

DS 32: Poster Session IV: Atomic layer deposition; Organic thin films; Organic Electronics and Photovoltaics; Organic Materials for Spintronics - from spinterface to devices; Thin film photovoltaic materials and solar cells

Time: Thursday 17:00–20:00

Location: Poster B2

DS 32.1 Thu 17:00 Poster B2

Regimes of leakage current in ALD-processed Al₂O₃ thin film layers — HOLGER SPAHR, JOHANNES REINKER, TIM BÜLOW, DIANA NANOVA, HANS-HERMANN JOHANNES, and WOLFGANG KOWALSKY — Technische Universität Braunschweig, Institut für Hochfrequenztechnik, Schleinitzstraße 22, 38106 Braunschweig

A recently known phenomenon at thin oxide layers with thicknesses below 40 nm is the increase of their breakdown electric field, called disruptive strength, when decreasing the layer thicknesses below 10 nm. This offers the possibility to examine the current - electric field characteristics to higher electric field strengths without an early electric breakdown.

In this contribution, we report on the identification of the current regime of trap free square law and the buildup of an S shaped current - electric field characteristic curve. This observation for ALD processed Al₂O₃ layers has not been mentioned in literature before. Additionally a modern model of space charge limited current (SCLC) was used to fit the S shaped characteristic and extract the associated parameters, such as mobility, density of states and the energy band gap between conduction band and trap state. In this context, it can be assumed, that the Poole-Frenkel effect does not play a significant role for the current increase after the trap filled limit (TFL).

DS 32.2 Thu 17:00 Poster B2

Barrier Properties of Nanolaminates Produced by ALD — BARBARA WEGLER^{1,2}, OLIVER SCHMIDT², and BERNHARD HENSEL¹ — ¹MSBT, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — ²Siemens AG, Corporate Technology, Erlangen, Germany

The water vapor transmission rate (WVTR) of the barrier layer is crucial for the lifetime of organic devices such as organic photo detectors (OPD) or organic light emission diodes (OLED). Up to now, the standard method is to glue a glass lid to the device. An alternative is to deposit nanolaminates by using atomic layer deposition (ALD) on the device. Promising results have been reported based on Al₂O₃/ZrO₂ with a WVTR of 3.2×10^{-4} g/(m² day).

Sputtered ZnSnOx is known to have low WVTRs. Depositing the barrier layers based on ALD nanolaminates instead of sputtering is expected to produce layers with even less defects.

The WVTR of ZnO/SnO and Al₂O₃/SnO nanolaminates has been obtained through the degradation of calcium to calcium oxide. The transparency of the resulting layers is measured by UV-Vis spectroscopy, as the transparency is an important factor for the efficiency of OPDs or OLEDs.

DS 32.3 Thu 17:00 Poster B2

Atomic Layer deposition of TiO₂ from TDMAT and H₂O: Evolution of microstructure and resulting resistance switching characteristics — SOLVEIG RENTROP¹, BARBARA ABENDROTH¹, THERESA MOEBUS¹, RALPH STROHMEYER¹, ALEXANDER SCHMID², and DIRK C. MEYER¹ — ¹Institut für Experimentelle Physik, TU Bergakademie Freiberg, Leipziger Str. 23, 09599 Freiberg — ²Institut für Angewandte Physik, TU Bergakademie Freiberg, Leipziger Str. 23, 09599 Freiberg

Atomic layer deposition (ALD) is a well-known technique used for the fabrication of thin oxide layers for high-k-dielectrics and resistive switching memory applications. Here, we present studies on the atomic layer deposition of TiO₂ from Tetrakis(dimethylamino)titan (TDMAT) and H₂O precursors in the substrate temperature range from 150 °C to 350 °C. The effects of the deposition temperature T_s and layer thickness d on the resulting anatase and rutile phase composition are investigated by grazing incidence X-ray diffraction. For T_s above 200 °C metastable anatase is always the first crystallized phase observed. At temperatures of 250 °C and higher anatase formation is always followed by the nucleation of rutile. Our results are summarized in a $T_s - d$ phase diagram. To determine the effect of the presence of crystalline phases on resistance switching performance, current-voltage characteristics are measured for Au-TiO₂-TiN capacitor structures with amorphous, partially and fully crystalline TiO₂ layers.

DS 32.4 Thu 17:00 Poster B2

Atomic layer epitaxy of Ruddlesden-Popper film structures prepared by MAD — FELIX MASSEL, SEBASTIAN HÜHN, MARKUS JUNGBAUER, MARKUS MICHELMANN, CAMILLO BALLANI, and VASILY MOSHNYAGA — I. Physikalisches Institut, Georg-August Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Ruddlesden-Popper (RP) phases can be described by the general formula $A_{n-1}A'_2B_nO_{3n+1}$, where A, A', and B are cations, O is oxygen, and n is the number of the layers of octahedra in the perovskite-like stack. When aiming at high values of n , conventional solid state synthesis produces mixtures of phases with different n and the parent perovskite rather than pure phases. Submonolayer deposition precision is a way to successfully grow single phase RP films. RP films were prepared by vacuum free metalorganic aerosol deposition (MAD), which has several advantages over physical deposition methods, especially a high oxygen pressure of $p(O_2) \approx 0.2$ bar. The films were prepared by controllable pulsed spray injections of A and B type precursor solutions into the MAD chamber. By means of optical ellipsometry, a layer-by-layer - i. e. A-O/B-O₂ - deposition was monitored in situ, giving early information on the film composition. Thin films of the $Sr_{n+1}Ti_nO_{3n+1}$ RP series were prepared for $n = 1, \dots, 4$. Further analysis of the films' structure and morphology was done by XRD and AFM. In order to achieve single phase RP samples, a fine tuning of precursor volumes, deposition temperature, deposition rate, and pulse delay time was found to be crucial for a successful synthesis. This work was supported by IFOX of the European Community's 7th Framework Programme.

DS 32.5 Thu 17:00 Poster B2

Organic molecular ion beam epitaxy of non-volatile molecules — GORDON RINKE¹, STEPHAN RAUSCHENBACH¹, and KLAUS KERN^{1,2} — ¹Max-Planck Institute for Solid State Research, Stuttgart, Germany — ²Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, Switzerland

Electrospray ion beam deposition (ES-IBD) was developed in our laboratory as a technique for the deposition of non-volatile molecules on well-defined surfaces in ultrahigh vacuum.[1, 2] ES-IBD is based on the creation of intact molecular ions or clusters by electrospray ionization, which are deposited on a surface as a mass selected hyperthermal beam. In contrast to evaporation, where neutral thermal particle beams are used, ES-IBD allows for the full control of the deposition process.

Here we show several examples of crystalline film growth using ES-IBD. Organic thin films are grown in layers or islands from high flux cluster beams.[3] Many other non-volatile molecules, including highly reactive species, form two-dimensional crystals on metal surfaces.

Our results show that, despite the significant differences, ES-IBD can achieve results equivalent to conventional epitaxy. The versatility and enhanced control of the deposition process shows a way towards novel coatings with unique properties.

[1] Small, 2006, 2, 540

[2] ACS Nano, 2009, 3, 2901

[3] Adv. Mater., 2012, 24, 2761-2767

DS 32.6 Thu 17:00 Poster B2

Dithiocarbamate Monolayers for Noble Metal Surface Functionalization — TOBIAS SCHÄFER¹, PHILIP SCHULZ^{1,2}, CHRISTIAN EFFERTZ¹, DANIEL GEBAUER¹, DOMINIK MEYER¹, RICCARDO MAZZARELLO³, and MATTHIAS WUTTIG¹ — ¹I. Inst. of Physics (IA), RWTH Aachen Univ. — ²Dept. of Elect. Engineering, Princeton Univ. — ³Inst. for Theoretical Solid State Physics, RWTH Aachen Univ.

Organic electronic devices like organic light emitting diodes, photovoltaics and thin-film transistors are well-known for their paramount technological potential. Nevertheless the need for improved electronic alignment and contact between the active organic layers and the metal electrodes remains a crucial issue. One promising approach is to modify the organic and metal interface by introducing a self-assembled monolayer (SAM) in between. In particular high work function noble metals impose the need for a dipolar interlayer to reduce the work

function to enhance electron injection into organic acceptor materials.

Here, we present dithiocarbamate (DTC) monolayers efficiently lowering the work function of noble metal surfaces by up to 2 eV, as can be measured by Photoelectron Spectroscopy (PES). This distinct work function reduction is modeled and explained by density functional theory computations (DFT) in a framework of interface dipoles. The interface dipoles stem from the formation of strong bond dipoles, intrinsic molecular dipoles and the high molecular packaging density. The latter can be experimentally verified by PES. The applicability of DTC-monolayers for enhancing electronic coupling was demonstrated in OTFT devices.

