

## O 37: Posters: Plasmonics, Electronic Structure and Spin-Orbit Interaction, Semiconductor and Insulator Surfaces, Nanostructures

Time: Tuesday 18:30–22:00

Location: P2

O 37.1 Tue 18:30 P2

**Free-standing gold nanoantennas for enhanced infrared spectroscopy** — ●CHRISTIAN HUCK<sup>1</sup>, ANDREA TOMA<sup>2</sup>, FRANK NEUBRECH<sup>1,3</sup>, and ANNEMARIE PUCCI<sup>1</sup> — <sup>1</sup>Kirchhoff-Institute for Physics, Heidelberg, Germany — <sup>2</sup>Istituto Italiano di Tecnologia (IIT), Genova, Italy — <sup>3</sup>4th Physics Institute and Research Center SCoPE, Stuttgart, Germany

Plasmon-polariton excitations of metal nanoparticles can couple to other excitations of similar energy, which gives rise to strong vibrational signal enhancement in the infrared. For a optimization with respect to the enhancement it is necessary to carefully design the optical properties of the antenna, e.g. by the geometry of the structure but also by the supporting substrate. Plasmonic nanostructures prepared on substrates with high refractive indices, such as silicon and zinc sulphide, feature lower quality factors, a lower extinction cross-section and a red-shifted resonance position compared to the low refractive index substrates glass and calcium fluoride. This behavior can be explained by induced screening charges in the substrate, leading to a more damped electron oscillation in the nanorods and thus to lower vibrational signal enhancements in SEIRS. In this contribution we present one way to reduce the undesirable influences of the substrate by fabricating elevated gold nanowires which are only partly in contact with the substrate. We show a comparison of the plasmonic response as well as the SEIRS activity between rods prepared by standard EBL and rods which were additionally treated with reactive ion etching to remove the silicon substrate around the hot-spots of the rods.

O 37.2 Tue 18:30 P2

**Thermal annealing of gold infrared nanoantennas** — ●JOCHEN VOGT<sup>1</sup>, FRANK NEUBRECH<sup>1,2</sup>, ANDREA TOMA<sup>3</sup>, and ANNEMARIE PUCCI<sup>1</sup> — <sup>1</sup>Kirchhoff-Institute for Physics, University of Heidelberg, Germany — <sup>2</sup>4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — <sup>3</sup>Italian Institute of Technology (IIT), Genoa, Italy

For the successful fabrication and application of plasmonic nanostructures, such as nanoantennas, proper material quality is indispensable. Often the material quality strongly affects the plasmonic properties of nanoantennas, which are essential for their application, e.g. for surface-enhanced infrared spectroscopy (SEIRS). In this work we demonstrate that thermal annealing can significantly improve the plasmonic properties of low quality polycrystalline nanowires, fabricated with standard electron beam lithography. Up to a certain temperature, thermal annealing leads to clear blue-shifts in resonance frequency accompanied by strong increases in extinction cross section. Beyond this limit, the annealing turns into a destruction of the nanowires due to the Rayleigh instability. In order to monitor the impact of thermal treatment on the morphology and the plasmonic properties, atomic force microscopy and microscopic infrared spectroscopy, respectively, were performed.

O 37.3 Tue 18:30 P2

**Mechanical control of plasmonic resonances** — ●ANJA LÖHLE, AUDREY BERRIER, and MARTIN DRESSEL — 1. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

The control of light-matter interactions in real time deepens our understanding of materials, in particular in the attractive field of plasmonics. The optical properties of plasmonic structures are influenced by geometrical parameters such as shape, size or ordering of the particles, as well as by the material properties of both the environment and of the resonant particle itself. This project proposes the investigation of the active control on plasmonic structures using mechanical stretching. We report on the mechanical tuning of the optical properties of different plasmonic systems, consisting of thin metallic layers or colloidal ensembles on top of a flexible substrate. The samples are uniaxially stretched to modify the inter-particle spacing or to induce changes in the geometry of the thin films. It is shown that it is possible to go from a conductive layer to an insulating regime and back to a conductive state by stretching the substrate and subsequent release of the strain. This is monitored by reflectance measurements associated to spectroscopic ellipsometry where models are applied to extract the complex permittivity of the layers. Understanding of the behaviour

of these novel, active materials is crucial to the development of novel technologies and emerging applications.

O 37.4 Tue 18:30 P2

**Magneto-optic surface plasmon resonance of Au/IrMn/Co/Au exchange biased layer systems** — ●SEBASTIAN KÜBLER, NICOLAS MÜGLICH, and ARNO EHRESMANN — Department of Physics, CINSaT, University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel

The magneto-optic surface plasmon resonance (MOSPR) in transverse geometry of glass/Au/IrMn/Co/Au/dielectric exchange biased (EB) thin film systems has been studied as a function of the Au-cap layer thickness for the dielectric air and water. The results show that it is possible to achieve either an optimal steepness of the reflectivity as compared to a glass/Au(48 nm)/dielectric layer system or to maximize the magneto-optic activity. As the Au-cap layer thickness is increased the magneto-optic activity is reduced whereas the steepness of the reflectivity in the range of the resonance is raised. The width of the reflectivity curves and the magneto-optic signals are broadened for thin Au capping layers. The presented results demonstrate that the EB system under investigation can be optimized by adjustment of the Au-cap layer thickness for SPR and MOSPR based biosensing applications.

O 37.5 Tue 18:30 P2

**Advantages of a quantum cascade laser for surface enhanced infrared spectroscopy** — ●ANTON HASENKAMPF, NIELS KRÖGER, ANNEMARIE PUCCI, and WOLFGANG PETRICH — Universität Heidelberg, Kirchhoff-Institut für Physik, INF 227, 69120 Heidelberg

The main tool for surface-enhanced infrared spectroscopy (SEIRS) is the Fourier transform infrared (FTIR) spectrometer with a global source. It allows spectroscopy of a sample over a broad spectral range, which in our case covers 1  $\mu\text{m}$  to 20  $\mu\text{m}$ . The disadvantage of this system is very low spectral power density of the global. This usually is compensated by long measurement times. In this work, we present measurements with an external cavity quantum cascade laser (QCL) with grating in Littrow configuration which is integrated into a scanning microscopy setup. The QCL enables spectral measurements in the range of 1140 to 1430  $\text{cm}^{-1}$ . The  $10^8$  times higher spectral power density as compared to a global reduces measurement time drastically. Also the detection with a deuterated triglycine sulfate (DTGS) instead of a nitrogen cooled mercury cadmium telluride (MCT) is possible. The tuning range of the QCL of 290  $\text{cm}^{-1}$  nicely matches the requirements of SEIRS since, for nanoantennas, the enhancement occurs over a limited spectral range of the same order.

O 37.6 Tue 18:30 P2

**Mueller matrix characterization of three-dimensional gold spiral nanostructures** — ●ELVIRA MBEKWE PAFONG, AUDREY BERRIER, BRUNO GOMPF, BETTINA FRANK, HARALD GIESSEN, and MARTIN DRESSEL — Physikalisches Institut and Research Center SCoPE, Pfaffenwaldring 57, 70550 Stuttgart

Mueller matrix (MM) spectroscopy is a powerful tool to characterize nanostructures as it provides both amplitude and phase information. The decomposition of the measured MM grants the extraction of all the optical parameters such as linear birefringence/dichroism and circular birefringence/dichroism. However, it is difficult to attribute effective parameters to artificial nanostructures, especially when they are three-dimensional (3D). A full characterization in a large frequency range and broad reciprocal space is therefore necessary. Along with angle-resolved transmission measurements to determine the spectral position and the dispersion of the resonant modes, we perform MM spectroscopy to obtain phase information and compare the optical behaviour to that of conventional crystals. The measured MM elements are compared with simulations based on general oscillator models taking into account the azimuthal and spectral positions of the resonances. We find that the 3D nanospirals exhibit a complex optical response that cannot be reproduced by basic optical properties such as birefringence or optical activity only. Spirals with different geometries are compared in order to extract the optical response intrinsic to their 3D nature. This study sheds light on the complex response of plasmonic nanostructures and is useful for future designs of novel optical devices.

O 37.7 Tue 18:30 P2

**Superlensing in n-doped GaAs investigated by near-field microscopy** — ●MARKUS FEHRENBACHER<sup>1</sup>, STEPHAN WINNERL<sup>1</sup>, HARALD SCHNEIDER<sup>1</sup>, JONATHAN DÖRING<sup>2</sup>, SUSANNE KEHR<sup>2</sup>, LUKAS M. ENG<sup>2</sup>, YONGHENG HUO<sup>3</sup>, OLIVER G. SCHMIDT<sup>3</sup>, KAN YAO<sup>4</sup>, YONGMIN LIU<sup>4</sup>, and MANFRED HELM<sup>1</sup> — <sup>1</sup>Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — <sup>2</sup>TU Dresden, Dresden, Germany — <sup>3</sup>Leibniz Institute for Solid State and Materials Research, Dresden, Germany — <sup>4</sup>Northeastern University, Boston, USA

It has been shown that materials with negative refractive index  $n$ , so-called metamaterials, can be exploited as perfect lenses characterized by a point-to-point projection. In the near-field regime where the distance between object and image is much smaller than the applied wavelength, negative permittivity is sufficient to create such super-resolution images. Those superlenses are based on heterostructures of different chemical composition, where the negative permittivity is induced by phonons. In contrast, in our sample this dielectric behavior is due to the electronic response of a doped GaAs layer sandwiched between two intrinsic layers. This is a simple and elegant way of producing a superlens as its resonant frequency can be controlled simply by varying the dopant level. In our experiments we investigate a sample with a charge carrier concentration tuned for superlensing at a  $20\mu\text{m}$  IR wavelength as explored using a free-electron laser.

O 37.8 Tue 18:30 P2

**Spectral properties of ordered nano-particle assemblies** — ●SIMON DICKREUTER, EMRE GÜRDAL, DIETER KERN, and MONIKA FLEISCHER — Institute for Applied Physics, Eberhard Karls University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Plasmonic nano-particles have proven to be useful for many applications like bio-sensing or near-field imaging. But due to their complex nature they are not yet fully understood. In this recently started project, the coupling between colloidal nano-particles is investigated. The plasmonic properties of single gold-colloids are well known, thus we chose gold-colloids as the building blocks for the fabrication of nano-particle assemblies. The techniques of e-beam lithography and diblock copolymer self-assembly are employed to fabricate ordered hole arrays, which can be filled with colloidal nano-particles by using capillary or convective self-assembly. This way controlled assembly of nano-particles inside the holes is possible. By choosing different geometries for the templates, one can fabricate oligomers consisting of a defined number of nano-particles. The assemblies are analyzed by dark-field spectroscopy to see how the coupling of several nano-particles affects the plasmonic resonances they exhibit. The methods of fabrication of the assemblies and first dark-field spectra will be presented.

O 37.9 Tue 18:30 P2

**Near-field optics of conductive ferroelectric domain walls** — ●DENNY LANG, SUSANNE C. KEHR, MATHIAS SCHRÖDER, ALEXANDER HAUSSMANN, and LUKAS M. ENG — IAPP, George-Bähr-Straße 1, 01069 Dresden

Ferroelectric domain walls (DWs) are planar interfaces of a few nm thickness that separate areas with different spontaneous polarizations. DWs show electric conductivity under certain conditions [1], e.g. when being illuminated by UV light, and thus are interesting as nanometer-scale optoelectronic devices [2]. We investigate the optical response of these topologically novel systems on the nm length scale by means of scattering-type scanning near-field optical microscopy (s-SNOM).

We inspect the domain wall conductivity in z-cut lithium niobate using different scanning probe methods. Firstly, we characterize the general domain structure by conventional piezoresponse force microscopy (PFM) in order to both allocate the exact DW position and quantify the magnitude of polarization in adjacent domains. Secondly, we measure the conductivity of a single DW rendered conductive by UV illumination with conductive atomic force microscopy (c-AFM). Thirdly, we study the optical response of the DW applying s-SNOM at visible and at infrared wavelengths. Here, we expect a near-field contrast since the DW constitutes a conductive singularity within a wide-bandgap insulator.

[1] M. Schröder et al., Adv. Funct. Mater. 22 (18), 3936-3944 (2012)

[2] A. Haussmann et al., Nano Lett. 9 (2), 763-768 (2009)

O 37.10 Tue 18:30 P2

**Self-assembly of gold nanoparticle structures** — ●EMRE GÜRDAL, SIMON DICKREUTER, DIETER KERN, and MONIKA FLEISCHER — Institute for Applied Physics, Eberhard Karls University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

In the last decade plasmonic nanoparticle assemblies took an important role in emerging nanotechnologies. Gold particles show resonances in the visible and infrared spectral range and exhibit a very strong near field in their close vicinity. This can be used e.g. for biosensing or optical antennas. Ordered arrays of such particles can be fabricated by using substrates with hole templates. There are several possibilities to fabricate such templates. E-beam lithography on the one hand which provides good control but is time consuming and costly, and the self-assembly of block-copolymers on the other, which is a larger area parallel process. We investigate the accumulation of gold nanospheres into the voids of either e-beam resist or diblock-copolymer layers. For the formation of cylindrical structures on top of a silicon substrate by diblock-copolymers selecting the optimum layer thickness is important. Furthermore it is a challenge to achieve a gold nanosphere monolayer in such cylindrical holes. An overview over different methods for fabricating gold nanosphere oligomers will be presented.

O 37.11 Tue 18:30 P2

**Optical Properties of Self-assembled Fluorescent and Metal Nanoparticle Arrays** — ●FRANZISKA BARHO, MARIO FEY, and PETER J. KLAR — Justus-Liebig-Universität Giessen, Germany

Localized plasmons in metal nanoparticles may influence the photoluminescence of adjacent fluorescent nanoparticles. Depending on the distance between the different nanoparticles, an enhancement of the photoluminescence signal as well as its quenching is possible. The influence caused by different arrangements of nanoparticles is going to be investigated.

The samples were prepared by electron beam lithography defining cavities in PMMA resist. Both types of nanoparticles, in our case gold particles, whose plasmon resonance frequency is located in the visible part of the spectrum, and fluorescent polystyrene spheres, were then placed into these structures by a horizontal dip coating process. With this self-assembling process, different arrangements of particles can occur which allow us to study their optical properties like the transmission and photoluminescence characteristics.

O 37.12 Tue 18:30 P2

**Optical Properties of Self-assembled Metal Nanoparticle Arrays** — ●MARIO FEY<sup>1</sup>, JAN KUHNERT<sup>2</sup>, SANGAM CHATTERJEE<sup>2</sup>, and PETER J. KLAR<sup>1</sup> — <sup>1</sup>Justus-Liebig-Universität Giessen, Germany — <sup>2</sup>Philipps-Universität Marburg, Germany

The investigation of the optical properties of metal nanoparticles has long been of interest in physics. Since these particles have particular properties as their size approaches the nanoscale, like tunable surface plasmon resonances, they can be employed in different research fields e.g. surface-enhanced Raman spectroscopy. To gain more insight into surface plasmons, self-assembled gold and silver nanoparticle arrays as well as single arrangements consisting of a few nanoparticles were investigated by optical transmission spectroscopy. The samples were fabricated by electron beam lithography and a horizontal dip-coating process. The former step enabled us to define cavities of different sizes and shapes in the PMMA resist deposited on glass substrates. Size and shape of the cavities allow one to control the number and arrangement of the nanoparticles assembled by the horizontal dip-coating process in the cavities. Thus different arrays or rather formations of metal nanoparticles (single particles, pairs of particles etc.) on glass were obtained. Optical transmission spectroscopy allowed us to investigate the surface plasmon resonances of arrays of metal nanoparticles depending on the formation of the metal particles.

O 37.13 Tue 18:30 P2

**GRIN lenses with plasmonic structures as compact elements for biosensing** — ●ANDREAS HERRER<sup>1</sup>, MICHAEL METZGER<sup>2</sup>, SABRINA RAU<sup>2</sup>, DOMINIK A. GOLLMER<sup>1</sup>, JULIA FULMES<sup>1</sup>, DAI ZHANG<sup>2</sup>, ALFRED J. MEIXNER<sup>2</sup>, GÜNTHER GAUGLITZ<sup>2</sup>, MARC BRECHT<sup>2</sup>, DIETER P. KERN<sup>1</sup>, and MONIKA FLEISCHER<sup>1</sup> — <sup>1</sup>Institute for Applied Physics, University of Tuebingen, Auf der Morgenstelle 10, 72076 Tuebingen, Germany — <sup>2</sup>Institute of Physical and Theoretical Chemistry, University of Tuebingen, Auf der Morgenstelle 10, 72076 Tuebingen, Germany

Light scattering by metallic nanostructures shows resonances at certain wavelengths which are due to the plasmonic properties of the structures. These resonances show a characteristic wavelength shift when the medium and thereby the refractive index in the range of the near field of the structures is changed. This can be used for the detection of molecules with high sensitivity. Nanostructures can be fabricated in defined shapes and sizes by standard electron beam lithography. It is however difficult to use this method on small or non-planar surfaces.

GRIN lenses are small glass cylinders with a diameter of only a few millimeters and a built-in radial gradient of the refractive index, which enables focusing of incident parallel light onto one of their plane surfaces. For structuring of GRIN lens surfaces we use a process in which gold nanostructures fabricated on silicon can be transferred directly onto the lenses. These structures are automatically in the focus when excited through the lens and therefore allow for compact sensing setups. The fabricated structures on GRIN lenses as well as their optical properties will be presented.

O 37.14 Tue 18:30 P2

**Plasmonic nanostructures for organic photovoltaic cells** — ●YAGMUR IPEK, DOMINIK A.GOLLMER, CHRISTOPHER LORCH, FRANK SCHREIBER, DIETER P. KERN, and MONIKA FLEISCHER — Institute for Applied Physics, Eberhard Karls University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

The topic of our research are OVP cells prepared by organic molecular beam deposition (OMBD). Diindenoperylen (DIP) [1] is used as the electron donor and Buckminster-Fullerene (C60) as the electron acceptor. The goal is to increase the efficiency of OPV cells by fabricating the transparent electrodes of OVP cells with plasmonic nanostructures, in particular gratings, such that the light harvesting properties of these cells may be improved. The plasmonic nanostructures are fabricated by electron-beam lithography or nanoimprint lithography. The OVP cells are measured via their current-voltage characteristics (I-V curve). Optical characterization of the structures by extinction measurements are compared with numerical simulations. An overview over the composition, different methods of nano fabrication and measurement methods of OVP cells will be presented.

[1] (J. Wagner et al., Adv. Funct. Mater.20 (2010) 4295)

O 37.15 Tue 18:30 P2

**Characterisation and Control of SPPs in silver waveguides using PEEM** — ●KELLIE PEARCE<sup>1,2</sup>, CHRISTIAN SPÄTH<sup>1</sup>, SOO HOON CHEW<sup>1,2</sup>, SEBASTIAN NOBIS<sup>1</sup>, JÜRGEN SCHMIDT<sup>1</sup>, and ULF KLEINEBERG<sup>1</sup> — <sup>1</sup>Department of Physics, Ludwig Maximilian University of Munich, Garching, Germany — <sup>2</sup>Max Planck Institute of Quantum Optics, Garching, Germany

Surface plasmon polaritons (SPPs) have garnered much interest because of their unique properties. They are able to travel at speeds comparable to that of light, whilst capable of being confined to dimensions much smaller than the diffraction limit. Potential applications rely on being able to fabricate, characterise and optimise SPP guiding structures.

