

## DS 44: Poster IV: Thin film photovoltaics; Organic electronics and photovoltaics (jointly with CPP, HL, O); Organic thin films; Trends in atomic layer deposition (Focused session)

Time: Friday 9:30–12:00

Location: Poster E

DS 44.1 Fri 9:30 Poster E

**Study of the optical properties of TiO<sub>2</sub> Thin Films prepared by rapid thermal oxidation** — WAFAA AL-KHAYAT<sup>1,2</sup> and GERHARD WILDE<sup>1</sup> — <sup>1</sup>Institute of Materials Physics, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — <sup>2</sup>College of Science, Al-Mustansiriyah University, Baghdad, Iraq

TiO<sub>2</sub> thin films were deposited by the thermal oxidation method on glass substrates at room temperature. The X-ray diffraction patterns indicate an amorphous structure of the TiO<sub>2</sub> thin films. The optical constants were characterized using the transmission spectra of the films obtained by uv-vis spectrophotometer. The optical band gaps were evaluated by the Tauc model. The optical properties of the thin films are discussed with respect of the film thickness and the oxidation condition.

DS 44.2 Fri 9:30 Poster E

**Inhomogeneities in charge carrier transport properties of Cu(In,Ga)Se<sub>2</sub> solar-cells** — MELANIE NICHTERWITZ<sup>1</sup>, CHRISTIAN KAUFMANN<sup>1</sup>, RAQUEL CABALLERO<sup>2</sup>, HANS-WERNER SCHOCK<sup>1</sup>, and THOMAS UNOLD<sup>1</sup> — <sup>1</sup>Helmholtz-Zentrum Berlin, Germany — <sup>2</sup>Universidad Autónoma de Madrid, Spain

In this study, electron beam induced current (EBIC) in the cross section configuration is used to characterize charge carrier transport in Cu(In,Ga)Se<sub>2</sub> (CIGSe)/CdS/ZnO solar-cells. It is shown that charge carrier transport properties are (i) generation dependent and (ii) grain specific, i.e. spatially inhomogeneous. Within some grains of the CIGSe absorber layer, the collected short circuit current is reduced significantly for electron beam irradiation such that there is no generation at the heterojunction. Charge carrier transport is generation dependent in these grains for all used electron beam currents, i.e. generation densities (low injection). In other grains however, charge carrier transport is only generation dependent for the highest used electron beam current. In conjunction with numerical simulations, these results are used to derive a model for the electronic band diagram of the heterojunction region of the solar cell. It is based on the assumption of (i) a thin layer with a high density ( $\approx 10^{17} \text{ cm}^{-3}$ ) of deep acceptor type defect states (p+ layer) and a lowered valence band maximum between the CIGSe and the CdS layer and (ii) donor type interface states at the p+ layer/CdS interface of some grains.

DS 44.3 Fri 9:30 Poster E

**Post-deposition optimization of LPCVD grown ZnO:B as front TCO in thin film silicon solar cells** — THOMAS BIENERT<sup>1</sup>, NLEG SERGEEV<sup>1</sup>, KARSTEN VON MAYDELL<sup>1</sup>, and CARSTEN AGERT<sup>1</sup> — NEXT ENERGY. EWE Forschungszentrum für Energietechnologie e.V., Oldenburg, Germany

Thin film solar cells with superstrate configuration have very specific requirements for optical and electrical properties of the front contact, like high transmittance and haze as well as a low sheet resistance. Transparent conductive oxides (TCO) have already been proven to be a good choice, but their optical and electrical properties can be improved even after the deposition by various means. The LPCVD grown ZnO:B TCO in this study has been treated with hydrochloric acid (HCl) and H<sub>2</sub>-plasma prior to the deposition of  $\mu\text{c-Si:H}$  and a-Si:H pin-cells. The influence of such a treatment on optical and electrical properties of the TCO was investigated. The performance of the cells deposited on original and treated TCO was determined. It is shown that both treatments can be used to improve the overall TCO's properties. It has been found the etching enhances surface topography and haze while H<sub>2</sub>-Plasma treatment decreases the sheet resistance significantly. The efficiency of both solar cell types ( $\mu\text{c-Si:H}$  as well as a-Si:H pin) deposited on optimized LPCVD ZnO:B was increased by enhancement of the fill factor and of the photocurrent.

DS 44.4 Fri 9:30 Poster E

**Photovoltaic energy conversion based on strongly correlated oxides** — BENEDIKT IFLAND<sup>1</sup>, GESINE SAUCKE<sup>2</sup>, JONAS NORPOTH<sup>1</sup>, JÖRG HOFFMANN<sup>1</sup>, and CHRISTIAN JOOSS<sup>1</sup> — <sup>1</sup>Institute of Materials Physics, University of Göttingen, Germany — <sup>2</sup>Institute for Condensed Matter Physics, University of Zürich, Switzerland

Materials with strong electron-electron or electron-phonon interaction offer promising opportunities in search for new fundamental mechanisms of light harvesting in solar cells via tuning their correlation interactions. We have studied two types of manganite-titanite pn-heterostructures, where p-doped manganites are deposited on single crystal substrate of n-type  $\text{SrTi}_{1-x}\text{Nb}_x\text{O}_3$  (STNO) via ion beam sputter deposition:  $\text{Pr}_{1-x}\text{Ca}_x\text{MnO}_3$  (PCMO) shows semiconducting behavior based on thermally assisted hopping of small polarons. In contrast,  $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$  (LSMO) exhibits band like "metallic" conductivity and ferromagnetic order. It may form a Schottky like junction in electrical contact with STNO. Current-voltage-characteristics of the oxide junction in a temperature range between 25 and 300 K show strongly rectifying behavior. Although both p-type manganites have no optical band gap at 300K, the junctions reveal a photovoltaic effect. The open circuit voltage increases with decreasing temperature up to several hundred millivolts. Experimental results are discussed with respect to conventional semiconductor models, taken also into account the non-linear mobility of polarons in the presence of an electric field.

DS 44.5 Fri 9:30 Poster E

**Physical vapor deposition of CdTe thin films at low temperature for solar cell applications** — CHRISTOPH HEISLER<sup>1</sup>, MICHAEL BRÜCKNER<sup>1</sup>, FELIX LIND<sup>1</sup>, CHRISTIAN KRAFT<sup>1</sup>, UDO REISLÖHNER<sup>1</sup>, CARSTEN RONNING<sup>1</sup>, and WERNER WESCH<sup>1</sup> — Institute of Solid State Physics, University of Jena, Max-Wien-Platz 1, D-07743 Jena

Cadmium telluride is successfully utilized as an absorber material for thin film solar cells. Industrial production makes use of high substrate temperatures for the deposition of CdTe absorber layers. However, in order to exploit flexible substrates and to simplify the manufacturing process, lower deposition temperatures are beneficial. Based on the phase diagram of CdTe, predictions on the stoichiometry of CdTe thin films grown at low substrate temperatures are made in this work. These predictions were verified experimentally using additional sources of Cd and Te during the deposition of the CdTe thin films at different substrate temperatures. The deposited layers were analyzed with energy-dispersive X-ray spectroscopy. In case of CdTe layers which were deposited at substrate temperatures lower than 200 °C without usage of additional sources we found a non-stoichiometric growth of the CdTe layers. The application of the additional sources leads to a stoichiometric growth for substrate temperatures down to 100 °C which is a significant reduction of the substrate temperature during deposition.

DS 44.6 Fri 9:30 Poster E

**Influence of the sintering process on the structure of Cu<sub>2</sub>ZnSnS<sub>4</sub> nanocrystal thin films** — KAI KORNUBER<sup>1</sup>, JAISSON KAVALLAKATT<sup>1,2</sup>, XIANZHONG LIN<sup>1</sup>, PATRYK KUSCH<sup>2</sup>, AHMED ENNAOUI<sup>1</sup>, and MARTHA C. LUX-STEINER<sup>1,2</sup> — <sup>1</sup>Helmholtz Center Berlin for Materials and Energy, Berlin, Germany — <sup>2</sup>Freie Universität Berlin, Berlin, Germany

Cu<sub>2</sub>ZnSnS<sub>4</sub> (CZTS) is a p-type emerging semiconductor solar absorber with optimal direct band gap energy of 1.5 eV and a large absorption coefficient above  $10^4 \text{ cm}^{-1}$ . It is structurally similar to Cu(In,Ga)Se<sub>2</sub> and contains only earth abundant, non-toxic elements. Recently promising energy conversion efficiencies of up to 10.1 % were demonstrated [D.Barkhouse, O.Gunawan, et. al, Prog. Photovolt: Res. Appl. (2011)]. So far, all preparation methods require an annealing step to improve the crystallinity. This process is not completely understood, suffering from the presence of secondary phases such as ZnS, Cu<sub>x</sub>SnS<sub>y</sub> and Cu<sub>x</sub>S. In this work, a solution based approach to prepare CZTS-nanoparticle ink was used for CZTS thin film deposition on Mo-coated glass and FTO. The processing under different temperatures and atmospheres (Ar, H<sub>2</sub>S) allowed to obtain compact film material. Combining X-ray diffraction and Raman spectroscopy as complimentary phase resolving techniques, identification of phases present in multi-phase CZTS thin films was accomplished. The results of the Raman- and XRD-analysis of the phases formed and the advantages of using these techniques are presented. Furthermore UV-Vis-spectroscopy was applied to investigate changes of the optical properties.

DS 44.7 Fri 9:30 Poster E

**Spectroscopic Characterization of Amorphous Silicon/Silicon Heterodiodes Prepared by DC Pulsed Magnetron Sputtering**— ●PHILIPP SCHÄFER<sup>1</sup>, FRANK NOBIS<sup>2</sup>, OVIDIU D. GORDAN<sup>1</sup>, HARTMUT KUPFER<sup>2</sup>, FRANK RICHTER<sup>2</sup>, and DIETRICH R. T. ZAHN<sup>1</sup> — <sup>1</sup>Semiconductor Physics, Chemnitz University of Technology — <sup>2</sup>Solid State Physics, Chemnitz University of Technology

Doped layers of hydrogenated amorphous silicon were prepared by dc magnetron sputtering onto oppositely doped crystalline silicon substrates. Defect levels of the thereby assembled heterostructure diodes were intensively studied using charge transient spectroscopy. During deposition the substrate temperature and hydrogen flow rate can be controlled individually. Energetic shifts of the defect levels occur with the variation of these key parameters. Furthermore, one can observe the influence of differently doped samples.

The influence of substrate temperature and hydrogen flow rate on the layer deposition is additionally studied by a variety of optical spectroscopy methods. Microstructure parameter as well as hydrogen content is derived from Si-H absorption in the infrared, while the Tauc-Lorentz band gap is derived from variable angle spectroscopic ellipsometry. Moreover, the parameters for which crystallization occurs were found by Raman spectroscopy. The combination of the variety of techniques provides a detailed insight in the optical, structural, and electrical properties of the samples studied.