DS 32.7 Thu 17:00 Poster B2

Electrical Characterization of Copper Phthalocyanine / Amorphous Silicon Hybrid Structures — ●EVELYN T. BREYER, DANIEL LEHMANN, and DIETRICH R. T. ZAHN — Semiconductor Physics, TU Chemnitz, 09107 Chemnitz, Germany

Organic-inorganic hybrid junctions combine the advantageous properties of organic and inorganic layers. The electrical properties of amorphous silicon (a-Si) strongly depend on the conditions during deposition, *e.g.* substrate temperature and hydrogen flow. By surface modification of the amorphous silicon it is intended to force copper phthalocyanine molecules to adopt a “lying down” orientation on the substrate, which favours electrical conduction through the vertical stack, and is therefore desired for photovoltaic devices.

Hydrogenated amorphous silicon (a-Si:H) was sputtered onto borosilicate glass with NiCr contact fingers by DC pulsed magnetron sputtering at a constant substrate temperature of 150 °C. Thin films of CuPc (nominal thickness up to 50 nm) were deposited onto the amorphous silicon by Organic Molecular Beam Deposition (OMBD) under high vacuum conditions (3×10^{-7} mbar). Finally, silver electrodes were thermally evaporated onto the cooled sample ($T \approx -150$ °C) without breaking the vacuum. Current-voltage measurements were performed *ex situ* directly after deposition under dark and illuminated conditions (solar simulator, AM 1.5). Temperature dependent I-V curves were recorded. Two types of current transport dominate in the chosen voltage range (-2V...2V): thermionic emission and space charge limited conduction (SCLC).

DS 32.8 Thu 17:00 Poster B2

A Systematic Growth Study of Thiazolothiazole Derivatives with Varying Deposition Parameters — ●SIMON SIEMERING, DANIEL GEBAUER, and MATTHIAS WUTTIG — I. Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany

Thiophene oligomers are an important class of organic semiconductors, which have considerable potential in thin film transistor (TFT) devices. Now we want to investigate their potential as an active layer in organic photovoltaic cells (OPC) and the first step is to understand the influence of different deposition parameters on thin film formation. In the framework of this study thin films of thiazolothiazole derivatives were deposited by organic molecular beam deposition (OMBD) on Indium Tin Oxide (ITO) substrates under high vacuum conditions. The influence of varying deposition rate, substrate temperature and film thickness on structure and morphology is studied with different methods. Atomic force microscopy measurements (AFM) determine the film roughness and correlation length. Film thickness and density are measured by X-ray reflectometry (XRR) while X-ray diffraction (XRD) yields the crystallinity and texture of the sample.

DS 32.9 Thu 17:00 Poster B2

Characterisation of Trap States in Transition Metal Phthalocyanine Thin Film Transistors — ●STEFAN KLAES, CHRISTIAN EFFERTZ, and MATTHIAS WUTTIG — I. Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany

The family of phthalocyanines is promising for novel organic thin film applications. Transition metal phthalocyanines exhibit very different charge carrier mobilities dependent on the transition metal even though their structural properties remain similar. The influence of the center metal atom on charge transport properties is not yet fully understood. To obtain a deeper understanding of electronic transport in organic thin film devices the charge carrier transport of several different transition metal phthalocyanines has been investigated. To do so SiO₂ bottom gate/Au top contact Organic Thin Film Transistors (OTFT) with different transition metal phthalocyanines as the active layers have been produced. Their properties like charge mobility, time-domain-effects and trap depth have been examined, in particular to determine the influence of trap states. Additionally DFT based model

calculations have been performed to gain a further insight into these phenomena.

DS 32.10 Thu 17:00 Poster B2

Growth Study of Organic Thin Films - Influence of Different Growth Conditions on Structure and Morphology — ●JANINA FELTER, DANIEL GEBAUER, and MATTHIAS WUTTIG — I. Institute of Physics (IA), RWTH Aachen University, D-52056 Aachen, Germany

The molecule N,N'-ditridecyl-3,4,9,10-perylene-tetracarboxylic diimide (PTCDI-13) is one of the few organic materials with good n-type conductivity. Hence this compound is attractive for the application in organic thin film transistors (OTFT). In order to optimize its thin film properties and to access the full potential of this molecule, the physical processes of growth and structure formation have to be investigated. In this work PTCDI-C13 films with a thickness varying from the submonolayer regime up to 60 nm have been deposited by organic molecular beam deposition (OMBD) on gold and SiO₂ surfaces. The deposition rate and the substrate temperature have been varied to study the influence of different growth conditions on structure and morphology. X-ray reflectometry (XRR) has been applied in order to measure thin film thickness and roughness. The crystallinity and texture have been determined by X-ray diffractometry (XRD), while the surface morphology has been investigated by atomic force microscopy (AFM).

DS 32.11 Thu 17:00 Poster B2

Initial steps of rubicene film growth on silicon dioxide — ●BORIS SCHERWITZL, WALTER LUKESCH, GÜNTHER LEISING, ROLAND RESEL, and ADOLF WINKLER — Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria

Studies of the initial stages of organic film growth are of great relevance for the use of organics in microelectronic devices, which became of increasing importance in a variety of applications. This contribution describes the behavior of rubicene film growth on silicon dioxide with respect to sample treatments under UHV conditions. Physical vapor deposition from a Knudsen cell was used to create films with varying thickness, from sub-monolayer up to multilayer range. The exact amount of evaporated material was determined by a quartz microbalance. A number of different analytical methods were used to examine sample and surface properties, namely Auger Electron Spectroscopy (AES) for chemical analysis, Thermal Desorption Spectroscopy (TDS) to determine desorption behavior and Atomic Force Microscopy (AFM) for a subsequent *ex-situ* analysis of the sample surface. It could be shown that rubicene initially forms two layers of flat-lying molecules, which will stand up and form islands at and above a certain coverage. Different desorption energies suggest that the binding of the organic molecules to the substrate material is not as strong as among the molecules themselves. Substrate conditions such as purity and roughness had no observable influence. AFM studies confirmed the dewetting of the initial layers under atmospheric conditions and showed desorption and diffusion processes happening at room temperature.

DS 32.12 Thu 17:00 Poster B2

Initial growth of ultra-thin films of pentacene on mica: Influence of water and substrate morphology — ●LEVENT TÜMBEK, ROMAN LASSNIG, and ADOLF WINKLER — Institute of Solid State Physics, Graz University of Technology, Austria

In recent years organic electronic devices (OFETs, OLEDs) became a highly active topic in surface science due to their novel properties. A full understanding and control of the formation of organic films is a requirement for improving existing devices and further innovation. This study describes the behavior of pentacene film growth on the model substrate mica under well controlled UHV conditions. Physical vapor deposition (PVD) was the method of choice to prepare films from sub-monolayers up to multilayers and a quartz micro balance was applied to determine the pentacene film thickness. Argon ion sputtering was used for modifying the surface morphology. For the characterization of the film and substrate XPS, AES, TDS and *ex-situ* AFM was applied. It can be shown by AFM that sputtering changed the film morphology from needle-like islands, composed of lying molecules, to dendritic islands, composed of standing molecules. In the former case a wetting layer could be identified by TDS. Furthermore, it can be demonstrated that pentacene film formation depends strongly on the partial pressure of water vapor present during deposition. Regarding the adsorption kinetics, TDS revealed that the initial sticking coefficient of pentacene on mica is smaller than unity.

DS 32.13 Thu 17:00 Poster B2

Weakly forbidden transitions in manganese(II)-phthalocyanine — •TOBIAS BIRNBAUM, CLAUDIA LOOSE, and JENS KORTUS — Institut für theoretische Physik, Leipziger Str. 23, 09599 Freiberg

Based on known theoretical models (for example [1]) we present a comparison of selection rules for optical transitions in porphyrins and phthalocyanines. We will focus on weakly forbidden transitions in manganese(II)-phthalocyanine and compare our results with experimental data [2].