To investigate potential waveguides, a technique is needed to observe plasmons with high spatial and temporal resolution. Photoemission microscopy (PEEM) is one such technique. Combining time-of-flight PEEM with two-photon photoemission enables plasmons and plasmon-induced hotspots to be mapped. We fabricate and examine various SPP-waveguides to determine the effect of waveguide geometry, composition, and laser polarisation on the generation, steering and focusing of SPPs in metal nano- and microstructures. Additionally we initiate first steps towards using the the carrier envelope phase of ultrashort pulses for plasmonic control.

O 37.16 Tue 18:30 P2

**Extraordinary optical transmission and cathodoluminescence in thin layers with subwavelength holes** — ●DAN-NHA HUYNH<sup>1</sup>, CHRISTIAN MATYSSEK<sup>1</sup>, and KURT BUSCH<sup>1,2</sup> — <sup>1</sup>Humboldt-Universität zu Berlin, Institut für Physik, AG Theoretische Optik und Photonik, Newtonstr. 15, 12489 Berlin, Germany — <sup>2</sup>Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin, Germany

We examine properties of nano-plasmonic thin layers utilizing a self-implemented Discontinuous Galerkin Time-Domain (DGTD) program package. Specifically, metal films including subwavelength and wavelength-scale holes lead to interesting optical properties due to the excitation of surface plasmons such as extraordinary optical transmission.

We quantitatively explore the complex plasmon dynamics in these systems via optical transmission, electron energy loss and cathodoluminescence computations.

O 37.17 Tue 18:30 P2

**Nonlinear optics with hybrid metal/dielectric nanostructures** — ●HEIKO LINNENBANK and STEFAN LINDEN — Physikalisches Institut, Universität Bonn, Germany

Particle plasmons, i.e., coherent excitations of the conduction band electrons, govern the optical properties of metallic nanostructures in the visible and in the near-infrared spectral region. Excitation of particle plasmons with ultrashort light pulses can give rise to a spatiotemporal concentration of the electromagnetic field in the vicinity of the metallic nanostructure. The intensity in these hot spots can exceed the incident intensity by orders of magnitude. Conversely, localized fields within these hot spots can be efficiently transferred to the far field. By carefully varying the geometry of the metallic nanostructures it is possible to tune their resonance and also to build structures with multiple resonances. In several studies it has been shown that gold nanostructures show a huge nonlinear response in terms of second and third harmonic generation to ultrashort light pulses. Here, we demonstrate that it is possible to influence the nonlinear emission of metallic nanoparticles by placing a dielectric material with a high second and third order nonlinear coefficient in the above mentioned hot spots. Furthermore, we show that the nonlinear processes can be tuned by building a metallic nanostructure which is not only resonant for the incoming light field but also for the generated field.

O 37.18 Tue 18:30 P2

**Optimizing arrangements of a few Au-nanoparticles for SERS applications** — ●KATHRIN KROTH, THOMAS SANDER, SABRINA DARMAWI, LIMEI CHEN, and PETER J. KLAR — JLU Gießen

Surface-enhanced Raman spectroscopy (SERS) allows one to detect analytes on single-molecule level. The electric field of the impinging excitation light as well as the locally scattered light can be enhanced by several orders of magnitude in the gaps between metal-nanoparticles. SERS-substrates out of Au-nanoparticles have been prepared by combining top down nanofabrication with self-assembly of nanoparticles. At first a periodical array of cavities with different size and shape was fabricated by electron beam lithography (EBL) on a silicon substrate out of PMMA. The Au-nanoparticles from colloidal suspensions were arranged inside the cavities by a horizontal dip-coating process. The number and the orientation of the Au-nanoparticles in the cluster can be controlled by the size and shape of the PMMA-cavity. For the characterization of the different nanoparticle arrangements by Raman-imaging, a Raman-active molecule was deposited on top of the SERS-substrates allowing to study enhancement effects with respect to the nanoparticle arrangements and the polarization of the excitation light.

O 37.19 Tue 18:30 P2

**Few-cycle laser photoelectron microscopy and spectroscopy using single-shot phase tagging technique** — ●SOO HOON CHEW<sup>1</sup>, ALEXANDER GLISERIN<sup>1</sup>, SEBASTIAN NOBIS<sup>1</sup>, FLORIAN SCHERTZ<sup>2</sup>, YINGYING YANG<sup>3</sup>, KELLIE PEARCE<sup>1</sup>, PETER GEISLER<sup>4</sup>, JÜRGEN SCHMIDT<sup>1</sup>, PETER HOMMELHOFF<sup>5</sup>, BERT HECHT<sup>4</sup>, MATTHIAS KLING<sup>1</sup>, and ULF KLEINEBERG<sup>1</sup> — <sup>1</sup>Faculty of Physics, Ludwig Maximilian University of Munich, 85748 Garching, Germany — <sup>2</sup>Institute of Physics, University of Johannes Gutenberg, 55128 Mainz, Germany — <sup>3</sup>Institute of Semiconductors, Haidian District, Beijing 100083, P. R. China — <sup>4</sup>Institute of Physics, University of Würzburg, 97074 Würzburg, Germany — <sup>5</sup>Department of Physics, University of Erlangen-Nürnberg, 91058 Erlangen, Germany

A single-shot phase-tagged time-of-flight-photoelectron emission microscope has recently been developed to investigate and control carrier-envelope phase (CEP) effects on tailored plasmonic nanostructures. First experiments measuring the CEP dependence on single gold nanoparticles on gold plane (NPOP) have been performed with 10 kHz few-cycle laser pulses via a multiphoton photoemission process. We report the results from calculations and observation of a CEP feature from the NPOP sample as well as the challenges of the experiments. We also address the possible solutions to improve the plasmonic sample quality and design for probing and control the plasmonic dynamics via the CEP effect. The experimental setup provides a versatile tool for both spatial-resolved and energy-resolved studies of the attosecond control of electrons in plasmonic nanostructures.

O 37.20 Tue 18:30 P2

**Transmission of surface plasmon polariton through nanometric constriction** — ●GOLALEH GHAFORI<sup>1</sup>, DANIEL BENNER<sup>2</sup>, JOHANNES BONEBERG<sup>3</sup>, PAUL LEIDERER<sup>4</sup>, and ELKE SCHEER<sup>5</sup> — <sup>1</sup>golaleh.ghafoori@uni.konstanz.de — <sup>2</sup>daniel.benner@uni.konstanz.de — <sup>3</sup>University of Konstanz — <sup>4</sup>University of Konstanz — <sup>5</sup>University of Konstanz

We study the excitation and propagation of surface plasmons polariton (SPPs) on a 4 micrometer wide gold stripe of thickness about 100nm.

For the excitation we use an optimized grating in the stripe. The surface plasmons propagate towards and across a constriction. We show that SPPs are transmitted with high probability across a constriction, with smallest lateral dimensions of atomic. For comparison we performed FDTD(Finite Difference Time Domain) simulations with Lumerical. We model a supported gold stripe in the same geometrical arrangement as the sample. These studies allow the determination of local intensities in experiments with mechanically controllable break-junctions under light irradiation [1].

O 37.21 Tue 18:30 P2

**Transmission of surface plasmon polariton through nanometric constriction** — ●GOLALEH GHAFORI<sup>1</sup>, DANIEL BENNER<sup>2</sup>, JOHANNES BONEBERG<sup>3</sup>, PAUL LEIDERER<sup>4</sup>, and ELKE SCHEER<sup>5</sup> — <sup>1</sup>golaleh.ghafoori@uni.konstanz.de — <sup>2</sup>daniel.benner@uni.konstanz.de — <sup>3</sup>University of Konstanz — <sup>4</sup>University of Konstanz — <sup>5</sup>University of Konstanz

We study the excitation and propagation of surface plasmons polariton (SPPs) on a 4 micrometer wide gold stripe of thickness about 100nm. For the excitation we use an optimized grating in the stripe. The surface plasmons propagate towards and across a constriction. We show that SPPs are transmitted with high probability across a constriction, with smallest lateral dimensions of atomic. For comparison we performed FDTD(Finite Difference Time Domain) simulations with Lumerical. We model a supported gold stripe in the same geometrical arrangement as the sample. These studies allow the determination of local intensities in experiments with mechanically controllable break-junctions under light irradiation [1].

O 37.22 Tue 18:30 P2

**Third Harmonic Spectroscopy of Polymer-Nanoantenna Hybrid Systems** — ●GELON ALBRECHT<sup>1,2</sup>, BERND METZGER<sup>1</sup>, SYBILLE ALLARD<sup>3</sup>, ULLRICH SCHERF<sup>3</sup>, and HARALD GIESSEN<sup>1</sup> — <sup>1</sup>4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, Stuttgart 70569, Germany — <sup>2</sup>Max Planck Institute for Solid State Research, Heisenbergstraße 1, Stuttgart 70569, Germany — <sup>3</sup>Bergische Universität Wuppertal, Gaußstraße 20, Wuppertal 42119, Germany

Nonlinear plasmonics [1] has gained a lot of interest lately due to its potential to tailor novel nonlinear optical materials. Plasmonics is a promising approach as it allows for nanofocusing electromagnetic energy into small spatial regions [2].

We perform third-harmonic (TH) spectroscopy using an 8 fs TiSa laser oscillator on polymer-covered gap-nanoantenna arrays made from gold. We use this hybrid system mainly for two reasons. First, antennas are an ideal system to transfer energy from the far-field of an electromagnetic wave to the near-field around the antenna, especially into the antenna gap region. Second, nonlinear polymers show a very large third-harmonic susceptibility. The combination of this two systems leads to a hybrid system which exhibits a strong wavelength-dependent resonant third-harmonic response function. Furthermore this response is sensitive to the gap size and to the plasmonic resonance of the antennas. [1] M. Kauranen and A.V. Zayats, Nat. Photonics 6, 737\*748 (2012) [2] M. Hentschel, T. Utikal, H. Giessen, and M. Lippitz, Nano Lett. 12, 3778-3782 (2012)

O 37.23 Tue 18:30 P2

**Impact of rotational symmetry on the nonlinear optical response of gold nanoantennas** — ●FRANZISKA ZEUNER<sup>1</sup>, SHUMEI CHEN<sup>2</sup>, GUIXIN LI<sup>3</sup>, SHUANG ZHANG<sup>2</sup>, and THOMAS ZENTGRAF<sup>1</sup> — <sup>1</sup>Department of Physics, University of Paderborn — <sup>2</sup>School of Physics & Astronomy, University of Birmingham, UK — <sup>3</sup>Department of Physics, Hong Kong Baptist University

The strength of a nonlinear optical response of natural materials is highly sensitive to their crystallographical symmetry. Because of the high interest in metamaterials and their potential in photonics, we want to investigate the impact of rotational symmetry on the nonlinear optical signal strength of plasmonic structures. By fabricating gold nanoantennas with four different rotational symmetries but the same plasmon resonance frequency, we are able to compare the symmetry induced change in the nonlinear optical response.

O 37.24 Tue 18:30 P2

**Surface plasmon enhanced chemiluminescence at metal surfaces using internal photodetection** — ULRICH HAGEMANN, FELIX BECKER, and ●HERMANN NIENHAUS — Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, D-

47048 Duisburg, Germany

Light emission during reactions on metal surfaces is generally quenched. If detectable at all the photon yield is low. The study presents data from two model reactions at low temperatures, i.e., the oxidation of Mg and the chlorination of K surfaces [1]. The metals are prepared as thin layers on a rough 5 - 200 nm Ag film grown on *p*-Si(111) surfaces. The Ag/Si(111) contact is used as a Schottky photodiode allowing an internal  $2\pi$  detection of the chemiluminescence photons. The photoyield can be enhanced up to an order of magnitude by varying the Ag film thickness. For Ag films in the thickness range between 30 and 50 nm, the yield shows characteristic maxima. The results can be explained by surface plasmon polaritons (SPP) in the Ag layer which are excited by the non-adiabatic chemical reaction on the Mg or K surface. The SPP decays radiatively into Si inducing the photocurrent. Model calculations are able to reproduce the observed yield maxima at certain Ag film thicknesses.

[1] F. Becker et al., JCP 138 (2013) 034710.

O 37.25 Tue 18:30 P2

**Sphere-based cantilever for SNOM** — ●CRITIAN GONZALEZ MORA, DANIELA BAYER, ELENA A. ILIN, EGBERT OESTESCHULZE, and MARTIN AESCHLIMANN — University of Kaiserslautern Erwin Schroedinger Str. 46 D-67663, Kaiserslautern

We present the development and first measurements with a new kind of cantilever sensors, which allow an enhanced transmission of light keeping the possibility to perform SNOM (Scanning Near-field Microscope) measurements in contact to the sample.

The characterization performed my measuring Au Nano-rings show a clear polarization dependence for the excited plasmons. These new cantilevers are a modification of the traditional aperture cantilevers for aperture based SNOM and consist, basically, of a glass micro-sphere at the apex of the tip of the sensor.

O 37.26 Tue 18:30 P2

**Photoluminescence study of SPP-supporting hybrid semiconductor-metal structures** — ●SÖREN KREINBERG<sup>1</sup>, MATTHIAS SALEWSKI<sup>1</sup>, LARS E. KREILKAMP<sup>1</sup>, ILYA A. AKIMOV<sup>1</sup>, CHRISTIAN SCHNEIDER<sup>2</sup>, SVEN HÖFLING<sup>2</sup>, MARTIN KAMP<sup>2</sup>, and MANFRED BAYER<sup>1</sup> — <sup>1</sup>Experimentelle Physik 2, Technische Universität Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund, Germany — <sup>2</sup>Lehrstuhl für Technische Physik, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

We study the optical properties of hybrid nanostructures comprising self-assembled InGaAs quantum dots (QDs) located in the direct vicinity from the surface which is covered with Au grating. The Au period is optimized in order to support the excitation of surface plasmon polaritons (SPP) by excitons in QDs emission and vice versa. Angle dependent transmission and reflection spectra show clear signatures of SPP resonances. We investigate SPP influence on exciton dynamics measured by means of time-resolved photoluminescence.

O 37.27 Tue 18:30 P2

**Towards superlens-based infrared near-field nanospectroscopy: imaging dielectric contrasts with  $\lambda/30$ -resolution** — ●PEINING LI<sup>1</sup>, TAO WANG<sup>1</sup>, BENEDIKT HAUER<sup>1</sup>, GENNADY SHVETS<sup>2</sup>, and THOMAS TAUBNER<sup>1</sup> — <sup>1</sup>I. Institute of Physics (IA), RWTH Aachen University, Aachen 52056, Germany — <sup>2</sup>Department of Physics and Center for Nano and Molecular Science and Technology, The University of Texas at Austin, Austin, Texas 78712, USA

Near-field superlenses present great capabilities for overcoming the diffraction limit [1], bringing new applications in optical lithography [2] and near-field imaging [3]. Here, using the combination of a silicon carbide superlens and scattering-scanning near-field optical microscopy (SL-SNOM), the infrared imaging of dielectric contrasts with a resolution of down to  $\lambda/30$  (about 350 nanometers) has been verified. This achieved resolution is an almost 2-fold improvement compared to state-of-the-art superlens results [3]. From quantifications of the superlens dispersion via near-field mapping of surface phonon polaritons (SPhPs), the physical mechanism behind the obtained ultra-high resolution is directly visualized to be the field enhancement by short- $\lambda$  SPhPs at the superlensing condition. Our results pave the way to superlens-based infrared spectroscopic applications for revealing vibration information of dielectric samples.

[1] J. B. Pendry, Phys. Rev. Lett. 85, 3966 (2000).

[2] N. Fang, et al., Science 308, 534 (2005).

[3] T. Taubner, et al., *Science* 313, 1595 (2006).

O 37.28 Tue 18:30 P2

**Plasmon Enhanced Fluorescence from Nanocrystals doped with Rare-earth Ions** — ●TOBIA MANCABELLI<sup>1</sup>, DAWID PIATKOWSKI<sup>2</sup>, NIKOLAI HARTMANN<sup>1</sup>, NINA MAUSER<sup>1</sup>, SEBASTIAN MACKOWSKI<sup>2</sup>, and ACHIM HARTSCHUH<sup>1</sup> — <sup>1</sup>Department Chemie & CENS, Ludwig-Maximilians-University, Munich, Germany — <sup>2</sup>Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Torun, Poland

We investigated the plasmonic enhancement of two-photon up-converted fluorescence of NaYF<sub>4</sub>:Er<sup>3+</sup>/Yb<sup>3+</sup> nanocrystals (NCs) for two different metallic structures. First we used NCs-decorated silver nanowires (NWs): a strong enhancement of the NC emission is observed for laser polarization parallel to the orientation of the NW, indicating that the silver NW is able to locally enhance absorption. Using Fluorescence Lifetime Imaging Microscopy we then observed a faster decay dynamics for NCs close to the NW, proving that the NC-plasmon interaction can increase the radiative decay rate of the rare-earth ions. This is further supported by angular-resolved emission patterns recorded in the Fourier plane [1] showing that the NCs can relax via coupling to the NW. Second we recorded fluorescence images of NCs at sub-diffraction spatial resolution using a sharp gold antenna tip [2]. The decay dynamics in presence of the tip was found to be faster consistent with what we observe in presence of silver NWs. This shows that plasmonic metal structures can be used to enhance absorption and emission in rare-earth doped NCs. [1] N. Hartmann, et al.; *ACS Nano*, 11, 2013. [2] N. Mauser, et al.; *Chem. Soc. Rev.*, 2013.

O 37.29 Tue 18:30 P2

**Active stabilization of a vector field synthesizer applied for spatiotemporal optical near-field control** — ●STANISLAW NICKEL, MICHAEL BIRLO, DOMINIK DIFFERT, and WALTER PFEIFFER — Department of Physics, University Bielefeld, 33615 Bielefeld, Germany

Ultrafast spatiotemporal optical near-field control in nanostructures and random scattering media requires full control of spectral amplitude and phase for both polarizations components. Conventional polarization pulse shapers that rely on a common optical path for both polarization components are limited and thus also allow only limited optical near-field control. Vector field synthesizers use independent pathways and thus are no longer restricted in their pulse shaping capabilities. However, because of the independent pathways interferometric stability of the whole setup is required. Here we demonstrate stable and reliable generation of polarization shaped pulses using a vector field synthesizer with active stabilization mechanism to correct the inherent mechanical instabilities of the setup because of vibrations and thermal drift. The phase between both pathways in the setup is detected by adding light from a cw laser diode operating at a wavelength just outside the fs-laser spectrum and measuring the output polarization. Using a piezo-driven wedge (pair) and an analog PID controller, the relative phase between both pathways is stabilized. With active stabilization the standard deviation is smaller than  $2\pi/50$ , i.e. 10 times improved compared to unstabilized operation, and no drift occurs over one hour.