DS 44.8 Fri 9:30 Poster E

**Photoluminescence of  $\text{CuIn}_x\text{Ga}_{1-x}\text{Se}_2$  absorbers and solar cells**— ●SVEN SCHÖNHERR<sup>1</sup>, JAKOB HAARSTRICH<sup>1</sup>, UDO REISLÖHNER<sup>1</sup>, CARSTEN RONNING<sup>1</sup>, and THORSTEN RISSOM<sup>2</sup> — <sup>1</sup>Institut für Festkörperphysik, Friedrich Schiller Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — <sup>2</sup>Helmholtz Zentrum Berlin für Materialien und Energie, Solar Energy Research, Institute for Technology, Lise-Meitner-Campus, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Photoluminescence (PL) has been studied on high-efficiency CdS/CIGS solar cells. The sample layers were illuminated by a HeNe-Laser in a PL setup with a spot size of 1mm and in a micro-PL ( $\mu\text{PL}$ ) setup, where the laser beam was focused by a microscope objective down to reach a spatial resolution of  $\sim 1 \mu\text{m}$  at the focal spot on the sample. The samples were mounted in a LHe flow cryostat and studied as a function of temperatures from 3.5 to 300 K.

Photoluminescence spectra were measured from the front and the back site of the  $\text{Cu}(\text{In,Ga})\text{Se}_2$  absorber layers and different peak energies were detected corresponding to the typical band-gap grading of CIGS solar cells. Additionally, the micro-PL measurements have shown a lateral peak shift, which could be interpreted as varying grains or by different luminescence radiation of grains and grain boundaries.

DS 44.9 Fri 9:30 Poster E

**Silicon Nanoparticle Sprayed Films and Their Characterization by Ellipsometry, Raman Spectroscopy, and Atomic Force Microscopy**— ●FALKO SEIDEL<sup>1</sup>, IULIA G. KORODI<sup>1</sup>, STEPHAN KOTH<sup>2</sup>, RONNY FRITZSCHE<sup>3</sup>, OVIDIU D. GORDAN<sup>1</sup>, REINHARD R. BAUMANN<sup>2</sup>, MICHAEL MEHRING<sup>3</sup>, and DIETRICH R.T. ZAHN<sup>1</sup> — <sup>1</sup>Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — <sup>2</sup>Institute for Print and Media Technology, Chemnitz University of Technology, D-09107 Chemnitz, Germany — <sup>3</sup>Coordination Chemistry, Chemnitz University of Technology, D-09111 Chemnitz, Germany

The growth of single crystal Silicon (c-Si) for photovoltaic applications is an expensive, high temperature requiring process. Regarding thin film solar cells less expensive processes such as spray coating would be advantageous. In this work dispersions of silicon nanoparticles (Si NP) having nominal sizes of 6 nm and 40 nm dispersed in a solution are sprayed on 0.1 mm thick molybdenum foils. The spraying setup works in a glovebox under nitrogen atmosphere and an in-line spectroscopic ellipsometer (SE) enables to investigate optical properties during film deposition. In order to obtain microcrystalline Silicon (mc-Si), an high energetic light flash sinters the accumulated Si NP. Raman spectroscopy probes the sintering process while atomic force microscopy (AFM) probes the surface morphology and roughness. Eventually, results of these three methods are presented and discussed in the light of the potential of spray coating for producing low cost, large area photovoltaic devices.

DS 44.10 Fri 9:30 Poster E

**Electrical Characterization of Doped a-Si:H/c-Si Heterojunc-****tions, Produced by Magnetron Sputtering** — ●FRANK NOBIS, HARTMUT KUPFER, PHILIPP SCHÄFER, DIETRICH R. T. ZAHN, and FRANK RICHTER — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz, Germany

We investigate thin films of doped hydrogenated amorphous silicon (a-Si:H) with respect to their application in photovoltaics. Currently, chemical vapour deposition is widely used for the formation of such films providing comparably low defect density and relatively high efficiency of dopants. Our method of choice is pulsed dc magnetron sputtering because this method is well suitable to realize a high-efficiency inline technology for solar cells formation. Thereby a key question in our investigations is the amount of electrically active dopants which can be achieved in the magnetron sputtered films.

We deposited doped a-Si:H films onto oppositely doped silicon wafers. Crucial deposition parameters like substrate temperature and hydrogen partial pressure were varied. The resulting heterojunctions were characterized with respect to electrical film properties and doping efficiencies. Under certain conditions very good rectification ratios of the produced pn-junctions were achieved. This finding is correlated with the doping efficiency in the amorphous films.

DS 44.11 Fri 9:30 Poster E

**Photoluminescence measurement of polycrystalline CdTe made of high purity source material**

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CdTe is a common material for thin film solar cells. However, the mainly used CdTe source material is known to contain a high number of intrinsic defects and impurities. In this work we investigate the defect structure of high purity CdTe by means of Photoluminescence, which is a common method to detect the energy levels of defects in the band gap of semiconductors. We used a 633nm HeNe-Laser at sample temperatures of 8 K. The examined samples were processed in a new vacuum system based on the PVD method. They yield significantly different spectra on as-grown samples compared to those measured on samples which are grown by the standard process, since the double peak at 1,55eV was hardly detectable and the A-center correlated transition vanished. Instead a peak at 1,50eV with pronounced phonon coupling was observed. The 1,50eV peak is known from other measurements but has not been characterized so far. The intention of this work is to characterize this new feature and the influence of post deposition treatments of the CdTe layers on the PL spectra.

DS 44.12 Fri 9:30 Poster E

**Deposition control of thin-film silicon solar cells by optical emission spectroscopy**— ●VITALIJ SCHMIDT<sup>1</sup>, WIEBKE HACHMANN<sup>1</sup>, STEFAN GRUSS<sup>2</sup>, HELMUT STIEBIG<sup>2</sup>, and ULRICH HEINZMANN<sup>1</sup> — <sup>1</sup>Fak. f. Physik, Uni Bielefeld, Germany — <sup>2</sup>Malibu GmbH & Co. KG

The improvement of the layer quality is one key factor to the overall efficiency of thin-film silicon solar cells. Plasma-enhanced chemical vapor deposition (PECVD) is a widely applied production process for microcrystalline silicon layers ( $\mu\text{c-Si}$ ). The  $\mu\text{c-Si}$  layer is used as a bottom cell material within a tandem stack.

Via in-situ spectroscopy we gain information on the deposition used as feedback for process control. The plasma emits light, characteristic for its composition. Research is done on the hydrogen dilution of silane as it affects the crystalline fraction of the grown layer. Observing the time development of the specific wavelengths for hydrogen and silane ( $\text{H}_\alpha$  at 656 nm and  $\text{SiH}^*$  at 414 nm) we determine the layer-thickness dependent crystallinity.

In order to achieve  $\mu\text{c-Si}$  layers with constant crystallinity we focus on monitoring and adjustment of the  $\text{SiH}^*/\text{H}_\alpha$ -ratio. This ratio can be used for a homogeneous  $\mu\text{c-Si}$  layer deposition.

DS 44.13 Fri 9:30 Poster E

**Growth of large-size-two-dimensional pentacene crystalline for high performance organic transistors**

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Organic field-effect transistors (OFETs) have been the focus of intense research in the last two decades. Several studies have been proposed to improve the field effect mobility, by optimizing the deposition of

organic semiconductor films and modifying surface properties of the gate insulators. The interface between gate dielectric and organic film plays an important role in field-effect behavior because the first two to three molecular layers next to the dielectric interface dominate the charge transport. Self-assembled monolayer (SAM) has been widely used to modify the gate electric surface (SiO<sub>2</sub>).

Here we demonstrate that the use of SiO<sub>2</sub> gate dielectric modified with a single molecular layer of PTCDI-C8 can yield a high-mobility organic semiconductor of pentacene. An average hole mobility about 1.71 cm<sup>2</sup>/VS is achieved, that is ten times higher than the mobility of devices fabricated on bare SiO<sub>2</sub> under the same fabrication conditions (0.15 cm<sup>2</sup>/VS) and it is also higher than that of the devices with OTS treated SiO<sub>2</sub>. The differences in film morphology and grain size obtained from AFM-Images and the X-ray diffraction patterns could be used to explain the high mobility resulting from the modification of SiO<sub>2</sub> with a single layer of PTCDI-C8.

DS 44.14 Fri 9:30 Poster E

**Use of PEDOT:PSS as Gate Electrode on a PMMA Gate Dielectric in Transparent Organic Field Effect Transistors —**

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Indium tin oxide (ITO) on glass was patterned to provide a transparent interdigitated source-drain electrode array. As an organic semiconductor, semitransparent 40 nm *pentacene* were prepared by physical vapor deposition (PVD) under fine vacuum conditions. As gate dielectric, a thin transparent polymer layer (500 nm) of *PMMA* (*poly(methylmethacrylate)*) was deposited by spin-coating on top of the *pentacene* layer. Finally, a layer of *PEDOT:PSS* was prepared by spin-coating and used as gate-electrode. The transistor structures were measured and as the characteristic properties the threshold voltage and the on/off ratio of the structures will be discussed.

DS 44.15 Fri 9:30 Poster E

**Doping and Phase Separation in Mixtures of Differently Substituted Phthalocyanines Measured in-situ During Film Growth —**

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Mixed films of the unsubstituted phthalocyaninato copper (*H<sub>16</sub>PcCu*) and its perfluorinated derivative (*F<sub>16</sub>PcCu*) with different molecular mixtures were prepared by co-evaporation and were analyzed in-situ by conduction measurements. High admixtures of *H<sub>16</sub>PcCu* in *F<sub>16</sub>PcCu* films disturbed the charge transport, presumably caused by phase separation and the presence of poorly conducting grains of *H<sub>16</sub>PcCu* in the conductive *F<sub>16</sub>PcCu* films. Very low admixtures increased the conductivity, indicating a successful doping of *F<sub>16</sub>PcCu* by *H<sub>16</sub>PcCu*. For pure thin films of *F<sub>16</sub>PcCu* well-defined crystal structures ( $\beta_{\text{bilayer}}$ -structure and  $\beta$ -structure) were determined in the literature and correlated to optical absorption bands. Optical transmission spectroscopy performed for the present films revealed the presence of these structures as expected for the pure films of *F<sub>16</sub>PcCu* and also for low admixtures of *H<sub>16</sub>PcCu* but a disturbance of the *F<sub>16</sub>PcCu* solid state structure was seen for increased admixtures of *H<sub>16</sub>PcCu*. The proportions of the  $\beta_{\text{bilayer}}$ -structure and the  $\beta$ -structure of *F<sub>16</sub>PcCu* were decreased indicating disturbance of the *F<sub>16</sub>PcCu* film growth by a large admixture of *H<sub>16</sub>PcCu*.

