

## DS 44: Postersession II

Time: Thursday 17:00–19:00

Location: P1C

DS 44.1 Thu 17:00 P1C

**Fascinating vanadium oxide nanostructured thin films for sensing applications** — ●MEGHA SINGH, PRABHAT KUMAR, and GADE B. REDDY — Thin Film Laboratory, Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016

Vanadium oxides (V-O) have enticed scientists and researchers due to their various properties offering wide optical band gap, good thermal and chemical stabilities. This makes oxides of vanadium, highly suitable, to be used in wide variety of devices applications including sensing. It is essential for any device to be employed in sensing applications to have high aspect ratio and surface area. We report the synthesis of vanadium oxide nanostructured thin films (NTFs) over wide area (400 mm<sup>2</sup>) using a novel technique plasma assisted sublimation process (PASP). Vanadium oxide NTFs were synthesized on glass substrates in N<sub>2</sub> plasma and N<sub>2</sub> gas. SEM micrographs show rod like morphology of microstructures with flake like nanostructures on the surface revealing very high surface area. HRTEM images of film revealed that flake like morphology as was observed in SEM, confirming results obtained on morphological studies. XRD and Raman spectroscopic studies confirm long range order in reduced V<sub>2</sub>O<sub>5</sub> (O/V ratio ~ 2.2) indicating structures are highly crystalline in nature. In absence of plasma, the crystallinity as well as surface morphology deteriorated, thereby indicating important role of plasma in microstructure, nanostructure as well as crystal structure of vanadium oxides NTFs with different stoichiometry. Hence, high surface area nanostructured thin films are obtained for sensing applications.

DS 44.2 Thu 17:00 P1C

**Plasma assisted synthesis of core-multishell nanostructured thin films** — ●PRABHAT KUMAR, MEGHA SINGH, and GADE B REDDY — Thin Film Laboratory, Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016

The ability to modify and tune the properties of core-multishell heterostructures nanoflakes (CMN) enables them to be used in wide range of applications. Firstly, we have carried out the sulfurization of MoO<sub>3</sub> nanostructured thin films using H<sub>2</sub>S/Ar plasma. XRD analysis shows that films after sulfurization have monoclinic MoO<sub>2</sub> and hexagonal MoS<sub>2</sub> phases. Maximum sulfurization is accomplished at 550°C in 60min. Core-shell was confirmed by the HR-TEM micrographs. XPS analysis shows that in all samples surface was completely sulfurized to form MoS<sub>2</sub> with good stoichiometry. From results, it was revealed that the depth of penetration of sulfur species in MoO<sub>3</sub>, converting it into MoS<sub>2</sub> increased with the increase in time and reduction of MoO<sub>3</sub> by hydrogen species was much more as compared to sulfur species. Secondly, core-shell heterostructures were treated in O<sub>2</sub> plasma for different durations of time. XRD and Raman analysis show that films after oxidation have MoO<sub>2</sub>, MoS<sub>2</sub> along with MoO<sub>3</sub>. HR-TEM micrographs revealed that nanoflake have acquired CMN. XPS analysis shows that surface consist of Mo oxidation states. The aim of this work is to achieve the appropriate growth conditions to obtain CMNs thin films on different substrates and to control their properties by using various reactive species environment of H<sub>2</sub>S/Ar and O<sub>2</sub> gas plasma.

DS 44.3 Thu 17:00 P1C

**Photo absorption of adsorbed azobenzene monolayers: impact of graphene substrate** — ●QIANG FU, CATERINA COCCHI, DMITRII NABOK, ANDRIS GULANS, and CLAUDIA DRAXL — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

To reveal the impact of a graphene substrate on the photo-absorption of azobenzene (AB), we investigate the optical spectra of both isolated and adsorbed AB monolayers within the framework of density-functional theory (DFT) and many-body perturbation theory (MBPT), as implemented in the full-potential all-electron code **exciting** [1]. In spite of weak hybridization, the optical excitations of AB monolayers are remarkably modulated. The excitation energies are affected via two counteracting mechanisms: Substrate polarization reduces the band-gap of the adsorbate, and enhanced dielectric screening weakens the attractive interaction between electrons and holes. The competition of the two effects give rise to a blueshift of peaks from intramolecular excitations and a redshift of peaks from intermolecular ones. Excitations corresponding to intermolecular electron-hole pairs,

which are dark in the isolated AB monolayers, are activated by the presence of graphene. Our results demonstrate that the photoswitching property of weakly adsorbed azobenzene undergoes notable changes on a carbon-based substrate.

[1] A. Gulans *et al.*, *J. Phys.: Condens. Matter* **26**, 363202 (2014).

DS 44.4 Thu 17:00 P1C

**Tuning excitons by 3D stacking of hexagonal boron nitride layers** — ●WAHIB AGGOUNE<sup>1,2</sup>, CATERINA COCCHI<sup>2</sup>, DMITRII NABOK<sup>2</sup>, KARIM REZOUALI<sup>1</sup>, MOHAMED AKLI BELKHIR<sup>1</sup>, and CLAUDIA DRAXL<sup>2</sup> — <sup>1</sup>Laboratoire de Physique Théorique, Faculté des sciences exactes, Université de Bejaia, 06000 Bejaia, Algérie — <sup>2</sup>Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

The opto-electronic properties of hexagonal boron-nitride (h-BN) are investigated from first principles, considering the five possible stacking arrangements obtained by translation of the two layers in the unit cell. We find the most stable structure in agreement with experiment [1] and with an earlier first-principles study [2]. All structures exhibit a quasi-particle gap, with values between 4.5 and 6 eV as calculated from the  $G_0W_0$  approach. From the solution of the two-particle Bethe-Salpeter equation an intense excitonic peak is found in the UV region for any stacking arrangement. Depending on the order of the h-BN layers, the lowest-energy excitation can be either bright or dark. We characterize the main optical excitations for all stacking arrangements and discuss them in the context of symmetry-induced selection rules. All calculations are performed using the **exciting** code [3], a full-potential all-electron package implementing the families of linearized augmented planewave methods.

[1] R. S. Pease, *Nature (London)* **165**, 722 (1950). [2] L. Liu *et al.*, *Phys. Rev. B* **68**, 104102 (2003). [3] A. Gulans *et al.*, *J. Phys. Condens. Matter.* **26**, 363202 (2014).

DS 44.5 Thu 17:00 P1C

**Diffusion in thin films** — ●MAX WOLFF<sup>1</sup>, GUNNAR PALSSON<sup>1</sup>, ANTON DEVISHVILI<sup>1</sup>, JOE DURA<sup>2</sup>, and BORIS TOPERVERG<sup>3</sup> — <sup>1</sup>Department for Physics and Astronomy, Uppsala University, Sweden — <sup>2</sup>National Institute for Standards and Technology, Gaithersburg, MD, USA — <sup>3</sup>Ruhr-University Bochum, Bochum, Germany

A surface imposes a singularity to materials, and with decreasing size of objects such as in nano-technology, they can dominate the physical properties. One apparent example of a surface effect is the reduction of the freezing temperature of ice in the surface layers, which allows skiing or skating on ice. Reflectometry is a powerful tool to explore interfaces and surfaces. More recently grazing incidence scattering techniques attracted more and more interest and in particular grazing incidence small angle scattering becomes more widely used to probe the interfacial structure of e.g. polymer systems. In the case of neutrons many studies suffer from limited incident flux. This applies even more for the case of neutron spectroscopy offering unique opportunities to probe dynamics in materials.

In this presentation the opportunities and challenges of grazing incidence neutron spectroscopy will be evaluated. Wave field enhancement in a potential well to access the study of dynamics in thin films and surfaces might be one possibility to overcome the limitations in neutron flux. The method will be discussed on the example of a thin film of vanadium loaded with hydrogen.

DS 44.6 Thu 17:00 P1C

**Particular electronic properties of F<sub>16</sub>CoPc: A decent electron acceptor material** — ●FLORIAN RÜCKERL, DANIEL WAAS, BERND BÜCHNER, and MARTIN KNUPFER — Leibniz Institute for Solid State and Materials Research Dresden, Institute for Solid State Research, Helmholtzstraße 20, D-01069 Dresden, Germany

Various interfaces with F<sub>16</sub>CoPc as one of the partners are characterized by a charge transfer across the interface and a concomitant reduction of the Co central atom in these molecules. We summarize recent photoemission spectroscopy results and compare those to the data from equivalent interfaces comprising F<sub>16</sub>CuPc. In the latter, the Cu center remains unchanged indicating the particular role of Co in F<sub>16</sub>CoPc as the electron accepting site.

DS 44.7 Thu 17:00 P1C

**Surface functionalization of WSe<sub>2</sub> by F<sub>16</sub>CoPc** — ●TOM KLAPROTH, FLORIAN RÜCKERL, ROMAN SCHUSTER, BERND BÜCHNER, and MARTIN KNUPFER — Leibniz Institute for Solid State and Materials Research Dresden, Institute for Solid State Research, Helmholtzstraße 20, D-01069 Dresden, Germany

We have investigated the electronic properties of WSe<sub>2</sub> surfaces covered by fluorinated cobalt phthalocyanine (F<sub>16</sub>CoPc) using photoemission spectroscopy. We show that a charge transfer occurs at this interface, which results in the creation of holes in the WSe<sub>2</sub> surface while the Co center of the phthalocyanine is reduced to Co(I). We observe a potential change in WSe<sub>2</sub> approaching the surface as a consequence of the induced positive charges near the surface. In addition, our data allow for a rough estimation of the induced charge density and suggest that the holes might be localized.