O 37.30 Tue 18:30 P2

**Strong-field gas excitation and EUV light generation in plasmonic nanostructures** — ●FREDERIK BUSSE, MURAT SIVIS, and CLAUDIUS ROPERS — IV. Physical Institute - University of Göttingen, Göttingen, Germany

Spatial confinement of electromagnetic fields in tailored plasmonic nanostructures allows for the enhancement of a variety of high-order nonlinear optical phenomena using low-energy laser pulses at MHz repetition rates. Here, we present a detailed study of extreme-ultraviolet (EUV) light generation in noble gases employing bowtie-antennas and tapered hollow waveguides for field-enhancement. In contrast to former expectations [1], we do not observe any signature of coherent high harmonic generation. Instead, we identify atomic and ionic fluorescence induced by multiphoton or strong-field gas excitation and ionization as the predominant mechanisms of EUV light generation in such plasmon-assisted scenarios [2, 3]. Furthermore, we discuss novel nonlinear effects such as the formation of a waveguide nanoplasma exhibiting a strong bistability, manifest as a pronounced intensity- and pressure-dependent hysteresis in the fluorescence signal. These observations lead to a deeper understanding of nanostructure-enhanced gas excitations and EUV light generation, representing an intriguing

link between strong-field physics, plasma dynamics and ultrafast nano-optics.

[1] S. Kim *et al.*, *Nature* **453**, 757 (2008).

[2] M. Sivas *et al.*, *Nature* **485**, E1 (2012).

[3] M. Sivas and C. Ropers, *Phys. Rev. Lett.* **111**, 085001 (2013).

O 37.31 Tue 18:30 P2

**Hydrogen-sensing with complex arrow-headed Au/Pd nanorods** — ●DOMENICO PAONE<sup>1</sup>, XINGCHEN YE<sup>2</sup>, NIKOLAI STROHFELDT<sup>1</sup>, ANDREAS TITTL<sup>1</sup>, CHRIS MURRAY<sup>2</sup>, and HARALD GIESSEN<sup>1</sup> — <sup>1</sup>4th Physics Institute and Research Center SCOPE, University of Stuttgart — <sup>2</sup>Department of Materials Science and Engineering, and Department of Chemistry, University of Pennsylvania

Sensitive and reliable hydrogen detection is a key safety requirement for industrial process monitoring and catalysis. Hybrid plasmonic nanoparticles combine highly-resonant noble metal nanoparticles with chemically sensitive materials to detect a variety of gases. Furthermore, chemically synthesized nanoparticles can be grown with high yield and thus at low cost. Here, we demonstrate hydrogen-sensing with arrow-headed Au nanorods that are covered with a small amount of palladium (Pd). The arrow-headed shape was chosen to maximize the plasmonic field enhancement at the tips of the gold nanorods, allowing them to detect very small hydrogen-induced changes in the adjacent Pd. We perform dark-field scattering measurements on single nanorods while exposing the sample to different concentrations of hydrogen in nitrogen carrier gas and find pronounced spectral shifts. In addition, we investigate nanorods with a variety of geometrical parameters and correlate them with the sensing performance. In future, our nanosensor platform will enable single particle sensing and spectroscopy of a variety of gases down to very low concentrations.

O 37.32 Tue 18:30 P2

**Hybrid Plasmonic Nanostructures: Characterization of Coupled Quantum Dot - Nanoantenna Systems** — ●CODY FRIESEN, MANUEL PETER, and STEFAN LINDEN — Physikalisches Institut, Universität Bonn, Nußallee 12, 53115 Bonn, Germany

This poster will provide an overview of the fabrication and characterization methods we use to investigate hybrid plasmonic nanostructures. Specifically, our structures consist of a quantum dot strongly coupled to a nanoscale gold dipole antenna.

The fabrication utilizes electron beam lithography, with a PMMA resist. First a PMMA mask defining the antennas is created, and gold evaporation is used to deposit the actual material. Following the structure fabrication a second PMMA mask is created that describes the areas for quantum dot deposition. A chemical linking process binds the quantum dots to the exposed substrate.

The antennas have resonances tuned to the excitation wavelength of the quantum dots ( $\lambda=780$  nm), which are pumped via a green laser. The red-shifted emission light of the dots is collected using a confocal microscope and fiber coupled either into a spectrometer or into a lifetime measurement device which uses a photodiode. The diode is used for dot lifetime and emission intensity measurements, while the spectrometer allows for the measurement of spectral shifts and changes in the spectral structure.

O 37.33 Tue 18:30 P2

**k-space polarimetry on an adiabatic nanofocusing near-field probe** — ●MARTIN ESMANN, SIMON F. BECKER, JENS H. BRAUER, PETERA GROSS, RALF VOGELGESANG, and CHRISTOPH LIENAU — Carl von Ossietzky Universität, 26111 Oldenburg, Germany

Adiabatic nanofocusing of surface plasmon polaritons (SPPs) propagating on tapered metallic waveguides bears great potential as a novel method for apertureless near-field scanning optical microscopy (SNOM) [1,2]. SPP wavepackets are excited on a grating-coupler and for an ideal cone-shaped waveguide come to a complete halt at the taper apex. Hence, a single point-dipole like light source is formed there. This, however, is only true for the lowest rotationally symmetric taper eigenmode [3]. Higher eigenmodes of the waveguide disturb the imaging process in SNOM as they radiate into the far field before reaching the taper end leading to unwanted background signals.

We have therefore developed and implemented a k-space imaging technique to analyse and separate contributions from the different eigenmodes [3]. Using Stokes polarimetry, we show that the symmetry of the lowest taper eigenmode gives rise to a radially polarized mode in k-space, which is clearly identified. Furthermore, we performed approach curve scans across metallic nanostructures to investigate the

influence of the near-field coupling between probe and sample on the polarization dependent intensity distribution in k-space.

[1] M. I. Stockman, PRL 93, 137404 (2004) [2] S. Schmidt et al., ACS Nano 6, 6040 (2012) [3] M. Esmann et al., BJ Nano 4, 603 (2013)

O 37.34 Tue 18:30 P2

**Pump-probe infrared near-field nanospectroscopy on germanium and silicon** — ●FREDERIK KUSCHEWSKI<sup>1</sup>, S.C. KEHR<sup>1</sup>, B. GREEN<sup>2</sup>, CH. BAUER<sup>2,3</sup>, M. GENSCH<sup>2</sup>, and L.M. ENG<sup>1</sup> — <sup>1</sup>Institut für Angewandte Photophysik, TU Dresden, 01062 Dresden, Germany — <sup>2</sup>Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — <sup>3</sup>Freie Universität Berlin, 14195 Dahlem, Germany

Scattering-type scanning near-field optical microscopy (s-SNOM) was applied to investigate the local infrared-optical properties of germanium, silicon and SiGe thin film in a pump-probe experiment below the diffraction limit. The novel combination of s-SNOM with pump-probe techniques allows us to study electron excitation processes at an ultimate temporal resolution and to investigate their decay behavior.

Our s-SNOM is based on a non-contact atomic force microscope. The optical near-field is demodulated at higher-harmonics, which is extended to a novel side-band demodulation technique that allows for the direct measurement of pump-induced effects. Pump excitation is exhibited with a Nd:YAG ps laser while near-field probing was carried out either by a cw CO<sub>2</sub> laser or by the tuneable FELBE free-electron-laser at the Helmholtz-Zentrum Dresden-Rossendorf (HZDR).

All three samples show a clear time-variable pump-effect in the near-field when being probed at  $\sim 10 \mu\text{m}$  wavelength. Image scans clearly proof the resolution far beyond the diffraction limit. The experiment provides a definite proof of the applicability of our approach for investigating ultrafast phenomena in the near-field.

O 37.35 Tue 18:30 P2

**Time-domain characterization of scattered fields from nanotextured thin film absorbers** — ●DOMINIK DIFFERT, STANISLAW NICKEL, and WALTER PFEIFFER — Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany

Recent investigations revealed that light trapping in localized photonic modes enhances absorption in thin film silicon solar cells with nanotextured interfaces. These localized modes can be detected and characterized by spectral interferometry of backscattered radiation if a sufficiently small illumination spot is chosen. Here we use dual channel spectral interferometry to fully characterize the temporal evolution of the backscattered light from fs laser materials processed amorphous silicon layers and nanotextured thin film silicon solar cells illuminated by ultra short laser pulses. Performing a 2D point to point surface scan of the backscattered light over the sample with a high resolution reveals localized photonic modes in both samples. Finally, the prospect to coherently control absorption in these modes by use time-reversed or adaptively optimized light pulses generated using a vector field pulse shaper is discussed.

O 37.36 Tue 18:30 P2

**Circular Plasmons in cross shaped nanoantennas** — ●MARTIN LEHR<sup>1</sup>, PETER KLAER<sup>1</sup>, XIAOFEI WU<sup>2</sup>, BERT HECHT<sup>2</sup>, FLORIAN SCHERTZ<sup>1</sup>, GERD SCHÖNHENSE<sup>1</sup>, and HANS JOACHIM ELMERS<sup>1</sup> — <sup>1</sup>Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, D-55099 Mainz, Germany — <sup>2</sup>Institut für Physik, Julius-Maximilians-Universität, Am Hubland, 97074 Würzburg, Germany

Optical near-fields generated by coupled plasmonic modes can have defined polarization states. In analogy to cross dipole antennas for radio waves, the cross-shaped arrangement of dipole nanoantennas investigated here concentrates not only intensity, but also the angular momentum of circularly polarized infrared light. The field enhancement of individual nanoantennas has been measured by the relative photoemission intensity using a photoemission electron microscope with front side illumination at grazing incidence and backside illumination at normal incidence. The analysis of the polarization dependence reveals the excitation of a unique circular plasmon mode. The strong confinement of angular momentum promises a strong coupling of the photon angular momentum to magnetic moments and to the spin of photo-emitted electrons.

Funded by DFG (EL172-16)

O 37.37 Tue 18:30 P2

**Implementation of Pulse Shaping in an Ultrafast confocal microscope** — ●KEVIN DONKERS, ALBERTO COMIN, RICHARD CIESIELSKI, and ACHIM HARTSCHUH — Ludwig Maximilians Univer-

sität München & CeNS

The area of ultrafast spectroscopy has been of interest for many years yet its application to microscopy has been hindered by the difficulty of focusing femtosecond laser pulses. The use of high numerical aperture objectives with such short, broadband pulses leads to the introduction of very large values of Group Delay Dispersion (GDD), as well as higher order derivatives of the phase, which can elongate a laser pulse from less than ten femtoseconds to several picoseconds.

We implemented a pulse shaping scheme using a Liquid Crystal Modulator (LCM) and Prism Compressor in a microscopy setup with NA=1.3 allowing us to control the phase and amplitude of a strongly focused ultrafast pulse. We first used Multiphoton Intrapulse Interference Phase Scans (MIIPS) to recover laser pulses close to their original pulse length. We then have developed an advanced scheme to improve this further and demonstrate the compensation of linear chirp introduced by glass, the effect on non-linear photoluminescence of graphene and the increase of second-harmonic generation on beta-barium borate.

O 37.38 Tue 18:30 P2

**Spatial and spectral near-field distributions of strongly coupled plasmons** — ●FLORIAN SCHERTZ, MARTIN LEHR, HANS-JOACHIM ELMERS, and GERD SCHÖNHENSE — Johannes Gutenberg Universität Mainz, Institut für Physik, Staudinger Weg 7, 55128 Mainz

The mutual interaction of plasmons results in a strongly enhanced and confined near-field in the interspace between the plasmon supporting structures. The spectral near-field distribution is known to deviate from the corresponding far-field characteristics for strongly coupled plasmons with interspace (gap) sizes in the sub-nm range [1]. To understand the origin of this difference, we calculated the phase distribution of the electric near-field of strongly coupled plasmons at specific excitation frequencies numerically. From the phase distribution the charge distribution at specific instants of time can be derived. The obtained multipole-like distribution of the near-field gives rise to a spatial-dependence of the near-field enhancement in the gap of the plasmon-supporting structures. The results are discussed for various systems of strongly coupled plasmons in dependence of characteristic parameters such as e.g. gap size, particle size and particle aspect ratio. [1] F. Schertz et al., Nano Lett. 12 (4), 1885, (2012).

O 37.39 Tue 18:30 P2

**Plasmonically enhanced Grätzel cells for photovoltaics** — ●JONAS SCHWENZER and HARALD GIESSEN — 4th Physics Institute and Research Center SCOPE, University of Stuttgart, Germany

Dye sensitized solar cells are one of the most promising alternatives to silicon-based solar cells. Improvements on these cells were achieved by changing the different components e.g. the titania layer, the dye, or the electrolyte. The rather low stability of these cells was improved by solid state hole transport materials instead of liquid electrolytes. Another promising step to improve the output power are plasmonic Grätzel-cells with incorporated silica coated gold-nanoparticles. We blend Au-SiO<sub>2</sub> nanoparticles with diameters of 150 nm and different shell sizes into the titania paste. The energy conversion efficiency was enhanced by 42% compared to cells with bare titania. Current voltage measurements showed that this enhancement is caused by an increase of the current while the open circuit voltage and the fill factor did not change significantly. Furthermore the study shows that the efficiency of the cell is higher if the silica shell is thinner. Another result of our work is the dependence of power conversion efficiency on the concentration of the nanoparticles.

O 37.40 Tue 18:30 P2

**Diffraction-limited few-cycle shaped laser pulses for plasmon microscopy** — ●SEBASTIAN GOETZ<sup>1</sup>, MONIKA PAWLOWSKA<sup>1</sup>, CHRISTIAN DREHER<sup>1</sup>, CHRISTIAN REWITZ<sup>1</sup>, ENNO KRAUSS<sup>2</sup>, PETER GEISLER<sup>2</sup>, GARY RAZINSKAS<sup>2</sup>, BERT HECHT<sup>2,3</sup>, and TOBIAS BRIXNER<sup>1,3</sup> — <sup>1</sup>Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — <sup>2</sup>Nano-Optics and Biophotonics Group, Experimentelle Physik 5, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — <sup>3</sup>Röntgen Center for Complex Material Systems (RCCM), Am Hubland, 97074 Würzburg, Germany

For the investigation of ultrafast processes on the nanoscale by far-field radiation, the temporal resolution of femtosecond laser pulses has to be combined with the spatial resolution of a high-NA microscope. Both resolutions need to be conserved when the incoming light field is manipulated, which is a prerequisite for the demanding concept of co-

herent control. These functionalities are implemented in our group by pairing confocal microscopy with phase and amplitude pulse shaping of few-cycle NIR pulses using an LCD pulse shaper in 4f single-pass geometry. The capability of the setup is demonstrated by investigating the influence on the diffraction-limited focus of LCD imperfections and spatio-temporal coupling. We examine the laser focus on plain gold surfaces and nanostructures by spectrally and spatially resolved analysis of reflections from the sample plane.

O 37.41 Tue 18:30 P2

**Infrared conductivity measurement of nanostructures** — ●ANNEMARIE PUCCI<sup>1,2,3</sup>, CHRISTIAN HUCK<sup>1</sup>, JOCHEN VOGT<sup>1</sup>, FABIAN HÖTZEL<sup>1</sup>, AKEMI TAMANAI<sup>1,2</sup>, JENS TROLLMANN<sup>1,2</sup>, and TOBIAS GLASER<sup>1,2</sup> — <sup>1</sup>Kirchhoff Institute for Physics (KIP), Heidelberg University, Heidelberg, GERMANY — <sup>2</sup>InnovationLab GmbH, Heidelberg, GERMANY — <sup>3</sup>Centre for Advanced Materials (CAM), Heidelberg University, Heidelberg, GERMANY

Nanostructures from materials with free charge carriers, as for example gold, ITO, and doped semiconductors, may show plasmonic absorption in the infrared, which allows conductivity measurement without electrical contacts. The electronic relaxation rate as a measure of crystalline quality can be separately derived from the spectra, even for nanowires.

O 37.42 Tue 18:30 P2

**Tuning the Localized Surface Plasmon Resonance in Silver Nanostructures prepared by Nanosphere Lithography** — ●STEFAN MORAS, OVIDIU D. GORDAN, and DIETRICH R. T. ZAHN — Semiconductor Physics, Technische Universität Chemnitz, D-09107 Chemnitz

Metallic nanoparticles and regular nanostructures attract great interest because of their unusual properties. The outstanding optical response of such structures stems from the Localized Surface Plasmon Resonance (LSPR) produced by oscillations of the electronic charge density under electromagnetic radiation. Recent advancements in producing ordered metallic objects at nanoscales enabled the use of LSPRs for light manipulation and made them a valuable tool for chemical and biological sensing experiments. Optical properties associated with LSPRs are determined by shape, size, structure, and local dielectric environment. In the present work we study the possibility to tune the LSPRs by changing the size and shape of ordered silver nanostructures. These structures were produced by nanosphere lithography. A close-packed monolayer of polystyrene nanospheres self-assembled at the air-water interface is transferred to arbitrary substrates like glass or silicon. After silver deposition and nanosphere removal only regular silver nanotriangles remain on the substrate. UV-Vis spectroscopy was used to determine the LSPR of these nanostructures on glass substrates. While nanostructures with a high aspect ratio lead to a blue shift with respect to the LSPR of lower aspect ratio structures such a blue shift can also be obtained by annealing.

O 37.43 Tue 18:30 P2

**Scanning near-field optical microscopy and nano-FTIR spectroscopy on sub-nanometer MoS<sub>2</sub> structures by using synchrotron radiation** — ●GEORG ULRICH<sup>1</sup>, PIOTR PATOKA<sup>1</sup>, PETER HERMANN<sup>2</sup>, ARIANA NGUYEN<sup>3</sup>, JOHN MANN<sup>3</sup>, ARNE HOEHL<sup>2</sup>, BURKHARD BECKHOFF<sup>2</sup>, LUDWIG BARTELS<sup>3</sup>, PETER DOWBEN<sup>4</sup>, GERHARD ULM<sup>2</sup>, and ECKART RÜHL<sup>1</sup> — <sup>1</sup>Physikalische und Theoretische Chemie, Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany — <sup>2</sup>Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, Berlin, 10587, Berlin, Germany — <sup>3</sup>Department of Chemistry, University of California Riverside, 0124 Pierce Hall, Riverside, California, U.S.A. 92521 — <sup>4</sup>Department of Physics and Astronomy, University of Nebraska, Lincoln, T. Jorgensen Hall, Lincoln, Nebraska, U.S.A. 68588-0299

We report on IR-spectromicroscopy on MoS<sub>2</sub> demonstrating the successful coupling of scattering type scanning near-field optical microscopy (s-SNOM) with a synchrotron radiation infrared source, provided by the electron storage ring Metrology Light Source (MLS). The technique provides high spatial resolution (<50 nm) spectromicroscopy in the infrared regime with chemical selectivity from nano-Fourier-transform-infrared (nano-FTIR) spectroscopy. The used synchrotron radiation has the advantage compared to lasers, that it covers the entire infrared regime, ranging from the near- to the far-infrared. The correlation of topographically well defined islands grown by chemical vapor deposition, as determined by atomic force microscopy, with the IR signature of MoS<sub>2</sub> is illustrated by s-SNOM the approach.