DS 44.16 Fri 9:30 Poster E

**Light-induced p-doping of P3HT and P3HT/Fulleren blends by oxygen studied by Photoelectron Spectroscopy —**

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Organic photovoltaic cells (OPVC) based on donor-acceptor blends present a quite new technique for environmental friendly energy conversion although their efficiency and lifetime is currently rather low compared to inorganic solar cells. Detailed understanding of the electronic properties and interface properties (e.g. electrodes or other organic materials) are required to increase efficiency and lifetime. We study the influence of oxygen and light (AM 1.5) on the energy level alignment of Poly(3-hexylthiophene) (P3HT) and P3HT/Fullerene blend films. The samples are alternately exposed to light and oxygen and then annealed. The electronic properties and interface properties are monitored subsequently by X-ray and ultraviolet photoelectron spectroscopy (XPS/UPS) in order to probe both changes in the electronic

structure and the chemical composition of the film. The exposure to light and oxygen leads to reversible and irreversible effects. The reversible effect is an oxygen induced p-doping of the semiconductor whereas the irreversible part is the photooxidation of the polymer which does not alter the electronic structure.

DS 44.17 Fri 9:30 Poster E

**Does NEXAFS provide valuable information on the electronic influence of functional groups? —**

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Motivated by their possible application in organic electronic devices a variety of systematically modified acene derivatives is nowadays investigated. A question that frequently arises is whether the introduction of functional groups (e.g. electronegative fluorine atoms) affects the electronic system by intramolecular dipoles or by direct interaction with the aromatic system. From an experimental point of view this question is not easy accessible, especially for thin films. Our approach is to employ NEXAFS as a versatile tool that gives insight into both: geometric and electronic structure. We investigated differently substituted molecules and addressed functional groups directly by conducting angular dependent NEXAFS experiments at the corresponding absorption K-edge (e.g. F1s, O1s, N1s). In order to interpret these spectra, we contrast them with carbon K-edge spectra of the aromatic backbone and provide a detailed analysis of the origin and dichroism of related resonances. This systematic use of NEXAFS enables us to give further insight into the electronic properties of derivatized acenes.

DS 44.18 Fri 9:30 Poster E

**The influence of typical degradative stresses on the constitutive parts of polymer/fullerene solar cells —**

•VIDA TURKOVIC, SEBASTIAN ENGMANN, ROLAND RÖSCH, HARALD HOPPE, and GERHARD GOBSCH — Technische Universität Ilmenau, Institut für Physik, Experimentalphysik 1, Weimarer Straße 32, 98693 Ilmenau

Improving the long time stability of organic photovoltaics is one of the key issues towards making them competitive with their inorganic counterparts. In order to separately investigate the degradation of the electrodes and the photoactive layer in thin film devices, we developed a simple approach based on ambient and inert atmosphere tests. The devices were characterized with standard spectroscopic measurements and electrical characterization, complemented by large-area imaging methods.

DS 44.19 Fri 9:30 Poster E

**Influence of triplet excitons on the performance and lifetime of polymer-based organic light-emitting diodes —**

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Although large progress has been made in the development of polymer-based organic light-emitting diodes (PLEDs), their lifetime still remains a problematic issue. One of the topics in PLEDs studied to a lesser extent is the influence of the high density of non-emissive triplet excitons on the device lifetime.

In this work, PLEDs with a poly(p-phenylene vinylene) (PPV) derivative are utilized. The influence of triplet excitons on the fatigue of the PLEDs is investigated by increasing their amount in the PPV film. Therefore, PPV singlet excitons are converted to triplets by mixing different concentrations of the triplet sensitizer platinum (II) octaethylporphine ketone (PtOEPK) into the PPV matrix. The increase in the triplet population is characterized by photoluminescence and photoinduced absorption measurements. Both  $t_{50}$  and  $t_{90}$  lifetimes of the diodes are drastically shortened in the presence of PtOEPK, which indicates that the additional triplets might be harmful to the diode stability and lifetime.

DS 44.20 Fri 9:30 Poster E

**Organic semiconductor devices in smart textiles: Challenges while approaching fibre shaped structures —**

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In the development of smart textiles already realized prototypes utilize embedded LEDs, displays or interactive communication devices based on inorganic semiconductor technology. Yet, these wearable smart textiles are not always comfortable since inorganic devices are stiff and rigid. On the other hand, organic electronic devices can be realized on flexible substrates employing very thin active layers of only about 100 nm thickness.

The aim of the present work is to process organic semiconductor based devices directly on fibre surfaces. This task is challenging as manufacturing related problems due to the cylindrical shape of the fibre substrates and their small diameter of about 0.2 mm have to be overcome. Here, we present our findings on the handling of fibre substrates in order to process working devices. In particular, the choice of proper fibre materials, ways to acquire smooth fibre surfaces and the structuring and encapsulation of fibre-shaped devices will be addressed. Additionally, methods to characterize the functionality of the devices will be presented.

DS 44.21 Fri 9:30 Poster E

**IR spectroscopy on metal oxide p-doped thin films of organic semiconductors** — •SVEN TENGELER<sup>1,4</sup>, TOBIAS GLASER<sup>1,4</sup>, SEBASTIAN BECK<sup>1,4</sup>, BERND LUNKENHEIMER<sup>2,4</sup>, DANIELA DONHAUSER<sup>3,4</sup>, and ANNEMARIE PUCCI<sup>1,4</sup> — <sup>1</sup>Universität Heidelberg, Kirchhoff-Institut für Physik, INF 227, 69120 Heidelberg — <sup>2</sup>Universität Mainz, Institut für Physikalische Chemie, Jakob Welder Weg 11, 55099 Mainz — <sup>3</sup>Technische Universität Braunschweig, Institut für Hochfrequenztechnik, Schleinitzstr. 22, 38106 Braunschweig — <sup>4</sup>InnovationLab GmbH, Speyerer Str. 4, 69115 Heidelberg

To understand the underlying mechanisms of electrochemical doping of organic semiconductors, we investigated thin films of the organic ambipolar charge-transport materials N,N'-bis(1-naphthyl)-N,N'-diphenyl-1,1'-biphenyl-4,4'-diamine ( $\alpha$ -NPD) and 4,4'-Bis(N-carbazolyl)-1,1'-biphenyl (CBP), each doped with the inorganic acceptor molybdenum oxide (MoO<sub>3</sub>). The doping efficiency of MoO<sub>3</sub> was analyzed for various doping concentrations and substrate temperatures using in-situ infrared spectroscopy in a UHV setup. We introduce our experimental setup, explain the measured spectra and compare them with DFT-calculations for the neutral as well as the charged matrix molecules in order to estimate the charge-generation efficiency.

Financial support by BMBF (project MESOMERIE) is gratefully acknowledged.

DS 44.22 Fri 9:30 Poster E

**IR spectroscopic studies on charge transfer in thin films of donor-acceptor complexes** — •SEBASTIAN BECK<sup>1,4</sup>, DIANA NANOVA<sup>2,4</sup>, ANDREAS FUCHS<sup>3,4</sup>, CHRISTIAN LENNARTZ<sup>3,4</sup>, TOBIAS GLASER<sup>1,4</sup>, MICHAEL KRÖGER<sup>2,4</sup>, and ANNEMARIE PUCCI<sup>1,4</sup> — <sup>1</sup>Universität Heidelberg, Kirchhoff-Institut für Physik, INF 227, 69120 Heidelberg — <sup>2</sup>Technische Universität Braunschweig, Institut für Hochfrequenztechnik, Schleinitzstr. 22, 38106 Braunschweig — <sup>3</sup>BASF SE, 67056 Ludwigshafen — <sup>4</sup>InnovationLab GmbH, Speyerer Str. 4, 69115 Heidelberg

In the ongoing development of organic electronic devices, new materials with adjustable properties are needed in order to meet different specific requirements. Prototypical examples are the charge transfer complexes (CT complexes) with the acceptor 7,7,8,8-Tetracyanoquinodimethan (TCNQ). In this study, the degree of charge transfer in thin films of organic CT complexes of TCNQ which were deposited via thermal evaporation was determined with infrared spectroscopy. We demonstrate a linear relationship between the shift in the energy of the CN-stretching mode of TCNQ and the charge transfer in the CT complexes. The measured correlation very well agrees with DFT calculations. For N-TCNQ we observe a splitting in the CN-stretching mode peak, which can be explained by the coupling of two modes and was confirmed by the calculations. In CT complexes with partial charge transfer the appearance of an electronic excitation is demonstrated.

Financial support by BMBF (project MESOMERIE) is gratefully acknowledged.

DS 44.23 Fri 9:30 Poster E

**Wavelength dependent pathways in the degradation of P3HT and PCPDTBT** — •ULF DETTINGER<sup>1</sup>, HOLGER HINTZ<sup>1</sup>, CATHARINA SESSLER<sup>1</sup>, HEIKO PEISERT<sup>1</sup>, HANS JOACHIM EGELHAAF<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>Konarka Technologies GmbH, Landgrabenstr. 94, D-90443 Nürnberg, Germany

Organic photovoltaic (OPV) present a promising and cost effective technology for the energy market of the future. Although the race for high efficiencies is still on the run, the stability of the single device materials becomes more and more important. Therefore photo degradation of P3HT and PCPDTBT thin films was investigated under both standard Air Mass 1.5 conditions and single wavelength illumination. The degradation of the materials was monitored using UV/VIS and FTIR transmission spectroscopy. Generally PCPDTBT exhibits an enhanced stability compared to the state of the art material P3HT. The effectiveness of the photo reaction does not follow the absorption spectrum in the case of P3HT suggesting a radical based mechanism which is not initiated by the polymer absorption[1].

[1] H. Hintz, H.J. Egelhaaf, L. Lüer, J. Hauch, H. Peisert, T. Chassé Chem. Mater., 2011, 23 (2), 145-154

DS 44.24 Fri 9:30 Poster E

**Influence of different additives to an organic hole conductor for hybrid photovoltaics** — •INGOLF SEGGER, ULRIKE KUCK, SASCHA HACKMANN, and MATTHIAS WUTTIG — I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

In recent years, remarkably high power conversion efficiencies have been reported for dye sensitized solar cells (DSSCs). Therefore they are considered as a promising candidate for market-relevant thin-film solar cells. However, high performance DSSCs usually employ a liquid iodide-based electrolyte as an essential component for dye regeneration which introduces significant drawbacks for commercialisation like thermal instability and the requirement for highly reliable sealing techniques.

It has been shown that the organic hole conductor 2,2',7,7'-tetrakis(N,N-di-p-methoxyphenylamine)-9,9'-spirobifluorene (spiro-OMeTAD) has the potential to replace the liquid electrolyte in DSSCs. In order to achieve high power conversion efficiencies in such solid-state DSSCs, different additives to spiro-OMeTAD like Lithium bis(trifluoromethylsulfonyl)imide (Li-TFSI) and pyridine derivatives are required. Both optical properties and the electronic structure of materials used in photovoltaics play an important role for device performance. Therefore in this study spiro-OMeTAD thin-films with the addition of those different essential additives were investigated by means of photoluminescence spectroscopy, UV-VIS absorption spectroscopy and photoemission spectroscopy.