DS 44.8 Thu 17:00 P1C

**Infrared studies of device relevant interfaces - energetic and morphological insights** — ●SABINA HILLEBRANDT<sup>1,2</sup>, SEBASTIAN BECK<sup>1,2</sup>, and ANNEMARIE PUCCI<sup>1,2</sup> — <sup>1</sup>Kirchhoff-Institut für Physik, Universität Heidelberg, Germany — <sup>2</sup>Innovationlab GmbH, Heidelberg, Germany

Organic electronic devices consist of stacked organic as well as inorganic materials and the device performance is mainly influenced by the interfaces of the layers. The investigation of charge generation, injection and transport at these interfaces is a major key to the basic understanding of the fundamental mechanisms in organic electronics. We use interface layers of metal oxides, i.e. nickel oxide (NiO) or molybdenum oxide (MoO<sub>3</sub>), and self-assembled monolayers (SAM) to engineer the surface of certain electrode materials in order to improve charge transport at the inorganic/organic interface. With their inherent dipole SAMs can improve the energetic alignment at the interface. Polarization dependent infrared spectroscopic studies reveal the orientation of such SAMs as well as the influence of the interlayers on the orientation of the subsequent organic semiconductor material like fluorinated zinc phthalocyanine (F<sub>4</sub>ZnPc). Additionally, supported by density functional theory (DFT) calculations, charge transfer between the electrode material and the organic semiconductor can be investigated, giving a deep insight into the energetic and morphological properties at the interface.

DS 44.9 Thu 17:00 P1C

**Co-crystal formation and HOMO-LUMO coupling in mixtures of organic semiconductors. Diindenoperylene (DIP), sexithiophene (6T) as donors and hexafluorotetracyanonaphthoquinodimethane (F<sub>6</sub>TCNNQ) as acceptor.** — ●GIULIANO DUVA<sup>1</sup>, PAUL BEYER<sup>2</sup>, TINO MEISEL<sup>2</sup>, ANDREAS OPITZ<sup>2</sup>, ALEXANDER HINDERHOFER<sup>1</sup>, ALEXANDER GERLACH<sup>1</sup>, and FRANK SCHREIBER<sup>1</sup> — <sup>1</sup>Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen (Germany) — <sup>2</sup>Humboldt-Universität zu Berlin, Department of Physics, Berlin (Germany)

Donor:acceptor (D:A) blended films of organic semiconductors [1] represent a technologically relevant class of materials. Studying the structural and optical properties of the mixtures resulting upon co-evaporation is mandatory to control the parameters that govern the final performances of the device. Here we compare two D:A pairs, respectively DIP:F<sub>6</sub>TCNNQ and 6T:F<sub>6</sub>TCNNQ. We investigate their structure via X-ray scattering and find the formation of a D:A co-crystal exhibiting  $\pi$ - $\pi$  stacking of the molecular components. Such structure correlates with the appearance of several new, sub-bandgap electronic transitions at energies specific for each combination. We discuss several models for charge-transfer, in particular a Hückel-like model for molecular orbitals [2], in order to relate the HOMO-LUMO energies of the compounds in the blend to the newly observed transitions. [1] A. Hinderhofer et al. Chem. Phys. Chem. 13 (2012), p.628. [2] H. Méndez et al. Angew. Chem. Int. Ed. 52 (2013), p.7751.

DS 44.10 Thu 17:00 P1C

**Interface formation of Titanium and Tantalum thin films onto LiNbO<sub>3</sub>** — ●UWE VOGEL<sup>1</sup>, STEFFEN OSWALD<sup>2</sup>, THOMAS GEMMING<sup>3</sup>, and JÜRGEN ECKERT<sup>4</sup> — <sup>1</sup>Helmholtz-Zentrum Berlin / IFW Dresden / TU Dresden — <sup>2</sup>IFW Dresden — <sup>3</sup>IFW Dresden / TU Dresden — <sup>4</sup>ÖAW / IFW Dresden / TU Dresden

We present results of detailed chemical interface analyses of sputtered Tantalum and Titanium thin films as potential adhesion and barrier layers onto cleaned SAW-substrate material (LiNbO<sub>3</sub>) with respect to

their temporal (up to 24 h) and thermal stability up to 600°C in vacuum. The main technique for surface clean is a special Helium plasma, the analysis is done using AR-XPS.

DS 44.11 Thu 17:00 P1C

**Photo-induced effects in hole-doped La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub> (0 < x ≤ 0.1) films probed by Raman spectroscopy** — ●CHRISTOPH MEYER, SEBASTIAN MERTEN, BERND DAMASCHKE, and VASILY MOSHNYAGA — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Perovskite manganite La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub> (LSMO) displays a variety of structural, electric and magnetic phases with different types of crystallographic distortions, e.g. the Jahn-Teller effect, manifesting themselves in colossal magnetoresistance effect and insulator-metal transition. To monitor and to disentangle the influence of light, temperature and doping on the structure, we grew series of hole-doped LSMO (0 < x ≤ 0.3) epitaxial thin films on LaAlO<sub>3</sub> (100) and MgO (100) substrates by metalorganic aerosol deposition and probed them by polarization-dependent Raman spectroscopy. The Raman spectra were studied as a function of the Sr content, temperature and laser power to determine a photo-induced effect. The emergence of the metallic phase, marked by the Raman mode at ~ 430 cm<sup>-1</sup> and a simultaneous suppression of the Jahn-Teller bands at ~ 510 cm<sup>-1</sup> and ~ 630 cm<sup>-1</sup> by increasing the laser power for the insulating LSMO films with 0 < x ≤ 0.1 was observed. The results are rationalized as a photo-induced shift towards metallic phase, equivalent to the increase of Sr-doping x > 0.15 in the LSMO phase diagram. Financial support by the DFG via project SFB 1073/B04 is gratefully acknowledged.

DS 44.12 Thu 17:00 P1C

**Defect induced photoluminescence of tungsten di-sulfide monolayers** — ●ASWIN ASAITHAMBI<sup>1</sup>, ROLAND KOZUBEK<sup>1</sup>, GUENTHER PRINZ<sup>1</sup>, FRANCESCO REALE<sup>2</sup>, CECILIA MATTEVI<sup>2</sup>, MARIKA SCHLEBERGER<sup>1</sup>, and AXEL LORKE<sup>1</sup> — <sup>1</sup>Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany — <sup>2</sup>Department of Materials, Imperial College London, London, UK

The intriguing electronic properties of graphene have renewed the interest in other 2D materials such as transition metal di-chalcogenides (TMDCs) monolayers. TMDCs, similar to graphite, have a layered structure with an indirect bandgap which becomes direct when only a monolayer is present. This leads to strongly enhanced photoluminescence (PL). However, unavoidable defects affect the opto-electronic properties of TMDC monolayers drastically, which makes it necessary to study and characterize their optical related properties.

In this contribution, we present highly sensitive, non-destructive, temperature and power dependent PL measurements to study the defects present in tungsten di-sulfide (WS<sub>2</sub>) monolayers. For this purpose, pristine samples of WS<sub>2</sub> were irradiated with Xe<sup>30+</sup> ions to additionally create defects in the monolayers. Low temperature spectra of pristine samples show two different peaks associated with free and defect-bound exciton recombinations. For higher temperature or power, only the free exciton recombinations dominate the spectrum. For the different defect densities created in the monolayers, we observed changes in the PL spectrum with regard to intensity and FWHM, which will be discussed and compared to data published in literature.

DS 44.13 Thu 17:00 P1C

**Growth of oxide microstructures by metalorganic aerosol deposition technique** — ●PHILIPP KSOLL, HANNES GÖDECKE, CHRISTOPH MEYER, MARIUS KEUNECKE, and VASILY MOSHNYAGA — I. Physikalisches Institut Göttingen, 37077 Göttingen, Friedrich-Hund-Platz 1

Microstructuring of thin films, usually processed by different lithography tools, is a crucial step for various device applications, e.g. semiconducting electronics, spintronics, photonics, etc. Metalorganic aerosol deposition (MAD) has been shown to be effective technique to grow complex oxide films of high quality. To avoid the complex oxide lithography we developed a MAD method to grow oxide microstructures with a line width down to 1  $\mu$ m. Recent material realizations include single, e.g. CuO<sub>x</sub>, and complex oxides, i.e. manganites La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub>. The microstructures were characterized by different types of microscopies, like Raman, atomic force, scanning electron and energy dispersion x-ray analysis. Financial support by the DFG via SFB 1073 (TP B04) is acknowledged.

DS 44.14 Thu 17:00 P1C

**Relation of sample stoichiometry and growth conditions in SrCoO<sub>3-δ</sub> thin films** — ●PATRICK SCHÖFFMANN<sup>1</sup>, SABINE PÜTTER<sup>1</sup>, JÜRGEN SCHUBERT<sup>2</sup>, WILLI ZANDER<sup>2</sup>, RÉNE HELLER<sup>3</sup>, MARKUS WASCHK<sup>4</sup>, PAUL ZAKALEK<sup>4</sup>, and THOMAS BRÜCKEL<sup>4</sup> — <sup>1</sup>Jülich Centre for Neutron Science (JCNS) am Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Garching — <sup>2</sup>Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich GmbH — <sup>3</sup>Helmholtz-Zentrum Dresden-Rossendorf — <sup>4</sup>Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH

Strontium cobaltite (SrCoO<sub>3-δ</sub>) exists in two topotactic phases, depending on the oxygen content. SrCoO<sub>3</sub> is a ferromagnetic metal (T<sub>C</sub>=305K) with perovskite structure while SrCoO<sub>2.5</sub> is an antiferromagnetic insulator (T<sub>N</sub>=570K) with brownmillerite structure.[1]

We aim at growing thin films of SrCoO<sub>3-δ</sub> via molecular beam epitaxy, and thus investigate the influence of growth conditions like the elemental deposition rate of Sr and Co, substrate temperature and oxygen pressure on the sample stoichiometry and surface topography.

For this, we employ in-situ electron diffraction to monitor the sample growth and ex-situ X-ray reflectometry and atomic force microscopy to investigate the structural properties. The stoichiometry is determined by Rutherford backscattering spectrometry.

We provide a comprehensive overview of the samples addressing the requirements to achieve a Sr:Co stoichiometry of 1:1.