We will present the results on optical mapping of MoS<sub>2</sub> monolay-

ers on SiO<sub>2</sub> gained with a tunable CO<sub>2</sub>-laser and the influence of such MoS<sub>2</sub> islands on SiO<sub>2</sub>-phonon resonance by means of nano-FTIR measurements with broadband synchrotron-radiation. The results suggest either a significant carrier concentration in MoS<sub>2</sub>, likely as a result of substrate interactions, or strong MoS<sub>2</sub>-SiO<sub>2</sub> substrate dipole interactions.

O 37.44 Tue 18:30 P2

**Enhancement of nonlinear optical effects by plasmonic nanoantennas** — ●NILS WEBER, THOMAS ZENTGRAF, and CEDRIK MEIER — University of Paderborn, Experimental Physics & CeOPP, Warburger Str. 100, 33098 Paderborn

The light-matter interaction for nonlinear processes is known to be rather weak. Consequently, high excitation powers are required for efficient light-light-interaction. Plasmonic nanostructures are a promising approach to achieve strong near-field enhancement.

In this work, silver split rings are used as plasmonic nanoantennas for the local enhancement of the electric field in a SiO<sub>2</sub>/ZnO/SiO<sub>2</sub>-microdisc, hence increasing the nonlinear optical response. The microdiscs are realized on a SiO<sub>2</sub>-Si(111) substrate by electron beam lithography, utilizing molecular beam epitaxy (MBE)-grown ZnO-layer as an optical emitter. With diameters ranging from 7 μm to 8 μm, the discs show whispering gallery modes with high quality factors of up to 5000. Furthermore, the electron beam lithography enables the patterning of nanostructures with high precision on top of the microdisc, allowing the deposition of silver split rings with outer diameters of 600nm in a concentric geometry. Finite-differences time-domain (FDTD) simulations show a strong enhancement of the electric field within the gap of the split rings in the near infrared. The optimization of the fabrication process as well as different sizes and geometries of nanoantennas are studied.

O 37.45 Tue 18:30 P2

**Scanning tunneling microscopy investigation of the phase change material Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub>** — ●JENS KELLNER<sup>1</sup>, CHRISTIAN PAULY<sup>1</sup>, MARCUS LIEBMANN<sup>1</sup>, ALESSANDRO GIUSSANI<sup>2</sup>, VOLKER DERINGER<sup>3</sup>, RAFFAELLA CALARCO<sup>2</sup>, RICHARD DRONSKOWSKI<sup>3</sup>, and MARKUS MORGENSTERN<sup>1</sup> — <sup>1</sup>II. Physikalisches Institut B, RWTH Aachen University and JARA-FIT, Germany — <sup>2</sup>Paul Drude Institut für Festkörperelektronik, Berlin, Germany — <sup>3</sup>Institute of Inorganic Chemistry, RWTH Aachen University, Germany

We investigated the phase change material GST-225. Despite the fact that GST is already commercially used, there is still no complete theory which can explain the ultra fast switching speed, the strong contrast and the high endurance of the Ge-Sb-Te alloys. One ingredient of such a theory is an atomic scale understanding of the electronic properties of GST.

Scanning tunneling microscopy (STM) measurements are used to achieve atomic resolution on metastable cubic GST. The STM data show the regular hexagonal Te lattice, which exhibits an additional irregular contrast. Comparison with DFT calculations reveals that subsurface defects create such contrast. For different subsurface arrangements of Ge, Sb and vacancies, simulated STM images show good agreement with experimental data. Scanning tunneling spectroscopy (STS) data revealed p-type doping and a band gap of 0.4 eV.

O 37.46 Tue 18:30 P2

**Solution of the GW-based quasiparticle-equation beyond the diagonal approximation: improvements in energies and wavefunctions** — ●FERDINAND KAPLAN<sup>1</sup>, MICHIEL VAN SETTEN<sup>2</sup>, and FERDINAND EVERS<sup>1</sup> — <sup>1</sup>Karlsruhe Institute of Technology — <sup>2</sup>Université catholique de Louvain

One of the most used approaches for the computational study of solids, nanoscale systems and molecules is the density functional theory (DFT). However, as is well known, DFT calculations of single particle excitation spectra, e.g. ionization potentials, often suffer from approximations in exchange correlations potentials. To systematically improve the estimation of quasi-particle energies for molecular system, we have implemented the so called GW method into a standard quantum chemistry package (*G<sub>0</sub>W<sub>0</sub>*-level). The approach represents a perturbative expansion of the many-body Green's function with respect to the screened interaction, *W*.

A central mathematical step in GW is the solution of the quasiparticle (qp-) equation. It finds the poles of the (approximate) many-body Greens function, that define the qp-energies. A common simplification in this procedure is to neglect all off-diagonal elements of the self-energy matrix, that enters the qp-equation. We investigate the

quantitative error associated with this approximation for a typical set of molecules and find significant effects. Including the off-diagonal terms the ionization potential experiences shifts (usually towards less binding) reaching 100mV or more.

O 37.47 Tue 18:30 P2

**Photoemission spectroscopy using high-order harmonics driven by a MHz fiber laser** — ●CHENG-TIEN CHIANG<sup>1,2</sup>, MICHAEL HUTH<sup>1</sup>, ANDREAS TRÜTZSCHLER<sup>1,2</sup>, JÜRGEN KIRSCHNER<sup>1,2</sup>, and WOLF WIDDRA<sup>2,1</sup> — <sup>1</sup>Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120, Halle(Saale), Germany — <sup>2</sup>Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120, Halle(Saale), Germany

We report a laboratory photoemission setup using high-order harmonic generation (HHG) as a light source driven by a fiber amplifier laser system at MHz repetition rate. The HHG light source consists of a compact generation chamber and a monochromator. Output of the fiber laser is expanded and focused in a tight focusing geometry into an argon or a xenon gas jet, producing vacuum ultraviolet light with photon energy from 16 to 40 eV. With this light source in combination with a time-of-flight electron spectrometer we demonstrate photon energy dependent photoemission experiments on a Ag(001) surface. Technical details of the setup will be presented.

O 37.48 Tue 18:30 P2

**Temperature-dependent scanning tunneling microscopy of Se-doped IrTe<sub>2</sub>** — ●MATTHIAS VOGT<sup>1</sup>, TOBIAS MAUERER<sup>1</sup>, PIN-JUI HSU<sup>1</sup>, WEIDA WU<sup>2</sup>, and MATTHIAS BODE<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — <sup>2</sup>Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA

We present variable-temperature scanning tunneling microscopy (STM) measurements of cleaved IrTe<sub>2-x</sub>Se<sub>x</sub> ( $x = 0.5$ ). A charge modulation period  $q = 1/6$  is observed at room temperature, 50 K, and 4 K. This observation is in accordance with the previously reported transition from a polymerized state above [1] to periodic dimer stripes below  $T_C \approx 400$  K [2]. The data are compared to undoped IrTe<sub>2</sub>, for which STM measurements revealed a  $1/5$  charge modulation below a much lower transition temperature ( $T_C = 275$  K) and convergence to the  $1/6$  ground state below a second transition at  $T_S = 180$  K [2]. The  $1/5$  modulation was interpreted as a soliton lattice and its alteration to  $1/6$  upon Se-doping can consistently be explained by a weakening of the Te-Te bonds by the more electronegative Se atoms, which also increases the transition temperature.

[1] Y. S. Oh *et al.*, Phys. Rev. Lett. **110**, 127209 (2013)

[2] P. J. Hsu *et al.*, arXiv:1311.3015v1 (2013)

O 37.49 Tue 18:30 P2

**Density functional study of GaN(0001)/AlN(0001) high electron mobility transistor structures** — JAKUB SOLTYS<sup>1</sup>, MARIA PTASIŃSKA<sup>1</sup>, ●JACEK PIECHOTA<sup>1</sup>, and STANISŁAW KRUKOWSKI<sup>1,2</sup> — <sup>1</sup>ICM, University of Warsaw, Pawińskiego 5a, 02-106 Warsaw, Poland — <sup>2</sup>Institute of High Pressure Physics, Polish Academy of Sciences, Sokolowska 29/37, 01-142 Warsaw, Poland

AlN/GaN high electron mobility transistor (HEMT) structures were theoretically investigated using the density functional theory (DFT). An existence of two-dimensional electron gas (2DEG), generated by strong polarization fields at the AlN/GaN interface, was confirmed by abinitio calculations. The potential profiles were analyzed for the HEMTs with different number of AlN layers, indicating that very thin AlN barrier could not provide a high density of carriers and good confinement of 2DEG. It was shown that for six AlN layers (thickness about 13Å), no electron gas is present as shown by the potential profile. In the investigated electronic structure, the band states associated with the two-dimensional electron gas were identified. It was shown that for a thicker AlN barrier, the occupancy of this states is higher, that is consistent with the available experimental data.

O 37.50 Tue 18:30 P2

**ab-initio investigation of topological states in  $\alpha$ -Sn surfaces** — ●SEBASTIAN KUEFNER, JUERGEN FURTHMUELLER, and FRIEDHELM BECHSTEDT — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany

The properties of topological insulators recently have been discussed with rising attention in solid state physics. Topological insulators are

insulating as a bulk material but exhibit metallic surface or edge states that are topologically protected and, therefore, are independent of orientation and passivation of interfaces or surfaces. Usually, the edge states show a Dirac-cone like dispersion. Mercury telluride has been proven to be a two dimensional topological insulator because of its inverted band structure. However, although  $\alpha$ -tin shows a very similar electronic structure, it is still under debate whether  $\alpha$ -tin is a topological insulator as well. We use density-functional theory based on a hybrid functional to investigate the electronic structure  $\alpha$ -Sn(001) surfaces and show the existence of a topological edge state close to the Fermi level.

O 37.51 Tue 18:30 P2

**Growth of epitaxial Bismuth films on vicinal Si(111)** — ●MONIKA JÄGER<sup>1</sup>, CHRISTIAN BRAND<sup>1</sup>, DANIEL LÜKERMANN<sup>1</sup>, SADDAM BANYOUDEH<sup>1</sup>, SERGEI SOLOGUB<sup>2</sup>, CHRISTOPH TEGENKAMP<sup>1</sup>, and HERBERT PFNÜR<sup>1</sup> — <sup>1</sup>Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — <sup>2</sup>Institute of Physics, National Academy of Sciences of Ukraine, Kyiv, Ukraine

Vicinal semi-metallic Bi-films are expected to reveal topologically protected edge states. In this study the growth of Bi-multilayer structures on Si(557) substrates has been investigated by LEED and STM. Thereby, wetting layer structures formed prior to the film deposition on Si(557) surfaces turned out to be crucial for epitaxial growth. Only in the presence of Bi-wetting layers well-ordered films can be grown. Depending on coverage of the Bi-wetting layers either stepped Bi(111) or Bi(110) have been found. In addition, Bi(221) surfaces have been obtained only on Bi-wetting layers formed by less than a monolayer. The formation of Si(335)-facets during formation of the wetting layers turns out to be essential for the growth of these structures.

O 37.52 Tue 18:30 P2

**Multichannel-Spin-Polarimetry for the Analysis of Spin-Transport in Metal-Organic Interfaces** — ●ERIK SCHAEFER<sup>1,2</sup>, DIMA KUTNYAKHOV<sup>1</sup>, GERD SCHÖNHENSE<sup>1,2</sup>, and HANS-JOACHIM ELMERS<sup>1,2</sup> — <sup>1</sup>Institut für Physik, Johannes Gutenberg-Universität, Staudinger Weg 7, D-55128 Mainz, Germany — <sup>2</sup>Graduate School Materials Science in Mainz, Staudinger Weg 9, D-55128 Mainz, Germany

The spin-resolved analysis of electronic properties of hybrid metal-organic interfaces is of great interest. Metal-organic materials are promising candidates for spintronic applications because of their advantageous properties and chemical flexibility.

Over the past decades, the various forms of photoemission experiments have become one of the standard measurement techniques in surface physics. In contrast to conventional photon optics, an effective spin polarisation analysis of a given electron beam is difficult. Since organic materials also tend to degrade within a short period, a massive reduction of spin-resolved data acquisition time is crucial.

The recently developed multichannel spin- and angle-resolved photoemission spectroscopy[1] solves this issue by enhancing the figure of merit by several orders of magnitudes, making the analysis of spin-transport (e.g. spin diffusion length) in metal-organic interfaces possible. Both, the analysis of the novel measurement technique and metal-organic interfaces will lead to new insights and prospects.

Funded by Stiftung Rheinland Pfalz für Innovation (project 1038)

[1] M. Kolbe *et al.*, Phys. Rev. Lett. **107**, 207601 (2011)

O 37.53 Tue 18:30 P2

**Electronic and magnetic properties of the MnO(001), FeO(001), CoO(001), and NiO(001) surfaces** — ●ANDREAS SCHRÖN and FRIEDHELM BECHSTEDT — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Due to their antiferromagnetic ordering, the 3d transition metal monoxides (TMOs) MnO, FeO, CoO, and NiO provide important benchmark materials for novel methods to investigate magnetic structures with atomic resolution. However, only little is known about the orientation of the local magnetic moments of the TM ions with respect to the bulk. The effect on the broken symmetry at surfaces, e.g. on the size and orientation of the local magnetic moments, has not been investigated yet.

We present *ab-initio* calculations of the TMO(001) surfaces in order to approach the open questions related to the reduced symmetry at their surfaces. The calculations have been performed in the framework of spin-polarized density functional theory (DFT). Exchange and correlation (XC) are treated within the local density approximation (LDA) and an additional on-site Coulomb interaction  $U$  acting on the



transition-metal 3d shells is included (LDA+U). Spin-orbit interaction is included self-consistently during all calculations and non-collinear arrangements are allowed.

We focus especially on the influence of the broken symmetry at the surface on the magnitude and orientation of the local magnetic moments of the 3d TM ions.

O 37.54 Tue 18:30 P2

**Photoemission calculations for surface states in 2DEGs within the models of  $\vec{k} \cdot \vec{p}$  theory** — ●MARKUS FLIEGER, JÜRGEN HENK, and INGRID MERTIG — Martin-Luther-Universität Halle-Wittenberg, Germany

Surface states in two-dimensional electron gases like Rashba-split and topological surface states attracted recently a lot of attention due to their unique electronic structure and spin texture. An appropriate method for investigating them is spin- and angle-resolved photoelectron spectroscopy (SPARPES).

These kinds of surface states are well described by model Hamiltonians which are derived within  $\vec{k} \cdot \vec{p}$  perturbation theory. We report on analyses for model Hamiltonians of systems with different symmetries in the process of photoemission. In addition, we compare theoretical intensities and spin polarizations of the photoelectrons with results from experiments and *ab initio* calculations.

O 37.55 Tue 18:30 P2

**Multi probe transport measurements on Bi<sub>2</sub>Se<sub>3</sub> thin films** — ●SEBASTIAN BAUER, PAUL GRAF, ROLF MÖLLER, and CHRISTIAN A. BOBISCH — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

Since their prediction, topological insulators (TIs) like Bi<sub>2</sub>Se<sub>3</sub> are very popular in condensed matter physics due to their peculiar electronic properties. At the surface of 3D TIs a conducting and spin polarized surface state evolves, which does not allow the direct backscattering of electrons [1]. We studied the transport field of a 4.5 QL thin Bi<sub>2</sub>Se<sub>3</sub> film by scanning tunneling potentiometry, an extended scanning tunneling microscopy (STM) technique which allows us to analyze the microscopic topography and the correlated microscopic electrochemical potential of the surface simultaneously [2]. The Bi<sub>2</sub>Se<sub>3</sub> film was prepared in-situ on a reconstructed Si(111)-( $\sqrt{3} \times \sqrt{3}$ )-Bi according to Zhang et al. [3]. On large scale measurements of the electrochemical potential we observe a lateral gradient of the electrochemical potential of the Bi<sub>2</sub>Se<sub>3</sub> surface. Both, the microscopic sheet conductance and the macroscopic sheet conductance of the 4.5 QL film agree well to other data from literature [4]. A thermovoltage signal at surface step edges indicates the local variation of the density of states [5].

[1] M. Z. Hasan, C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010). [2] A. Bannani, C. A. Bobisch, R. Möller, Rev. Sci. Instrum. 79, 083704 (2008). [3] G. Zhang, et al., Appl. Phys. Lett. 95, 053114 (2009). [4] A. A. Taskin et al., Phys. Rev. Lett. 109, 066803 (2012). [5] T. Zhang et al., Phys. Rev. B. 87, 115410 (2013).

O 37.56 Tue 18:30 P2

**Specular reflection of spin-polarized electrons from W(001) spin-filter crystal in a larger range of scattering energies and angles** — ●D. KUTNYAKHOV<sup>1</sup>, H.J. ELMERS<sup>1</sup>, G. SCHÖNHENSE<sup>1</sup>, C. TUSCHE<sup>2</sup>, J. KIRSCHNER<sup>2</sup>, S. BOREK<sup>3</sup>, J. BRAUN<sup>3</sup>, J. MINÄR<sup>3</sup>, and H. EBERT<sup>3</sup> — <sup>1</sup>Institut für Physik, Johannes Gutenberg-Universität Mainz — <sup>2</sup>MPI für Mikrostrukturphysik, Halle — <sup>3</sup>Department Chemie, Physikalische Chemie, Universität München

Extending our previous work on the novel imaging spin-filter technique based on electron diffraction from W(001) in the specular (00)-LEED spot [1,2], we studied the scattering energy (E) and angle of incidence (theta)-landscape of the spin sensitivity S, and reflectivity I/I<sub>0</sub>. The setup includes a spin-polarized GaAs electron source and a rotatable delayline detector for spatially-resolving detection. We measured the intensity and spin asymmetry of the specularly reflected beam for a large range of energies and angles of incidence of spin-polarized primary electrons. Resulting energy-angular landscape show rather good agreement with theory (relativistic layer KKR SPLEED code [3,4]). The results identify several regions of high asymmetry and figure of merit. These regions open a path for the development of the multichannel spin-filter for electron spectroscopy and momentum microscopy with higher performance. Funded by BMBF (05K13UM1).

[1] C. Tusche et al., APL 99 (2011) 032505; [2] M. Kolbe et al., PRL 107 (2011) 207601; [3] R. Feder in Polarized Electrons in Surface Physics (World Scientific, Singapore, 1985); [4] H. Ebert et al., Rep. Prog. Phys. 74, 096501 (2011)

O 37.57 Tue 18:30 P2

**Growth morphology of thin films on the metallic and oxide surfaces** — ●ALEKSANDER KRUPSKI — Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom.