DS 44.25 Fri 9:30 Poster E

**Transient spectroscopic studies of high performance PTB7-PCBM films for organic photovoltaics: the effect of processing additive and fullerene absorption** — •CLARE DYER-SMITH, HANNAH MANGOLD, and FRÉDÉRIC LAQUAI — Max-Planck Institut für Polymerforschung, Mainz, Germany

Photovoltaic blends of the thienothiophene-benzodithiophene polymer PTB7 with PC70BM have shown power conversion efficiencies exceeding 7%. Using transient absorption spectroscopy, we study the photoexcitation dynamics in PTB7:PC70BM and PTB7:PC60BM blend films across more than six orders of magnitude in time and across the entire spectral range from the visible to the near-infrared. We observe a fast spectral relaxation in the blend film, as well as a spectral relaxation in the pristine polymer emission detected using picosecond time-resolved fluorescence spectroscopy. We assign the latter to energetic disorder in the polymer, while the assignment of the former is the subject of ongoing investigation. Secondly, we characterize the dynamics of excited states in the heretofore unreported time range from 1 to 100 ns, crucial for the understanding of charge separation and recombination in organic solar cells. Our studies indicate that the use of the processing additive di-iodooctane produces longer lived charges in blend films, despite the presence of a more finely interpenetrating blend morphology and therefore a larger interfacial area. We also study the effect of varying the fullerene acceptor in the blend film to investigate the contribution of light absorption in the fullerene component to charge generation in the solar cell.

DS 44.26 Fri 9:30 Poster E

**Metallic nano-particles embedded in small molecule organic solar cells (OSCs) : Optical and electrical effects.** — •TILL HOHEISEL, ANDREAS HILLE, ANDRÉ MERTEN, MORITZ RIEDE, LUKAS M. ENG, and KARL LEO — IAPP, TU Dresden

OSCs have the potential to provide electrical energy in a resource saving way by combining small material consumption with low temperature production processes in comparison to silicon solar cells. The thickness and absorption in OSCs is currently limited by the mobil-

ity of photo-generated excitons. We have systematically investigated the effect of plasmon active metallic nano-structures for enhancing the electromagnetic field close to the absorbing layers. We show that enhanced absorption inside typical organic solar cell material single layers is due to metallic nano-particles. The electrical effects of metallic nano-particles inside vacuum processed small molecule solar cells are investigated by varying the distance between the nano-particle layer and the absorber layer.

DS 44.27 Fri 9:30 Poster E

**I-V Characteristics of Copper Phthalocyanine Based Laterally Stacked Devices Fabricated by Semiconductor Processing** — ●J. GHOSH<sup>1</sup>, D. REUTER<sup>1</sup>, M. RENNAU<sup>1</sup>, K. HILLER<sup>1</sup>, G. SALVAN<sup>1</sup>, M. FRONK<sup>1</sup>, D.R.T. ZAHN<sup>1</sup>, C. C. BOF BUFON<sup>1,2</sup>, and O. SCHMIDT<sup>1,2</sup> — <sup>1</sup>Chemnitz University of Technology, Germany — <sup>2</sup>Institute for Integrative Nanosciences, IFW Dresden, Germany

This work presents a new approach of fabricating arrays of electrodes, separated by sub-micrometer gaps allowing the systematic investigation of electric properties of organic semiconductors. The laterally stacked devices are fabricated by using a trench isolation technique for separating different electrical potentials, as it is known for micro-machining technologies like Single Crystal Reactive Ion Etching and Metallization (SCREAM). The essential part of this process is the patterning of sub-micrometer trenches onto the silicon substrate in a single lithographic step. Afterwards, the trenches are refilled by SiO<sub>2</sub> to allow the precise tuning of the electrode separation gap. The metal electrodes are formed via magnetron sputtering. This technological approach allows us to fabricate device structures with a transport channel length in the range of 100-250 nm by conventional photolithography. In this experiment, three different metals like Au, Co, and Ni were used as the electrode materials, while copper phthalocyanine, being deposited by thermal evaporation in high vacuum, was employed as the organic semiconductor under evaluation. The correlation, observed between the current across the junction and the gap between the electrodes, can be explained by the space charge limited current model.

DS 44.28 Fri 9:30 Poster E

**Vibrational analysis of thin Zinc Tetraphenylporphyrin films on Si(111)** — ●STEPHAN PETER KATE<sup>1</sup>, KARSTEN HINRICHS<sup>1</sup>, NORBERT ESSER<sup>1</sup>, JÖRG RAPPICH<sup>2</sup>, and SIMONA POP<sup>1</sup> — <sup>1</sup>Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Albert-Einstein Str. 9, Berlin, 12489, Germany — <sup>2</sup>Helmholtz-Zentrum für Materials and Energy GmbH, Kekulestraße 5, Berlin, 12489, Germany

The presented work includes micro-Raman spectroscopy for the analysis of the vibrational modes of the ZnTPP (Zinc Tetraphenylporphyrin) thin films. Resonant Raman spectra are taken with the 458 nm (2.71 eV) Ar-laser line which is located in the spectral range of the B-band. The Raman frequencies are compared for samples with different film thicknesses and ZnTPP crystalline powder. A systematic shift with increasing film thickness is observed for some vibrational modes while others are not affected by the film thickness. The changes in the vibrational bands are discussed with respect to symmetry and in the vibration involved parts of the molecules.

DS 44.29 Fri 9:30 Poster E

**Optical and structural properties of organic heterostructures: PTCDA and SnPc on Au(111)** — ●KRISTIN WACHTER, MARCO GRUENEWALD, MATTHIAS MEISSNER, FALKO SOJKA, ROMAN FORKER, and TORSTEN FRITZ — University of Jena, Institute of Solid State Physics, Max-Wien-Platz 1, 07743 Jena, Germany

The optical and structural properties of organic heterostructures of ultrathin 3,4,9,10-perylenetetracarboxylic-dianhydride (PTCDA) and tin(II)-phthalocyanine (SnPc) films grown on the reconstructed Au(111) surface were investigated by Differential Reflectance Spectroscopy (DRS), Low Energy Electron Diffraction (LEED) and Scanning Tunneling Microscopy (STM) under ultra-high vacuum conditions. The film growth was carried out by organic molecular beam epitaxy (OMBE). In our optical spectra we find clear indications for a strong interaction between the substrate and the first monolayer SnPc and PTCDA, respectively. The overlying PTCDA, however, decouples from the first monolayer. Furthermore, from LEED measurements we conclude a commensurate structure of a SnPc monolayer film on Au(111) at room temperature.

DS 44.30 Fri 9:30 Poster E

**Interface analysis of aluminum doped zinc oxide sputtered on copper phthalocyanine thin films** — ●CATHY JODOCY, IN-

GOLF SEGGER, PATRICK RIES, and MATTHIAS WUTTIG — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Organic electronics have attracted considerable attention due to their wide range of possible applications as well as their suitability for inexpensive and highly scalable processing techniques. Optoelectronic devices like organic solar cells and organic light-emitting diodes with a transparent top electrode are of interest since they allow a larger variety of organic-inorganic layer systems including semitransparent stacks.

We have deposited the transparent conductive oxide (TCO) material aluminum doped zinc oxide (ZnO:Al) as a top cathode above an organic layer. Copper phthalocyanine (CuPc) is an excellent material for the use as a donor in organic heterojunctions in organic solar cells. Furthermore its very rigid crystal structure is supposed to prevent degradation upon the impact of high kinetic energy particles generated during sputter deposition of the TCO. For the deposition of the ZnO:Al thin films we have used a dc magnetron sputtering process whereby layers with an excellent performance can be produced at low temperatures.

In this study a detailed investigation of the interface between sputtered ZnO:Al and the underlying CuPc layer is presented. The influence of sputter damage in the organic layer is characterized with photoelectron spectroscopy and x-ray diffraction measurements.

DS 44.31 Fri 9:30 Poster E

**Study of excited states and a model for exciton-polaron interaction in P3HT** — ●SHINE PHILIP<sup>1</sup>, KLAUS MÜLLER<sup>1</sup>, MATTHIAS RICHTER<sup>1</sup>, MARINUS KUNST<sup>2</sup>, and DIETER SCHMEISSER<sup>1</sup> — <sup>1</sup>Brandenburgische Technische Universität Cottbus, Angewandte Physik-Sensorik, 03046 Cottbus, Germany — <sup>2</sup>Helmholtz-Zentrum Berlin, Institut für Solare Brennstoffe (E-I6), Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Organic semiconductors efficiently harvest light in the region of the solar spectrum due to a high absorption/extinction coefficient. In our work we study the electronic structure and the charge carrier dynamics of polymeric organic semiconductor regioregular poly(3-hexylthiophen-2,5-diyl) (P3HT), an ideal p-type semiconductor and a widely used conjugated polymer, and blends with the fullerene derivative phenyl-C61-butyric acid methyl ester (PCBM), an electron acceptor material. The study was done with the help of time resolved microwave conductivity (TRMC) for contactless investigation of bulk carrier dynamics, optical spectroscopy, ultraviolet photoelectron spectroscopy (UPS) and high resolution X-ray absorption spectroscopy (XAS) which investigates excited states of rr-P3HT. From the data obtained we could infer the positions of the valence and conduction band, the existence of two excitons as well as the co-existence of one dimensional and two dimensional polarons. Based on our spectroscopic data we propose a model in which the scattering of virtual polarons and excitons are shown to create mobile polaronic charge carriers.

DS 44.32 Fri 9:30 Poster E

**Influence of pre-structuring on self-organized pattern formation at organic-metal interfaces - experiment vs. modeling** — ●FLORIAN SZILLAT and S.G. MAYR — Leibniz-Institut fuer Oberflächenmodifizierung, Translationszentrum fuer regenerative Medizin und Fakultät fuer Physik und Geowissenschaften der Universität Leipzig, 04318 Leipzig

Self-organized pattern formation observed during physical vapor deposition of organic materials on inorganic substrates leads to characteristic structure evolution up to film thicknesses of some tens of nanometers. By employing a combined experimental-computational approach we demonstrate the capability of a continuum model to describe structure evolution during poly(bisphenol A)carbonate deposition on rough copper surfaces [1]. The next step on the route to computer-assisted interface engineering is carried out by modeling poly(bisphenol A)carbonate deposition on pre-structured copper surfaces by means of stochastic rate equations. These predictions are compared with experiments on physical vapor deposition experiments with pre-patterned copper substrates, which are subsequently analyzed with atomic force microscopy. This allows conclusions on the underlying physical processes. This project is funded by the German BMBF, PTJ-BIO, Grant Number: 0313909.