[1]C.K. Xie et al., Appl. Phys. Lett 99, 052503 (2011)

DS 44.15 Thu 17:00 P1C

**Large area graphene on silicon by carbon ion implantation in copper and subsequent transfer** — ●JAN LEHNERT<sup>1</sup>, DANIEL SPEMANN<sup>1</sup>, STEPHAN MÄNDL<sup>1</sup>, HAMZA HATAHET<sup>1</sup>, ARON VARGA<sup>1</sup>, and BERND RAUSCHENBACH<sup>1,2</sup> — <sup>1</sup>Leibniz Institute of Surface Modification (IOM), Leipzig, Germany — <sup>2</sup>Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany

Despite of many research efforts on graphene it still attracts much interest due to its promising properties. Especially for practical applications it is necessary to produce large area and high quality graphene films which is still a challenge. In this work we present a synthesis method by use of ion beam implantation, annealing and subsequent transfer. Cu foils (cm in size) which were pre-annealed at 950 °C for 2h and analysed by SEM, AFM, XRD and XPS measurements before and after annealing have been implanted with 35 keV carbon ions with a fluence of  $1 \times 10^{16} \text{ cm}^{-2}$  at room temperature and subsequently annealed at 850 °C for 2h to form graphene layers on the Cu surface. Afterwards, the graphene was transferred to a SiO<sub>2</sub>/Si substrate by a PMMA free chemical etching process in which the Cu foils were removed by exposure to a mixture of iron(III) chloride (FeCl<sub>3</sub>) and hydrochloric acid (HCl). Raman spectroscopy at room temperature after the transfer show nearly defect-free monolayer graphene. Furthermore, SEM and AFM measurements were performed to investigate the size and quality of the synthesised graphene. No graphene was observed on unimplanted samples that were treated with the same annealing procedure.

DS 44.16 Thu 17:00 P1C

**Morphology and adsorption of organic thin films on MgO/Ag(100)** — ●SABRINA PECHMANN, DANIEL SCHULTHEISS, and RAINER H. FINK — Physical Chemistry II, FAU Erlangen-Nuremberg, Erlangen, Germany

Over recent years a vast field of new technological applications for organic thin films on defined and tunable metal-oxide surfaces has gained increasing attention. These systems allow investigation by various electron or photon based techniques, which would be impossible for bulk metal-oxides due to potential charging. Epitaxial MgO/Ag(100) was chosen as model system, as both bulk structures exhibit a comparatively small lattice mismatch [1], which reduces the amount of defects. Growth could be observed in-situ by LEEM, stoichiometry and thin film properties were checked by XPS and LEED-IV. It could be shown, that MgO can be modified by electrons and photons, enabling to tune the surface properties. The MgO surface serves as substrate for semiconducting organic molecules with large, extended pi-systems. For our studies cobalt (II) octaethylporphyrin, its free base equivalent, PTCDA and dihexylquaterthiophene were chosen, as all those systems grow in different, highly ordered manners. Therefore their long-range ordered superstructure could be determined by LEED, whereas NEXAFS dichroism offered insight into the molecular orientation. Further-

more, it was possible to metalize octaethylporphyrin by the underlying magnesium [2]. This work is funded by the funCOS research unit (FOR 1878, DFG). [1] Valeri, S. et al., Surf. Sci. 507-510, 311-317, 2002 [2] Schneider, J. et al., Chem. Eur. J. 22, 1744-1749, 2016

DS 44.17 Thu 17:00 P1C

**Electrical Characterization of Silver Thin Films for Optimization of Low-Emissivity Glass-Coatings** — ●JULIAN MERTENS, ROLAND SITTNER, and MATTHIAS WUTTIG — 1. Physikalisches Institut A, RWTH Aachen

The increasing use of large window areas in modern architecture makes the improvement of efficient low-emissivity coatings indispensable. Therefore the key property to optimize transparent thin film layer stacks used for glass coatings is given by the infrared reflectance. As the infrared reflectance of the corresponding thin film is directly linked to the goodness of electrical conductivity, it is mandatory to gain an understanding of the dominant scattering mechanisms in metallic thin films that dominate conductivity. Due to its lowest bulk-resistivity, silver is the element of choice. To improve the infrared reflectance of silver thin films different layer systems were used and improved over the last twenty years. However, it is still not understood what kind of scattering mechanisms are responsible for the huge increase of specific sheet resistance as the layer thickness decreases. Mayadas and Shatzkes developed a theory which combines diffusive interface scattering, as well as electron scattering at grain boundaries in a total picture, which makes it possible to distinguish between both scattering mechanisms. To apply this approach, the resistivity of thin silver films, deposited on different seed-layers by DC Magnetron Sputter Deposition, is fitted to said theory. The results enable to separate both scattering mechanisms and help to improve the development of layer stack optimization methods.

DS 44.18 Thu 17:00 P1C

**Recombination prefactor in organic bulk heterojunction solar cells** — ●JĘDRZEJ SZMYTKOWSKI — Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Gdańsk, Poland

In this work, we report on theoretical studies of reduced bimolecular recombination in organic donor-acceptor bulk heterojunction structures. The values of the Langevin recombination prefactor have been calculated as a function of several quantities, including temperature, external electric field and charge carrier concentration. In addition, an effect of exciton-charge carrier interaction has been taken into account to describe changes of this prefactor. We have also investigated an influence of disorder on the nongeminate recombination in organic systems with an exponential density of states. Presented results can explain mechanisms which cause a loss of photocurrent in organic solar cells.

DS 44.19 Thu 17:00 P1C

**Self-Assembly of Di-lithium Phthalocyanine on Different Surfaces** — ●NHUNG N.T.T.<sup>1,3</sup>, LARS S.<sup>2</sup>, HA N.T.N.<sup>2</sup>, and MICHAEL H.<sup>2</sup> — <sup>1</sup>IFW Dresden — <sup>2</sup>TU-Chemnitz — <sup>3</sup>Duy Tan University, Vietnam

Metal phthalocyanines (MPc) behave as semiconductors in their pure form. Therefore doping MPc thin films by oxidizing the ligands and creating an open shell can considerably increase their electrical conductivity [1-2]. These doped organic thin films may play an crucial role in developing new effective materials for nano-devices like insulator-metal-insulator transistor [3] or light emitting devices [4].

In addition, self-assembly structures of di-lithium phthalocyanine (Li2Pc), which have been used as electrolyte in an all-solid state electrochemical cell, lead to a pronounced electric field dependence of the lithium ion transport in channel formation process [5].

Here the self-assembly of Li2Pc on different crystalline surfaces will be investigated by means of scanning tunneling microscopy (STM) in ultra-high vacuum. In the first part Li2Pc is grown by organic molecular beam deposition (OMBD) on Au(111) surface to prepare a crystalline thin film. To get more information on the adsorption process, a small amount of this molecule has been doped at the F16CoPc thin films on Au(111) and HOPG substrates. STM results collected at low temperatures as well as molecular manipulating of Li2Pc by applying voltage pulses to the STM tip illustrate the deposition behavior of Li2Pc. All of the research was performed in TU-Chemnitz.

DS 44.20 Thu 17:00 P1C

**Microstructure and Stress Gradients in Diamond Films Revealed by Cross section X-ray nanodiffraction** — ●NICOLAS WÖHRL<sup>1</sup>, HADWIG STERNSCHULTE<sup>2</sup>, MANFRED BURGHAMMER<sup>3</sup>, JU-

RAJ TODT<sup>4</sup>, and JOZEF KECKES<sup>4</sup> — <sup>1</sup>Faculty of Physics and CENIDE, University of Duisburg- Essen, Lotharstr. 1, 47057 Duisburg, Germany — <sup>2</sup>Hochschule Augsburg, Fakultät für Allgemeinwissenschaften, Augsburg, Germany — <sup>3</sup>ESRF, Grenoble, France — <sup>4</sup>Erich Schmidt Institut and Montanuniversität Leoben, Leoben, Austria

Ultrananocrystalline diamond (UNCD) films consist of small randomly oriented diamond grains embedded in an amorphous C:H matrix. Usually, the grain size is determined by X-ray diffraction (XRD) or transmission electron microscopy revealing information only from the total UNCD film or only locally from selected areas with low statistics, respectively. In this work we present the first cross section X-ray nanodiffraction study of diamond multi-layers with varying grain size from microcrystalline to UNCD. For the cross section study the samples have been cut in thin slices by FIB. The X-ray nanodiffraction was performed in transmission geometry at the ESRF in Grenoble using X-ray beam of 30nm in a diameter adjusted parallel to the Diamond-Si interface and the sample scanned in steps from the interface to the growth surface. The 2D XRD patterns recorded by a CCD detector were used to evaluate depth gradients of texture, grain sizes and residual stress in the diamond crystals. The results show complex gradients of microstructure and stresses. [1] J. Keckes et al., Scripta Materialia 67 (2012) 748

DS 44.21 Thu 17:00 P1C

**In-depth analysis of nanomorphology in thin films of 6,13-dihydro-6,13-diazapentacene** — •XIAOYAN DU<sup>1</sup>, LISA MÜLLER<sup>2</sup>, NICOLAI BURZLAFF<sup>2</sup>, and RAINER H. FINK<sup>1</sup> — <sup>1</sup>Physical Chemistry 2 and ICMM Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) Egerlandstr. 3, 91058 Erlangen, Germany — <sup>2</sup>Inorganic Chemistry, Department of Chemistry and Pharmacy Friedrich-Alexander-University Erlangen-Nuremberg Egerlandstr. 1, 91058 Erlangen, Germany

6,13-Dihydro-6,13-diazapentacene (DHDAP) is one of the important pentacene derivatives due to its ability to be easily derivatized, or its environmental stability and its solubility. The performance of organic field-effect transistors (OFETs) based on DHDAP has been found to be extremely sensitive to the substrates nature and temperature, which induces different polymorphs. We employ several complementary microspectroscopic probes to investigate the structure of thermally evaporated films evaporated at different conditions. Detailed analysis of atomic force microscopy (AFM), scanning transmission X-ray microscopy (STXM) and resonant soft X-ray scattering (RSOXS) reveals the dependence of the crystalline domain size on the film preparation conditions. Angle-resolved near edge x-ray absorption fine structure (NEXAFS) spectroscopy sheds lights on the molecular orientation of the molecules close to the substrates. Thus, the structure-property relations offer further insights into the transport properties of the respective OFETs devices. This work is funded by the DFG within GRK 1896.