[1] M. Gouterman, J. Mol. Spec. 6, (1961), 138

[2] M. Fronk et al., PRB 79, (2009), 235305

DS 32.14 Thu 17:00 Poster B2

The influence of molecular tilt angle on the absorption spectra of pentacene:perfluoropentacene blends — •KATHARINA BROCH, CHRISTOPH BÜRKER, JOHANNES DIETERLE, ALEXANDER GERLACH, and FRANK SCHREIBER — Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

The understanding of the optical properties of organic semiconductor blends is not only crucial for the optimization of opto-electronic devices but also of relevance for fundamental research, since it sheds light on intermolecular interactions within the films. The absorption spectra of mixed systems can be influenced by different effects, such as charge-transfer interactions within a donor-acceptor system [1,2] or structural disorder [3,4]. Using spectroscopic ellipsometry and near-edge X-ray absorption fine structure spectroscopy (NEXAFS) we investigate equimolar mixtures of perfluoropentacene (PFP) and pentacene (PEN) grown at diverse substrate temperatures. Depending on the preparation conditions, the absorption spectra exhibit significant differences. By determining the molecular tilt angles from the NEXAFS-data and by comparing our results with the structural order and the morphology [5], we discuss the effects of film structure and molecular orientation on the optical properties. [1] F. Anger et al., J.Chem.Phys., **136**, 054701 (2011); [2] K. Broch et al., Phys.Rev.B., **83**, 245307 (2011); [3] A. Aufderheide et al., Phys.Rev.Lett, **109**, 156102 (2012); [4] K. Broch et al., *in preparation*; [5] A. Hinderhofer et al., J.Chem.Phys., **134**, 104702 (2011); [6] A. Hinderhofer and F. Schreiber, Chem.Phys.Chem., **13**, 628 (2012)

DS 32.15 Thu 17:00 Poster B2

IR spectroscopic studies of p-doped thin films of organic semiconductors — •SEBASTIAN BECK^{1,2}, DAVID GERBERT^{1,2}, MARKUS GÖLZ^{1,2}, TOBIAS GLASER^{1,2}, and ANNEMARIE PUCCI^{1,2} — ¹Universität Heidelberg, Kirchhoff-Institut für Physik, INF 227, 69120 Heidelberg — ²InnovationLab GmbH, Speyerer Str. 4, 69115 Heidelberg

In this study, the underlying mechanisms and effects of doping were investigated by means of infrared spectroscopy. We examined doped and undoped thin films of organic semiconductors, such as 4,4'-Bis(N-carbazolyl)-1,1'-biphenyl (CBP), whereas different organic (e.g. 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ)) and inorganic (e.g. molybdenum oxid (MoO₃)) materials were used as acceptor.

The additional charge on donor and acceptor molecules in doped systems leads to specific changes in the absorption spectra compared to the spectra of undoped thin films. From the appearance of new vibrational bands, spectral shifts, and broad electronic absorptions, information about the morphological, electronic and molecular properties of the thin films was obtained, for example, on the different segregation of organic and inorganic acceptor materials and the different degree of charge transfer between donor and acceptor.

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DS 32.16 Thu 17:00 Poster B2

Electrical characterization of selected matrix dopant systems via U-I measurements — •MARKUS GÖLZ^{1,4}, DANIELA DONHAUSER^{2,4}, ERIC MANKEL^{3,4}, WOLFRAM JAEGERMANN^{3,4}, and WOLFGANG KOWALSKY^{1,2,4} — ¹Kirchhoff-Institut für Physik, Universität Heidelberg — ²Technische Universität Braunschweig — ³Technische Universität Darmstadt — ⁴Innovation Lab GmbH, Heidelberg

Understanding the electrical effects of doping of organic materials is necessary to produce efficient organic devices, such as OLEDs or organic solar cells. The electrical conductance of selected matrix dopant

systems is investigated via current - voltage (I-V) measurements. Typical matrices are α -NPD(NPB), CuPc and CBP. F4-TCNQ and HATNA-F6 are used as dopants. The samples are made by thermal coevaporation under UHV conditions. The electrical measurements are carried out at room temperature and atmospheric conditions.

Specifically the α -NPD: F4-TCNQ (2.7%) samples show an increase of the conductance of a factor of ten compared to the undoped matrix. Furthermore, the space-charged-limited-current region (SCLC) in the doped matrix is shifted to higher voltages. It sets in at approximately 1.5 V compared to 0.1 V in the undoped matrix.

DS 32.17 Thu 17:00 Poster B2

Interface properties of polar phthalocyanines on silver substrates — •MALGORZATA POLEK, FOTINI PETRAKI, FLORIAN LATTEYER, HEIKO PEISERT, and THOMAS CHASSÉ — University of Tuebingen, Institute of Physical Chemistry, Auf der Morgenstelle 18, 72076 Tuebingen, Germany

Phthalocyanines (Pcs) are promising materials for various devices like light-emitting diodes, field effect transistors and solar cells. In this context, polar Pcs are of particular interest, e.g. due to their different growth properties and the variation of the chemical reactivity. Chemical reactions at interfaces could be a route for the tuning of both electronic interface properties and the molecular orientation.

We study interface properties between polar Pcs and silver using X-ray photoelectron spectroscopy (XPS), Ultraviolet photoelectron spectroscopy (UPS) as well as optical spectroscopies. We focus on VOPc, VOPcF₁₆, GaClPc and AlClPc. For some interfaces a clear indication for a chemical interaction was found.

DS 32.18 Thu 17:00 Poster B2

Investigation of the electronic structure of cobalt phthalocyanine films on MnO substrates by X-ray Photoemission Spectroscopy — •MATHIAS GLASER, HEIKO PEISERT, and THOMAS CHASSÉ — Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Auf der Morgenstelle 18, 72076 Tübingen

Interactions at the interface between transition metal phthalocyanines (TMPc) and metal substrates affect electronic properties of adsorbed organic molecules in many cases [1,2]. Besides metals, transition metal oxide thin films are promising substrates for applications of TMPcs; studies of these interfaces however are rare. It is known that epitaxially grown ultrathin transition metal oxide films on metals show unique chemical physical properties depending e.g. on the film thickness [3,4]. In addition, charging effects in photoemission can be avoided. In this work we investigate the electronic structure of cobalt phthalocyanine on MnO ultrathin films epitaxially grown on Ag(001) using x-ray photoelectron spectroscopy.

[1] F. Petraki H. Peisert, I. Biswas, U. Aygül, F. Latteyer, A. Vollmer, T. Chassé, J. Phys. Chem. Letters 1 (2010), 3380.

[2] F. Petraki . Peisert, I. Biswas, T. Chassé, J. Phys. Chem. C 114 (2010), 17638.

[3] M. Nagel , I. Biswas, P. Nagel, E. Pellegrin, S. Schuppler, H. Peisert, T. Chassé, Phys. Rev. B 75 (2007), 195426.

[4] S. Altieri L.H. Tjeng, G.A. Sawatzky, Thin Solid Films 400 (2001), p.9.

DS 32.19 Thu 17:00 Poster B2

In-situ X-ray reflectivity of the formation of OTS-SAMs on amorphous SiO₂ and quartz — •HANS-GEORG STEINRÜCK¹, MICHAEL KLIMCZAK¹, STEFAN GERTH¹, ANDRE BEERLINK², and ANDREAS MAGERL¹ — ¹Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen Nürnberg , Germany — ²Hamburger Synchrotronstrahlungslabor am Deutsches Elektronen-Synchrotron DESY, Germany

To gather further insight into the correlation between the structure of (C₁₇H₃₇Cl₃Si, OTS) self-assembled monolayers and the nature of the substrate [1] we compared in-situ the growth of OTS-SAMs on amorphous SiO₂ and crystalline quartz (001) via specular X-ray reflectivity. These measurements were performed at the high resolution diffraction beamline P08, DESY

As the striking difference between these two substrates we note that the dominant reflection minima remain at a constant q value for amorphous SiO₂ albeit with increasing amplitude over time, indicating that the molecules attach in an island growth mode (similar to the findings of Richter et al. [2]), whereas for crystalline quartz the corresponding minima shift to lower q_z -values signaling an increasing layer thickness during the coating as expected for a random growth mode [3].

[1] Steinrueck, H. G.; Klimczak, M.; Gerth, S.; Magerl, A. submitted

2012

[2] Richter, A. G.; Yu, C. J.; Datta, A.; Kmetko, J.; Dutta, P. *Physical Review E* 2000, 61, 607-615.

[3] Mirji, S. A. *Surface and Interface Analysis* 2006, 38, 158-165.

DS 32.20 Thu 17:00 Poster B2

X-ray reflectivity study on the growth of a porphyrin monolayer — JULIA MÜLLER, ●HANS-GEORG STEINRÜCK, and ANDREAS MAGERL — Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen Nürnberg, Germany

We investigated the growth of a metallo porphyrin ($C_{45}H_{28}CoN_4O_2$, CoP) self-assembled monolayer on amorphous SiO_2 via X-ray reflectivity. The fractional coverage of the sample was examined as a function of the reaction time in solution and was determined by multiplying the electron density with the thickness of the monolayer, which both increase with reaction time until saturation. The thickness, corresponding molecular tilt and electron density of the fully covered substrates compare with the findings of Griffith et al. [1].

Langmuir isotherms state that the rate of surface reactions is given as: $\frac{d\theta}{dt} = k_a(1-\theta)C - k_d\theta$. Integration of this equation gives the time dependence of the fractional coverage. Fitting this to the experimental data yields the adsorption rate constant for CoP on amorphous SiO_2 at the given concentration of about 0.8mM.

[1] Griffith, M. J.; James, M.; Triani, G.; Wagner, P.; Wallace, G. G.; Officer, D. L. *Langmuir* 2011, 27, 12944-12950.