In this work we briefly review recent investigations concerning growth morphology of thin metallic films on the Mo(110) and the Ni<sub>3</sub>Al(111) surfaces, and Fe and Copper Phthalocyanine (C<sub>32</sub>H<sub>16</sub>N<sub>8</sub>Cu) on the Al<sub>2</sub>O<sub>3</sub>/Ni<sub>3</sub>Al(111) surface. Comparison of Ag, Au, Sn, and Pb growth on the Mo(110) surface has shown a number of similarities between these adsorption systems except surface alloy formation that has only observed in the case of Sn and Au. In the Pb/Mo(110) and Pb/Ni<sub>3</sub>Al(111) adsorption systems selective formation of uniform Pb island heights during metal thin film growth has been observed and interpreted in terms of quantum size effects. Furthermore, our studies showed that Al<sub>2</sub>O<sub>3</sub> on Ni<sub>3</sub>Al(111) exhibits a large superstructure in which the unit cell has a commensurate relation to the substrate lattice. In addition, Copper Phthalocyanine chemisorbed weakly onto an ultrathin Al<sub>2</sub>O<sub>3</sub> film on Ni<sub>3</sub>Al(111) and showed a poor template effect of the Al<sub>2</sub>O<sub>3</sub>/Ni<sub>3</sub>Al(111) system. In the case of iron cluster growth on Al<sub>2</sub>O<sub>3</sub>/Ni<sub>3</sub>Al(111) the nucleation sites were independent of deposition temperature, yet cluster shape showed a dependence. In this system, Fe clusters formed a regular hexagonal lattice on the Al<sub>2</sub>O<sub>3</sub>/Ni<sub>3</sub>Al(111).

O 37.58 Tue 18:30 P2

**Structure and manipulation of h-BN on Ir(111)** — ●DOMENIK M. ZIMMERMANN, ULRIKE A. SCHRÖDER, and THOMAS MICHELY — II. Physikalisches Institut, Zülpicher Str. 77, Universität zu Köln

The formation of high quality hexagonal, 2D boron nitride (h-BN) through thermal decomposition of borazine (B<sub>3</sub>N<sub>3</sub>H<sub>6</sub>) on Ir(111) is investigated by scanning tunneling microscopy (STM).

As growth methods chemical vapor deposition (CVD) and temperature programmed growth (TPG, room temperature adsorption followed by annealing) are applied in the temperature range from 1000 K to 1400 K. In contrast to graphene, the morphology depends strikingly on the growth method applied, resulting in nearly perfect, large h-BN flakes (CVD) or percolation networks with nanoscale holes (TPG).

Unlike graphene, h-BN consists of two distinct sublattices, made up of B and N atoms, respectively. Exchanging B and N atoms results in two different domains, that are observed with STM. We investigate the preferred domain orientation depending on growth temperature and growth method.

The monolayer is further treated in the electric field of the STM tip. Periodic, 2-dimensional defect structures are achieved by tip-induced manipulation. A threshold bias voltage for this nanomesh creation is obtained and the manipulation probability is investigated as a function of tunneling parameters.

O 37.59 Tue 18:30 P2

**Properties of ultrathin Pb layers on the Ni<sub>3</sub>Al(111) studied by AES/LEED/STM/DFT** — ●KATARZYNA MIŚKÓW and ALEKSANDER KRUPSKI — Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom.

The morphology, atomic and electronic structure of ultrathin Pb layers deposited on the Ni<sub>3</sub>Al(111) face in ultrahigh vacuum at the substrate temperature, ranging from 200 K to 950 K, were investigated with the use of Auger electron spectroscopy (AES), low-energy electron diffraction (LEED), directional elastic peak electron spectroscopy (DEPES), scanning tunnelling microscopy (STM). Density functional theory calculations (DFT) with the use of CASTEP code were used to describe atomic and electronic structure of the Pb/Ni<sub>3</sub>Al(111) system. The analysis of AES and STM measurements indicate that two-dimensional growth of the first Pb monolayer wetting layer takes place. For T = 200 K, lead on the Ni<sub>3</sub>Al(111) grows layer-by-layer, while for T = 300 K flat three atomic-layer-high islands seem to grow after the completion of the first lead monolayer. Above 350 K, the Stranski-Krastanov growth mode is observed. The ordered LEED patterns are observed. Above  $\theta > 1.0$  ML, a three-dimensional growth of the Pb islands was observed with a strongly preferred atomic-scale magic height (N), hexagonal shape and flat-tops. At coverage  $\theta = 3.5$  ML, only islands containing N = 3, 5, 7 and 11 atomic layers of Pb are observed. At the higher coverage  $\theta = 5.5$  ML, three types of regular hexagonal islands with side lengths of 25, 30 and 45 nm are observed. Furthermore, three different island adsorption configurations were observed.

O 37.60 Tue 18:30 P2

**Growth study of nickel nanoislands on Ir(111)** — ●STEFAN WIL-

FERT, LYDIA EL-KAREH, and MATTHIAS BODE — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We have investigated the growth of Ni nanoislands on Ir(111) by means of low-temperature scanning tunneling microscopy (STM) and spectroscopy (STS). Both, iridium and nickel, exhibit a fcc crystal structure in the bulk with a lattice mismatch of about 8%. Ni deposition at room temperature initially leads to equally spread islands with a diameter of about 10 nm. The early onset of 3D islands nucleation is observed. After a post-annealing process we observe coalescence into larger hexagonally shaped islands up to 40 nm in diameter while maintaining the 3D island character.

O 37.61 Tue 18:30 P2

**XPD structure determination of HfSi<sub>2</sub> islands grown on Si(110) surfaces** — •FRANK SCHÖNBOHM<sup>1,2</sup>, TOBIAS LÜHR<sup>1</sup>, DOMINIQUE HANDSCHAK<sup>1,2</sup>, PHILIPP ESPETER<sup>1,2</sup>, CHRISTOPH KEUTNER<sup>1,2</sup>, ULF BERGES<sup>1,2</sup>, and CARSTEN WESTPHAL<sup>1,2</sup> — <sup>1</sup>Fakultät Physik - Technische Universität Dortmund, Otto-Hahn-Str. 4, D 44221 Dortmund, Germany — <sup>2</sup>DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D 44227 Dortmund, Germany

Perspective replacement candidates of the SiO<sub>2</sub> gate dielectrics in MOSFETs are the so-called *high-k* materials like HfO<sub>2</sub>. The thermal stability of thin HfO<sub>2</sub> films on Si(110) surfaces plays an important role during the production process and was studied by means of x-ray photoelectron spectroscopy (XPS) and photoelectron diffraction (XPD). The sample was stepwise annealed within the temperature range from 500°C up to 770°C. XPS spectra of the Si 2p, Hf 4f, and O 2s signal were recorded as a function of the annealing temperature. The measurements indicate a stable HfO<sub>2</sub>-film for temperatures up to 730°C. Further annealing at temperatures up to 770°C removed the oxygen completely from the sample and the remaining Hf was bound to the substrate forming HfSi<sub>2</sub>. SEM investigations of the surface showed that the HfSi<sub>2</sub> is arranged in islands at the surface. An XPD pattern of the Hf 4f signal was recorded in order to investigate the internal atomic structure of the HfSi<sub>2</sub> islands. The experimental diffraction pattern was compared to simulated pattern resulting in a structure model for the HfSi<sub>2</sub> islands.

O 37.62 Tue 18:30 P2

**Structural and optical investigations of organic-organic heterosystems** — •JULIA PEUKER, FALKO SOJKA, MATTHIAS MEISSNER, MARCO GRUENEWALD, ROMAN FORKER, and TORSTEN FRITZ — University of Jena, Institute of Solid State Physics, Max-Wien-Platz 1, 07743 Jena, Germany

Here, we report on the epitaxial growth of quaterylene (QT) on one monolayer of hexabenzocoronene (HBC) on graphene, epitaxially grown on silicon carbide (SiC(0001)). During the deposition the change of the optical properties is observed with Differential Reflectance Spectroscopy (DRS). This *in-situ* method provides information on the interaction of the molecular transition dipoles and a possible charges transfer. It is also used for the control of the layer thickness to get a well-defined structure. The resulting structure is characterized by Low Energy Electron Diffraction (LEED). Finally, other heterostructures serve as comparison.

It is already known that an organic interlayer can change the interaction between the substrate, here epitaxial graphene, and the subsequently deposited molecules drastically. This effect can be used for electronic decoupling. [R. Forker, D. Kasemann, T. Dienel, C. Wagner, R. Franke, K. Müllen, and T. Fritz, *Adv. Mater.* **2008**, 20, 4450 - 4454.]

O 37.63 Tue 18:30 P2

**Growth of coronene-layers on reactive and inert substrates** — •TOBIAS HUEMPFNER, FALKO SOJKA, MARCO GRUENEWALD, ROMAN FORKER, and TORSTEN FRITZ — Friedrich-Schiller-University Jena, Institute of Solid State Physics, Max-Wien-Platz 1, 07743 Jena, Germany

Here we report on the growth of ultrathin coronene-layers on different substrates deposited via Organic Molecular Beam Epitaxy (OMBE) under ultra-high vacuum conditions. On the one hand we used reactive substrates like Ag(111) and Au(111), on the other hand inert substrates like mica. The differences in the optical properties due to the molecule-substrate interactions were observed *in situ* during the deposition using Differential Reflectance Spectroscopy (DRS) [1].

The resulting molecular structures of the coronene-films are characterized with Low Energy Electron Diffraction (LEED) as well as Scanning Tunneling Microscopy (STM) for metallic and Atomic Force Microscopy (AFM) for inert substrates, respectively, at about 1 K.

A layer system consisting of potassium-chloride (KCl) on a Ag(100) surface gains special interest as a substrate for this molecule, because KCl-layers seem to be easy to prepare on this surface [2]. Moreover, STM investigations are still possible due to the metal-crystal below the KCl-layer, although the coronene still grows electronically decoupled from the Ag(100) surface.

[1] R. Forker *et al.*, *Annu. Rep. Prog. Chem., Sect. C: Phys. Chem.*, **2012**, 108, 34-68.

[2] M. Müller *et al.*, *Surface Science*, **2011**, 605, 1090-1094.

O 37.64 Tue 18:30 P2

**Growth of epitaxial Bi<sub>1-x</sub>Sb<sub>x</sub> films** — •JULIAN KOCH, PHILIPP KRÖGER, HERBERT PFNÜR, and CHRISTOPH TEGENKAMP — Leibniz Universität Hannover, Inst. für Festkörperphysik, Appelstr. 2, 30167 Hannover

The alloy Bi<sub>1-x</sub>Sb<sub>x</sub> was the first 3D topological insulator to be discovered. Depending on the relative concentrations of Bi and Sb the surface states can be tuned between topologically trivial and nontrivial (e.g. see PRB 83, 201104(R)). The fundamental difference of these states can be probed in principle by surface transport. However, in order to identify these different regimes, control of the film quality as well as the atomic defect structure is mandatory. *In-situ* epitaxy is a well established concept to grow such high-quality films.

In this study this material class was epitaxially grown by co-deposition on Si(111) substrates and investigated by means of low energy electron diffraction. Films of different stoichiometry ranging from  $x = 0.07 - 0.3$  have been grown by co-deposition at various temperatures and correlated with their lattice constants. In order to achieve epitaxial growth of (111)-oriented Bi<sub>1-x</sub>Sb<sub>x</sub>-films a buffer layer is necessary which has been realized by growth of 10 bilayer Bi. Growth of contiguous Bi<sub>1-x</sub>Sb<sub>x</sub>-films with single domain structures succeeds for deposition temperatures below 400 K. At higher temperatures the film is ruptured accompanied by segregation of Sb as confirmed by XPS.

O 37.65 Tue 18:30 P2

**Surface investigation of ceria films on Si(111) after post deposition annealing** — •ROBERT OELKE<sup>1</sup>, WANJA SPIESS<sup>1</sup>, HENRIK WILKENS<sup>1</sup>, MARVIN H. ZOELLNER<sup>2</sup>, GANG NIU<sup>2</sup>, THOMAS SCHROEDER<sup>2,3</sup>, and JOACHIM WOLLSCHLÄGER<sup>1</sup> — <sup>1</sup>Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany — <sup>2</sup>IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — <sup>3</sup>BTU Cottbus, Institute of Physics, Konrad-Zuse-Str.1, 03046 Cottbus, Germany

CeO<sub>2</sub>(111) films are a promising candidates in the field of microelectronics due to their high dielectric constant and the very small lattice mismatch in respect to Si(111). Furthermore, CeO<sub>2</sub> films can be used as model systems to study its catalytic properties. The generation of oxygen vacancies is of particular interest since they have a strong influence on the catalytic, as well as, the electronic properties.

Therefore, we present a post deposition annealing study of several CeO<sub>2</sub>(111) films grown on hex-Pr<sub>2</sub>O<sub>3</sub>/Si(111) system. Films with thicknesses in the range of 8 to 250 nm are annealed under UHV conditions. After each annealing step low energy electron diffraction measurements combined with spot profile analysis (SPA-LEED) are performed.

Several superstructures are formed at elevated temperatures indicating a periodic order of oxygen vacancies during reduction. Spot profile analysis show that the crystalline quality increases with higher film thickness.

O 37.66 Tue 18:30 P2

**Constructive electromigration of indium on silicon(111)** — •PAUL GRAF, ALEXANDER M. BERNHART, MARK R. KASPERS, CHRISTIAN A. BOBISCH, and ROLF MÖLLER — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

Electromigration (EM) is the material transport driven by an electron current or by an electric field [1]. This process is technically very important for thin/small conductors in electronic devices (e.g. CPUs) since the dimension of such structures reach the range of 10 nm or less. Here, we investigate *in situ* the EM of Indium on a Si(111) surface using a four probe scanning tunneling microscope (STM) and a scanning electron microscope (SEM). We study the indium induced

surface reconstruction on Si(111) [2] with  $\mu\text{m}$ -scaled indium islands. To apply an electric field in parallel to the surface two tips make contact to islands. Using the SEM we observe the formation of additional In islands in between the contacted islands, which results from the material transport from the indium reconstruction. In contrast to the usual destructive EM, we use this transport to form Indium wires; the method may become a starting point for the directed growth of small electronic networks.

- [1] R. Landauer and W. Woo, Phys. Rev. B 10, p. 1266 (1974).  
 [2] Eli Rotenberg et al., Phys. Rev. Lett. 91, 246404 (2003).

O 37.67 Tue 18:30 P2

**In situ control of step formation on Si(100) in process gas ambient** — ●SEBASTIAN BRÜCKNER<sup>1,2</sup>, OLIVER SUPPLIE<sup>1,2</sup>, PETER KLEINSCHMIDT<sup>2,3</sup>, HENNING DÖSCHER<sup>2</sup>, ANJA DOBRICH<sup>2</sup>, and THOMAS HANNAPPEL<sup>1,2,3</sup> — <sup>1</sup>Helmholtz-Zentrum Berlin, Institut Solare Brennstoffe und Energiespeichermaterialien, D-14109 Berlin — <sup>2</sup>TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, D-98693 Ilmenau — <sup>3</sup>CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, D-99099 Erfurt

Double-layer step formation on Si(100) substrates is a crucial prerequisite for antiphase-domain free III-V heteroepitaxy. Si(100) preparation in hydrogen process gas ambient, which is commonly employed for Si and III-V device preparation, differs strongly from preparation in ultra-high vacuum due to strong interaction between H<sub>2</sub> and the Si surface. In situ surface characterization by reflection anisotropy spectroscopy allowed us to study and control the domain formation of Si(100) surfaces directly in dependence on process parameters during MOVPE preparation. Here, we show that energetically and kinetically driven step formation on Si(100) compete depending on MOVPE process conditions. While preparation of vicinal substrates at low H<sub>2</sub> pressure leads to predominant (2×1) surface reconstruction with D<sub>B</sub> steps (i.e. dimer rows perpendicular to step edges), preparation at high H<sub>2</sub> pressure resulted in a predominant (1×2) reconstructed surface with D<sub>A</sub> steps (dimer rows parallel to step edges). On nearly exact Si(100), Si monolayer removal in H<sub>2</sub> ambient results in an oscillating A- and B-type majority domain formation.

O 37.68 Tue 18:30 P2

**SPA-LEED studies on structure and morphology of Ce<sub>x</sub>Pr<sub>1-x</sub>O<sub>2</sub> films** — ●WANJA SPIESS<sup>1</sup>, HENRIK WILKENS<sup>1</sup>, MARVIN H. ZOELLNER<sup>2</sup>, GANG NIU<sup>2</sup>, THOMAS SCHROEDER<sup>2,3</sup>, and JOACHIM WOLLSCHLÄGER<sup>1</sup> — <sup>1</sup>Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany — <sup>2</sup>IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — <sup>3</sup>BTU Cottbus, Institute of Physics, Konrad-Zuse-Str.1, 03046 Cottbus, Germany

Rare earth oxides (REOs) are in the focus of research for several catalytic applications, e.g. the three-way automotive exhaust catalysis. Lattice oxygen directly participates in these surface redox reactions based on the Mars-van-Krevelen mechanism. Therefore, the structural properties of the REOs and especially oxygen vacancies have a strong impact on the catalytic reactivity and selectivity. In addition, the intermixing of different REOs gives further opportunity of tuning the catalytic properties. We present a post deposition annealing study of mixed Ce<sub>x</sub>Pr<sub>1-x</sub>O<sub>2</sub> films grown on Si(111) using SPA-LEED (spot profile analysis at low energy electron diffraction) to control structural properties. Several crystalline structures are stabilized at moderate temperatures while at high temperatures silicide is formed. Spot profile analysis of the fundamental diffraction spot reveals a strong correlation between surface morphology (atomic steps) and the stoichiometry of the films.

O 37.69 Tue 18:30 P2

**Two-Photon Photoemission from magnesium oxide** — ●REBECCA PÖSCHEL, ANDREJ CLASSEN, and THOMAS FAUSTER — Lehrstuhl für Festkörperphysik, Staudtstr. 7, D-91058 Erlangen

We prepared MgO by evaporating magnesium on a well-defined Ag(100) single-crystal surface kept at 473 K in 10<sup>-7</sup> mbar oxygen. Thin films of different thicknesses between 0.25 and 10 monolayers (ML) were deposited on the crystal. The samples were studied by two-photon photoelectron spectroscopy (2PPE) (1.55 eV and 4.65 eV) and by vacuum ultra-violet (VUV) photoelectron spectroscopy (21.2 eV). The work function decreases with increasing thickness and reaches a value of 3.14 eV for 10 ML. The image potential states of Ag(100) are seen for MgO coverages up to 1 monolayer. Between 1 and 2.5 ML the 2PPE spectra are rather structureless and make MgO an ideal substrate for the study of unoccupied electronic states of adsorbed

molecules.

O 37.70 Tue 18:30 P2

**Growth and magnetic properties of ultrathin iron oxide films on MgO(001) and STO(001)** — ●NICO PATHÉ, OLGA SCHUCKMANN, TOBIAS SCHEMME, MATTHÄUS WITZIOK, KARSTEN KÜPPER, and JOACHIM WOLLSCHLÄGER — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück

In this work, ultrathin iron oxide films were reactively grown on MgO(001) and STO(001) at 250 °C depositing Fe in 5·10<sup>-6</sup> mbar oxygen. Previous to this, NiO interlayers were reactively grown on both materials at 250 °C and an oxygen partial pressure of 10<sup>-5</sup> mbar. All samples were investigated via X-RAY PHOTOELECTRON SPECTROSCOPY (XPS) and X-RAY ABSORPTION SPECTROSCOPY (XAS). The surface structures were determined by LOW ENERGY ELECTRON DIFFRACTION (LEED) and the magnetic properties of the films were analyzed with MAGNETO-OPTIC KERR EFFECT (MOKE) and X-RAY MAGNETIC CIRCULAR DICHROISM (XMCD). XPS data show that stoichiometric magnetite was grown on all surfaces. This result was confirmed by the expected ( $\sqrt{2} \times \sqrt{2}$ )R45° superstructure obtained in LEED measurements. XMCD results indicate that the substrate has a strong influence on the critical film thickness, where stoichiometric magnetite occurs. All ironoxide films were found to be ferrimagnetic and most of them show a fourfold magnetic in-plane anisotropy in MOKE studies.