DS 44.22 Thu 17:00 P1C

**Epitaxial thin films of the high-*k* dielectric SrZrO<sub>3</sub>** — •CORINNA MÜLLER, PATRICK SALG, ALDIN RADETINAC, PHILIPP KOMISSINSKIY, and LAMBERT ALFF — Technische Universität Darmstadt, Germany

SrZrO<sub>3</sub> has an orthorhombic perovskite crystal structure with a pseudocubic lattice constant of 4.101 Å, a high-*k* dielectric constant (~ 22), a large optical bandgap (~ 5.8 eV), and a low oxygen diffusion constant of 10<sup>-12</sup> cm<sup>2</sup>s<sup>-1</sup> [1,2]. We have investigated the growth of SrZrO<sub>3</sub> thin films fabricated by pulsed laser deposition onto GdScO<sub>3</sub> substrates at a substrate temperature of 630-700 °C, laser fluence of 0.32-0.98 J/cm<sup>2</sup>, and oxygen partial pressure below 10<sup>-8</sup> Torr. X-ray diffraction measurements reveal that the crystal structure of SrZrO<sub>3</sub> is rather stable against variation of the growth parameters. The 20-70 nm thick films are relaxed and show lattice parameters close to the SrZrO<sub>3</sub> bulk values. It is investigated how the Sr:Zr cation stoichiometry of the films depends on laser fluence which is important as Sr and Zr vacancies act as acceptor defects [2].

[1] P. A. Langjahr *et al.*, Mater. Res. Soc. Symp. Proc. **401**, 109 (1996). [2] L. Weston *et al.*, Phys. Rev. B **89**, 184109 (2014).

DS 44.23 Thu 17:00 P1C

**Dopant-Drift in Organic Semiconductors in Dependence of Different Parameters** — •SEON-YOUNG RHIM<sup>1,3</sup>, LARS MÜLLER<sup>1,2,3</sup>, VIPILAN SIVANESAN<sup>1,3</sup>, DONGXIANG WANG<sup>1</sup>, JAKOB BERNHARDT<sup>1,3</sup>, and WOLFGANG KOWALSKY<sup>1,2,3</sup> — <sup>1</sup>InnovationLab Heidelberg — <sup>2</sup>Institute for High-Frequency Technology, TU Braun-

schweig — <sup>3</sup>Kirchhoff Institute for Physics, Heidelberg University

The increase in the electrical conductivity of organic semiconductors by doping enables the fabrication of organic electronic devices with high performance. We show that besides the already known dopant diffusion due to a concentration gradient, the dopants are subject to a drift caused by certain operating conditions. In this study we use I(V)-Curve measurements, optical microscopy and spatially resolved infrared spectroscopy for the investigation of the dopant movement. For the device preparation different solution-processable organic hole conducting host-materials as Poly(3-hexylthiophen-2,5-diyl) (P3HT) and p-dopants as 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ) were utilized. In dependence of the applied voltage and respective current we observe the formation of an undoped region which we analyze in terms of dopant concentration and other operational parameters. Furthermore we compare the conventional doping in solution to the recently applied sequential doping method. The spatial control of the doped and undoped region within an organic semiconductor can be used to produce passive electronic devices with simple structures. As example we introduce a passive resistor and a non-volatile memory device.

DS 44.24 Thu 17:00 P1C

**Perforation of CVD silicon nitride by AgAl alloy formation** — •KATHARINA KRÜGEL, TOBIAS URBAN, and JOHANNES HEITMANN — Institut für Angewandte Physik, TU Bergakademie Freiberg, Freiberg, Germany

The alloying of Al and Ag on dielectric silicon nitride layer (Si<sub>3</sub>N<sub>4</sub>), deposited by Chemical Vapor Deposition on <100> Silicon substrates, was investigated. Ag and Al were deposited in variable proportions with overall thickness of 1 μm by Physical Vapor Deposition on the Si-substrate with Si<sub>3</sub>N<sub>4</sub> layers of 80 and 100 nm thickness. This setup is similar to industrial photovoltaic application.

The samples were tempered with Rapid Temperature Processing up to 1000 °C. By microscopy square-shaped hollows within the metal layer for annealing temperatures higher than 800 °C were shown. By preparation of a Focused Ion Beam-cut and following Scanning Electron Microscope investigation a local perforation of the Si<sub>3</sub>N<sub>4</sub> layer was observed. Below this region a pyramidal etching spike is formed with an angle of 52.3° which is equal to the angle between the <100> and <111> plane. These spikes were filled with an intermetallic phase consisting of fcc AgAl- and hcp Ag<sub>2</sub>Al-phase with local silicon precipitations. The formation of this etching pits can be proven by resistance measurement between metal and silicon. With increasing temperature an electrical contact was formed due to the local etching of the dielectric layer.

Usually Si<sub>3</sub>N<sub>4</sub> has a high chemical and thermal stability. For the first time an etching of the passivation layer only by AgAl was observed.

DS 44.25 Thu 17:00 P1C

**Ti<sub>2</sub>AlN and Ti<sub>2</sub>AlC MAX-phase synthesis by multilayered PVD coatings** — •FRANK BURMEISTER<sup>1</sup>, LUKAS GRÖNER<sup>1</sup>, EBERHARD NOLD<sup>1</sup>, EDUART REISACHER<sup>1</sup>, FRANCESCO COLONNA<sup>2</sup>, ALEXANDER FROMM<sup>1</sup>, FRANK MEYER<sup>1</sup>, and CHRIS EBERL<sup>1</sup> — <sup>1</sup>Fraunhofer IWM, Freiburg, Deutschland — <sup>2</sup>Freiburger Materialforschungszentrum, Freiburg, Deutschland

Mn+1AX<sub>n</sub> phases belong to a group of ternary nitrides or carbides, where M denotes an early transition metal, A denotes mostly a group III or IVA element and X is either nitrogen or carbon. Due to the presence of strong covalent MX bonds and weak ionic MA bonds, these materials often exhibit a high corrosion resistance as well as good electrical conductivity and thermal stability. The phase synthesis and their suitability for industrial applications, e.g. as protective and/or conductive coatings has been studied for crystalline films by others. However, these properties are strongly influenced by the material's microstructure and phase composition. To investigate the evolving microstructure of polycrystalline Ti<sub>2</sub>AlN and Ti<sub>2</sub>AlC coatings, AlN-Ti and Al-TiC multilayers were deposited by reactive sputtering using either nitrogen or methane as reactive gases, followed by a subsequent annealing step at 700 °C in vacuum. In this way, coatings with a dominant M<sub>2</sub>AX-phase component were synthesized successfully. The coating's properties were examined by elemental and phase analysis using XPS, XRD and Raman spectroscopy. The investigations revealed a prominent texture in the coating's microstructure which was ascribed to the multilayered deposition.

DS 44.26 Thu 17:00 P1C

**Effects of Molecular Orientation in Acceptor-Donor Inter-**

**faces between Pentacene and C<sub>60</sub> and Diels-Alder Adduct Formation at the Molecular Interface** — ●TOBIAS BREUER, ANDREA KARTHÄUSER, and GREGOR WITTE — Philipps-Universität Marburg, Germany

Interfaces between pentacene and Buckminster-Fullerene (C<sub>60</sub>) have attracted interest due to their application as oligomeric acceptor/donor model system for organic solar cells. As the actual device characteristics in such implementations are crucially controlled by the interface structure, detailed investigations of this interface on a molecular level are mandatory. In this study we analyze the influence of the orientation of the pentacene molecules in highly-ordered crystalline bottom layers on the characteristics of such internal interfaces. We show that the interface structure is driven by temperature-controlled diffusion of C<sub>60</sub> molecules to the pentacene step-edges in the case of uprightly-oriented pentacene. For lying pentacene in the bottom layer, no step-edge decoration is observed while the wetting of the pentacene layer is enhanced. Furthermore, the stability of the interface against intercalation and re-orientation has been analyzed by means of NEXAFS spectroscopy, showing that the orientation of the pentacene molecules at the interface remains unchanged. Instead, we observe strong indication for chemical modification of the molecular entities by the formation of Diels-Alder adducts between C<sub>60</sub> and pentacene.

[1] T. Breuer et al., *Adv. Mater. Interfaces*, 3, 1500452 (2016).

DS 44.27 Thu 17:00 P1C

**Combinatorial research on thin film Bi-W-Mo-O-N electrocatalysts for solar water splitting** — ●MONA SCHERBECK<sup>1</sup>, RAMONA GUTKOWSKI<sup>2</sup>, WOLFGANG SCHUHMAN<sup>2,3</sup>, and ALFRED SCHUHMAN<sup>1,3</sup> — <sup>1</sup>Chair for MEMS Materials, Institute for Materials, Ruhr-Universität Bochum, Universitätsstraße 150, D-44780 Bochum, Germany — <sup>2</sup>Analytical Chemistry-Center for Electrochemical Sciences (CES) — <sup>3</sup>Materials Research Department, Ruhr-Universität Bochum, Universitätsstraße 150, D-44780 Bochum, Germany

The discovery of novel photoabsorbers for solar water splitting with improved properties e.g. photocorrosion resistance, high photocurrents and photovoltages is an important topic. In this contribution, results on Bi-W-Mo-O-N n-type photoelectrodes synthesized by combinatorial reactive magnetron co-sputtering are presented. The material libraries were deposited by varying the sputtering parameters e.g. reactive gas flow, sputtering pressure and temperature to identify dependencies of sputtering parameters on the properties of the thin film material libraries. To further characterize the properties of the material libraries the crystal structure, composition, optical properties, and photoelectrochemical performance were measured with high-throughput methods. The functional properties of these material libraries are correlated to their structure, composition, and processing in phase diagrams.