DS 32.21 Thu 17:00 Poster B2

Optical and Magneto-optical Characterisation of Thin Films of Functionalised Tetra-phenyl-porphyrines — FRANK LUNGWITZ, CAROLA MENDE, ●MICHAEL FRONK, HEINRICH LANG, DIETRICH R.T. ZAHN, and GEORGETA SALVAN — Chemnitz University of Technology, Faculty of Natural Sciences

Metal-organic complexes are of strong interest as active materials e.g. in organic spintronic devices. Assembling these complexes as thin films on surfaces in a well defined way is an important step towards the goal of constructing such devices. In the present work we chose the group of tetra-phenyl-porphyrines (TPP) which are in terms of size just at the limit to be evaporable in vacuum in order to obtain films with very homogeneous thickness. The molecules were functionalised by short side groups such as the methoxy group and the central metal ion was varied in order to check the impact of these modifications on the dielectric and magneto-optical properties of the films prepared by organic molecular beam deposition (OMBD) onto silicon and gold substrates. The investigations utilised the techniques Variable Angle Spectroscopic Ellipsometry and Magneto-Optical Kerr Effect spectroscopy. The optical constants obtained from ellipsometry were compared to UV-VIS data taken from material in solution and the degree of uniaxial optical anisotropy and the magneto-optical data were used to estimate the molecular arrangement on the substrates. It was found that on silicon the molecular porphyrine backbone encloses a slightly smaller angle with the substrate surface than on gold.

DS 32.22 Thu 17:00 Poster B2

Controlling molecular orientation of Azaacene relatives of pentacene by substrate-choice — ●MICHAEL KLUES¹, TOBIAS BREUER¹, JULIUS KÖGEL², JÖRG SUNDERMEYER², and GREGOR WITTE¹ — ¹Physics Department, Philipps Uni. Marburg, 35032 Marburg — ²Chemistry Department, Philipps Uni. Marburg, 35032 Marburg

Nitrogen substitution of the central ring of pentacene suggests to supply a chemical more robust but almost iso-electronic molecular compounds. However, previous studies revealed for such diaza-pentacene (DAP) an entire different crystal structure than for pentacene as well as a poor charge carrier mobility. By contrast dihydrodiazapentacene (DHDAP) resembles the crystalline packing of pentacene and exhibits excellent charge carrier mobility although this hydrogenation is expected to break the conjugation [1]. To gain deeper insight into the electronic and structural properties of these various acenes, thin films of all compounds were studied by means of XPS, NEXAFS and XRD. Moreover, different substrates were used since this allows a control of the molecular orientation. XPS data signify an instability of DAP during the evaporation process and suggests a degradation which could be an explanation for the poor charge carrier mobility, in addition to the disadvantageous crystal structure.

[1]Qian Miao. N-heteropentacenes and n-heteropentacenequinones: From molecules to semiconductors. *SYNLETT*, (3):326-336, 2012

DS 32.23 Thu 17:00 Poster B2

Fabrication of Ag-TCNQ nanowires — ●MARKUS BARANOWSKI and MICHAEL HUTH — Physikalisches Institut, Johann Wolfgang Goethe-University, Frankfurt am Main, Germany

A method is presented which allows to grow silver-tetracyanoquinodimethan (Ag-TCNQ) nanowires by utilizing porous aluminum oxide (Al_2O_3) templates. Ag-TCNQ nanowires are interesting because of their unique electric properties. They exhibit a reproducible I-V hysteresis which shows electrical switching [1]. Promising application of the Ag-TCNQ nanowires are therefore memory devices. The Ag-TCNQ nanowires are fabricated by sputtering Ag on one side of porous Al_2O_3 templates and subsequent covering of the Ag surface with an adhesive. Afterwards a solution reaction of TCNQ solute in acetonitrile is used to obtain the Ag-TCNQ nanowires. With this technique simultaneous fabrication of nanowires with 200nm diameter and a length of up to $15\mu m$ can be achieved.

[1]:K. Xiao et al. *Adv. Funct. Mater.* 2008, 18, 3043-3048

DS 32.24 Thu 17:00 Poster B2

Vibrational properties of fluorinated rubrene in thin films — ●FALK ANGER¹, REINHARD SCHOLZ², ALEXANDER GERLACH¹, and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen — ²Institut für Angewandte Photo-physik, TU Dresden, 01069 Dresden

One possibility of tuning the electronic properties of organic molecules is the substitution of hydrogen end groups by fluorine. Vibrational spectroscopy can be used to obtain information about the conformation of the molecules as well as intermolecular coupling in thin films. Rubrene ($C_{42}H_{28}$) has been shown to be a suitable semiconductor for applications, for which numerous experimental efforts have been made. In this study, we present FT-IR and Raman spectra of thin films of partly ($C_{42}H_{14}F_{14}$) and completely ($C_{42}F_{28}$) fluorinated rubrene. We analyse the single component-films using DFT calculations and discuss different vibrational modes. Finally, we analyse mixtures of Rubrene, $C_{42}H_{14}F_{14}$, and $C_{42}F_{28}$ to investigate the effect of the molecular environment.

[1] F. Anger *et al.*, *submitted* (2012)

[2] T. Breuer *et al.*, *J. Phys. Chem. C* **116**, 14491-14503 (2012)

DS 32.25 Thu 17:00 Poster B2

Energy level alignment at interfaces between low-band-gap polymers and C60 — ●MILUTIN IVANOVIC¹, HEIKO PEISERT¹, INES DUMSCH², MICHAEL FORSTER², ULRICH SCHERF², and THOMAS CHASSÉ¹ — ¹Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Tübingen, Germany — ²Makromolekulare Chemie und Institut für Polymertechnologie, Bergische Universität Wuppertal, Wuppertal, Germany

In electronic devices based on organic materials, the properties of interfaces are as important as the organic substances itself. Bulk heterojunctions (BHJ) play a crucial role in several devices, such as organic light emitting devices (OLEDs), organic field-effect transistors, and organic photovoltaic devices (OPVs). As example, in bulk heterojunction solar cells the interface between the donor and the acceptor material determines the ability for charge separation and the maximal reachable open circuit voltage. We study electronic properties of interfaces between low band gap (LBG) polymers (promising candidates for donor materials in OPVs) and C60 (model molecule for the acceptor material). We focus on the LBG polymers PCPDTBT, Si-PCPDTBT, PCPDTBBT and Benzosenadiazole-based low band gap polymers. C60 films were evaporated on doctor blade casted polymer films in UHV. The interfaces were studied using X-ray photoemission spectroscopy (XPS) and Ultraviolet photoemission spectroscopy (UPS).

DS 32.26 Thu 17:00 Poster B2

Investigation of electronic and structural properties of cobalt phthalocyanine on graphene interlayers on Ni(111) — ●HILMAR ADLER, JOHANNES UIHLEIN, HEIKO PEISERT, MALGORZATA POLEK, FOTINI PETRAKI, and THOMAS CHASSÉ — Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 18, 72076 Tübingen, Germany

Transition metal phthalocyanines (TMPcs) gained increasing attention due to their tunable properties, and therefore their application in light-emitting diodes, field-effect transistors and solar cells. Most recently, the interface between TMPcs and metal substrates raised additional interest due their important role in spintronic nanodevices. Depend-

ing on the substrate TMPcs may show strong interactions at the interface.[1] The molecule-substrate interaction at the interface can be further tuned by insertion of a buffer layer. Graphene with its exciting electronic properties is an ideal candidate for such layers. Cobalt phthalocyanine as a representative of TMPcs was investigated on Ni(111) with a graphene buffer layer by scanning tunneling microscopy. The results are compared to X-ray photoelectron spectroscopy measurements and X-ray absorption spectroscopy studies.

(1) F. Petraki, H. Peisert, U. Ayg ul, F. Latteyer, J. Uihlein, A. Vollmer, T. Chass e, J. Phys. Chem. C 2012, 116, 11110-11116.

DS 32.27 Thu 17:00 Poster B2

The effects of oxygen exposure on copper phthalocyanine thin films — •TOMOKI SUEYOSHI^{1,2}, MASAKI ONO¹, HIROSHI TOMII³, MASAKAZU NAKAMURA³, and NOBUO UENO¹ — ¹Graduate School of Advanced Integration Science, Chiba University, Japan — ²Peter Gr unberg Institut (PGI-3), JARA, Forschungszentrum J ulich, Germany — ³Graduate School of Engineering, Chiba University, Japan

The exposure of organic semiconductor thin films to gas atmospheres, such as O₂, water vapor, and air, has been reported to influence their electronic properties. The gas exposure consequently results in a short lifetime and low performance of organic devices under ambient atmosphere. Such effects have been discussed from a viewpoint of electronic properties of organic layers in relation to chemical interactions between organic molecules and gas molecules. However, there is little known about the correlation between the gas exposure effects and structural properties of organic thin films.