O 37.71 Tue 18:30 P2

**Electronic structure of the polar ZnO(0001) surface with Ga and N substitution: A density functional theory study** — ●JACEK PIECHOTA<sup>1</sup>, JAKUB SOŁTYS<sup>1</sup>, and STANISŁAW KRUKOWSKI<sup>1,2</sup> — <sup>1</sup>ICM, University of Warsaw, ul. Pawińskiego 5a, 02-106 Warszawa, Poland — <sup>2</sup>Institute of High Pressure Physics, Polish Academy of Sciences, ul. Sokolowska 29/37, 01-142 Warsaw, Poland

An extensive theoretical investigation of the polar ZnO(0001) surface, with Ga and N substitution for Zn and O, respectively, was performed. It was shown that some extra bands, located near the valence-band maximum, emerge due to dangling bonds existing at nonsaturated O or Zn layers. These dangling bonds were subsequently saturated by the hydrogen atoms. The surface related electron bands were then calculated for slabs where the Zn atom was substituted by the Ga atom, or the O atom by the N atom. In all cases, for different distances between the surface atoms and hydrogen saturation atoms the electric field within the ZnO slab was computed. It was demonstrated that the slab polarization depends on the distance between the slab surfaces and the hydrogen atoms. The Fermi level is pinned at both faces of the slab, and this fact determines the electric field within the slab. Also, the properties of the ZnO(0001) surface, as a function of the Fermi energy of the system, were examined. The obtained results were compared with experimental and other theoretical data.

O 37.72 Tue 18:30 P2

**Electronic properties and optical response of nonpolar GaN surfaces** — ●MARC LANDMANN, EVA RAULS, and WOLF GERO SCHMIDT — University of Paderborn, Germany

In nonpolar or semipolar GaN, the hexagonal c axis is orthogonal or inclined to the growth direction, in order to eliminate or limit the internal piezoelectric and spontaneous polarization fields that inherently limit the performance of optoelectronic devices. [1] We have calculated the electronic structure of the semipolar m-plane GaN(1-100) and a-plane GaN(11-20) surfaces within density functional theory (DFT). The band gap underestimation of (semi)local density functionals is corrected by a non-local Heyd-Scuseria-Ernzerhof (HSE) type hybrid-functional with an adjusted fraction of exact exchange. Surface characteristic states and their microscopic origin are identified in the calculated surface band structure and density of states. While the complex dielectric functions of GaN bulk and surface slabs, calculated within the independent particle approximation (IPA) on the HSE hybrid functional DFT level of theory, fail to reproduce prominent near band-edge features of the optical response, the inclusion of excitonic effects via solution of the Bethe-Salpeter equation for Coulomb correlated electron-hole pairs reproduces the experimentally observed spectral features. The optical anisotropies of the semipolar surfaces are investigated by calculation of the reflection anisotropy spectroscopy (RAS) [2] spectra and discussed alongside experimental data.

- [1] J. Schörmann et al., Appl. Phys. Lett. 89 (2006) 131910.  
 [2] W. G. Schmidt, phys. Stat. sol. (b) 242 (2005) 2751.

O 37.73 Tue 18:30 P2

**Adsorption of PTCDA on KCl and NaCl surfaces** — ●HAZEM ALDAHAK, WOLF GERO SCHMIDT, and EVA RAULS — Theoretische Physik, Universität Paderborn

In recent years, various highly regular supramolecular architectures of self-organized molecules on crystals have been designed and used in the bottom-up device technology. In the past, metal surfaces have frequently been used as substrate. However, metal substrates induce screening and quenching effects and thus hamper the detailed spectroscopy of the adsorbed overlayer. In contrast, molecular adsorption on ionic crystals like sodium or potassium chloride opens the possibility to study electronically decoupled molecules. Here we present density-functional theory calculations on the adsorption of single PTCDA molecules on KCl and NaCl (100) surfaces. Thereby, the adsorption on flat surfaces as well as on stepped substrates has been investigated. In order to understand and rationalize the adsorption mechanisms leading to the formation of these structures, a large variety of interface geometries was studied and analyzed with respect to the contribution of ionic, covalent and van-der-Waals interactions between adsorbates and substrates. The influence of the substrate and bonding mechanism on the molecular electronic structure has been investigated in detail and compared with the experimental data available. The calculation of the potential energy surface (PES) allows us to determine the activation energy for the mobile molecules on the surface.

O 37.74 Tue 18:30 P2

**Liquid Crystal Adsorption on Lithium Niobate (0001) Surfaces** — ●CHRISTIAN BRAUN, SIMONE SANNA, EVA RAULS, and WOLF GERO SCHMIDT — Lehrstuhl für Theoretische Physik, Universität Paderborn, Paderborn, Germany

LiNbO<sub>3</sub> (LN) is a man-made ferroelectric with an extraordinary high spontaneous polarization of 0.7 C/m<sup>2</sup>. The polarization creates a net electric field outside of the LN crystal, which can be locally patterned by switching ferroelectric domains. This opens the possibility for selective molecular adsorption, in particular of polarizable molecules, at the LN surface. Liquid crystals are highly interesting adsorbates, as their optical properties are easily manipulated by electrical or magnetic fields. Indeed, they are currently employed for the realization of modern displays, as well as in other optic and opto-electronic devices. Therefore, the detailed knowledge of the adsorption mechanisms of liquid crystal on LN, as well as the understanding of the influence of the ferroelectric substrate on the molecular ordering, would be highly desirable. In order to model the interaction of liquid crystals with ferroelectric surfaces, we have investigated the adsorption of 4-*n*-octyl-4'-cyanobiphenyl (8CB) molecules at the LN(0001) surfaces from *first-principles*. The adsorption energy and configuration are found to be both strongly polarization and coverage dependent. Van der Waals interactions, accounted for by Grimme-type corrections to the total energy, are found to yield a major contribution to the bond strength and influence the adsorbate orientation.

O 37.75 Tue 18:30 P2

**Heat induced passivation of CuInSe<sub>2</sub> surfaces: A strategy to optimize the efficiency of chalcopyrite thin film solar cells?** — HARRY MÖNIG<sup>1,2</sup>, ●DAVID LOCKHORN<sup>1,2</sup>, NABI AGHDASSI<sup>1</sup>, ALEXANDER TIMMER<sup>1,2</sup>, CHRISTIAN A. KAUFMANN<sup>3</sup>, RAQUEL CABALLERO<sup>4</sup>, HELMUT ZACHARIAS<sup>1,2</sup>, and HARALD FUCHS<sup>1,2</sup> — <sup>1</sup>Physikalisches Institut, Westfälische Wilhelms-Universität, Münster, Germany — <sup>2</sup>CeNTech, Center for Nanotechnology, Münster, Germany — <sup>3</sup>Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — <sup>4</sup>Departamento de Física Aplicada, Universidad Autónoma de Madrid, Madrid, Spain

Despite the success of chalcopyrite thin film solar cells, many open questions concern the complex defect physics at the interface between the n-type window layer and the p-type absorber, which crucially determines the device efficiency. Therefore, our study addresses this issue by scanning tunneling spectroscopy, photoelectron, and inverse photoelectron spectroscopy. After removing oxides by a KCN treatment and subsequent UHV annealing at 280°C, a complete passivation of defect levels is observed, which goes along with a type inversion and an enlarged band gap at the surface. Therefore, this sample state consolidates three exclusively beneficial properties, which potentially minimize interface recombination losses and increase the open circuit voltage in completed devices. In contrast, oxidation of the surface by annealing in air reduces the surface band bending and creates a high density of charge compensated defect levels.

O 37.76 Tue 18:30 P2

**A density functional theory study of the structural and electronic properties of the GaN(000-1) surface** — ●JACEK PIECHOTA<sup>1</sup>, MARIA PTASIŃSKA<sup>1</sup>, JAKUB SOLTYŚ<sup>1</sup>, and STANISŁAW KRUKOWSKI<sup>1,2</sup> — <sup>1</sup>ICM, University of Warsaw, Pawińskiego 5a, 02-106 Warsaw, Poland — <sup>2</sup>Institute of High Pressure Physics, Polish Academy of Sciences ul. Sokolowska 29/37, 01-142 Warsaw, Poland

Nitrogen terminated GaN(000-1) surface was studied using the density functional theory (DFT). It was shown that some extra bands, located near the valence-band maximum, emerge due to dangling bonds existing at nonsaturated N or Ga surfaces, respectively. These dangling bonds were subsequently saturated by the hydrogen atoms. The surface related electron bands were calculated for different distances between the surface atoms and hydrogen saturation atoms. The electric field within the GaN slab was computed, showing that the slab polarization depends on the distance between the slab surfaces and the hydrogen atoms. The Fermi level is pinned at both faces of the slab, and this fact determines the electric field within the slab. Also, the properties of the GaN(000-1) surface, as a function of the Fermi energy of the system, were examined. The obtained results were compared with experimental and earlier theoretical investigations data.

O 37.77 Tue 18:30 P2

**The interaction of benzaldehyde with water-saturated Si(001)** — ●SEBASTIAN FREY, DANIEL LAUMANN und ULRICH KÖHLER — Ruhr-Universität, Bochum, NRW

In the last years the interaction between organic compounds and silicon got importance regarding the connection of organic and inorganic conductors in semiconductor technology. Particular interest lies on molecules containing conjugated  $\pi$ -electrons, since they often act as organic (semi-)conductors. The adsorption of Benzaldehyde (BAH) on Si(100)-2x1 surfaces can be used as a model system to understand the interaction of aromatic species with semiconductor surfaces. In technology the Si dimers are mostly saturated with O adatoms or OH-groups due to contact with water molecules. We investigated the bonding between BAH and such dimers with HR-EELS to further understand the adsorption mechanism and to clarify the role of H- and OH-terminated Si. Water, deuterium, hydrogen and hydroxyl saturated and unsaturated Si was exposed to normal and deuterium labeled BAH to check whether the H adatom or the OH group is involved in the adsorption process.

O 37.78 Tue 18:30 P2

**Poly(phenylene-ethynylene)s and related bichromophoric molecules on HOPG: An STM study** — ●STEFAN-S. JESTER, KLAAS REMMERSEN, DANIELA SCHMITZ, and SIGURD HÖGER — Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Conjugated polymers have attracted increased attention in the last decades due to their interesting optical and electronic properties. We have recently synthesized and investigated model dimers of conjugated oligomers, linked in a macrocyclic scaffold. Two monodisperse conjugated oligomers of distinct chain length, based on phenylene-ethynylene-butadiynylene entities, are intramolecularly connected by two rigid clamp units, providing a defined distance and alignment in parallel. The lengths and distances of the chromophores are synthetically defined and adjustable with atomic-scale precision. Self-assembled monolayers (SAMs) of the compounds at the solid/liquid interface of highly oriented pyrolytic graphite (HOPG) and 1,2,4-trichlorobenzene (TCB) are studied by scanning tunneling microscopy (STM) with submolecular resolution. The results provide understanding about the shape and structure of the compounds. [1] S.-S. Jester, A. Idelson, D. Schmitz, F. Eberhagen, S. Höger *Langmuir* **2011**, *27*, 8205; [2] S. Liu, D. Schmitz, S.-S. Jester, N. J. Borys, S. Höger, J. M. Lupton *J. Phys. Chem. B* **2013**, *117*, 4197; [3] S.-S. Jester, D. Schmitz, F. Eberhagen, S. Höger, *Chem. Commun.* **2011**, *47*, 8838.

O 37.79 Tue 18:30 P2

**Imaging and controlling organic molecule adsorption on metal plated silicon surfaces: formation and structure of organic-silicide monolayers** — ●PAVEL SHUKRYNAU, MARIUS TOADER, LARS SMYKALLA, and MICHAEL HIETSCHOLD — 1 Institute of Physics Technische Universität Chemnitz, Reichenhainer Straße 70, D-09107 Chemnitz, Germany.

We have employed variable temperature scanning tunneling microscopy (STM) to follow the adsorption of fluorinated cobalt-phthalocyanine (F16CoPc) on Fe plated silicon 7\*7 reconstructed sur-

face. The coverage of F16CoPc varied from 0.05 up to 3 monolayers (ML). At coverage more than a monolayer the surface is completely covered with roundly shaped 3D clusters of typical size of  $\sim 1$  nm. Each cluster has lobe-like pattern that may suggest that they consist of several perpendicular standing phthalocyanine molecules. Tunneling spectra taken over each individual lobe within a cluster reveal small energy gap, showing semiconductor-like behavior of constituent parts. The general structure of the surface, i.e., shape of the step edges, remains unchanged, however, the cluster coverage/cluster size is substrate dependent. The interplay between the electronic and structural properties of molecular layers and transition metal silicide is the key to tune the functionalities of hybrid organic-semiconductor interfaces.

O 37.80 Tue 18:30 P2

**Barium titanate: A promising candidate for the use of oxide-based electronics.** — ●PETER LUTZ<sup>1,2</sup>, SEBASTIAN FIEDLER<sup>1,2</sup>, CHUL-HEE MIN<sup>1,2</sup>, HENDRIK BENTMANN<sup>1,2</sup>, and FRIEDRICH REINERT<sup>1,2</sup> — <sup>1</sup>Experimentelle Physik VII, Universität Würzburg, 97074 Würzburg, Germany — <sup>2</sup>Gemeinschaftslabor für Nanoanalytik, Karlsruher Institute für Technologie KIT, 76021 Karlsruhe, Germany

Barium titanate (BTO) belongs to the material class of transition metal oxides which recently arouse a great deal of attention because of their multifunctional character and the rich physics occurring especially at oxide interfaces [1,2]. BTO is a particularly interesting oxide material showing ferroelectric properties and several structural phase transitions as a function of temperature [3,4]. One idea is to use this material as a substrate for thin films and to modify the film properties through the electric polarization direction. This requires detailed knowledge of the surface electronic and structural properties. To this end we investigate the influence of different preparation processes on the surface properties of BTO using tunneling spectroscopy (STM/STS), electron spectroscopy (XPS/UPS) and electron diffraction (SPALEED). We focus in particular on the processes for the evolution of oxygen vacancies at the surface in regard of their influence on the electronic structure and of their function in the formation of thin layers on the substrate.

[1] H. Y. Hwang et al., *Nature Mat.*, 11, 103 (2012) [2] C. H. Ahn et al., *Nature*, 424, 1015 (2003) [3] R. E. Cohen, *Nature*, 358, 136 (1992) [4] W. Zhong et al, *PRL*, 73, 1861 (1994)

O 37.81 Tue 18:30 P2

**Structure determination of CdO(100): A combined quantitative LEED and DFT study** — ●JAMES MUDD<sup>1</sup>, KATARZYNA MIŚKÓW<sup>1</sup>, JACOPO ARDINI<sup>2</sup>, GEORG HELD<sup>2</sup>, ALEKSANDER KRUPSKI<sup>1</sup>, and CHRIS MCCONVILLE<sup>1</sup> — <sup>1</sup>Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom. — <sup>2</sup>Department of Chemistry, University of Reading, Reading, RG6 6AD, United Kingdom

Cadmium oxide (CdO) is a transparent conducting oxide, with potential applications in solar cells and gas sensing. In addition it exhibits interesting surface electronic properties including electron accumulation resulting in a quantized 2D electron gas (Q2DEG), despite this there have so far been no studies of the surface structure of CdO. The surface structure of CdO(100) has been determined by quantitative low-energy electron diffraction LEED I(V) analysis and density functional theory (DFT) calculations. An analysis of LEED I(V) spectra from the CdO(100) surface has been performed by comparing measured intensities with data calculated using an automated CLEED program package. All DFT calculations have been performed with the CASTEP code (Cambridge Sequential Total Energy Package) using a plane-wave pseudopotential formalism.

O 37.82 Tue 18:30 P2

**Structure determination of TiO<sub>2</sub>(001) – (4 × 1) surface using quantitative low-energy electron diffraction** — ●KATARZYNA MIŚKÓW<sup>1</sup>, JAMES MUDD<sup>1</sup>, JACOPO ARDINI<sup>2</sup>, SEAN MCMITCHELL<sup>1</sup>, GEORG HELD<sup>2</sup>, CHRIS MCCONVILLE<sup>1</sup>, and ALEKSANDER KRUPSKI<sup>1</sup> — <sup>1</sup>Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom. — <sup>2</sup>Department of Chemistry, University of Reading, Reading, RG6 6AD, United Kingdom

Titanium (TiO<sub>2</sub>) is a non-toxic, wide band-gap semiconductor with three different crystal polymorphs (brookite, rutile and anatase). Systems based on TiO<sub>2</sub> have a large variety of possible applications including photocatalysis, heterogeneous catalysis, electrochromic devices and solar cells for hydrogen and electric energy production. Here we report a quantitative structural determination of the anatase TiO<sub>2</sub>(001)-(4×1)

surface with the use of low energy electron diffraction. An analysis of LEED I(V) spectra from the (4×1) surface has been performed by comparing measured intensities with data calculated using the automated CLEED program.

O 37.83 Tue 18:30 P2

**CO on NiO(001)** — ●JOSEF GRENZ, ALEXANDER SCHWARZ, and ROLAND WIESENDANGER — Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, 20355 Hamburg, Germany

Tips functionalized with CO molecules have recently been used in AFM studies to enhance the resolution to the submolecular level [1]. While investigating single CO molecules with metallic tips on different substrates various studies observed a ring-like structure (e.g. [2]). Since metallic tips should always exhibit a dipole moment [3] and CO, at least in the gas phase, also possesses a dipole moment, we attribute the observed contrast pattern to an interplay between attractive van-der-Waals and repulsive electrostatic dipole-dipole interactions. The latter should become relevant before the Pauli repulsion, which can be probed at even smaller distances.

In this contribution a detailed analyses of CO adsorbed on the bulk insulator NiO(001) will be shown. Adsorption sites, diffusion and the possibility to quantify the magnitude of the dipole moment via imaging and spectroscopy will be discussed.

[1] L. Gross, *et al.*, *Science* **325**, (2009) 1110.

[2] Z. Sun, *et al.*, *Phys. Rev. Lett.* **106**, (2011) 046104.

[3] G. Teobaldi, *et al.*, *Phys. Rev. Lett.* **106**, (2011) 216102.