DS 44.28 Thu 17:00 P1C

**The novel Kiel high flux X-ray diffractometer for heavy loads and with focusing option** — ●FINN CHRISTIANSEN, JOCHIM STETTNER, and OLAF MAGNUSSEN — Institut für experimentelle und angewandte Physik Kiel, Universität Kiel

We present a novel X-ray diffractometer, installed at the Kiel rotating anode microfocus X-ray lab source, which is characterized by a flexible and massive design of all components and high X-ray flux. The instrument is especially dedicated for in-situ investigations of solid surfaces, solid-solid and liquid-solid interfaces in complex sample environments (e.g. vacuum and plasma chambers up to 250 kg). Additionally, the diffractometer provides a vertical focusing option for spatially resolved measurements, microcrystals and measurements under grazing incidence with enhanced flux on the sample.

Two different modes are available: In the "high flux mode" a Multilayer Montel mirror provides a vertically and horizontally collimated beam with a diameter of  $\approx 2$  mm with  $4.3 \cdot 10^8$  Ph/s. The white beam background and CuK $\beta$  contributions are strongly suppressed. In the "vertical focusing mode", an additional multilayer mirror, located close to the sample, reduces the spot size at the sample position to  $2(h) \times 0.1(v)$  mm<sup>2</sup>.

Key parameters for both operational modes like flux, resolution and spot size at the sample position were determined quantitatively. Additionally, we present first X-ray data of model systems, e.g. ZnO surfaces and microcrystals in order to demonstrate the performance of this instrument.

DS 44.29 Thu 17:00 P1C

**Influence of Microstructure on the Amorphous to Crystalline Phase Transition in the Phase-Change Material GST124**

— ●CARL-FRIEDRICH SCHÖN, NIKITA POLIN, MATTHIAS M. DÜCK, CHRISTOPH PERSCH, and MATTHIAS WUTTIG — I. Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany

Phase-change materials (PCM) are a promising candidate for universal memory, as their optical reflectivity and electrical resistivity change considerably along the nanosecond scale transition between the amorphous and the crystalline state. Because this phase transition is the foundation of device functionality, significant effort has been devoted to its understanding. The microstructure of PCM thin films has been found to heavily impact the properties of the phase transition in GST124. While the investigation of microstructural defects is not relevant for application, it might yield new insights into the fundamental mechanisms of the phase transition.

In this work, the microstructure of GST124 thin films is varied and characterized utilizing x-ray reflectivity (XRR) and scanning electron microscopy (SEM). The effects of the microstructure on the film's properties are then measured by x-ray diffraction (XRD), while the phase transition is investigated with a laser setup featuring a high and low power laser combination, enabling the measurement of the materials reflectivity during crystallization. A higher gas pressure causes an increased incorporation of voids as well as an increased minimum energy to crystallize the sample. This energy shift can be attributed to the change of microstructure, as subsidiary effects can be excluded.

DS 44.30 Thu 17:00 P1C

**Texture Optimization and Structure-Property Relationships in Chalcogenide Thin Films** — ●MATTHIAS MAXIMILIAN DÜCK, STEFAN JAKOBS, TOBIAS SCHÄFER, CAROLIN JACOBI, FELIX LANGE, and MATTHIAS WUTTIG — I. Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany

Chalcogenides along the pseudobinary line between GeTe and Sb<sub>2</sub>Te<sub>3</sub> are currently gaining much attention, since a number of interesting properties can be attributed to certain members of that material group. Amongst these compounds, phase-change materials, thermoelectric materials, topological insulators and superconductors are found. Especially for the latter two, a large correlation between functionality and film quality has been observed. With the incorporation of a new sputter setup in a UHV cluster tool featuring a variety of analytic capabilities, access to a large parameter space for the deposition of chalcogenide systems was gained. This allows to push the boundaries in terms of film quality achieved in the sputter process. That way, a compromise between the strengths of MBE (film quality) and sputter deposition (industrial relevance) is found. This study focuses on the optimization of phase-change material thin films with respect to film quality and texture. The films are thoroughly characterized by a variety of methods, enabling the detailed investigation of film quality, texture and structure-property relationships.

DS 44.31 Thu 17:00 P1C

**On the Role of the Interface on the Growth of a Stabilized Bilayer Framework System** — ●ALEXANDER MÄNZ, MICHAEL KOTHE, and GREGOR WITTE — Molekulare Festkörperphysik, Fachbereich Physik, Philipps-Universität Marburg, Renthof 7, 35032 Marburg

The nonplanar,  $\pi$ -conjugated PAH titanyl-phthalocyanine (TiOPc) is known for exceptional optical and electronic properties. To utilize and optimize TiOPc based thin film devices a detailed understanding of interface related growth is of great importance. This study links characteristics of initial growth of the TiOPc bilayer framework, deposited via organic molecular beam deposition (OMBD) with the morphology of TiOPc multilayer systems on various substrates. In a first step, the molecular arrangement of TiOPc on Au(111) and Ag(111) substrates from monolayer to multilayer regime is characterized by scanning tunneling microscopy (STM). Consecutively, we analyze the morphology and crystallinity of TiOPc multilayers by means of atomic force microscopy (AFM) and X-ray diffraction (XRD). After completion of the first bilayer on Au and Ag substrates, dewetting leads to formation of separated islands with height of multiples of the bilayer, which are stabilized by the alternating orientation of the titanyl units. Comparative analyses for thin films grown on KCl and HOPG substrates show a similar behaviour, while somewhat different polymorphs were identified in thicker films.

DS 44.32 Thu 17:00 P1C

**Development of a new method to probe the electronic structure of organic photovoltaic materials in a bulk heterojunction** — ●VINCENT LAMI<sup>1,2</sup>, PAUL E. HOPKINSON<sup>1,2</sup>, and YANA

VAYNZOF<sup>1,2</sup> — <sup>1</sup>Kirchhoff Institute for Physics, Heidelberg University, Germany — <sup>2</sup>Centre for Advanced Materials, Heidelberg University, Germany

Organic photovoltaic (OPV) cells have attracted remarkable interest as a possible alternative to conventional inorganic technologies. The performance of an OPV device is largely determined by the alignment of the electronic energy levels of its individual components. Despite the importance of energetics, the understanding of the energy level evolution within the device is still limited. Consequently, energy level diagrams of OPVs are typically constructed by measuring the energy levels of the individual materials, without taking into account the interactions between them. Herein, we demonstrate the development of a new experimental technique based on ultra-violet photoemission spectroscopy that allows us to measure the progression of both the energy levels and material composition within the photovoltaic active layer. Our preliminary results obtained on a variety of organic materials are very promising and demonstrate the effectiveness of our new technique.

DS 44.33 Thu 17:00 P1C

**Morphological studies of Squaraine-Fullerene blend films** — ●ANGELIKA MADERITSCH<sup>1</sup>, OLIYA SADRILLAIEVNA ABDULLAEVA<sup>1</sup>, MATTHIAS SCHULZ<sup>2</sup>, ARNE LÜTZEN<sup>2</sup>, JÜRGEN PARISI<sup>1</sup>, and MANUELA SCHIEK<sup>1</sup> — <sup>1</sup>Energy and Semiconductor Research Laboratory, Institute of Physics, University of Oldenburg, Germany — <sup>2</sup>Kekulé Institute of Organic Chemistry and Biochemistry, Rheinische-Friedrich-Wilhelms-University of Bonn, Germany

Organic photoelectric materials are promising candidates for the development of biocompatible artificial photoreceptors. Currently, we are investigating a photoactive layer consisting of an anilino-squaraine donor (SQIB), a small molecular model organic semiconductor, blended with a fullerene acceptor (PCBM). After annealing at high temperatures the crystalline film shows two distinct structural motifs with different properties.<sup>1</sup> SEM and TEM are applied to gain a deeper insight to the morphology of the photoactive layer. TEM samples are prepared via floating and FIB-milling providing cross section lamellae. The predominant structure (platelets) shows a rather flat surface partly with elongated pinholes and borders between different crystalline orientations. The discontinuously localised second structure (ferns) is less homogeneous and significantly rougher. Voids between ferns seem to consist of very thin PCBM film. The results are compared to those of other methods like AFM, XRD and optical microscopy.

(1) Abdullaeva et al., Langmuir 2016 32 (33), 8533-8542, DOI:10.1021/acs.langmuir.6b02085

DS 44.34 Thu 17:00 P1C

**Investigation of Disorder Related Electrical Properties in the Pseudo-Binary Line SnTe-PbTe** — ●JOHANNES REINDL<sup>1</sup>, ALEXANDER ROCHOTZKI<sup>1</sup>, ZHENG ZHEN<sup>1</sup>, STEFAN JAKOBS<sup>1</sup>, and MATTHIAS WUTTIG<sup>1,2</sup> — <sup>1</sup>Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — <sup>2</sup>JARA-FIT, RWTH Aachen University, 52056 Aachen, Germany

The solid solutions of the chalcogenides SnTe and PbTe have been thoroughly investigated in the past under the premise of infrared applications, which exploit the small band gap that can be tuned with stoichiometry [1]. Of additional interest is the shift from p-type conduction in SnTe to n-type conduction of PbTe that can be described with a band inversion in SnTe and the crossing of the bands at a specific composition of the alloys [1]. In recent years the investigation of topological insulator states has led to the insight that topology is pivotal in this material system and thus SnTe single crystals have been found to be topological crystalline insulators [2].

For industrial applications of the aforementioned effects it would be beneficial to shift from physical vapor deposition fabrication of single crystals to large scale production processes, like sputtering. However, the unique physical properties might get lost due to the formation of structural defects. This general increase of disorder and the subsequent influence on some key electrical properties will be investigated, with special focus on the region of the band crossing.