Here, we demonstrate that the effects of O₂ gas exposure depend on the molecular packing structure of organic thin films. We investigated electronic states of a copper phthalocyanine (CuPc) thin film on graphite before and after O₂ exposure using ultrahigh-sensitivity ultraviolet photoelectron spectroscopy. The highest occupied molecular orbital state of CuPc with a lying-down molecular orientation was not affected by 1 atm O₂ exposure while that of CuPc with a tilted-up orientation shifted toward the Fermi level after the exposure. The O₂ exposure effects may originate from a weak disorder in the molecular packing structure induced by O₂ diffusion into the film.

DS 32.28 Thu 17:00 Poster B2

Recombination in organic donor-acceptor bulk heterojunction solar cells — •J EDRZEJ SZMYTKOWSKI — Department of Chemistry, University of Florida, Gainesville, USA — Faculty of Applied Physics and Mathematics, Gda nsk University of Technology, Gda nsk, Poland

Recombination of generated charge carriers is a dominant mechanism which causes loss of photocurrent and limits the achievement of high efficiencies in organic solar cells. In this work, we present new theoretical model of bimolecular recombination in organic bulk heterojunction photovoltaic devices. Based on analysis of excitons annihilation on polarons near interface between donor and acceptor materials, we have derived analytical formula to describe the reduced Langevin recombination, which is typically observed in such molecular systems. The model explains the dependence of recombination coefficient with charge carrier concentration and also the origin of higher orders of nongeminate recombination. In addition, we discuss the light intensity dependence of polaron concentration.

DS 32.29 Thu 17:00 Poster B2

The drying process of spin coated polytriarylamine and poly(3-hexylthiophene) thin films studied by IR spectroscopy — •MICHAEL SENDNER, JENS TROLLMANN, and ANNEMARIE PUCCI — Kirchhoff-Institut f ur Physik der Universit at Heidelberg

Solution processed organic semiconductor thin films are attracting increasing interest due to the possible low cost production in a roll-to-roll printing process. However the drying of such films is not well understood yet. We analyze the drying process of spin coated polytriarylamine (PTAA) and poly(3-hexylthiophene) (P3HT) films on silicon substrates in a time frame from minutes to hours after production. For this purpose we are looking at characteristic vibrational modes of the solvents, excited by mid infrared light, as well as at film morphology. Further knowledge of the drying process will offer the possibility to control important parameters of the film formation during processing. Funding by BMBF (Polytos) is gratefully acknowledged.

DS 32.30 Thu 17:00 Poster B2

Degradation processes in naphthalene diimide n-type and flexo printed polytriarylamine p-type organic field effect

transistors studied by IR ellipsometry and electrical characterizations — •JENS TROLLMANN, MICHAEL SENDNER, and ANNEMARIE PUCCI — Kirchhoff-Institut f ur Physik der Universit at Heidelberg

Degradation processes in organic field effect transistors is a subject not well studied yet. Especially for printed layers there is few data available. We compare variations in mid-infrared (IR) ellipsometrical spectra of evaporated naphthalene diimide thin films with changes in the electrical properties of transistors after degradation by water vapour and heat (65 C, 85%rH). Furthermore we investigate flexo printed polytriarylamine layers degraded under the same conditions. The variations of vibrational modes of atomic bonds during degradation reveal morphological and chemical changes in organic thin films causing losses in electrical performance. Based on this information procedures to avoid serious losses can be developed. Funding by BMBF (Polytos) is gratefully acknowledged.

DS 32.31 Thu 17:00 Poster B2

Organic heterojunctions for photovoltaic applications - How does structure influence performance? — •INGOLF SEGGER, STEFAN KLAES, ULRIKE KUCK, DOMINIK MEYER, CHRISTIAN EFFERTZ, and MATTHIAS WUTTIG — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Organic donor-acceptor heterojunctions are arguably the most promising system for the use as active layers in organic solar cells. Their key feature is a very efficient exciton dissociation at the interface between donor and acceptor which is crucial for device operation. Hence, one way towards high performance organic solar cells is the enlargement of the interface area, which can be achieved by simultaneous processing of donor and acceptor in order to deposit bulk heterojunctions. For certain donor-acceptor combinations significant performance improvements for bulk heterojunctions over simple bi-layer systems have already been demonstrated.

For this study we have produced small molecule bi-layers and bulk heterojunctions based on Copper Phthalocyanine as a donor and C₆₀ as well as PTCDI-C₁₃ as acceptor materials. The structure of the resulting films can be tuned over a wide range by employing different substrate temperatures during evaporation in ultrahigh vacuum. Here we present our results on the influence of structural properties on absorption, charge transport and device performance which were investigated by means of x-ray diffraction, optical spectroscopy and electrical measurements.

DS 32.32 Thu 17:00 Poster B2

Tailoring Contacts in Organic Transistors by Dithiocarbamate Monolayers — •DOMINIK MEYER, CHRISTIAN EFFERTZ, FRANZISKA MARTIN, INGOLF SEGGER, DANIEL GEBAUER, and MATTHIAS WUTTIG — Institute of Physics (IA), RWTH Aachen University, 52066 Aachen, Germany

It is well-known that the device performance of organic field-effect transistors (OFETs) strongly depends on the device geometry: Top-contact bottom-gate (TCBG) transistors usually show much better current on-to-off ratios and higher charge carrier mobilities than bottom-contact bottom-gate (BCBG) transistors. This deficiency can primarily be attributed to the difference in the electric field distribution. However, the ability to modify metal S/D-contacts with self-assembling monolayers (SAMs) is solely provided by BC OFETs. SAMs may have a direct impact on charge carrier injection barriers by changing the work function of the metal contact. We have reported previously that the work function of gold can be lowered by 2 eV with dithiocarbamate SAMs. This decrease has been attributed to the formation of an interface dipole¹. Hence the question arises: Is it possible to improve BCBG OFETs by minimizing the charge injection barrier employing dithiocarbamate SAMs as S/D-contact modification? In this study we present the influence of dithiocarbamate SAMs on charge transport and trap state distributions in BCBG OFETs and compare them to unmodified TCBG OFETs for different n- and p-type organic semiconductors.

¹P. Schulz et al., 2011 MRS Fall Meeting & Exhibit U13.17

DS 32.33 Thu 17:00 Poster B2

Investigation of the interface between aluminum-doped zinc oxide sputtered on copper phthalocyanine thin films. — •CATHY JODOCY, CAROLIN JACOBI, and MATTHIAS WUTTIG — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Organic based electronic devices are of considerable interest because of their wide range of possible applications and commercial potential. In optoelectronic devices such as organic solar cells, organic thin film transistors and organic light emitting diodes a transparent conductive top contact can be deposited onto an organic film. These inorganic/organic interfaces are responsible for injection or collection of charge carriers. Hence an understanding of the electronic structure of the interface region is crucial to improve the performance of these devices. In this study, thin films of the transparent conductive oxide (TCO) aluminum-doped zinc oxide (ZnO:Al) are deposited onto organic semiconductor layers by a dc magnetron sputtering process. Copper phthalocyanine (CuPc) is used as the organic donor material. Due to its very rigid crystal structure, it is supposed to withstand the impact of high kinetic energy particles generated during sputter deposition of the TCO. A detailed investigation of the interface between aluminum-doped zinc oxide and copper phthalocyanine is presented. The influence of the sputter deposition of the TCO layer onto the organic thin film is characterized with x-ray photoelectron spectroscopy and x-ray diffraction measurements.

DS 32.34 Thu 17:00 Poster B2

Interface Analysis of Thermally Evaporated Thin Noble Metal Films on PTCDI-C13 — ●CAROLIN C. JACOBI, DANIEL GEBAUER, RÜDIGER M. SCHMIDT, CHRISTINA M. M. GUNTERMANN, CATHY JODOCY, CHRISTIAN EFFERTZ, and MATTHIAS WUTTIG — I. Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany

In recent years optoelectronic devices based on organic thin-films have gained considerable interest. They offer a wide range of possible applications and have advantageous properties such as flexibility, applicability to large areas and low production costs. The performance of devices such as organic light emitting diodes (OLED), organic field effect transistors (OFET) or organic solar cells (OSC) depends critically on the interfaces between the different layers, e.g. the organic layer and the metal electrodes. In this study, thin noble metal top contacts (Gold and Silver) have been thermally evaporated with varying film thickness and different deposition rates on N,N*-ditridecyl-3,4,9,10-perylene-tetracarboxylic diimide (PTCDI-C13), which is a promising n-type material for OFETs, because it exhibits a high electron mobility. A detailed investigation of the interface between the noble metal contact and the underlying PTCDI-C13 layer is presented. We have characterized the influence of metal evaporation on the organic layer with photoelectron spectroscopy (PS) and Rutherford backscattering spectroscopy (RBS). The morphology of the metal top layer has been investigated by scanning electron microscopy (SEM).