O 37.84 Tue 18:30 P2

**Characterization of the adlayer formation of CO on the NaCl(100) surface based on diffuse LEED intensities** — ●JOCHEN VOGT and BIRGIT VOGT — Chemisches Institut der Uni Magdeburg, Magdeburg, Germany

Changes of the diffuse background in low-energy electron diffraction patterns can be used to characterize the stages of adlayer formation on well-ordered surfaces. Using the MCP-LEED technique, such experiments are also possible with bulk insulators without extensive surface charging. Although a helium atom diffraction study reported a  $p(1 \times 1)$  symmetry of the system CO/NaCl(100) at temperatures above 35 K [1], superstructure features of the low-temperature  $p(2 \times 1)$  phase are visible in LEED diffraction patterns well above this temperature. At 40 K, the subtraction of subsequently recorded LEED patterns reveals the formation of a diffuse background in the initial stages of the adlayer growth, consistent with an earlier proposed adsorption of CO at isolated sites [2]. The superstructure peels off from the background at a coverage of about half a monolayer. With the intention to develop a structure model of the disordered adsorbate, we present calculated diffraction patterns based on energy optimized local geometries. [1] D. Schmicker, J. P. Toennies, R. Vollmer, H. Weiss, *J. Chem. Phys.* **95** (1991), 9412 [2] C. Noda, G. E. Ewing, *Surf. Sci.* **240** (1990), 181

O 37.85 Tue 18:30 P2

**Pentacene adsorption and oxidation on a cobalt oxide bilayer film** — ●MARINA SCHULER, PASCAL FERSTL, LUTZ HAMMER, and M.ALEXANDER SCHNEIDER — Lehrstuhl f. Festkörperphysik, FAU Erlangen-Nürnberg, 91058 Erlangen

As a prototypical example of the adsorption of functional organic molecules on an oxide surface we investigate pentacene on a bilayer of CoO epitaxially grown on Ir(100) [1] by STM and TDS in UHV. At 300 K the molecules adsorb flat-lying and a maximum areal density of 0.66 molecules per nm<sup>2</sup> is obtainable before multi-layer growth sets in. For single-layer coverage we observe a well-defined rotational alignment of the molecules with respect to the crystallographic axes of the CoO layer. The lateral binding configuration, in contrast, is variable on the atomic scale, since the molecules always bridge many inequivalent sites of CoO. From the absence of any lateral long-range order of the molecular film even after annealing to 400 K we conclude that the molecule-substrate interaction is dominating.

Pentacene starts to get oxidized by the CoO film already at 420 K, the molecules decompose into CO<sub>2</sub>, H<sub>2</sub>O, CO and H<sub>2</sub>. In the beginning of the reaction the oxide layer gradually transforms into ordered sub-oxide structures. At higher temperatures and lower oxygen content of the cobalt oxide layer the dominant reaction products shift from CO<sub>2</sub> and H<sub>2</sub>O to CO and H<sub>2</sub>. We note that the sub-oxides can be reoxidised in the same temperature regime, hence a full catalytic cycle of molecule oxidation is achievable.

[1] C. Tröppner, et al., *PRB* **86**, 235407 (2012)

O 37.86 Tue 18:30 P2

**Preparation and characterization of phenylphosphonic acid self-assembled monolayers on ZnO substrates** — ●ALEXANDRA OSTAPENKO and GREGOR WITTE — Molekulare Festkörperphysik, Philipps-Universität Marburg, Renthof 7,35032 Marburg, Germany

Metal oxides are promising materials for fabrication of organic/inorganic hybrid structures. Surface functionalization by means of self-assembled monolayers (SAMs) is a promising approach to tailor their electronic interface properties or to fixate molecular chromophores. However, in contrast to widely used SAMs on gold surfaces, the molecular interaction and stability of such films on metal oxides have been much less studied. Here we report on the formation, thermal stability and molecular orientation of phenylphosphonic acid (PPA) SAMs on the Zn- and O-terminated basal planes of ZnO crystals that were studied by combining x-ray photoelectron spectroscopy (XPS), near edge x-ray absorption fine structure spectroscopy (NEXAFS) and thermal desorption spectroscopy (TDS). In addition the effect of OH-precoating on the adsorption was studied and the film ordering on pristine and defective ZnO surfaces was compared.

O 37.87 Tue 18:30 P2

**Superoxide and peroxide chemical states of adsorbed molecular oxygen on rutile TiO<sub>2</sub> (110) surface** — ●HIKMET SEZEN, ALEXEI NEFEDOV, and CHRISTOF WÖLL — Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

TiO<sub>2</sub> is a highly attractive material due to its unique electron storage and transfer capabilities. In order to generate versatile chemical and physical interactions with the surface of TiO<sub>2</sub>, molecular oxygen was chosen because of its singlet and triplet electronic configurations. However, these properties of O<sub>2</sub> have already been utilized as photo-oxidizing agent or electron scavenger, 1-2 the nature of superoxide and peroxide states of molecule oxygen especially on metal oxide surfaces has not yet been understood. In this contribution, we demonstrate spectroscopic evidences about present of superoxide and peroxide species on rutile TiO<sub>2</sub> (110) surface from both laboratory-based ultraviolet and X-ray photoelectron spectroscopies, and synchrotron-based X-ray photoelectron and near edge X-ray absorption fine structure spectroscopies.

1. I.X. Green, and J.T. Yates, The Journal of Physical Chemistry C 114, 11924 (2010). 2. M.A. Henderson, M. Shen, Z.-T. Wang, and I. Lyubnitsky, The Journal of Physical Chemistry C 117, 5774 (2013)

O 37.88 Tue 18:30 P2

**Water dissociation on  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>(1102)** — ●SEBASTIAN WLOSCZYK<sup>1</sup>, HARALD KIRSCH<sup>1</sup>, JONAS WIRTH<sup>2</sup>, MARTIN WOLF<sup>1</sup>, PETER SAALFRANK<sup>2</sup>, and R. KRAMER CAMPEN<sup>1</sup> — <sup>1</sup>Fritz-Haber-Institut, Abt. Physikalische Chemie, 14195 Berlin, Germany — <sup>2</sup>Universitaet Potsdam, Institut fuer Chemie, 14476 Potsdam OT Golm, Germany

Alumina surfaces are ubiquitous in technologically relevant applications and a useful model system for more complicated, environmentally abundant, aluminosilicate phases. Because their properties change dramatically on interaction and reaction with water, water/Alumina chemistry has been studied, both experimentally and theoretically, for decades. In this work, we study the interaction of heavy water (D<sub>2</sub>O) with the  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>(1102) surface under ultra high vacuum (UHV) conditions. In-situ preparation of the carbon-free, well defined single crystal surfaces is checked by low energy electron diffraction (LEED) and Auger electron spectroscopy (AES). Hydroxylation of the Al<sub>2</sub>O<sub>3</sub>(1102) in UHV is performed by dosing D<sub>2</sub>O seeded in Helium with a molecular beam source (MBS). For characterization we employ vibrationally resonant sum frequency generation (VSF) spectroscopy to probe the OD stretch response of interfacial species and thermal desorption spectroscopy (TDS). The aim of the study is to investigate the adsorbate/substrate interaction and understand the effect of surface morphology on the hydroxylation process.

O 37.89 Tue 18:30 P2

**Preparation of single bismuth atoms on the silicon (111)-(7x7) surface** — ●ALEXANDER KÖLKER<sup>1,2</sup>, MATTHIAS ELTSCHKA<sup>1</sup>, CAROLA STRASSER<sup>1</sup>, MARKUS ETZKORN<sup>1</sup>, CHRISTIAN AST<sup>1</sup>, and KLAUS KERN<sup>1,3</sup> — <sup>1</sup>Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — <sup>2</sup>Westfälische Wilhelms-Universität Münster, Fachbereich Physik, 48149 Münster, Germany — <sup>3</sup>Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Exploiting the nuclear spin for qubits is a possible route towards the

realization of quantum computing. Bi in Si is a promising donor based quantum system due to the combination of its large nuclear spin ( $I = 9/2$ ) and large hyperfine splitting that could be resolved by inelastic electron tunneling spectroscopy (IETS) [1].

In preparation of such a measurement we have investigated Bi in the sub monolayer regime on the Si (111)-(7x7) surface by scanning tunneling microscopy (STM). We observe the formation of isolated Bi impurities on the surface. Increasing the temperature of the Si sample during the evaporation of Bi we have observed a smaller height of the Bi atoms on the Si (111)-(7x7) surface, which indicates a stronger bound state of Bi atoms to the surface. First steps have been carried out to study the electronic properties of both systems at room temperature.

The ultimate goal is to observe single nuclear spin flips with an STM. As this energy scale is extremely small, we will investigate this using an STM operating at 15 mK for high energy resolution.

[1] F.Delgado Phys. Rev. Lett. 107, 076804 (2011)

O 37.90 Tue 18:30 P2

**Characterization of mass selected silver clusters produced in a supersonic nozzle expansion** — ●JENS-CHRISTIAN MEYER, DAVID ENGEMANN, and HEINZ HÖVEL — Fakultät Physik / DELTA, Technische Universität Dortmund, 44227 Dortmund

The structures and properties of clusters are located in between molecules and solids and their properties are strongly dependent on their size.

Silver-cluster with a diameter distribution of  $2R = 2 \pm 0.6$ nm are produced in a cluster apparatus with a supersonic nozzle expansion source [1] and deposited into various matrices. These clusters are characterized by UV/VIS-spectroscopy, transelectron-microscopy (TEM) and small angle x-ray scattering technique (SAXS) to determine their structure.

To investigate in detail how the properties of silver-clusters are related to their size, a mass selector will be implemented to our cluster source. With an electric field, ionized clusters will be deflected dependent on their size.

[1] H. Hövel; S. Fritz; A. Hilger; U. Kreibig; M. Vollmer, Width of cluster plasmon resonances: Bulk dielectric functions and chemical interface damping. Phys.Rev.B, 48, 18178, 1993.

O 37.91 Tue 18:30 P2

**Photovoltage on Metallic and Semiconducting Surfaces in Vicinity of Metallic Nanostructures** — ●KEVIN OLDENBURG, KRISTIAN SELL, STEFAN POLEI, SYLVIA SPELLER, and INGO BARKE — University of Rostock, Institute of Physics, 18051 Rostock, Germany

The effect of the local environment on the dynamics of electron-hole generation and decay is investigated by means of spatially resolved photovoltage measurements. For metallic surfaces such as Si(111)-(7x7) and Si(111)-(5x2)-Au a surprisingly low metal content results in saturation of the coverage-dependent photovoltage [1]. Experiments in progress include the comparison to samples with non-metallic surface states where pronounced spatial variations are expected. An experimental setup is presented that enables measurements at 405 nm wavelength, such that saturation conditions can be efficiently achieved with low thermal load. This is important to understand the spatial distribution of charge carriers at semiconducting surfaces in contact with clusters and metallic nanostructures.

[1] K. Sell, et al., Phys. Stat. Sol. (b) 247, 1087 (2010).

O 37.92 Tue 18:30 P2

**Growth and characterization of ultrasmall cobalt nanoislands on Cu(111)** — ●DAVID GOHLKE and JASCHA REPP — Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany

The ability to manipulate the magnetic properties of individual molecules and atoms is greatly affected by the substrate on which they rest. By adding nanoscale ferromagnetic regions to normal metal, one can vary the magnetic landscape for these adsorbates. It has previously been shown that Co adsorbed on the Cu(111) surface can self-assemble into spin-polarized triangular islands with lateral sizes between 5 and 30 nm. Here, we present a modified growth procedure for forming Co islands on this surface. By depositing metal on a cryogenic-temperature copper surface before annealing to room temperature, islands smaller than 5 nm are formed. These Co nanoislands bridge the size regime from the isolated adatom and few-atom clusters to the larger Co islands previously studied. Scanning tunneling microscopy (STM) allows for clear topographic characterization as well

as a detailed examination of the electronic states of these islands, showing a continuation of the previously published downward trend in the energy of the highest occupied electronic state with decreasing island size.

O 37.93 Tue 18:30 P2

**Ab initio transport calculations of copper junctions in the presence of hydrogen chloride** — ●PAUL SCHNÄBELE<sup>1</sup>, RICHARD KORYTÁR<sup>1</sup>, ALEXEI BAGRETS<sup>1</sup>, AXEL GROSS<sup>3</sup>, and FERDINAND EVERS<sup>1,2</sup> — <sup>1</sup>Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76344 Eggenstein-Leopoldshafen, Germany — <sup>2</sup>Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — <sup>3</sup>Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

Understanding nanoscale transport in the presence of a solvent is an important challenge in electrochemistry. To this end, we investigate transport properties of single-atom Copper junctions surrounded by hydrogen chloride. The components of this environment are partially adsorbed on the surface of the junction. In a first step we relax the geometry using density functional theory. (The chloride coverage is obtained from reference-calculations for flat surfaces [1].) This helps us to improve our understanding of the chemical bonds that occur in this situation. Furthermore, the optimized structure provides the basis for the investigation of transport properties. The calculations rely on a non-equilibrium Green's function (NEGF) approach and are implemented in the AITRANSS package that is being developed in our group [2,3]. We show that the solvent has a significant impact on the transmission and density of states.

[1] T. Roman, A. Groß, Phys. Rev. Lett. **110**, 156804 (2013)

[2] A. Arnold, F. Weigend, F. Evers, J. Chem. Phys. **126**, 174101 (2007)

[3] A. Bagrets, J. Chem. Theory Comput. **9**, 2801 (2013)

O 37.94 Tue 18:30 P2

**Controlled electromigration of copper wires and copper thin films** — ●JULIA HAUSER<sup>1</sup>, JAKOB SCHWICHTENBERG<sup>1</sup>, MICHAEL MARZ<sup>1</sup>, CHRISTOPH SÜRGER<sup>1</sup>, HILBERT V. LÖHNEYSEN<sup>1,2</sup>, and REGINA HOFFMANN-VOGEL<sup>1</sup> — <sup>1</sup>Karlsruher Institut für Technologie, Physikalisches Institut und DFG-Center for Functional Nanostructures, D-76131 Karlsruhe — <sup>2</sup>Karlsruher Institut für Technologie, Institut für Festkörperphysik, D-76021 Karlsruhe

Controlled electromigration (EM), i.e., thinning of a metallic wire by cyclic voltage ramping, offers the possibility to fabricate nanocontacts with gaps of a few nanometers in size [1]. We have investigated controlled EM of freely suspended Cu wires under ambient and UHV conditions. We are able to thin the contact down to a conductance of a few conduction quanta  $G_0 = 2e^2/h$ , in some cases even to  $G_0$ . The onset of the EM follows multiple constant-power curves, as reported earlier [1,2]. Under ambient conditions, we find a negative curvature of the envelope in the first cycles of the EM process before entering the constant-power envelope, which is not observed in UHV. Additionally, we have performed EM on thin Cu films on SiO<sub>2</sub> substrates under ambient conditions as well, in order to study the effect of the sample geometry on EM. We find that the films show qualitatively the same behavior as the 'ambient' wires. From the maxima of conduction histograms we infer preferred conduction values, whose number in the range of  $0 < G \lesssim 10G_0$  depends on the initial thickness of the film.

[1] D. R. Strachan et al., Appl. Phys. Lett. **86**, 043109 (2005).

[2] D. Stöffler et al., Phys. Rev. B **85**, 033404 (2012).

O 37.95 Tue 18:30 P2

**Structural Transition in Atomic Chains Driven by Transient Doping** — ●STEFAN POLEI<sup>1</sup>, PAUL SNIJDERS<sup>2</sup>, STEVE ERWIN<sup>3</sup>, FRANZ HIMPEL<sup>4</sup>, KARL-HEINZ MEIWES-BROER<sup>1</sup>, and INGO BARKE<sup>1</sup> — <sup>1</sup>Department of Physics, University of Rostock, D-18051 Rostock, Germany — <sup>2</sup>Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — <sup>3</sup>Center for Computational Materials Science, Naval Research Laboratory, Washington, DC 20375, USA — <sup>4</sup>Department of Physics, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA

Transient, non-equilibrium electronic phases are of great interest for various fields of physics, as they open the door to hidden states of matter that are not accessible by static measurements. In this contribution we present scanning tunneling microscopy (STM) measurements of a reversible structural transition on Si(553)-Au from a 1x3 ground state to a 1x2 excited state upon electron injection from the tip to the surface [1]. It is shown that the 1x2 phase is created by temporary doping

of the atom chains. Random telegraph fluctuations between two levels of the tunneling current provide direct access to the dynamics of the phase transition. An intriguing observation is the unusual temperature behavior that results in easier excitation at lower temperatures. As a consequence, the 1x3 ground state is not accessible by STM at low temperatures (e.g. T=5K). In a broader context this implies that a phase observed using STM at the lowest possible temperatures may not be the ground state of the system.

[1] Polei et al., PRL **111**, 156801 (2013)

O 37.96 Tue 18:30 P2

**Vibration modes of Si(111)-(7x7) and various reconstructed Au/Si(111) surfaces, studied by Raman spectroscopy** — MARTIN LIEBHABER<sup>1</sup>, UTZ BASS<sup>1</sup>, ●JEAN GEURTS<sup>1</sup>, JOCHEN RÄTHEL<sup>2</sup>, EUGEN SPEISER<sup>2</sup>, SANDHYA CHANDOLA<sup>2</sup>, ARNE BAUMANN<sup>2</sup>, and NORBERT ESSER<sup>2</sup> — <sup>1</sup>Universität Würzburg, Physikalisches Institut, Experimentelle Physik III, 97074 Würzburg — <sup>2</sup>Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., 12489 Berlin

Ordered submonolayers of adsorbate atoms on semiconductor surfaces constitute a playground for electronic correlation effects, which are tightly connected with the local atomic arrangement and the corresponding vibration modes. We applied polarized Raman spectroscopy to Au-covered Si(111) surfaces, either with  $(5 \times 2)$  or with  $(\sqrt{3} \times \sqrt{3})$  reconstruction, and to clean Si(111)-(7x7) surfaces for reference. On the latter ones, six surface vibration modes appear between 7.7 meV and 52.1 meV, with different polarization dependence. Upon Au coverage, they are quenched and replaced by new modes, governed by the specific Au reconstruction. For  $(5 \times 2)$ , five low-frequency Au-induced vibration modes emerge (3.2 meV to 18.7 meV). The  $(\sqrt{3} \times \sqrt{3})$  Au reconstruction shares two of them, but also shows two new peaks in the same range. For the clean Si(111) (7x7) surface, these results should enable refined calculations of the dynamic properties of the DAS structural model. For the Au-covered surfaces, the reconstruction-specific vibrations may help to clarify the atomic geometry, extending the base for more sophisticated calculations of atomic and orbital properties of ordered adatom arrangements for correlated-electron systems.