[1] Dimmock, J. O. et al., Phys. Rev. Lett. 16, 1193 (1966)

[2] Xu, S.-Y. et al., Nat. Commun. 3, 1192 (2012)

DS 44.35 Thu 17:00 P1C

**Surface reconstruction in STO: Experimental and theoretical optical constants** — ●B. KATTER<sup>1</sup>, V. B. ZABOLOTNYI<sup>1</sup>, C. SCHÜSSLER-LANGEHEINE<sup>2</sup>, E. SCHIERLE<sup>2</sup>, L. DUDY<sup>1</sup>, O. KIRILMAZ<sup>1</sup>,

S. MACKE<sup>4</sup>, M. W. HAVERKORT<sup>3</sup>, and V. HINKOV<sup>1</sup> — <sup>1</sup>Universität Würzburg — <sup>2</sup>Helmholtz-Zentrum Berlin für Materialien und Energie — <sup>3</sup>Universität Heidelberg — <sup>4</sup>Max-Planck-Institut Stuttgart

Transition metal oxides, like all crystalline solids, can show reconstruction effects at their surface due to breaking of the crystal symmetry. In *SrTiO<sub>3</sub>* missing oxygen at the surface lifts the orbital degeneracy and effectively lowers the symmetry from *O<sub>h</sub>* to *D<sub>4h</sub>*, which leads to anisotropy of the optical constants in the surface layer. We have implemented a matrix formalism to study *SrTiO<sub>3</sub>* with surface reconstruction using resonant X-ray reflectometry. This allows us to extract the optical constants of the anisotropic system from experimental data. These in turn can be compared to crystal field calculations, which helps to understand the orbital reconstruction on a microscopic level.

DS 44.36 Thu 17:00 P1C

**Substrate roughness effect on c-axis preferred orientation of ZnO layers** — SEBNEM YAZICI, ●MARIANA V.G.OLIVEIRA, and MATTHIAS WUTTIG — I. Institute of Physics, Physics of New Materials, RWTH Aachen University, 52056 Aachen, Germany

Improved TCO materials are needed for a range of applications, such as photovoltaics and flat panel displays. Understanding how to control the production processes and thus structure and properties is of fundamental importance. In this work, we have investigated how the roughness of the substrate affects the c-axis texture formation of ZnO thin films. To obtain the substrates, SiN<sub>x</sub> under layers were deposited on Si wafers, before ZnO layer deposition. Rough SiN<sub>x</sub> was a good candidate due to its amorphous structure, avoiding epitaxy influence. The roughness dependence of SiN<sub>x</sub> layers on different operating pressures and thickness were investigated. Generally, thicker films and films that were deposited at higher operating pressures ended up with higher roughness values. Layers of ZnO with thickness of 50nm were deposited onto 10, 20, 30 nm thick SiN<sub>x</sub> layers and on bare Si wafer as a reference sample. Structural characterization using X-ray diffraction (Bragg-Brentano, rocking curve) was carried out to compare the reference and rough underlayer samples.

DS 44.37 Thu 17:00 P1C

**Combined local electrical and optical measurements of individual semiconductor nanosheets** — ●ANDREAS KOLDITZ, CHRISTIAN STRELOW, TOBIAS KIPP, and ALF MEWS — University of Hamburg, Institute of Physical Chemistry, Grindelallee 117, 20146 Hamburg, Germany

Tin(II) sulfide or tin(II) selenide are very attractive IV-VI semiconductor materials because of the natural abundance and low toxicity. In particular, two-dimensional (2D) nanosheets of these materials are promising for photovoltaics as well as for light-emitting applications. We investigate the optical and electrical characteristics of individual 2D nanosheets by combining scanning electrostatic force microscopy (EFM) and Kelvin probe force microscopy (KPFM) with electrical transport and fluorescence measurements. This combination allows us to investigate the effect of band bending on the photo current and also the effects of external charging on the fluorescence properties of individual structures. In first EFM measurements on SnSe nanosheets under local illumination we observed a separation of the photoexcited electrons and holes within the nanosheets. In detail the EFM measurements showed positive excess charges at the excitation area and negative excess charges distributed everywhere else.

DS 44.38 Thu 17:00 P1C

**Interactions at the interface of Cobalt phthalocyanine and graphene covered metal surfaces: Influence of fluorination of CoPc** — ●DAVID BALLE, MALGORZATA POLEK, REIMER KARSTENS, PETER GRÜNINGER, HILMAR ADLER, THOMAS CHASSÉ, and HEIKO PEISERT — Institute of Physical and Theoretical Chemistry, Auf der Morgenstelle 18, 72076 Tuebingen, University of Tuebingen, Germany

The unique electronic, optical and magnetic properties of transition metal phthalocyanines (TMPc) have recently led to increasing research efforts and make them suitable candidates for possible organo-electronic devices. Interactions at interfaces, like charge transfers, can drastically change said properties, though, and need to be carefully investigated.

Graphene buffer layers present an effective way to manipulate or prevent such transfer processes. To function as such a buffer layer, interaction between the graphene layer and the substrate must be controlled, though. Properties of strongly bound and coupled graphene on Ni(111) are severely affected, while an intercalated, uncoupled graphene

layer can influence interactions between the substrate and the organic layer. Variations of other electronic interface parameters, such as fluorination of the phthalocyanines, also have an impact, leading to a persisting interaction at the interface for CoPcF<sub>16</sub> while the corresponding interaction is blocked for CoPc on intercalated graphene on Nickel.

Investigations were carried out using mainly X-ray absorption and photoemission spectroscopies (XAS, PES).

DS 44.39 Thu 17:00 P1C

**Study of manganites with Resonant X-ray Reflectivity** — ●MICHAEL DETTBARN<sup>1</sup>, VOLODYMYR B. ZABOLOTNYI<sup>1</sup>, ABDUL-VAKHAB TCAKAEV<sup>1</sup>, BENJAMIN KATTER<sup>1</sup>, JORGE ENRIQUE HAMANN-BORRERO<sup>2</sup>, KIRILL MILLER<sup>1</sup>, MICHAEL ZAPP<sup>1</sup>, ANDREAS HERKLOTZ<sup>3</sup>, DIANA RATA<sup>4</sup>, ENRICO SCHIERLE<sup>5</sup>, FEIZHOU HE<sup>6</sup>, RONNY SUTARTO<sup>6</sup>, KATHRIN DÖRR<sup>4</sup>, JOCHEN GECK<sup>7</sup>, GEORGE A. SAWATZKY<sup>8</sup>, MICHAEL SING<sup>1</sup>, RALPH CLAESSEN<sup>1</sup>, and VLADIMIR HINKOV<sup>1</sup> — <sup>1</sup>Universität Würzburg and Röntgen Center for Complex Material Systems (RCCM), Würzburg — <sup>2</sup>IFW, Dresden — <sup>3</sup>ORNL, Oak Ridge, USA — <sup>4</sup>Martin-Luther-Universität Halle-Wittenberg, Halle — <sup>5</sup>HZB, Berlin — <sup>6</sup>CLS, Saskatoon, Canada — <sup>7</sup>TU Dresden, Dresden — <sup>8</sup>UBC, Vancouver, Canada

Perovskite manganites such as LaMnO<sub>3</sub> are known to reveal a non-trivial behavior of the manganese L-edge resonant absorption, due to a complicated interplay between Hund's first rule, spin-orbit coupling and crystal field splitting. Using Resonant X-ray Reflectivity (RXR), together with cluster calculations, we study the optical properties of LaMnO<sub>3</sub> and Pr<sub>0.5</sub>Ca<sub>0.5</sub>MnO<sub>3</sub> samples. We are investigating the resonant behavior of the Mn ions depending on varying mechanisms such as doping, oxygen stoichiometry overshoots and distortions of the MnO<sub>6</sub> octahedra, the latter being induced by either the Jahn-Teller effect or epitaxial strain. The layer-resolved nature of RXR enables us to derive the separate concentrations of the Mn valencies, which allows for different conclusions about interfacial correlation effects in the presence of orbital and magnetic ordering.

DS 44.40 Thu 17:00 P1C

**Photoluminescence imaging of few-layer transition metal dichalcogenides** — ●VICTOR FUNK, MICHAEL FÖRG, and ALEXANDER HÖGELE — Ludwig-Maximilians-Universität, München, Deutschland

Transition metal dichalcogenides (TMDs) are novel two-dimensional semiconductor materials with unique optoelectronic properties (1). A crucial step in the fabrication of mono- and multilayer TMD devices is the classification of the number of layers of TMD crystals exfoliated on a polydimethylsiloxane (PDMS) stamp for transfer (2). We report a simple and reliable method for the identification of individual monolayers by means of two-dimensional photoluminescence imaging. Our technique, established for four representative materials of TMD semiconductors and calibrated with layer-sensitive Raman spectroscopy, enables rapid characterization of the crystal layer thickness prior to subsequent transfer onto target substrates.

(1) T. Cao et al., Nature Communications, 3, 887 (2012) (2) A. Castellanos-Gomes et al., 2D Materials, 1, 2053 (2014)

DS 44.41 Thu 17:00 P1C

**Photo-Degradation studies of PDTSTzTz (KP115) for application in OVP** — ●ANDREAS FRÜH<sup>1</sup>, ULF DETTINGER<sup>1</sup>, HEIKO PEISERT<sup>1</sup>, HANS-JOACHIM EGELHAUF<sup>2</sup>, and THOMAS CHASSÉ<sup>1</sup> — <sup>1</sup>Eberhard-Karls-University, Institute for Physical and Theoretical Chemistry, Auf der Morgenstelle 18, D-72076 Tübingen, Germany — <sup>2</sup>Belectric OPV GmbH, Landgrabenstr. 94, D-90443 Nürnberg, Germany

Organic photovoltaic (OPV) offers a possible solution for the future energy demands and combines challenging design requirements with flexibility. On the other hand the limited life time of such devices remains a challenge. UV-Vis and FTIR spectroscopy as well as AFM and REM microscopy were used to study the photo-oxidation of the Low-Band-Gap Polymer Poly[4,4'-bis(2-ethylhexyl)dithieno[3,2-b:2',3'-d]silole]-2,6-diyl-alt-[2,5-bis(3-tetradecylthiophen-2-yl)thiazole-[5,4-d]thiazole-1,8-diyl] (PDTSTzTz) as pristine film and blended with PC[60]BM. For pristine PDTSTzTz films in ambient air, an UV induced radical mechanism was recently suggested [1]. In this work we study the photo-oxidation in dry synthetic air as a function of the wavelength of the light and compare the results to irradiation under standard Air Mass 1.5 conditions. The results point to a different degradation mechanism for lower wavelengths. The degradation of the

different monomer units of the polymer backbone as well as the side chains is monitored by IR spectroscopy. [1] H. S. Silva et al., J. Mater. Chem. A, 4 (2016) 15647-15654.