DS 32.35 Thu 17:00 Poster B2

Influence of PCBM on the stability of the LBG Polymer PCPDTBT — ●ULF DETTINGER¹, HEIKO PEISERT¹, HANS-JOACHIM EGELHAAF², and THOMAS CHASSÉ¹ — ¹Eberhard-Karls-University Tübingen, Institute for Physical and Theoretical Chemistry, Auf der Morgenstelle 18, D-72076 Tübingen, Germany — ²Belectric OPV GmbH, Landgrabenstr. 94, D-90443 Nürnberg, Germany

Organic photovoltaic (OPV) incorporates an auspicious technology for the rising energy costs of the future. While aspiring for devices with higher efficiencies, the stability of the device materials is getting more and more important. It was observed, that the electron acceptor (EA) in bulk-heterojunction solar cells can affect the stability significantly [1]. We study the influence of the commonly used EA material PC[60]BM on the stability of the promising Low-Band-Gap Polymer PCPDTBT under illumination of standard Air Mass 1.5 conditions. The Photo-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. Different mechanisms for the influence of PC[60]BM on the stability of both donor materials are discussed.

[1] A. Dupuis et al. Eur. Phys. J. Appl. Phys., 2011, 56, 34104

DS 32.36 Thu 17:00 Poster B2

Orientation and self organization properties of new low band-gap polymers — ●UMUT AYGÜL¹, DAVID BATCHELOR², ULF DETTINGER¹, FLORIAN LATTEYER¹, MILUTIN IVANOVIC¹, HEIKO PEISERT¹, and THOMAS CHASSÉ¹ — ¹Eberhard Karls Universität Tübingen, Institut für Physikalische und Theoretische Chemie — ²Karlsruher Institut für Technologie, Institut für Synchrotron Strahlung

In polymer based organic solar cells so called "Low Band-Gap" (LBG)

polymers with their alternating electron-deficient and electron-rich subunits are promising donor components. The orientation and the electronic properties of these polymers play an important role in device performance and therefore a detailed understanding is necessary. The orientation was investigated via angular dependent NEXAFS (Near Edge X-Ray Absorption Fine Structure) measurements of the Sulfur K-edge as for 1s absorption edges the analysis of transitions into π^* molecular orbitals enables a relatively simple and direct determination of the molecular orientation. Obviously both the chemical and geometrical structure of the polymers determines the ability for self-organization. Consequently we studied the orientation of the LBG polymers PCPDTBT, Si-PCPDTBT and PCPDTBBT. Furthermore the influence of the acceptor molecule PCBM on the self organization properties of these polymers was studied by NEXAFS measurements of donor/acceptor blend films with varying amount of PCBM. In some cases a subsequent annealing step increases the ability for self-organization significantly.

DS 32.37 Thu 17:00 Poster B2

Comparative experimental and theoretical NEXAFS-study of Acenes and Azaacenes — ●MICHAEL KLUES¹, KLAUS HERMANN², and GREGOR WITTE¹ — ¹Physics Department, Philipps Uni. Marburg, 35032 Marburg — ²Theory Department, Fritz Haber Institute, 14195 Berlin

NEXAFS is a powerful tool to investigate the electronic structure of molecules and can also be used to determine the molecular orientation. However, these analyses require a precise assignment of the occurring resonances, which can be provided by modern ab-initio DFT calculations implemented e.g. in the StoBe package [1]. In this study we have measured the C1s- and N1s NEXAFS signatures of various acenes (benzene and anthracene, pentacene), aza-acenes and their hydrogenated derivatives which were compared with StoBe-based calculations. By comparing spectra of acenes and aza-acenes, we carve out the influence of the higher core charge of nitrogen on the molecular electronic structure. While this effect is quite small, a distinct effect occurs upon hydrogenation of the aza-species because the conjugation of the pi-system is reduced so that the resulting signature can be described by a superposition of a dihydropyrazine and sideways attached small acenes. [1] K. Hermann, L.G.M. Pettersson, et al. Stobe-demon version 3.1. 2011

DS 32.38 Thu 17:00 Poster B2

Domain dimensions, in-plane orientation and chemical contrast at the nanoscale: X-ray spectromicroscopy studies of organic molecules and polymers — ●ANTON ZYKOV¹, ROBERT STEYRLEUTHNER², MARCEL SCHUBERT³, TAYFUN METE³, KONSTANTINOS FOSTIROPOULOS³, PETER GUTTMANN³, STEPHAN WERNER³, KATJA HENZLER³, GERD SCHNEIDER³, DIETER NEHER², and STEFAN KOWARIK¹ — ¹Inst. of Physics, HU Berlin — ²Inst. of Physics, University of Potsdam — ³HZB, Berlin

Transmission X-ray microscopy (TXM) at the U41-TXM beamline at BESSY, Berlin was carried out to study polymers and molecules used for different organic optoelectronic devices. We investigate the polymers P3HT and P(NDI2OD-T2), which are photoactive materials for organic solar cells, and diindenoperylene (DIP) heterostructures as applied in OFET's. The films were deposited by spin-coating and OMDB under variation of the preparation conditions, e.g. choice of solvent, blend ratio, post-annealing temperatures and film thickness. The dimensions of domains ranging from 40 to 500nm were analyzed with the TXM resolution of ~30nm at the C K-edge. By measurements of the polarization dependency we obtain information about the orientation of polymer backbones and molecules in the domains, which strongly influences their optoelectronic properties. Due to the difference in the x-ray absorption energies of the used materials we got chemical contrast of blends at a nanoscale. These results will be correlated with the properties of the materials and conclusions will be drawn regarding the processes influencing the efficiency of the devices.

DS 32.39 Thu 17:00 Poster B2

Electronic structure derived from SXPS of TiO₂/C₆₀ and AZO/C₆₀ as model electron extraction interfaces in inverted organic solar cells — ●PHILIP RECKERS¹, SARA TROST², THOMAS RIEDL², THOMAS MAYER¹ und WOLFRAM JAEGERMANN¹ — ¹Technische Universität Darmstadt — ²Bergische Universität of Wuppertal

We present first results of our study on inverted organic solar cells (IOSC) using synchrotron induced photoelectron spec-

troscopy (SXPS). A typical device structure is ITO/TiO₂/PCBM:P3HT/MoO₃/Ag. The low work-function (LWMO) transparent metal oxide conductors TiO₂ or AZO act as electron extraction layer and MoO₃, with its high work-function (HWMO) as hole extractor. IV-characteristics using TiO₂ show photovoltaically unfavourable s-shape while AZO shows good diode characteristic. As PCBM cannot be evaporated without destruction, we investigate the model interface TiO₂/C60 and compare the derived interface band diagram to AZO/C60. The LWMOs were deposited ex-situ via ALD. The acceptor C60 was evaporated stepwise onto the LWMO. Band diagrams for the pristine materials and for the hetero-junctions are derived from SXPS spectra taken at BESSY II. The used energy gaps are derived from UV-Vis absorption spectra. The CBM/LUMO offset for TiO₂/C60 is 100 meV, and for AZO/C60 is 300meV with the LUMO above the conduction band maxima. Thus there is no offset at the TiO₂/C60 interface that was suspected to cause the unfavourable s-shaped IV-characteristic observed in the IOSC using PCBM.

DS 32.40 Thu 17:00 Poster B2

Ultrafast Photodynamics of the Indoline Dye D149 Adsorbed to Porous ZnO in Dye-Sensitized Solar Cells — ●NADINE HEMING^{1,2}, EGMONT ROHWER¹, CHRISTOPH RICHTER³, CHRISTIAN LITWINSKI⁴, DERCK SCHLETTWEIN³, and HEINRICH SCHWOERER¹ — ¹Laser Research Institute, Stellenbosch University, South Africa — ²Leibniz Institute for Solid State and Materials Research Dresden, Dresden University of Technology, Germany — ³Institute for Applied Physics, Justus-Liebig-Universität, Gießen, Germany — ⁴Chemistry Department, Rhodes University, South Africa

Research in the field of dye-sensitized solar cells (DSCs) has been driven by a desire to develop versatile, sustainable and affordable sources of electrical energy. We investigate photoinduced electron transfer dynamics between surface-adsorbed Indoline D149 and porous ZnO as used in working electrodes of dye-sensitized solar cells via femtosecond transient absorption spectroscopy. In the transient absorption spectra of dye D149 in solution, we found lifetimes of the excited state absorption (ESA) of 300 ± 50 ps. The absorption spectra of the dye adsorbed to ZnO shows a faster component, which is severely quenched to decay times of 150 ± 20 fs and can be assigned to the electron-transfer from the dye molecules to the semiconductor. Transient absorption spectroscopy was also conducted on the working electrode in contact with different electrolytes. The adsorption bands of the oxidized dye molecules show regeneration times in the excess of 1 ns and are shortened by the presence of electrolytes.