[1] F. Szillat and S. G. Mayr, Phys. Rev. B 84, 115462 (2011)

DS 44.33 Fri 9:30 Poster E

**Comparison of Structural Properties of Layers of Different Phthalocyanines on Reconstructed GaAs(001) Surfaces** —

•LINDA RIELE<sup>1,2</sup>, BENJAMIN BUICK<sup>1</sup>, IHOR M. KUPCHAK<sup>3</sup>, BJORN-OVE FINLAND<sup>4</sup>, PATRICK VOGT<sup>2</sup>, and WOLFGANG RICHTER<sup>1</sup> — <sup>1</sup>Università di Roma Tor Vergata, Rome, Italy — <sup>2</sup>TU Berlin, Berlin, Germany — <sup>3</sup>V. Lashkaryov Institute of semiconductor physics NAS, Kyiv, Ukraine — <sup>4</sup>Dept. of Electronics and Telecommunications, NTNU, Trondheim, Norway

The conductivity of organic layers depends crucially on the orientation and ordering of the molecules. Depending on the specific application in optoelectronic or electronic devices, a controlled growth of these layers on inorganic substrates is therefore desired. In this work we present a comparison of Raman scattering experiments of layers (up to 20 nm thick) of planar Cu phthalocyanines, and non-planar Pb phthalocyanines deposited on  $c(4 \times 4)$  and  $(2 \times 4)$  reconstructed surfaces of GaAs(001). The dependence of the molecular order on the surface reconstruction is analyzed by measuring the intensity of the Raman peaks as a function of sample rotation. We observe periodic intensity changes of the Pc vibrational modes with the rotation angle. These periodic changes have a fixed relation to the GaAs substrate phonons. This is an indication for well ordered Pc layers with a fixed geometrical relation to the substrate implying an epitaxial-like growth mode. DFT calculations allow a symmetry assignment of the vibrational modes ( $A_1$ ,  $B_1$ ,  $B_2$ , etc.) and allow consequently model calculations with the different Raman tensors.

DS 44.34 Fri 9:30 Poster E

**Interrelation between Substrate Roughness and Thin-Film Structure of Functionalized Acenes on Graphite** — •TOBIAS BREUER<sup>1</sup>, INGO SALZMANN<sup>2</sup>, JAN GÖTZEN<sup>1</sup>, MARTIN OEHZELT<sup>2</sup>, ANTONIA MORHERR<sup>1</sup>, NORBERT KOCH<sup>2</sup>, and GREGOR WITTE<sup>1</sup> — <sup>1</sup>AG Molekulare Festkörperphysik, Philipps-Universität Marburg, D-35032 Marburg — <sup>2</sup>Institut für Physik, Humboldt-Universität zu Berlin, D-12489 Berlin

We analyzed the growth of differently modified pentacenes (perfluoropentacene (PFP) and pentacenetetrone (P-TET)) on graphite and demonstrate that both, the resulting morphology and the crystalline structure of the films, critically depend on the microroughness of the substrate. On well-ordered highly oriented pyrolytic graphite (HOPG) surfaces prepared by exfoliation, both molecular materials form exceptionally smooth films, which consist of large-area molecularly flat islands yielding an overall low roughness. Interestingly, in these films molecules adopt a recumbent orientation, while on defective substrates, created by brief ion sputtering, the molecules adopt an upright orientation and form nonconnected islands exhibiting a significantly increased film roughness. Our study not only underlines the possibility to prepare very smooth films on a weakly interacting substrate but also emphasizes the importance of a proper substrate preparation and the significance of precise knowledge of substrate-surface properties to control the resulting structure of organic films.

[1] J. Götzén et al., Phys. Rev. B 81, 0854406 (2010).

[2] T. Breuer et al., Cryst. Growth Des. 11, 4996 (2011).

DS 44.35 Fri 9:30 Poster E

**Investigation of the structure and electronic alignment of PTCDI-C13 thin films on metal surfaces** — •DANIEL GEBAUER, PHILIP SCHULZ, DOMINIK MEYER, and MATTHIAS WUTTIG — I. Institute of Physics (IA), RWTH Aachen University, D-52056 Aachen, Germany

N,N'-Ditridecylperylene-3,4,9,10-tetracarboxylic diimide (PTCDI-C13) is a promising acceptor material for organic solar cells. To fully utilize the potential of this material, the growth of thin films of PTCDI-C13 has been studied. Particular attention has been devoted to understanding the electronic and chemical properties of the interface between the organic layer and the metal contact. The interaction between the PTCDI-C13 and the metal strongly influences the charge carrier transport mechanisms and thus the efficiency of the solar cell. In this study thin films of PTCDI-C13 with a thickness varying from single monolayers up to 20 nm, have been evaporated on Au, Ag, Cu and Al surfaces. The energy level alignment between the valence band of each metal and the frontier molecular orbitals of the subsequently deposited organic layer has been determined by Ultraviolet Photoelectron Spectroscopy (UPS). The chemical bonding is investigated by X-ray Photoelectron Spectroscopy (XPS). Finally, the nature of the interaction between the organic layer and the metal surface has been determined from the formation of interface states and the position of the energy levels.

DS 44.36 Fri 9:30 Poster E

**A multitechnique investigation of substituted pentacene**

**nanorods** — •SABINE-ANTONIA SAVU<sup>1</sup>, SIMON SCHUNDELMAIER<sup>1</sup>, SABINE ABB<sup>1</sup>, CHRISTINA TÖNSHOFF<sup>2</sup>, HOLGER F. BETTINGER<sup>2</sup>, MARIA BENEDETTA CASU<sup>1</sup>, and THOMAS CHASSÉ<sup>1</sup> — <sup>1</sup>Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Tübingen, Deutschland — <sup>2</sup>Institut für Organische Chemie, Universität Tübingen, Tübingen, Deutschland

We report our investigation on nanorods of two newly synthesized substituted pentacenes by using X-ray photoemission spectroscopy (XPS), near edge X-ray absorption fine structure (NEXAFS) spectroscopy, and atomic force microscopy (AFM). The nanorods were deposited on Au(111). We have analyzed the photoemission spectra in detail by using a fitting procedure. XPS thickness dependent spectra show a different screening of the core-hole at the interface, while NEXAFS investigations suggest a molecular arrangement similar to what reported for pentacene thin films. In addition, the morphology of the nanorods has been investigated by using AFM, evaluating the nanorod characteristics also from a statistical point of view.

DS 44.37 Fri 9:30 Poster E

**FePc/metals: Influence of the 3d-open shell on the interface properties** — •FOTINI PETRAKI<sup>1</sup>, HEIKO PEISERT<sup>1</sup>, FLORIAN LATTEYER<sup>1</sup>, UMUT AYGÜL<sup>1</sup>, JOHANNES UIHLEIN<sup>1</sup>, ANTJE VOLLMER<sup>2</sup>, and THOMAS CHASSÉ<sup>1</sup> — <sup>1</sup>Universität Tübingen, IPTC, Auf der Morgenstelle 18, 72076 Tübingen, Germany — <sup>2</sup>Helmholtz Zentrum Berlin für Materialien und Energie, Elektronenspeicherring BESSY II, Albert-Einstein-Str. 15, 12489 Berlin, Germany

The present work is focused on transition metal phthalocyanines (TM-Pcs) and in particular, on iron phthalocyanine (FePc), a two dimensional MPC where the central atom is a Fe<sup>2+</sup> ion. The magnetic properties of such molecules depend strongly on the electronic configuration of the central metal atom, and in particular, the occupation of the 3d-related states. Recent studies, on TMPcs (TM: Co, Mn) by X-ray absorption (XAS) and resonant photoemission spectroscopy (ResPES) revealed a quite strong interaction between the TM and metallic substrates through charge transfer towards the 3d unoccupied electronic states. The investigation of FePc/ Au(100) and FePc/ Ag(111) interfaces by XAS and ResPES confirmed strong interactions also at these interfaces. The detailed electronic configuration however, depends on the substrate under consideration. Effects of chemical changes during the interface formation in terms of different oxidation state for the Fe-ion were detected also by XPS, confirming the partial filling of the 3d-open shell of Fe from electrons coming from the metallic substrate. From resonant PES measurements at the Fe-edge information on the local electronic structure of the occupied orbitals was also obtained.

DS 44.38 Fri 9:30 Poster E

**Ultrathin oligothiophene films for organic electronics applications** — •NINA ARZT<sup>1</sup>, BENEDIKT RÖSNER<sup>1</sup>, ANDREAS SPÄTH<sup>1</sup>, NORMAN SCHMIDT<sup>1</sup>, HANNES SCHULZ<sup>2</sup>, and RAINER FINK<sup>1</sup> — <sup>1</sup>Universität Erlangen-Nürnberg, Department Chemie u. Pharmazie, Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen, Germany — <sup>2</sup>Universität Erlangen-Nürnberg, Department Chemie u. Pharmazie, Theoretische Chemie, Egerlandstr. 3, 91058 Erlangen, Germany

Oligothiophenes are attracting major attention due to their potential application as semiconducting material for cheap, flexible and large-area electronic devices such as organic field effect transistors [1]. For their successful preparation homogenous and highly ordered thin films of the semiconductor material are required. We have successfully studied two different kinds of oligothiophenes with respect to their local arrangements. From low-energy electron diffraction (LEED) we deduce long-range ordered films of flat-lying molecules when deposited on Ag(100) single crystals. In contrast, the utilization of Si<sub>3</sub>N<sub>4</sub> membranes, small domains are observed in scanning transmission X-ray microspectroscopy (STXM). Furthermore, NEXAFS studies using the PoLux-STXM installed at the Swiss Light Source offers more direct insight into the electronic structure of these microcrystalline films. We discuss the crystal growth properties considering the specific interface interactions. The work is funded by the BMBF, project 05 K10WEA.

[1] M. Halik, H. Klauk, U. Zschieschang, G. Schmid, S. Ponomarenko, S. Kirchmeyer, W. Weber, Adv. Mater., 2003, 15, 917-922.

DS 44.39 Fri 9:30 Poster E

**Nucleation of Perylene films on SAM-covered Gold Surfaces** — •ANDRÉ PICK and GREGOR WITTE — Molekulare Festkörperphysik, Philipps-Universität Marburg, Germany

Previous studies have demonstrated the ability to control the nucle-

ation of organic semiconductor films on a micron scale by patterning of silicon dioxide substrates by means of micro contact printing of self-assembled monolayers. In that way arrays of organic micro-crystallites have been fabricated that are well suited for the fabrication of organic field-effect transistors (OFETs) [1]. It was found that the roughness of stamped domains of the used octadecyltrichlorosilane (OTS), the chemical termination and the mechanical contrast are critical parameters for selective crystal nucleation. To analyze microscopic mechanisms of this nucleation more qualitatively, we have studied the initial stage of growth of perylene (PER) films on gold surfaces that were pre-treated with aliphatic organothiol SAMs of various chain length and different chemical termination. Substrates were coated by the SAMs either homogeneously or selectively by using micro-contact printing. PER films were prepared by molecular beam deposition under vacuum conditions and the resulting film structures were characterized by means of atomic force microscopy. Moreover, to study the influence of substrate roughness these experiments have been carried out on single crystalline Au(111)/mica and poly-crystalline gold substrates. The observed variety of PER structures indicate that the actual film thickness of the thiol layer is an important parameter which will be discussed.