DS 44.42 Thu 17:00 P1C

**Preparation of Epitaxial PMN-PT Films on Si-based Templates for Electrocaloric Studies** — ●ROBERT KUHR<sup>1,2</sup>, MICHAEL MIETSCHKE<sup>1,2</sup>, CHRISTIAN MOLIN<sup>4</sup>, SYLVIA GEBHARDT<sup>4</sup>, MATTHIJN DEKKERS<sup>3</sup>, KORNELIUS NIELSCH<sup>1,2</sup>, and RUBEN HÜHNE<sup>1</sup> — <sup>1</sup>IFW Dresden, Germany — <sup>2</sup>Technische Universität Dresden, Germany — <sup>3</sup>Solmates B.V., Enschede, Netherlands — <sup>4</sup>Department of Smart Materials and Systems, Fraunhofer Institute for Ceramic Technologies and Systems, Dresden, Germany

Ferroelectric materials that show a strong electrocaloric (EC) effect near a phase transition are subject of current research. These materials show a temperature change when applying an electric field adiabatically which makes them suitable for solid state coolers. One prominent example are Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>-PbTiO<sub>3</sub> (PMN-PT) compounds, which show a high EC effect over a broad temperature range close to room temperature. An integration of these materials into semiconductor architectures might open up new opportunities for cooling sensors or other device structures.

Therefore, epitaxial 0.9PMN-0.1PT films were grown on (001)-oriented SrTiO<sub>3</sub> buffered Si wafers by pulsed laser deposition with conducting interlayers as electrodes. Epitaxy, phase purity and surface topography were studied using XRD and AFM. The ferroelectric properties were determined by temperature dependent global polarization measurements as well as local piezo response force microscopy.

DS 44.43 Thu 17:00 P1C

**Simulating Interferometric Spectra using Multiple Matrix Methods** — ●KAI ALEXANDER SCHWENZFEIER<sup>1</sup>, ANDREAS ERBE<sup>2</sup>, and MARKUS VALTNER<sup>3</sup> — <sup>1</sup>MPIE, Düsseldorf, Germany — <sup>2</sup>NTNU, Trondheim, Norway — <sup>3</sup>TU-BAF, Freiberg, Germany

The analytical equations used for evaluating Surface Forces Apparatus (SFA) data were derived on the basis of a number of simplifications, but the actual impact of these simplifications is largely unknown. Especially the influence of mirror materials has completely been neglected.

By simulating SFA spectra for different interferometer layouts and different mirror materials and analysis of those spectra using the analytical equations it is possible to estimate the relative error done by using those equations.

The optical properties of the mirror material have a great impact on the peak shape as well as position of the resulting interference patterns. Especially with 10-20 nm thin mirrors and gold as mirror material the determination of the fringe order as one integral part of the analytical equations breaks down.

Our findings illustrate the need to reevaluate SFA data with respect to mirror materials and thicknesses with a suitable analysis tool. We developed a new software tool based on multiple matrix methods, that addresses these issues and allows the simulation of interferometer pattern based on the physical properties of the interferometer layers. Our simulation tools can be applied not only to SFA analysis but to general interferometry applications with white light.

DS 44.44 Thu 17:00 P1C

**X-Ray Reflectivity Investigation of Structure and Kinetics of Photoswitchable Lipid Monolayers** — ●MALTE JACOBSEN<sup>1</sup>, KUNTAL CHATTERJEE<sup>1</sup>, BJÖRN HAUSHAHN<sup>1</sup>, CHEN SHEN<sup>1,2</sup>, SVEN FESTERSEN<sup>1</sup>, JONAS WARIAS<sup>1</sup>, BENJAMIN RUNGE<sup>1</sup>, FRANZISKA REISE<sup>3</sup>, THISBE LINDHORST<sup>3</sup>, BEATE MARIA KLÖSGEN<sup>2</sup>, OLAF MAGNUSSEN<sup>1,4</sup>, and BRIDGET MURPHY<sup>1,4</sup> — <sup>1</sup>Institute for Experimental and Applied Physics, CAU Kiel, Germany — <sup>2</sup>SDU Odense, Denmark — <sup>3</sup>Institute of Organic Chemistry, CAU Kiel, Germany — <sup>4</sup>Ruprecht Haensel Laboratory, CAU Kiel, Germany

The mechanical and dynamic properties of phospholipid membranes are important for biological functions such as switching of embedded proteins. To investigate these biologically relevant properties we study model systems in which amphiphilic photoswitchable glycoconjugates have been integrated into biomimetic phospholipid membranes. The structure and kinetics of the switching process in a lipid Langmuir film are measured using Langmuir isotherms and in situ X-ray reflectivity at LISA diffractometer P08, PETRA III. We have modified glycolipids to contain an azobenzene photoswitch between the chain and head group and successfully embedded them in a monolayer of DPPC. We can reversibly change the azobenzene-glycolipid orientation between trans- and cis-conformation by illumination with UV and blue light.



Strong changes in membrane conformation upon switching have been observed, and a critical point has been discovered above which the membrane expands rather than compresses upon switching. This work is funded by SFB 677 and BMBF 05K13FK2.

DS 44.45 Thu 17:00 P1C

**Investigation of Charge Carrier Distribution in OLEDs by Means of Photoluminescent Molecular Probes** — ●THOMAS FERSCHKE<sup>1</sup>, LARS JÄGER<sup>2</sup>, WOLFGANG BRÜTTING<sup>2</sup>, and JENS PFLAUM<sup>1,3</sup> — <sup>1</sup>Experimental Physics VI, Julius Maximilian University, 97074 Würzburg — <sup>2</sup>Institute of Physics, University of Augsburg, 86135 Augsburg — <sup>3</sup>ZAE Bayern, 97074 Würzburg

The charge carrier distribution in organic thin film devices is essential for optimizing their operation characteristics. Recently, it has been shown that these current densities can be determined by means of photoluminescence (PL) studies on single guest dye molecules. [Nothaft M. *et al.*, *ChemPhysChem* **12**, 2590–2595 (2011)] Here, this concept is applied to common Alq<sub>3</sub>/α-NPD OLEDs by utilizing molecular dopant ensembles in combination with μ-PL. Tetraphenylidibenzoperiflanthene (DBP) is intentionally embedded as dopant (0.1 v-%) via co-evaporation at defined positions within the Alq<sub>3</sub> emission layer. Upon charge injection an effective reduction in the DBP PL is observed which can be attributed to electron - exciton interaction. The macroscopic current density related to the respective PL reduction scales with the distance from the injecting electrode in qualitative agreement with a SCLC model. The validity of this model and thus, variations in vertical charge carrier distribution are studied as a function of current density as well as of temperature. Since at reverse bias PL quenching of DBP near the Alq<sub>3</sub>/α-NPD interface is observed, a comparative study of the interfacial charge density is performed by means of integral impedance spectroscopy. [Brütting W. *et al.*, *Org. Electron.*, **2**, 1-36 (2001)]

DS 44.46 Thu 17:00 P1C

**Introducing band gap states in MoS<sub>2</sub> monolayers by triangular defects** — TOMMY LORENZ<sup>1</sup>, ●ANDRÉ NIEBUR<sup>1,2</sup>, SIBYLLE GEMMING<sup>2,3</sup>, ARTUR ERBE<sup>2</sup>, and GOTTHARD SEIFERT<sup>1</sup> — <sup>1</sup>Theoretical Chemistry, TU Dresden, 01062 Dresden, Germany — <sup>2</sup>Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden - Rossendorf e.V., 01314 Dresden, Germany — <sup>3</sup>Theoretical Physics, Faculty of Sciences, TU Chemnitz, 09107 Chemnitz, Germany

Triangular defects in MoS<sub>2</sub> monolayers and their influence on the crystal and electronic structure have been studied using the density-functional based tight-binding (DFTB) method. Systems with different defect sizes and concentrations have been compared to find out how these parameters affect the electronic properties of MoS<sub>2</sub> monolayers. The density of states (DOS) calculations show the presence of additional states in the HOCO-LUCO-Gap of pristine MoS<sub>2</sub> even for small defects in a low concentration. Band structure calculations and orbital plots characterize these states as localized mid-gap states. From the projected densities of states can be seen that these states mainly arise from d-orbitals of the molybdenum atoms at the defect edges and their number increases with an increasing defect size. Due to the fact that the molybdenum d-states dominate the valence and conduction band edges of MoS<sub>2</sub>, the additional states which arise in the band gap may impact the electronic transport through the layer. Analyses of the orbital's degree of (de-) localization show that this influence seems to be quite small for low defect concentrations but increases for higher ones.

DS 44.47 Thu 17:00 P1C

**Time-resolved THz spectroscopy on 1T-TaS<sub>2</sub>** — ●SIMON LANGE<sup>1</sup>, LARA WIMMER<sup>1</sup>, GEORG HERINK<sup>1</sup>, KAI ROSSNAGEL<sup>2</sup>, and CLAUS ROPERS<sup>1</sup> — <sup>1</sup>4th Physical Institute - Solids and Nanostructures, University of Göttingen, Friedrich-Hund-Platz 1, Germany — <sup>2</sup>Institute for Experimental and Applied Physics, University of Kiel, Leibnizstraße 15, Germany

Transition metal dichalcogenides (TMDCs) are a highly interesting class of materials due to their two-dimensional behaviour, which leads to multiple phenomena, like Mott and Peierls transitions, superconductivity and charge and spin density waves. A prominent representative of TMDCs, 1T-TaS<sub>2</sub>, shows various different charge density wave (CDW) phases associated with periodic lattice distortions.

