Theoretical intensity distributions were obtained using multiple scattering (MS) calculations [2]. In calculations different scattering orders were taken into account. An R-factor analysis of experimental and theoretical patterns reveals a significant role of the higher scattering order leading to the defocusing effect along the closest-packed rows of atoms. A contribution of particular sample layers to the recorded signal as well as application of the total electron mean free path instead of so far used values of the inelastic mean free path in calculated MS intensities are discussed.

[1] S. Mróz, M. Nowicki, Surf. Sci. 297 (1993) 66.
[2] I. Morawski, M. Nowicki, Phys. Rev. B 75 (2007) 155412

O 95: Special Talk Theodore Postol

Time: Friday 13:15–14:00 Location: H 0105

The US Missile Defense and Its European Components - Implications for European Security

O 96: Invited Talk Klaus Wandelt

Time: Friday 14:00–14:45 Location: HE 101

Invited Talk O 96.1 Fri 14:00 HE 101
Electrochemical Surface Science — •Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn

An important trend in surface science is to expand the investigations to more complex surfaces in UHV and/or surfaces in more realistic ambients like gas atmospheres or liquids. Based on a combination of in-situ (cyclic voltametry, electrochemical scanning tunneling microscopy, infrared spectroscopy and X-ray diffraction) as well as ex-situ methods (low energy electron diffraction, synchrotron X-ray- and Auger electron spectroscopy, ion scattering) various processes at single crystal copper electrode surfaces in contact with electrolytic solutions have been investigated and will be discussed in this presentation. Specific examples are ion-induced surface reconstruction, thin film growth, surface compound formation, and selfassembly of organic layers. Whenever possible comparison to relevant systems in UHV will be made.

O 97: Invited Talk Charles Campbell

Time: Friday 14:45–15:30 Location: HE 101

Invited Talk O 97.1 Fri 14:45 HE 101
Energetics of Metal Atom Adsorption on Surfaces of Oxides and Polymers — •Charles Campbell — University of Washington, Seattle, WA, USA

Heats of adsorption of metal atoms have been measured calorimetrically on clean MgO(100), CeO2(111) and polymer surfaces. These directly probe the thermodynamics that control molecular beam epitaxy (MBE), particle nucleation and film growth. A pulse of metal vapor from a chopped atomic beam adsorbs onto an ultrathin sample's surface, causing a transient temperature rise detected by a pyroelectric polymer ribbon touching the sample. The differential heat of adsorption and sticking probability are measured versus coverage up through multilayer coverages. Complimentary information on the film morphology and electronic structure is provided by ion scattering spectroscopy, AES, work function measurements and DFT calculations. The data provide the metal-substrate bond energy (BE), the adhesion energy and the interfacial energy. Defect sites are important strong-binding nucleation sites for metal cluster growth, and these can be produced and controlled by electron and ion bombardment. For polymer surfaces, the metal atoms have two main reaction pathways in dynamic competition: diffusion below the surface, where they bind strongly to reactive functional groups, and nucleation of 3D metal clusters on the surface.