[1] A.L. Briseno et al., *Nature* Vol. 444, 913 (2006)

DS 44.40 Fri 9:30 Poster E

**Structural properties of molecular mixtures of pentacene and diindenoperylene** — •ANTJE AUFDERHEIDE<sup>1</sup>, KATHARINA BROCH<sup>1</sup>, JIŘÍ NOVÁK<sup>1</sup>, ALEXANDER HINDERHOFER<sup>1</sup>, ROBERTO NERVO<sup>2</sup>, RUPAK BANERJEE<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>ESRF, 6 Rue Jules Horowitz, BP 220, 38043 Grenoble Cedex 9, France

We investigate mixtures of pentacene (PEN) and diindenoperylene (DIP) with different mixing ratios using x-ray reflectivity (XRR) and grazing incidence x-ray diffraction (GIXD). With a multilayer model we fit the reflectivity data including the first-order Bragg peak. Furthermore, we determine the coherent island size from the GIXD peak widths. Using the results of the in- and out-of-plane measurements we determine the ordering behavior which changes with the mixing ratio [1] and compare it with mixtures of similar molecules [2,3]. A first approach to a phenomenological description of the mixed film structure is made.

[1] A. Aufderheide et al., in preparation [2] A. Hinderhofer et al., *J. Chem. Phys.*, **134**, 104702 (2011). [3] J. P. Reinhardt et al., in preparation

DS 44.41 Fri 9:30 Poster E

**Impact of the 3d-electronic states of nickel and manganese phthalocyanines on electronic interface properties to metal substrates** — •JOHANNES UIHLEIN<sup>1</sup>, UMUT AYĞÜL<sup>1</sup>, FOTINI PETRAKI<sup>1</sup>, FLORIAN LATTEYER<sup>1</sup>, PATRICK HOFFMANN<sup>2</sup>, ANTJE VOLLMER<sup>2</sup>, HEIKO PEISERT<sup>1</sup>, and THOMAS CHASSÉ<sup>1</sup> — <sup>1</sup>Universität Tübingen, IPTC, Auf der Morgenstelle 18, 72076 Tübingen, Germany — <sup>2</sup>Helmholtz Zentrum Berlin für Materialien und Energie, Elektronenspeicherring BESSY II, Albert-Einstein-Str. 15, 12489 Berlin, Germany

In recent years there has been growing interest in the field of thin organic semiconducting films due to their successful application in optical and electronic devices. Transition-metal phthalocyanines (TMPc) are a promising class of organic semiconductors with remarkable electronic and magnetic properties and they are capable candidates for future applications. The electronic configuration of the central metal atom strongly affects the electronic properties of such molecules in thin films and of corresponding interfaces [1]. Interactions at the interface between transition-metal phthalocyanines (MnPc, NiPc) and single-crystalline metal substrates (Au(100), Ag(111)) are studied using X-ray absorption (XAS) and photoemission spectroscopy. In all cases, charge transfer processes from metallic substrates to the metal 3d levels of the phthalocyanine are found. However, the detailed electronic situation depends clearly on the system under consideration.

[1] F. Petraki et. al., *J. Phys. Chem. C* **115** (2011), 21334-21340.

DS 44.42 Fri 9:30 Poster E

**Impact of Annealing of Structural, Optical and Electrical Properties of CoPc thin films** — HUSAM EL-NASSER<sup>1</sup>, •DOMINIK MEYER<sup>2</sup>, PHILIP SCHULZ<sup>2</sup>, CHRISTIAN EFFERTZ<sup>2</sup>, and MATTHIAS WUTTIG<sup>2</sup> — <sup>1</sup>Departement of Physics, Al al-Bayt University, Mafraq-Jordan — <sup>2</sup>I. Institute of Physics (IA), RWTH Aachen University, Germany

Organic materials are well known for their high potential as cost-efficient alternatives in the field of thin film based optoelectronic devices. Especially the wide range of possible materials offers promising opportunities to tailor crucial optical and electronic properties of the functional layers. Metal-phthalocyanines are commonly employed as p-type semiconducting layer in organic electronics. Yet the choice of the central metal atom has significant impact on the inter- and intramolecular characteristics. In this study we investigate structural, optical and electrical properties of cobalt-phthalocyanine (CoPc) as an alternative to the regularly used CuPc and ZnPc with a wide range of analytical setups. The XRD diffraction pattern present CoPc to be of high crystal order with a single sharp peak at  $2\theta = 6.9^\circ$  corresponding to an interlayer spacing of  $d = 12.72 \text{ \AA}$ . Subsequent annealing revealed an increase of the mean grain size from 11 nm to 26 nm for the as deposited and annealed samples, respectively. The effect of annealing to optical constants as well as the charge carrier mobility is analyzed. Finally, we conclude on the impact of annealing affects to improve the suitability of this molecule for optoelectronic applications and to understand the driving forces in thin film formation and charge transport.

DS 44.43 Fri 9:30 Poster E

**Influence of chemical transformation on molecular orientation and surface texture of aluminium and gallium phthalocyanines thin films** — •FLORIAN LATTEYER<sup>1</sup>, TAMARA BASOVA<sup>2</sup>, VITALY KISELEV<sup>3</sup>, HEIKO PEISERT<sup>1</sup>, and THOMAS CHASSÉ<sup>1</sup> — <sup>1</sup>Universität Tübingen, IPTC, Auf der Morgenstelle 18, 72076 Tübingen, Germany. — <sup>2</sup>Nikolaev Institute of Inorganic Chemistry SB RAS, 630090 Novosibirsk, Russia. — <sup>3</sup>Institute of Chemical Kinetics and Combustion SB RAS, 630090 Novosibirsk, Russia.

The chemical transformation of aluminium and gallium phthalocyanines (AlClPc and GaClPc) in thin films to the mu-(oxo)dimers (PcAl)2O and (PcGa)2O has been investigated. IR, Raman, and XPS spectroscopies, as well as quantum chemical computations (DFT) were employed to study the structure of the films before and after annealing. It has been found that the annealing of AlClPc and GaClPc thin films in the presence of humidified nitrogen resulted in the formation of the corresponding mu-(oxo)dimers (PcAl)2O and (PcGa)2O. On the other hand, the annealing of the same films in the presence of oxygen led, beside to the formation of mu-(oxo)dimers, to a partial degradation and consequently to a parallel reaction. The structure changes of the thin films during annealing were studied using in situ Raman spectroscopy and AFM technique. Both, the initial AlClPc film and the obtained mu-(oxo)dimer (PcAl)2O film formed after annealing were disordered. At the same time, the molecules of the mu-(oxo)dimer (PcGa)2O formed out of GaClPc turned out to form a preferential standing orientation with respect to the substrate surface.

DS 44.44 Fri 9:30 Poster E

**In situ X-ray diffraction on mixed pentacene - perfluoropentacene thin films** — •CHRISTIAN FRANK<sup>1</sup>, JIŘÍ NOVÁK<sup>1</sup>, ALEXANDER GERLACH<sup>1</sup>, ALEXANDER HINDERHOFER<sup>1</sup>, ROBERTO NERVO<sup>2</sup>, KATHARINA BROCH<sup>1</sup>, GIOVANNI LIGORIO<sup>1</sup>, and FRANK SCHREIBER<sup>1</sup> — <sup>1</sup>Institut für Angewandte Physik, Universität Tübingen, Germany — <sup>2</sup>ESRF, Grenoble, France

Using X-ray diffraction [1] and optical spectroscopy [2] we have studied binary mixtures on SiO<sub>x</sub>, consisting of pentacene (PEN) and perfluorinated-pentacene (PFP). For films with different mixing ratios we investigate the coexistence of the two mixed PEN:PFP phases together with the phases of the pure molecules. We show, that the  $\sigma$ -phase, with its long molecular axis oriented nearly perpendicular to the substrate is thermally stable, whereas the appearance of the  $\lambda$ -phase with its molecules lying flat, is induced by low temperatures. Based on previous results [1,3], the growth of these films is studied in real-time to measure the evolution of the coherent island size for both phases: We find that for PFP<sub>1</sub>:PEN<sub>2</sub>-mixtures the nucleation of the  $\lambda$ -phase is significantly retarded compared to PFP<sub>2</sub>:PEN<sub>1</sub>-mixtures. The study is complemented with a temperature series of pure PFP and post-growth measurements. [1] A. Hinderhofer, C. Frank, T. Hosokai, A. Resta, A. Gerlach, and F. Schreiber, *J. Chem. Phys.* **134** (2011), 104702. [2] K. Broch, U. Heinemeyer, A. Hinderhofer, F. Anger, R. Scholz, A. Gerlach, and F. Schreiber, *Phys. Rev. B* **83** (2011), 245307. [3] S. Kowarik, A. Gerlach, S. Sellner, F. Schreiber, L. Cavalcanti, and O. Konovalov, *Phys. Rev. Lett.* **96** (2006), 125504.

DS 44.45 Fri 9:30 Poster E

**Interface Effects on Soret Band Excitations in Magnesium-**



**Tetraphenylporphyrin Thin Films observed by Second-Harmonic Generation Spectroscopy** — ●JAN METJE, KLAUS STALLBERG, and WINFRIED DAUM — Institute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld

MgTPP films with thicknesses from 10 to 40 nm evaporated in UHV conditions on fused silica were studied using optical second-harmonic generation (SHG), UV-VIS absorption spectroscopy and AFM. The SHG spectra of the films exhibit two resonances in the spectral region of the Soret band of the molecule ( $S_0 \rightarrow S_2$ ) at 2.95 eV and at about 2.7 eV. The 2.95 eV band agrees in energy with that of MgTPP molecules dissolved in benzene, indicating the presence of weakly interacting molecules. The 2.7 eV SHG band is strongly red-shifted with respect to the Soret band of the aggregated bulk molecules of the film, for which our UV-VIS spectra show an absorption band at 2.81 eV. SHG spectra from films deposited on oxidized Si(100) allow us to relate the SHG strength of the porphyrin bands to that of the silicon  $E_1$  interband transitions. The comparatively weak porphyrin SHG signals indicate an interface effect. The low energy of 2.7 eV in comparison to the bulk transition energy points to strongly interacting molecules presumably located at the  $\text{SiO}_2/\text{MgTPP}$  interface.