DS 32.41 Thu 17:00 Poster B2

Spin properties of the interface between cobalt and metal-quinolines — ●SABINE STEIL¹, ANDREA DROGHETTI², NICOLAS GROSSMANN¹, STEFANO SANVITO², MIRKO CINCHETTI¹, and MARTIN AESCHLIMANN¹ — ¹Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — ²School of Physics and CRANN, Trinity College Dublin, 2, Ireland

In metallorganic complexes it is expected that the metal atom plays a central role in determining the molecule electronic structure and thus the magnetic properties of hybrid interfaces formed with ferromagnetic metals. This is well known in the case of metal-phthalocyanines (MPc). In fact, recent experiments [1] have demonstrated that strong changes in the spin polarization of the MPc/cobalt interface can be induced by properly choosing the central metal atom. This is a fundamental knowledge for the design of future organic spintronics devices. As aluminium quinoline (Alq₃) is a prominent molecular candidate used in spin-valve systems [2], we investigated the effect of substituting the Al atom with either gallium or indium. The electronic structure of the molecules as well as the properties of the interfaces formed with ferromagnetic cobalt were study both, experimentally, by using different photoemission spectroscopy methods and, theoretically, with density functional theory calculations. The results will be discussed focusing on the application of different quinolines in spin-valve devices.

[1] S. Lach et al. *Advanced functional Materials* 22, 989 (2011)

[2] V. A. Dediu et al., *Nature Mater.* 8, 707 (2009)

DS 32.42 Thu 17:00 Poster B2

Towards Rolled-up Spintronic Devices - Effect of Water on Permalloy and CoPc Layers — ●PETER RICHTER¹, MARIA ESPERANZA NAVARRO FUENTES², FRANK LUNGWITZ¹, MICHAEL FRONK¹, DANIEL GRIMM², OLIVER G. SCHMIDT², DIETRICH R.T. ZAHN¹, and GEORGETA SALVAN¹ — ¹Semiconductor Physics, TU Chemnitz, 09126

Chemnitz, Germany — ²Institute for Integrative Nanosciences, IFW Dresden, 01069 Dresden, Germany

Using the technique of rolled-up nanotubes, we aim to manufacture spintronic devices made from cobalt phthalocyanine molecules (CoPc) sandwiched between ferromagnetic layers. A thin CoPc layer is deposited on top of a permalloy (Py) electrode by organic molecular beam deposition. To ensure a soft and secure contact, the top electrode is formed by a nickel layer, which is the outer part of a strain engineered nanomembrane that rolls up onto the structure. The roll-up process is triggered by exposing the system to water and thus dissolving a sacrificial germanium oxide contact layer. This preliminary study determines the effect that water will have on the magnetic and optical properties of Py and CoPc. Therefore, Py and CoPc/Py layers on Si were characterized by means of spectroscopic ellipsometry, reflection anisotropy spectroscopy as well as magneto-optical Kerr-effect spectroscopy and magnetometry - once for the fresh samples and once after exposing them together with GeO₂ to water for 4 hours. The results obtained demonstrate that an oxide layer grows on Py. The CoPc layers become optically thicker, possibly due to water incorporation. The magnetic coercivity of both layers, however, remains unchanged.

DS 32.43 Thu 17:00 Poster B2

Investigation of the influence of graphene interlayers on the interaction between cobalt phthalocyanine and Ni(111) by X-ray photoemission and absorption spectroscopies — ●JOHANNES UIHLEIN¹, HEIKO PEISERT¹, MATHIAS GLASER¹, MALGORZATA POLEK¹, HILMAR ADLER¹, FOTINI PETRAKI¹, RUSLAN OVSYANNIKOV², MAXIMILIAN BAUER², and THOMAS CHASSÉ¹ — ¹Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 18, 72076 Tübingen, Germany. — ²Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Elektronenspeicherring BESSY II, Albert-Einstein-Str. 15, 12489 Berlin, Germany.

The interactions appearing at interfaces between transition metal phthalocyanines (TMPCs) and metal substrates play an important role for electron transportation processes in optoelectronic devices and spintronic nanodevices. These molecule-substrate interactions also can drastically influence the magnetic properties of the adsorbed molecules. However, these interactions might be tuned by the insertion of an interfacial buffer layer in between the metal substrate and the adsorbed molecules. With its outstanding electronic properties, graphene promises to be an excellent candidate for the tuning of interface properties. Its influence on the interactions between cobalt phthalocyanine and a Ni(111) single crystal surface has been investigated by X-ray photoemission and absorption spectroscopies.

DS 32.44 Thu 17:00 Poster B2

Properties of Phthalocyanine Heterojunctions for the Application as Molecular Spintronic Materials — ●TORSTEN HAHN — Institut für Theoretische Physik, TU Freiberg, Germany

Recently charge and spin transfer at an interface between two well known transition metal phthalocyanines: MnPc and F16CoPc was observed [1]. The resulting partially charged species MnPcδ⁺ and F16CoPcδ⁻ show different electronic properties compared to their bulk counterparts. Density Functional Theorie investigations her with experimental photoelectron spectroscopy measurements reveal that the transferred charge is substantially confined to the two transition metal centers and that a hybrid state is formed between the two types of phthalocyanines. The impact of those findings on charge and spin transport of the heterojunction coupled to different contact materials is discussed. Additional current-voltage characteristics calculated within the non-equilibrium green functions formalism (NEGF) reveal clear predictions about the spin-filter properties of this novel material.

[1] S. Lindner et. al, *Phys. Rev. Lett.* 109, 027601 (2012).

DS 32.45 Thu 17:00 Poster B2

Determined Molecular Orientation of Terbium Diphthalocyanine Thin Films by Ellipsometry and Magneto-optical Kerr Effect Spectroscopy — ●P. ROBASCHIK¹, M. FRONK¹, S. KLYATSKAYA², M. RUBEN^{2,3}, D.R.T. ZAHN¹, and G. SALVAN¹ — ¹TU Chemnitz, 09126 Chemnitz, Germany — ²KIT, 76344 Eggenstein-Leopoldshafen, Germany — ³ICPMS, 67034 Strasbourg, France

The detection and control of the molecular growth mode is a key prerequisite for fabricating opto-electronic and future spintronic devices. Thin films of the single molecule magnet (SMM) terbium diphthalocyanine, which are successfully deposited by organic molecular beam deposition on silicon substrates covered with native oxide, are inves-

tigated by means of variable angle spectroscopic ellipsometry (VASE) and magneto-optical Kerr effect (MOKE) spectroscopy at room temperature. The molecular orientation was determined from the degree of uniaxial anisotropy of the optical constants. A numerical analysis of the energy dispersion of the real and imaginary part of the complex magneto-optical Kerr rotation angle in the 1.7 eV to 5.0 eV spectral range allows the magneto-optical material constant, the so-called Voigt constant, to be determined. The amplitude of the Voigt constant provides a more sensitive measure for the molecular orientation in thin films than spectroscopic ellipsometry. While VASE and MOKE are able to yield quantitative results for the molecular angle, MOKE can even resolve slight relative differences. The organic molecules in a thin film below 10 nm were found to have molecular planes close to parallel to the silicon substrate and the tilt angle increases in thicker films.

DS 32.46 Thu 17:00 Poster B2

Electro-optical characterization of CIGS solar cells with varied absorber compositions — ●ALEXANDER KUSCH, MICHAEL OERTEL, DAVID STOLL, UDO REISLÖHNER, and CARSTEN RONNING — Institut für Festkörperphysik, Physikalisch-Astronomische Fakultät, Friedrich-Schiller-Universität Jena, Helmholtzweg 3, 07743 Jena, Germany

The results of the electro-optical characterization of sequentially processed Cu(In, Ga)Se₂ solar cells are presented. The first step of the sequential absorber layer forming process is the deposition of a multi-layer system containing copper, indium and gallium on top of a molybdenum back contact. Both the multi-layer system and the back contact are deposited by DC-magnetron sputtering. In the second step this metallic precursor is reactively annealed in two steps in a selenium vapour atmosphere where it is converted to an about 2 μm thick CIGSe absorber layer. Electro-optical measurements of solar cells with such prepared absorber layers show strong variations in the resulting characteristics for different precursor compositions. The efficiency of gallium free cells can vary by up to 20% as a function of the [Cu]:[In] ratios in the range of 0.75 < [Cu]:[In] < 0.95. The distribution and share of gallium within the absorber was varied and the impact on solar cell performance was investigated.