Here, we present an optical pump/terahertz probe setup in a transmission geometry for characterizing the ultrafast response of materials in the spectral range of 0.5 to 3 THz and at temperatures between 130 to 300 K.

Using this setup, in temperature-dependent measurements, we ob-

serve the phase transition between the commensurate (C) and nearly-commensurate (NC) charge density wave phases and its hysteresis in a 1T-TaS<sub>2</sub> thin film. We identify three characteristic phonon modes in the insulating C phase, which vanish in the metallic NC phase [1]. In time-resolved measurements (see also Ref. [2]), we optically induce this transition and track the evolution of the phonon modes.

[1] L. Gasparov, *Phys. Rev. B*, **66**, 094301 (2002)

[2] N. Dean *et al.*, *Phys. Rev. Lett.* **106**, 016401 (2011)

DS 44.48 Thu 17:00 P1C

**Ultrafast laser-triggered electron emission from diamond coated metal tips** — ●ALEXANDER TAFEL, PETER HOMMELHOFF, and JÜRGEN RISTEIN — Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen

Sharp metal tips are widely used in electron microscopy as cold cathodes utilizing the outstanding beam quality of field emitted electrons from a nm sized virtual source. Nanocrystalline diamond with negative electron affinity exhibits excellent electron field emission properties and allows nm thin coating. The combination of the unique properties of sharp tips and nanodiamond are used in this work for building a high brightness femtosecond electron source.

Tungsten tips are etched electrochemically with resulting tip radii < 20 nm. Nanodiamond seeding is used to achieve high nucleation densities required for thin but dense films. Diamond films are grown using microwave enhanced chemical vapour deposition.

Ultrafast electron emission from diamond coated samples is investigated by few-cycle infrared pulses. Here, we present first experimental results and compare electron emission from diamond coated tips to bare tungsten tips.

The goal of this research is to develop a source of ultrashort and intense electron bunches for use in 4-D electron microscopy, dielectric laser acceleration and ultrafast electron diffraction.

DS 44.49 Thu 17:00 P1C

**Improving the photovoltaic performance of hybrid photovoltaics by inorganic interfacial modification** — ●YVONNE J. HOFSTETTER<sup>1,2</sup>, PAUL E. HOPKINSON<sup>1,2</sup>, ARTEM A. BAKULIN<sup>3</sup>, and YANA VAYNZOF<sup>1,2</sup> — <sup>1</sup>Kirchhoff-Institut für Physik, Ruprecht-Karls-Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany — <sup>2</sup>Centre for Advanced Materials, Ruprecht-Karls-Universität Heidelberg, Im Neuenheimer Feld 225, 69120 Heidelberg, Germany — <sup>3</sup>Cavendish Laboratory, Cambridge University, JJ Thomson Ave, Cambridge, UK

Bilayer organic-inorganic hybrid photovoltaic devices offer the possibility to modify the organic-inorganic interface, and thus to influence the efficiency of photo-induced charge separation. Various organic modifiers have been investigated, whereas inorganic modifiers have remained unconsidered for the most part. Here, we introduce an inorganic modifier, caesium carbonate, as an interlayer in a model poly(3-hexathiophene)/ZnO system. Upon modification, we observe an improved energy level alignment at the hybrid interface resulting in a significantly increased open circuit voltage, and suppressed formation of interfacial bound charge pairs resulting in reduced interfacial recombination losses and an increased short circuit current. These improvements add up to a twelve fold enhancement in power conversion efficiency which demonstrates the significant potential of applying inorganic modifiers in hybrid photovoltaics to improve the performance.

DS 44.50 Thu 17:00 P1C

**Combinatorial Synthesis of Ni-based Nanoparticles by Sputtering into Ionic Liquids** — ●CHRISTINA EBERLING, GESA ZAHN, CHRISTOPH SOMSEN, and ALFRED LUDWIG — Institute for Materials, Ruhr-Universität Bochum, 44780 Bochum, Germany

Nanomaterials are of great interest for different applications, especially for catalysis, for example in fuel cells. To realize low-cost hydrogen fuel cells, commonly used rare and expensive metals must be replaced by new potential catalysts. High-throughput and combinatorial approaches offer a good possibility to identify promising material combinations in a fast and efficient way. By using combinatorial co-sputter deposition techniques, unary, binary and multinary metal alloys nanoparticles (NPs) can be synthesized with different composition. As a substrate, we use a micromachined cavity array wafer. The cavities are filled with an ionic liquid (IL) that can be handled under vacuum conditions due to its very low vapour pressure. In first experiments, we focused on the fabrication of Ni-based alloy NPs with different compositions in the IL 1-Butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([BMim][Tf<sub>2</sub>N]), espe-



cially Ni-Co and Ni-Mn. Transmission electron microscopy (TEM) measurements show that non-agglomerated, crystalline NPs with a diameter of 3 to 6 nm could be synthesized. In addition, thin films were deposited under the same sputtering conditions and analysed using energy dispersive X-ray spectroscopy (EDX) and X-ray diffraction (XRD) in order to compare elemental distribution and crystal structure of thin films with those of NPs.

DS 44.51 Thu 17:00 P1C

**Understanding Epitaxial Growth of Perfluoropentacene on Graphite** — ●FELIX WIDDASCHECK and GREGOR WITTE — Molekulare Festkörperphysik, Philipps-Universität Marburg, Renthof 7, D-35032 Marburg, Germany

Understanding and controlling the growth of organic molecular films is crucial for their use in optoelectronic devices. A common approach is to use different substrates in order to mediate the growth and control the orientation and polymorph in the film. Therefore, the substrate-molecule interface is of particular importance as this controls the initial stage of film growth. In this regard an interesting model system are perfluoropentacene (PFP) films which grow epitaxially on graphite and exhibit a new, substrate induced  $\pi$ -stacked polymorph. [1, 2] Here, we report on a STM study of the PFP/Graphite interface and the initial stage of film growth. Using single crystalline graphite and tip assisted removing of PFP molecules the adlayer structure and the azimuthal orientation of the first two monolayers were determined with high precision. It is found that the first monolayers act as a precursor for further growth, already resembling the multilayer structure, while a dislocation pattern was identified, which is attributed to the misfit between the locally dense packed film and the substrate lattice.

[1] I. Salzman et al., ACS Nano (2012), 6, 10874

[2] R. Félix et al., Cryst. Growth Des., Article ASAP, DOI: 10.1021/acs.cgd.6b01117

DS 44.52 Thu 17:00 P1C

**Growth of pinholes in metal electrodes of organic photovoltaic cells** — ●DANIEL FLUHR<sup>1</sup>, BURHAN MUHSIN<sup>2</sup>, ROLF ÖTTKING<sup>2</sup>, ROLAND RÖSCH<sup>2</sup>, STEFAN KRISCHOK<sup>1</sup>, and HARALD HOPPE<sup>2</sup> — <sup>1</sup>Institute of Physics, Technische Universität Ilmenau, 98693 Ilmenau, Germany — <sup>2</sup>Center for Energy and Environmental Chemistry Jena (CEEC Jena) & Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, 07743 Jena, Germany

Lifetime is still a major problem of organic photovoltaic (OPV) cells. There are many reasons for solar cell degradation varying from shunts induced by impurities or electromigration over photoinduced oxidation of active layer materials to corrosion and delamination of the metal contact both induced by oxygen or water ingress. One issue concerns so-called pinholes through the metal back electrode of the device. These pinholes offer pathways for ingress of water and oxygen which may attack the metal-organic interface by introducing delamination through formation of insulating metal oxides or hydrogen evolution.

As charge injection and extraction is suppressed at delaminated areas, the active area taking part in power conversion - and hence the overall efficiency becomes reduced. We investigated the influence of different environmental conditions on the reduction of the active area of the OPV cell. Spatially resolved measurements give information on location and size of insulated areas induced by pinholes in the metal back contact. Time resolved measurements during degradation of the devices revealed the dynamics and rate of growth of these individual defects.

DS 44.53 Thu 17:00 P1C

**3D-Analysis of InGaN-Quantum Wells** — ●MAXIMILIAN RIES — Schwarzschildstraße 8

Modern LEDs (light emitting diodes) are frequently made of III-nitride structures, with applications ranging from lightning, optoelectronics to life sciences and health care. To allow excellent performances, complex heterostructures must be fabricated with high precision. This study introduces a 3D analysis based on Raman and photoluminescence (PL) spectroscopy of InGaN quantum well (QW) structures. Simultaneous excitation and measurement of PL and Raman modes with a home-built setup allow for non-destructive and efficient determination of QW thickness and In-content, providing valuable information on device performance.

DS 44.54 Thu 17:00 P1C

**Development of quantitative Reflectance Anisotropy Microscopy** — ●TIMO SEEMKE, EUGEN SPEISER, JOHANNES FALKENBURG, MACIEJ D. NEUMANN, and NORBERT ESSER — Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Department Berlin, Schwarzschildstraße 8, 12489 Berlin, Germany

Reflectance anisotropy microscopy (RAM) is a technique that monitors the optical anisotropy of surfaces with spatial resolution and provides information about crystal orientation and local strain on the surface.

Often, technologically relevant materials are not transparent, thus transmittance based polarization- or phase microscopy methods are not an option for measuring spatially resolved, low amplitude surface anisotropy. Common reflectance based methods depend on beam-splitting elements that do not fully conserve polarization states. Other common methods make use of a Foster prism polarizing beamsplitter, that detect only the depolarization by the surface and do not measure the anisotropy quantitatively. A third widely used approach is to separate the incoming and outgoing light beam by using a small angle of incidence to the surface, which severely limits the use of high spatial resolution optics.

We present a new RAM setup for quantitative and spatially resolved measurements of optical anisotropy with a signal to noise ratio comparable to common, non-spatially resolved Reflectance Anisotropy Spectroscopy (RAS) methods. Spatial resolution in the micrometer range was achieved in a spectral range from UV to near IR. RAM measurements on wide-bandgap oxide- and nitride-semiconductors surfaces as well as on periodic microstructures will be discussed.