Work supported by the NTH School for Contacts in Nanosystems

DS 44.46 Fri 9:30 Poster E

**BioRef - the new, versatile reflectometer at HZB** — ●MARCUS TRAPP<sup>1</sup>, MARTIN KREUZER<sup>2</sup>, MARKUS STROBL<sup>3</sup>, MICHAEL GRUNZE<sup>1</sup>, REINER DAHNT<sup>1</sup>, and ROLAND STEITZ<sup>2</sup> — <sup>1</sup>Universität Heidelberg — <sup>2</sup>Helmholtz Zentrum Berlin — <sup>3</sup>European Spallation Source AB

The BioRef reflectometer was built in collaboration between the University of Heidelberg and the Helmholtz Zentrum Berlin (HZB). It offers the unique possibility to combine neutron reflectivity and in situ ATR-FTIR measurement on a sample at the same time. Despite these unique features an upgrade of the instrument is in progress in order to expand its capabilities even further.

The upgrade in progress will increase the available wavelength resolution up to 11% at a constant  $\Delta\lambda/\lambda$  and will allow to resolve lateral structure with high resolution using the spin echo resolved grating incidence technique (SERGIS).

The recent development of the instrument as well as further perspectives will be presented.

DS 44.47 Fri 9:30 Poster E

**Investigation of the electronic properties of FePc by photoemission spectroscopy** — ●QURATULAIN TARIQ, SUSI LINDNER, and MARTIN KNUFFER — IFW Dresden, HelmholtzStr. 20, 01069 Dresden

Recently there has been much interest in the fundamental processes at the interfaces involving organic semiconductors and metals, since they represent a key factor in nearly all important aspects of device performance. Transition metal phthalocyanines have already obtained substantial attention of researchers due to many different potential applications in organic light emitting diodes, organic field effect transistors, organic photovoltaic cells and organic spintronic devices. Surface and interface analytical studies have generated critical insight into these fundamental processes at the interfaces. We investigate the electronic properties of iron phthalocyanine on noble metal single crystals using x-ray photoemission spectroscopy and valence band ultra-violet photoemission spectroscopy.

DS 44.48 Fri 9:30 Poster E

**Spin-coating of Metal-organic Structures and (Magnetooptical Characterization** — ●FRANK LUNGWITZ<sup>1</sup>, MICHAEL FRONK<sup>1</sup>, FREDERIK SCHLEIFE<sup>2</sup>, DIETRICH R.T. ZAHN<sup>1</sup>, and GEORGETA SALVAN<sup>1</sup> — <sup>1</sup>Physics Department, Chemnitz University of Technology, Chemnitz, Germany — <sup>2</sup>Chemistry Department, Universität Leipzig, Leipzig, Germany

Optical and magneto-optical characterization of molecular complexes is an important tool for the development of molecular spintronic devices. The technique of spin-coating for preparing thin films ( $\sim 50$  nm to 100 nm) is often used for molecules which are not stable at higher temperatures required for preparation techniques like organic molecular beam deposition (OMBD). Here the spin-coating process is optimized for several organic molecules with multiple metal centres.

The silicon substrates are coated with a solution of the investigated material in a solvent, e.g. methanol. To prevent or at least minimize external influences the spin-coating process is performed in a glove-box under nitrogen atmosphere.

The first step of characterization is to determine the actual film thickness and the optical constants of the material using variable angle spectroscopic ellipsometry (VASE). In addition, layer properties like roughness, inhomogeneity, or optical anisotropy are derived from the VASE data. The polar magneto-optical Kerr effect measurements are used to determine magnetic properties and the Voigt constant of the material.

DS 44.49 Fri 9:30 Poster E

**Influence of metal nanoparticles on the optical properties of molecular thin films** — ●VERENA KOLB<sup>1</sup>, NADEZDA TARAKINA<sup>2</sup>, JOCHEN MANARA<sup>4</sup>, ANDRÉS GUERRERO MARTÍNEZ<sup>3</sup>, and JENS PFLAUM<sup>1,4</sup> — <sup>1</sup>Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — <sup>2</sup>Experimental Physics III, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — <sup>3</sup>Departamento de Química Física, Universidade de Vigo, 36310 Vigo, Spain — <sup>4</sup>ZAE Bayern, D-97074 Würzburg

Utilization of plasmonic effects at metal nanoparticle surfaces provides an interesting approach to modify the optical properties of molecular thin films and thereby, to enhance their effective absorption. This enhancement is caused by an increase of the near-field component and the scattering of incident light and might be applied in e.g. organic photovoltaic (OPV) cells. In this contribution we present our latest results on synthesis and characterization of metallic nanoparticles. Silver nanocubes were prepared by wet-chemistry from  $\text{CF}_3\text{COOAg}$ -precursor. Complementary structural investigation by TEM, REM and X-ray confirmed the cubic morphology and single crystallinity. By UV-VIS spectroscopy the characteristic spectral features related to the plasmonic resonances of the nanoparticles were identified. Finally, the particles were embedded in an ITO/PEDOT:PSS/DIP layer structure, in analogy to standard OPV architectures, to analyze their influence on optical properties of the active molecular layer by Raman-spectroscopy.

DS 44.50 Fri 9:30 Poster E

**Organophosphonate monolayer functionalization of planar and nano-porous aluminum oxide** — ●ANSHUMA PATHAK<sup>1</sup>, BJÖRN BRAUNSCHWEIG<sup>2</sup>, ACHYUT BORA<sup>1</sup>, HONGDAN YAN<sup>3</sup>, PETER LEMMENS<sup>3</sup>, WINFRIED DAUM<sup>4</sup>, and MARC TORNOW<sup>1</sup> — <sup>1</sup>IHT, TU Braunschweig, Germany — <sup>2</sup>LFG, University of Erlangen-Nuremberg, Germany — <sup>3</sup>IPKM, TU Braunschweig, Germany — <sup>4</sup>IEPT, TU Clausthal, Germany

Self-assembled monolayers (SAMs) of molecules on metal oxides are of increasing interest for organic electronics. We have deposited SAMs of aliphatic organophosphonates on different aluminum oxide substrates, including sapphire, polycrystalline  $\text{Al}/\text{Al}_2\text{O}_3$  and nano-porous, amorphous aluminum oxide (AAO). Water contact angles in the range 95–120° and AFM measurements with RMS roughness down to  $\sim 0.2$  nm revealed homogeneous SAM formation. We used FTIR and Sum Frequency Generation (SFG) spectroscopy to investigate the molecular ordering of the layers. The positions of the asymmetric and symmetric  $\text{CH}_2$  vibrational peaks determined by FTIR were below  $2918\text{ cm}^{-1}$  and below  $2850\text{ cm}^{-1}$ , respectively, indicating densely packed, crystalline layers. Remarkably, we observed only very small or even no intensity of  $\text{CH}_2$  peaks in the SFG spectra on sapphire and AAO. We conclude that the molecules in these SAMs are highly organized, practically in an all-trans conformation.

Work supported by the NTH School for Contacts in Nanosystems and by the Braunschweig International Graduate School of Metrology (IGSM).

DS 44.51 Fri 9:30 Poster E

**Raman Spectroscopy on Potassium Doped Manganese Phthalocyanine Thin Films** — ●MICHAEL LUDEMANN<sup>1</sup>, BENJAMIN MAHNS<sup>2</sup>, OVIDIU D. GORDAN<sup>1</sup>, MARTIN KNUFFER<sup>2</sup>, and DIETRICH R.T. ZAHN<sup>1</sup> — <sup>1</sup>TU Chemnitz, 09126 Chemnitz, Germany — <sup>2</sup>IFW Dresden, 01069 Dresden, Germany

Alkali metals are well known as electron donors due to their strongly electropositive character. On the other hand, phthalocyanines are a known class of very stable organic molecules. Here, the influence of potassium intercalation on manganese phthalocyanine (MnPc), an archetype magnetic molecule, is investigated by *in situ* Raman spectroscopy. MnPc thin films ( $\leq 10$  nm) are prepared by organic molecular beam deposition (OMBD) in ultra-high vacuum (UHV) conditions and potassium is evaporated afterwards. Charge transfer from the potassium atoms to MnPc leading to negatively charged MnPc molecules is clearly observed by pronounced spectral changes in the Raman spectra. In combination with theoretical results the amount of



charge per molecule was analysed.

DS 44.52 Fri 9:30 Poster E

**Ellipsometry and UPS-IPS Measurements on MnPc Layers on Silicon** — •FRANCISC HAIDU, DANIEL LEHMANN, MICHAEL FRONK, GEORGETA SALVAN, and DIETRICH R. T. ZAHN — Chemnitz University of Technology, Semiconductor Physics, D-09107 Chemnitz, Germany

Spectroscopic Ellipsometry (SE) is an elegant technique to monitor in situ changes in the optical response of thin films. Moreover, physical quantities, e.g. optical constants and optical band gap can be determined from the data evaluation. The transport band gap can be determined using the combination of Ultraviolet Photoelectron Spectroscopy (UPS) with Inverse Photoelectron Spectroscopy (IPS). Phthalocyanines, in general, are well known for their physical and chemical stability. Manganese Phthalocyanine (MnPc), in contrast, has high affinity towards oxygen. MnPc thin films were studied by in situ SE and UPS in combination with IPS. Monitoring by SE was performed during thermally evaporating onto Si substrates and during exposure of the MnPc films to air, clean oxygen, and nitrogen, respectively. We see changes in the optical response due to oxidation. The optical band gap as obtained from the SE data is compared to the transport gap derived from UPS-IPS measurements.

DS 44.53 Fri 9:30 Poster E

**Protective Layer on Indexable Inserts** — •DUSTIN FISCHER, MARIO ESCHNER, JAN GLÜHMANN, CHRISTINE LORENZ, ANDREAS NEIDHARDT, CHRISTEL REINHOLD, ULLRICH REINHOLD, MICHAEL SCHNEEWEISS, and HANS-DIETER SCHNABEL — Westsächsische Hochschule Zwickau, University of Applied Sciences, Leupold-Institut, 08056 Zwickau, Germany

The use of uncoated indexable inserts and micro tools is a common procedure for cutting metals. In order to achieve an effective removal of material, a uniform abrasion is required at the cutting edge of the tool. Despite great thermal resistance of the tool there is a high risk of oxidation at high temperatures so that the sealing of the inserts is indicated. An aluminium oxide ( $\text{Al}_2\text{O}_3$ ) coating performed by Atomic Layer Deposition is a method to positively influence the cutting parameters as well as the wear and tear.

DS 44.54 Fri 9:30 Poster E

**Optical Properties of Alucone Thin Films and Composite Materials** — •LILIT GHAZARYAN, ADRIANA SZEGHALMI, ERNST-BERNHARD KLEY, and ANDREAS TÜNNERMANN — Institute of Applied Physics, Friedrich Schiller University, Jena, Germany

Atomic layer deposition (ALD) is a powerful thin film coating technique that allows to precisely controlling the film thickness of inorganic coatings based on sequential self-limiting surface reactions. Similar to ALD, molecular layer deposition (MLD) enables growing completely organic or organic-inorganic hybrid polymer thin films typically using bi- or multifunctional monomers. One class of such hybrid polymers alucones had been recently grown with MLD using trimethylaluminium (TMA) as inorganic and ethylene glycol (EG) as organic constituent. In this contribution we have investigated the optical properties of alucone thin films prepared by MLD for possible applications as low refractive index optical coatings. The refractive index of the film can be precisely controlled through the composition of the coating. Using various bifunctional organic precursors it is possible to adjust the refractive index of the coating film in a controlled manner. Hybrid organic/inorganic nanolaminates have been deposited with ALD aluminium oxide and MLD alucone layers. By calcination of alucone layers at elevated temperatures it is possible to tune the refractive index of the coating to desired value. These films may find application in graded refractive index optical elements.