O 37.97 Tue 18:30 P2

**Unusual resistance-voltage dependence of ultra-high vacuum-electromigrated nanojunctions** — DOMINIK STÖFFLER<sup>1</sup>, ●MICHAEL MARZ<sup>1</sup>, BIRGIT KIESSIG<sup>2</sup>, TIHOMIR TOMANIC<sup>1</sup>, HILBERT V. LÖHNEYSEN<sup>1,2</sup>, and REGINA HOFFMANN-VOGEL<sup>1</sup> — <sup>1</sup>Karlsruher Institut für Technologie, Physikalisches Institut und DFG-Center for Functional Nanostructures, D-76131 Karlsruhe — <sup>2</sup>Karlsruher Institut für Technologie, Institut für Festkörperphysik, D-76021 Karlsruhe

Clean and well-defined electronic contacts in the nanometer-size range are one prerequisite for single-molecule-based electronics. Controlled electromigration (EM) [1], especially in ultra high vacuum (UHV), allows the preparation of sufficiently small and clean metallic contacts. Here we present measurements of the voltage dependence of the electrical resistance  $R(V)$  subjected to EM in UHV. For large  $R$  values an unexpected decrease of  $R(V)$  with increasing bias is observed. Comparing with simple model calculations, we tentatively ascribe this behavior to tunneling in parallel to ohmic nanocontacts. In addition, we observe field emission, which additionally supports the idea that tunneling occurs in EM experiments performed in UHV.

[1] D. R. Strachan et al., Appl. Phys. Lett. **86**, 043109 (2005).

O 37.98 Tue 18:30 P2

**Oligothiophene nanorings as electron resonators for whispering gallery modes** — ●GAËL REECHT<sup>1</sup>, HERVÉ BULOUP<sup>1</sup>, FABRICE SCHEURER<sup>1</sup>, VIRGINIE SPEISSER<sup>1</sup>, FABRICE MATHEVET<sup>2</sup>, and GUILLAUME SCHULL<sup>1</sup> — <sup>1</sup>IPCMS, Strasbourg, France — <sup>2</sup>Laboratoire de Chimie des Polymères, Paris, France

Recently, conjugated molecular wires were investigated using scanning tunneling microscopy (STM) [1]. These studies showed that the electronic structure of these oligomers can be approximated by a (nearly) free electron gas confined to a 1D box. Using a recent "on-surface" synthesis method [2], we obtained oligothiophene nanowires and nanocycles on a Au(111) surface. The electronic properties of these structures were energetically and spatially resolved using scanning tunneling spectroscopy (STS). This study reveals large differences between the electronic properties of the linear and cyclic structures. These differences find their origin in the close-ended nature of the cyclothiophene resonances which must be treated with periodic boundary conditions. A more detailed analysis shows that cyclothiophene must be considered

as a ribbon (i.e., having an effective width) rather than a purely 1D structure. A fascinating consequence is that the molecular nanorings act as whispering gallery mode resonators for electrons, opening the way for new applications in quantum electronics [3].

- [1]. Wang, S and al. *Phys. Rev. Lett.*, 106, 206803 (2011)
- [2]. Grill, L and al., *Nature Nano*, 2, 687 (2007)
- [3]. Reece, G and al. *Phys. Rev. Lett.*, 110, 056802 (2013)

O 37.99 Tue 18:30 P2

**Composite wire metamaterial for broadband infrared super-lensing** — ●MIKE PRÄMASSING, TOBIAS MASS, and THOMAS TAUBNER — I. Institute of Physics, RWTH Aachen University

Superlenses can either consist of natural [1] or metamaterials and enable subwavelength imaging beyond Abbes diffraction limit. Thereby, the evanescent near-fields are preserved and subwavelength information is transported [2]. We investigate a composite wire metamaterial consisting of parallel aligned metallic nanowires in a dielectric host medium. Its superlensing effect originates from strongly anisotropic optical properties [3,4]. Our theoretical investigations of the imaging properties concern the mid-infrared spectral range from 1 - 10 $\mu$ m. Furthermore we provide first fabrication attempts by means of electrochemical deposition [5].

- [1] Taubner et al. *Science* **2006** 313(5793) 1595.
- [2] Li et al. *ACS nano* **2012** 6(11), 10107-10114.
- [3] Belov et al. *Phys. Rev.* **2006** E73, 056607.
- [4] Elser et al. *Appl. Phys. Lett.* **2006** 89(26), 261102-261102.
- [5] Noginov et al. *Appl. Phys. Lett.* **2009** 94(15), 151105.

O 37.100 Tue 18:30 P2

**Characterisation of Boron-doped Silicon Nanowires** — ●STEFAN WEIDEMANN<sup>1</sup>, MANFRED RAMSTEINER<sup>2</sup>, ANNA MOGILATENKO<sup>3</sup>, KLAUS RADEMANN<sup>4</sup>, and SASKIA F. FISCHER<sup>1</sup> — <sup>1</sup>Neue Materialien, Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — <sup>2</sup>Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin, Germany — <sup>3</sup>Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, 12489 Berlin, Germany — <sup>4</sup>Nanostructured Materials, Institut für Chemie, Humboldt-Universität zu Berlin

Nanostructures of silicon possess a high surface to volume ratio and reveal new intrinsic properties like decreased thermal conductivity [1], which make them interesting for catalytic applications and electronic devices. Measuring simultaneously thermal and electronic transport properties of individual, structurally characterised, silicon nanowires still remains a challenge. Here we prepare silicon nanowires by the two-step metal-assisted chemical etching (MACE) [2].

In dependence of the boron doping concentration we obtain nanowires with lengths up to 110  $\mu$ m (undoped Si,  $\rho > 1$  k $\Omega$ cm), 90  $\mu$ m (medium doped,  $\rho = 14 - 23$   $\Omega$ cm) and about 40  $\mu$ m (highly doped Si,  $\rho < 0.01$   $\Omega$ cm), with smooth, rough and porous surfaces, respectively. Fabrication on wafer scale is feasible. Surface and structural properties of nanowire ensembles and individual nanowires are investigated by scanning and transmission electron microscopy and Raman spectroscopy.

- [1] A. I. Hochbaum *et al.*, *Nature* 451, 163 (2008)
- [2] Z. Huang *et al.*, *Adv. Mater.*, 23, 285-308 (2011)

O 37.101 Tue 18:30 P2

**Improving the performance of MW-CNT-based via interconnect systems - a conductive-AFM study** — ●MARIUS TOADER<sup>1</sup>, HOLGER FIEDLER<sup>2</sup>, SASCHA HERMANN<sup>2</sup>, STEFAN E. SCHULZ<sup>2,3</sup>, THOMAS GESSNER<sup>2,3</sup>, and MICHAEL HIETSCHOLD<sup>1</sup> — <sup>1</sup>Technische Universität Chemnitz, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany — <sup>2</sup>Technische Universität Chemnitz, Center for Microtechnologies, D-09126 Chemnitz, Germany — <sup>3</sup>Fraunhofer Institute for Electronic Nano Systems (ENAS), D-09126 Chemnitz, Germany

We have studied via interconnect systems based on vertically aligned multi-walled carbon nanotubes (MW-CNTs) grown on a copper-based metal line. Using c-AFM the corresponding overall performance can be accurately estimated based on the resistance of individual CNTs [1] in good agreement with the classical electrical measurements. By tuning the top metallic layer within the conductive line the corresponding CNT/metal contact quality could be considerably improved. Moreover, an improved performance as a result of exposure to HF vapours was observed as well.

- [1] H. Fiedler, M. Toader, S. Hermann, R. D. Rodriguez, E. Sheremet, M. Rennau, S. Schulze, T. Waechter, M. Hietschold, D.R.T.

Zahn, S. E. Schulz and T. Gessner; *Microelectron. Eng.* 2013 (<http://dx.doi.org/10.1016/j.mee.2013.07.007>).

O 37.102 Tue 18:30 P2

**A Ruler for the Nanoworld: Scatterometry at the PTB** — ●VICTOR SOLTWISCH, ANTON HAASE, JAN WERNECKE, and FRANK SCHOLZE — Physikalisch-Technische Bundesanstalt

The continuous shrinking in feature size in industrial application is a huge challenge under metrology aspects. In- and ex-situ metrology solutions are needed which are fast enough, non-destructive and have capabilities for 3D structures. The PTB operates several Beamlines at BESSYII and the new MLS, with different endstations designed for highest accuracy of scatterometric measurements. EUV and GISAXS scatterometry is a part of the optical scatterometry (OCD) solutions. EUV scatterometry is designed for the next step in photolithography in the semiconductor industry with wavelengths around 13.5 nm. Scattering from surfaces enables to reconstruct geometric parameters from nm structured surfaces. The study of off-specular scattering from multilayers gives insight in the interface roughness. We present several practical application of different scatterometric experiments which were performed at the PTB.

O 37.103 Tue 18:30 P2

**Silicene on Ag(111): Reconstructions and first tests of laser-induced non-thermal deposition** — ●SILKE HATTENDORF<sup>1</sup>, CHRISTIAN KALUPKA<sup>2</sup>, MARTIN REININGHAUS<sup>2</sup>, MARCO PRATZER<sup>1</sup>, and MARKUS MORGENSTERN<sup>1</sup> — <sup>1</sup>II. Institute of Physics B and JARA-FIT, RWTH Aachen — <sup>2</sup>Chair for Laser Technology, RWTH Aachen

Silicene, a buckled 2D honeycomb structure made of silicon, was predicted to be stable and exhibit an Dirac cone like graphene[1].

So far, it has been grown on Ag(111)[2], Ir(111)[3] and ZrB<sub>2</sub>[4]. However, due to strong hybridization with the underlying substrate the Dirac cone is most likely strongly distorted and the silicene states are pushed far into the valence and conduction band[5] making it mandatory to transfer it to a less interacting substrate.

Silicene was grown on Ag(111) at rates between 0.05 and 0.16 ML/min and at a substrate temperature of 200-250°C. The atomic structure was studied by scanning tunneling microscopy (STM) revealing the known reconstructions (e.g. 4 x 4,  $\sqrt{13} \times \sqrt{13}$ )[2].

We tried to transfer the silicene to mica using laser-induced non-thermal deposition [6]. However, possibly due to the strong interaction between the silver and silicene surfaces, this was not successful so far.

- [1] S. Cahangirov *et al.*, *PRL* 102, 236804 (2009).
- [2] P. Vogt *et al.*, *PRL* 108, 155501 (2012).
- [3] L.Meng *et al.*, *Nano Lett.* 13, 685 (2013).
- [4] A. Fleurence *et al.*, *PRL* 108, 245501 (2013).
- [5] Y.Yuan *et al.*, *Arxiv*:1310.2420.
- [6] M.Reininghaus, *APL* 100, 151606(2012).

O 37.104 Tue 18:30 P2

**Automated spray coating process for the fabrication of large-area opaline structures on textured substrates** — ●DANIELA SCHNEEVOIGT<sup>1</sup>, FREDERIK BUB<sup>1</sup>, ALEXANDER SPRAFKE<sup>1</sup>, and RALF WEHRSPHORN<sup>1,2</sup> — <sup>1</sup>Martin-Luther-Universität, Halle-Wittenberg, Deutschland — <sup>2</sup>Fraunhofer IWM, Halle, Deutschland

3D photonic crystals, such as opaline structures, have been shown to have a high potential to increase the efficiency of solar cells by enabling advanced light management concepts. Our automated process for the spray induced self-assembly of large-area artificial opals presents a low-cost technique, which complies with the demands of the photovoltaic industry for the integration of such structures [1]. The process is based on spraying a dispersion of monodisperse nanoscaled colloids onto a substrate and subsequent crystallization of a 3D photonic crystal.

Here, we report on the successful fabrication of artificial opaline structures, such as opals and inverted opals, via spray coating on textured substrates.

With the intention to integrate opaline structures as back reflectors in  $\mu$ c-Si thin film solar cells, the crystallization of extensive artificial opals on different  $\mu$ c-Si surface textures was analyzed. The inversion of the opals was achieved with a conformal deposition of Al:ZnO (by atomic layer deposition) and a subsequent wet-chemical removal of the colloids. The optical, structural and electrical characteristics of these opaline structures were examined.

- [1] Sprafke, A., Schneevoigt, D., Seidel, S., Schweizer, S. L., Wehrspohn, R., *Optics Express*, 21(26): 528, (2013).

O 37.105 Tue 18:30 P2



**Fabrication and application of nanosecond laser-induced surface nanostructures on polyimide** — ●LUKAS BAYER<sup>1,2</sup>, PIERRE LORENZ<sup>1</sup>, MARTIN EHRHARDT<sup>1</sup>, KLAUS ZIMMER<sup>1</sup>, and LUTZ ENGISCH<sup>2</sup> — <sup>1</sup>Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstraße 15, 04315 Leipzig, Germany — <sup>2</sup>Hochschule für Technik, Wirtschaft und Kultur Leipzig, P.O. Box 301166, 04251 Leipzig, Germany

The formation of nanostructures on polymers, produced by laser irradiation near the ablation threshold, is well-known. In the last 20 years, the influence of laser parameters on the resultant structures has been manifold studied. However, applications for this kind of constant and good manageable surface structures are hardly known. In this study, the fabrication and application of KrF excimer laser-induced 3-D conical surface structures on polyimide is presented. The properties of the laser-induced surface structures that are dependent on the laser parameters are analysed by optical and scanning electron microscopy (SEM). Furthermore, some applications of these surface structures are presented. Particularly in the field of product safety there are many opportunities to bring these structures to use. There are both low and high security features possible. A low security feature could be a microscopic QR-code containing any desired data. For high security applications it is also possible to create pictures with very high resolution. In this case, the resolution is much higher than in conventional printing technologies.

O 37.106 Tue 18:30 P2

**Nanostructuring of stainless steel by pulsed laser interference lithography** — ●LUKAS GRÖNER, MARTIN STÄRK, ELKE SCHEER, and JOHANNES BONEBERG — Universität Konstanz, BW

In pulsed laser interference lithography a laser pulse is divided into several beams which are recombined on the sample to be structured. Due to interference one gets a periodic pattern of high and low intensities. Therefore samples will get hot only in the high intensity regions. We show that this temperature modulation leads to a change in etching resistance which can be used to structure stainless steel surfaces with periods in the micrometer range and depths up to several hundreds of nanometers. As the experiments show not all stainless steel types are usable for this process.

O 37.107 Tue 18:30 P2

**Processing and characterization of photonic crystals on flexible substrates for light absorption enhancement in solar cells** — ●FREDERIK BUB<sup>1</sup>, DANIELA SCHNEVOIGT<sup>1</sup>, ALEXANDER SPRAFKE<sup>1</sup>, and RALF WEHRSPHON<sup>1,2</sup> — <sup>1</sup>Martin-Luther-Universität, Halle-Wittenberg, Germany — <sup>2</sup>Fraunhofer IWM, Halle, Germany

The success of the photovoltaic technology depends highly on two opposing improvements: saving material and therefore costs and increasing efficiency. One easy and cheap way to solve this conflict of interests is an advanced light management with photonic crystals to increase the light path in the absorber material.

Thus, we developed a production method for photonic crystals on flexible substrates based on a spray coating technique. The main advantage of this procedure is the fast assembly of photonic crystals consisting of polymeric colloids and the creation of a light management device separated from the solar-cell production line which allows easy integration into existing cell concepts. [1]

We produced photonic crystals respectively artificial opals on flexible substrates such as aluminum foil. The quality of the crystals was characterized optically, spectroscopically and mechanically. In detail we investigated the crystallization behavior of the artificial opals on flexible substrates by electron microscopy and analyzed the optical reflection. The stability and adhesion of the opaline films were qualified by applying mechanical stress to the flexible substrate.

[1] Sprafke, A, Schnevoigt, D, Seidel, S., Schweizer, S., Wehrspohn, R; Opt. Expr., 21(26): 528, (2013)

O 37.108 Tue 18:30 P2

**Simulation of ballistic glancing angle deposition** — ●CHRISTOPH GRÜNER, STEFAN G. MAYR, and BERND RAUSCHENBACH — Leibniz Institute of Surface Modification, Leipzig, Germany

Computer simulations can be a powerful tool to investigate physical

vapor deposition processes. While molecular dynamics simulations can provide information about short range effects, long range effects have to be treated with different simulation techniques. Glancing angle deposition (GLAD) is based on the long range self-shadowing, which appears when a vapor beam reaches a substrate at a highly oblique condition [1]. This leads to the growth of a highly porous thin film, composed of many free-standing nanostructures. For a realistic modeling of this shadowing effect very large numbers of particles and large cell dimensions are required. Handling this large number of particles is very computationally intensive, so that on-lattice simulations are a common tool. However, this ballistic growth process is highly sensitive to the geometrical correctness of the simulation. Tanto et al. [2] have shown, that a simple approach, using cubic particles on a cubic lattice, introduces significant errors to the results of such simulations. A deeper investigation of these effects and a discussion of their impact on the modeling of the GLAD process are presented. Further a 'work-around' is proposed, that nearly eliminates the presented effects while it not increases the computation time to much.

[1] J.M. Nieuwenhuizen, H.B. Haanstra, Philips Tech. Rev. 27 87 (1966).

[2] B. Tanto, C. F. Doiron, T.-M. Lu, Phys. Rev. E 83, 016703 (2011).

O 37.109 Tue 18:30 P2

**A comparison of evaporation and sputter glancing angle deposition** — ●XUBIN LU, CHRISTOPH GRÜNER, JENS BAUER, and BERND RAUSCHENBACH — Leibniz Institute of Surface Modification, Leipzig, Germany

It is well known, that different physical vapor deposition techniques lead to different micro structures of the deposited thin films. Particle energy and angular distribution during the process are the main factors influencing the growth behavior. While these parameters and their effects are well investigated for normal incidence deposition, the situation is much more unclear for oblique and glancing angle deposition (GLAD). Here the substrates normal and the incoming particle beam form a nearly right angle. This results in the growth of separated nanostructures, that form a porous thin film [1]. This process is mainly based on a self-shadowing effect between neighboring nucleation sites and later nanostructures. This self-shadowing during the growth is influenced by the divergence of the particle beam, while the shape of the individual nanostructures is sensitive to surface diffusion effects. A comparison of electron beam evaporation and sputter GLAD is shown, investigating growth speed and porosity of the film as well as size and tilt angle of the individual nanostructures.

[1] J.M. Nieuwenhuizen, H.B. Haanstra, Philips Tech. Rev. 27 87 (1966).

O 37.110 Tue 18:30 P2

**Structural and mechanical properties of graphene and polycrystalline carbon membranes** — ●MAXIMILIAN AMMON, YURI KOVAL, MICHAEL ENZELBERGER-HEIM, CHRISTIAN STEINER, and SABINE MAIER — Department of Physics, University of Erlangen-Nürnberg, Germany

Thin carbon membranes show interesting physical properties and are therefore promising materials for a variety of applications on the nano-scale ranging from chemical sensors to resonators. Here we discuss the structural and mechanical properties of two types of carbon membranes based on atomic force microscopy experiments in ambient condition. In one hand, we investigated the structure of electrochemically etched graphene membranes with an average graphene thickness of around 2-3 monolayers and a diameter of up to 30  $\mu\text{m}$ . The morphology of these membranes shows a strong buckling with apparent heights of several tens of nanometers, which can be quantifiably connected to the pre-stress of the graphene after the growth on SiC at high temperatures. [1] On the other hand we studied polycrystalline carbon membranes with thicknesses down to about 3 nm obtained by the graphitization of polymers after low-energy ion irradiation. We determined the stiffness and Young's-Modulus of such polycrystalline membranes by force distance spectroscopy.

[1] D. Waldmann et al. ACS Nano, 7, 5, 4441-4448 (2013).