DS 44.55 Fri 9:30 Poster E

**Optical Properties of Alucone Thin Films and Composite Materials** — •LILIT GHAZARYAN, ADRIANA SZEGHALMI, ERNST-BERNHARD KLEY, and ANDREAS TÜNNERMANN — Institute of Applied Physics, Friedrich Schiller University, Jena, Germany

Atomic layer deposition (ALD) is a powerful thin film coating technique that allows to precisely controlling the film thickness of inorganic coatings based on sequential self-limiting surface reactions. Similar to ALD, molecular layer deposition (MLD) enables growing completely organic or organic-inorganic hybrid polymer thin films typically using bi- or multifunctional monomers. One class of such hybrid polymers

alucones had been recently grown with MLD using trimethylaluminium (TMA) as inorganic and ethylene glycol (EG) as organic constituent. In this contribution we have investigated the optical properties of alucone thin films prepared by MLD for possible applications as low refractive index optical coatings. The refractive index of the film can be precisely controlled through the composition of the coating. Using various bifunctional organic precursors it is possible to adjust the refractive index of the coating film in a controlled manner. Hybrid organic/inorganic nanolaminates have been deposited with ALD aluminium oxide and MLD alucone layers. By calcination of alucone layers at elevated temperatures it is possible to tune the refractive index of the coating to desired value. These films may find application in graded refractive index optical elements.

DS 44.56 Fri 9:30 Poster E

**Guided mode resonance sensors for monitoring film nucleation in atomic layer deposition** — •ADRIANA SZEGHALMI, HAIYUE YANG, ERNST BERNHARD KLEY, and ANDREAS TÜNNERMANN — Institute of Applied Physics, Friedrich Schiller University, Jena, Germany

Thin films produced by atomic layer deposition (ALD) have interesting electrical, optical, catalytic applications. It is well known that the film growth rate in the ALD process is constant, and the ALD film thickness can be precisely controlled through the number of ALD cycles. However, the effect of the substrate surface on the nucleation of the ALD layers is generally unexplored. The surface chemistry will influence the adsorption of the precursors. Depending on the surface material, the film growth might be constant, substrate-inhibited, or substrate-enhanced. The main challenge in the study of ALD film nucleation is the development of in situ detection methods with atomic sensitivity to trace very small amounts of film growing on the substrate surface. Here, we developed guided mode resonance grating (GMRG) sensors for the in situ detection of sub-nm thin coatings. The nucleation of  $\text{TiO}_2$  on  $\text{Al}_2\text{O}_3$  surface has been monitored. The GMRG sensor indicates the formation of ca. 4 Ångström titania on the alumina surface after two cycles, and a constant growth rate (ca. 0.4 Ångström/cycle) afterwards. Hence, the number of reactive sites on the  $\text{Al}_2\text{O}_3$  surface (OH groups) is much larger than on  $\text{TiO}_2$ . The coverage of alumina with titania is rapidly completed within the first two cycles. The titania layer is already continuous at a film thickness of 4 Ångström.

DS 44.57 Fri 9:30 Poster E

**Atomic Layer Deposition of Strontium Titanate using TDMAT and AbsoluteSr** — •SOLVEIG RENTROP, THERESA MOEBUS, BARBARA ABENDROTH, and DIRK C. MEYER — TU Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Straße 23, 09596 Freiberg

Atomic layer deposition (ALD) is a well-known technique used for binary systems in industry. Ternary oxides are desirable for high-k-dielectrics und resistive switching memories. Here we present preliminary studies on deposition of  $\text{SrTiO}_3$  as a model system for ternary oxides. The used precursors in the ALD system are TDMAT, AbsoluteSr and  $\text{H}_2\text{O}$ . At this we have succeeded optimized  $\text{TiO}_2$  layers in a temperature range from 323K up to a maximum temperature of 593 K, whereby the purge time for a deposition at 593 K has to be a little higher. At time we are going to optimize  $\text{SrO}$  layers. Because of the TDMAT temperature limit and the fact that AbsoluteSr is only reactive from 573 K, the precursors merely overlap in this range. Fabrication of  $\text{SrTiO}_3$  may be facilitated by using StarTi as a precursor since it has an ALD window with temperatures better comparable to AbsoluteSr.

DS 44.58 Fri 9:30 Poster E

**Variation of the growth behavior of copper oxide deposited via ALD on thermally pretreated CNTs** — •MARCEL MELZER<sup>1</sup>, THOMAS WAECHTLER<sup>1,2</sup>, STEVE MUELLER<sup>2</sup>, HOLGER FIEDLER<sup>2</sup>, SASCHA HERMANN<sup>1,2</sup>, RAUL D. RODRIGUEZ<sup>3</sup>, ALEXANDER VILLABONA<sup>3</sup>, ANDREA SENDZIK<sup>3</sup>, ROBERT MOTHES<sup>4</sup>, STEFAN E. SCHULZ<sup>1,2</sup>, THOMAS GESSNER<sup>1,2</sup>, DIETRICH R.T. ZAHN<sup>3</sup>, MICHAEL HIETSCHOLD<sup>3</sup>, and HEINRICH LANG<sup>4</sup> — <sup>1</sup>Fraunhofer Institute for Electronic Nano Systems (ENAS), Technologie-Campus 3, D-09126 Chemnitz, Germany — <sup>2</sup>Center for Microtechnologies, Chemnitz University of Technology, D-09107 Chemnitz, Germany — <sup>3</sup>Institute of Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — <sup>4</sup>Institute of Chemistry, Chemnitz University of Technology, D-09107 Chemnitz, Germany

For a number of applications, carbon nanotubes (CNTs) need to be functionalized by metallic or metal oxide thin films or nanoparticles. The current work is therefore considered with the thermal atomic layer deposition (ALD) of  $\text{Cu}_x\text{O}$  from the liquid  $\text{Cu(I)}$   $\beta$ -diketonate  $[(^n\text{Bu}_3\text{P})^2\text{Cu}(\text{acac})]$  and wet oxygen at  $135^\circ\text{C}$  on carbon nanotubes. Since high quality CNT surfaces are chemically inert, a pretreatment is required. For this reason the influence of different thermal oxidations onto the subsequent  $\text{Cu}_x\text{O}$  ALD was investigated. Depending on the oxidation either the growth of particles or a rather layer like growth was observed. The  $\text{Cu/C}$  ratio measured via EDX reaches its maximal values for a pretreatment with oxygen. This suggests that the used precursor couples to oxygen surface groups.

DS 44.59 Fri 9:30 Poster E

**Investigation of Linear Dichroism in ALD layers of  $\text{TiO}_2$**   
— •CHITTARANJAN DAS, MATTHIAS STÄDTER, MASSIMO TALLARIDA, and DIETER SCHMEISSER — Brandenburgische Technische Universität, Konrad Wachsmann Allee, 17, 03046, Cottbus, Germany

Titanium dioxide is on the most studied material due to its wide range of applications in various fields such as self cleaning, photocatalysis, solar cell, water splitting, bio-implants, etc. In order to increase its efficiency in water splitting and solar cell, it is necessary to understand the crystal structure and electronic properties in thin films. In our approach we are investigating the X-ray linear dichroism (XLD) of thin layers of  $\text{TiO}_2$ . XLD studies have been done in multiferroics, antiferromagnetic, and ferromagnetic materials, but a very less amount of work have been done in studying XLD effect of  $\text{TiO}_2$  thin films. These layers are grown by in-situ atomic layer deposition (ALD) system and are investigated with X-ray absorption spectroscopy (XAS) at BESSY II, Berlin. ALD is a promising technique to grow thin films on different

substrates conveniently due to its uniform deposition property. XAS study will also help us to better understand the interfacial electronic properties of thin films of  $\text{TiO}_2$ .

DS 44.60 Fri 9:30 Poster E

**Atomlagenabscheidung von Antimonoxid** — •BODO KALKOFEN<sup>1</sup>, MAX KLINGSPORN<sup>2</sup>, BERND GARKE<sup>3</sup> und EDMUND BURTE<sup>1</sup> — <sup>1</sup>IMOS, Otto-von-Guericke-Universität Magdeburg — <sup>2</sup>IHP, Frankfurt (Oder) — <sup>3</sup>IEP, Universität Magdeburg

Dünne Schichten aus Antimonoxid wurden mittels Atomlagenabscheidung (ALD) auf Silicium aufgewachsen. Antimonoxid dient als Dotierstoff für Zinnoxid-Halbleiter, besitzt einen hohen optischen Brechungsindex und wird als Katalysator eingesetzt. Als Ausgangsstoffe für die Abscheidung wurden Triethylantimon ( $\text{SbEt}_3$ ) und Ozon eingesetzt. Typische Prozessparameter waren:  $\text{SbEt}_3$ : 15ms/5s/8s (Puls-/Einwirk-/Spülzeit),  $\text{O}_3$ : 3s/1s/13s; die Abscheidetemperaturen lagen im Bereich von  $50^\circ\text{C}$  bis  $250^\circ\text{C}$ . Die Schichtdicken und optischen Parameter wurden mittels spektroskopischer Ellipsometrie bestimmt. Die Schichten wurden weiterhin durch XPS, ToF-SIMS, SEM und HR-TEM analysiert, und die Stabilität der Schichten gegenüber Säureeinwirkung und bei Hochtemperaturprozessen wurde untersucht. Schichtwachstum wurde ab einer Temperatur von  $100^\circ\text{C}$  beobachtet. Im Bereich von  $100^\circ\text{C}$  bis  $250^\circ\text{C}$  stieg das Wachstum pro Zyklus linear mit T an und lag bei  $250^\circ\text{C}$  bei  $0,65\text{\AA}$ . Dabei konnten sehr homogene Schichten abgeschieden werden ( $1,6\text{\AA}$  Min/Max-Variation bei  $7,5\text{nm}$  Schichtdicke auf  $150\text{mm}$ -Substrat). Die Analysen zeigten ein Interface von ca.  $1,5\text{nm}$   $\text{SiO}_2$  auf dem eingangs mit HF gereinigten Silicium unter den Schichten, die polykristalline Bereiche trotz der geringen Wachstumstemperaturen aufwiesen, was die gefundene hohe chemische Beständigkeit der Schichten gegenüber verschiedenen Säuren erklären kann.