DS 32.47 Thu 17:00 Poster B2

Spatially-resolved measurements of charge carrier lifetimes in CdTe solar cells — ●MARTIN KRAUSSE¹, CHRISTIAN KRAFT¹, HANNES HEMPEL¹, VOLKER BUSCHMANN², TORSTEN SIEBERT², CHRISTOPH HEISLER¹, WERNER WESCH¹, and CARSTEN RONNING¹ — ¹Friedrich-Schiller-Universität Jena, Physikalisch-Astronomische Fakultät, Max-Wien-Platz 1, 07743 Jena, Germany — ²PicoQuant GmbH, Rudower Chaussee 29, 12489 Berlin, Germany

The lifetime of the minority charge carriers in polycrystalline Cadmium Telluride (pc-CdTe) for solar cell applications is a crucial material parameter and has been determined by analysis of the decay curves of the luminescence signal. Both the lateral and transversal distribution of the carrier lifetime on the surface and in the bulk of pc-CdTe material as well as the respective solar cell characteristics were measured as a function of the deposition technique, the activation treatment and the incorporation of additional group-V elements. The results are compared to prior studies.

It was found, that an activation process passivates grain boundaries and increases the carrier lifetime, which is then higher at the p-n junction than at the surface. Furthermore, nitrogen and phosphorus doping of the CdTe absorber material influences the charge carrier lifetime. The results show that the spatial resolved measurement of the carrier lifetime in pc-CdTe gives an important insight to the charge carrier dynamics of the material.

DS 32.48 Thu 17:00 Poster B2

Investigation of physical properties of doped ZnTe thin films for solar cell applications — ●WAQAR MAHMOOD — Thin Films Technology Research Laboratory, COMSATS Institute of Information Technology

Zinc telluride thin films were deposited on to glass substrate using close spaced sublimation technique. The thickness of these films was optimized by deposition time. Cu & Ag doped thin films of same thickness were considered for comparative study. XRD pattern showed polycrystalline ZnTe thin films with preferred orientation (111) having cubic phase. ZnTe thin films were immersed in Ag (NO₃)₂ and Cu (NO₃)₂ solution for different times varying from 05 min to 20 min respectively. The temperature of dopant solutions were kept at 600C ± 50C throughout the doping process. Post annealing of doped ZnTe thin films was done at 3500C for 1 hour under vacuum of 10-4 mbar. In

XRD spectra, the crystallite size was increased after silver and copper immersion. SEM with EDX indicated the change in grain size of as-deposited and doped samples with compositional analysis of Cu and Ag in ZnTe thin films. Optical study showed the change of energy band gap in doped samples with as deposited ZnTe also %T decreases after immersion. Resistivity of as deposited ZnTe thin films was about 106 Ω-cm. which was reduced upto 68.97 Ω-cm after Cu immersion. The resistivity was reduced up to 104 Ω-cm after Ag immersion. Raman spectra showed TO and LO modes also it was used to check the crystallinity of un-doped and doped ZnTe samples.

DS 32.49 Thu 17:00 Poster B2

optical investigation of kesterite and CIGS solar cell absorber layers — ●DAVID SPERBER¹, CHRISTOPH KRÄMMER¹, CHAO GAO¹, MANUEL LÖW², THOMAS SCHNABEL², ERIK AHLWEDE², MICHAEL POWALLA², HEINZ KALT¹, and MICHAEL HETTERICH¹ — ¹Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — ²Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), Stuttgart, Germany

CIGS is a well-established absorber material for thin film solar cells and efficiencies above 20% have been demonstrated. Due to its abundant components kesterite Cu₂ZnSn(S,Se)₄ is a very promising alternative. However optical properties and the band structure of this material are still not entirely understood. We investigate kesterite solar cells and absorbers using modulation spectroscopy techniques. The results of temperature dependent electroreflectance and photoreflectance measurements to detect fundamental and higher optical transitions will be presented and discussed.

DS 32.50 Thu 17:00 Poster B2

preparation of Cu₂ZnSn(S,Se)₄ thin films and solar cells by chemical bath deposition — ●CHAO GAO¹, THOMAS SCHNABEL², ERIK AHLWEDE², MICHAEL POWALLA^{2,3}, HEINZ KALT¹, and MICHAEL HETTERICH¹ — ¹Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — ²Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart, Germany — ³Light Technology Institute (LTI), Karlsruhe Institute of Technology (KIT)

Cu₂ZnSn(S,Se)₄ (CZTSSe) is a promising absorber material for thin-film solar cells. It has the suitable optical band-gap for photovoltaic energy conversion, a high optical absorption coefficient, and all its constituent elements are abundant and non-toxic. Here we show a low-cost aqueous solution approach to prepare Cu₂ZnSn(S,Se)₄ thin films: SnS/CuS/ZnS precursor layers were prepared by chemical bath deposition firstly and then the precursor films were selenized in a graphite box under inert gas atmosphere. By optimizing the fabrication parameters, CZTSSe thin films with good quality could be obtained. The films were characterized by XRD, SEM, EDX, etc. Finally, first CZTSSe solar cells could be fabricated the properties of which will be discussed in our contribution.

DS 32.51 Thu 17:00 Poster B2

Flash Lamp Annealing of Spray Coated Silicon Nanoparticle Films — ●DANIEL BÜLZ, FALKO SEIDEL, IULIA G. TOADER, RONNY FRITZSCHE, BENJAMIN BÜCHTER, ALEXANDER JAKOB, ROY BUSCHBECK, MICHAEL MEHRING, HEINRICH LANG, and DIETRICH R. T. ZAHN — TU Chemnitz, 09126 Chemnitz, Germany

Flash lamp annealing (FLA) of spray coated silicon nanoparticles (Si NP) is considered as a low cost alternative for thin film solar cell fabrication. In this work the effect of FLA on Si NP films produced with varying number of spray cycles is investigated by Raman spectroscopy, scanning electron microscopy, and electrical characterization. The Si NPs are dispersed in ethanol or tetrahydrofuran + di-N-methylpyrrole-silane [H₂Si(NMP)₂], the latter being a silicon precursor. The organosilicon acts as glue between the Si NPs in order to achieve more compact spray coated films. The suspensions are sprayed onto a preheated substrate (molybdenum sheets and hydrogen passivated doped silicon wafers). Then the samples are treated by FLA (energy: 6,37 J/cm²; pulse time: 900 μs; flash lamp system provided by Dresden Thin Film Technology) varying the number of flashes. The whole procedure takes place in a glove box under nitrogen atmosphere to prevent oxidation. A sputtered Ni-Cr alloy reveals ohmic contact behaviour on the FLA treated spray coated Si NP films. It turns out, that adding a silicon precursor to the Si NP suspension improves the effect of FLA on spray coated films. The Si NPs are more contiguous within the films and the amount of fused Si NPs is larger than for films sprayed from pure Si NP suspensions.

DS 32.52 Thu 17:00 Poster B2

Plasma induced nitrogen incorporation in CdTe-layers for solar cell applications — ●MARTIN SALGE, CLAUDIA SCHNITZER, CHRISTOPH HEISLER, CHRISTIAN KRAFT, and WERNER WESCH — Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 3, 07743 Jena, Germany

CdTe is a promising absorber material for solar cells considering its direct band gap of 1.5 eV. CdTe solar cells feature low production costs per watt and reach efficiencies of about 17 % on a laboratory scale. The intrinsic p-type doping level of CdTe used for solar cell application is typically 10^{14} cm^{-3} . However, the efficiency can be increased further by raising the doping level by several orders of magnitude [1]. Using group-V-elements as a dopant on tellurium lattice sites is one possibility to achieve an increase in carrier concentration. Thereby, nitrogen is a promising material because in CdTe it creates doping energy levels within the band gap close to the valence band edge. In this experiment nitrogen ions were incorporated by a plasma source simultaneously to the physical vapor deposition of the CdTe-layer. Several source parameters during the absorber deposition were varied and their effects on the solar cell characteristics were studied. It was found that the solar cell characteristics and the p-type doping of CdTe absorber layers decrease significantly with increasing acceleration voltage of the N-ions. Possible reasons for that are under investigation.

[1] Sites, J. R. und J. Pan, Thin Solid Films, 515:6099, 2007

DS 32.53 Thu 17:00 Poster B2

Modulated charge separation across disordered TiO₂ / In₂S₃ hetero-junctions — ●ALBERT JUMA, ANAHITA AZARPIRA, CHRISTIAN-HERBERT FISCHER, and THOMAS DITTRICH — Helmholtz-Centre-Berlin for Materials and Energy, Hahn-Meitner-Platz 1, 14109 Berlin, Germany.

Charge separation across hetero-junctions between disordered wide gap semiconductors and suitable inorganic absorbers play a decisive role for the development not only of nanocomposite solar cells. Extremely thin coatings of Cl-free and Cl-containing In₂S₃ (In₂S₃:Cl) layers were prepared by spray ion layer gas reaction (ILGAR) on nanoporous TiO₂ (np-TiO₂). Charge separation in FTO/np-TiO₂/In₂S₃:Cl, FTO/In₂S₃:Cl, FTO/np-TiO₂ / In₂S₃ and FTO/In₂S₃ systems has been investigated by modulated surface photovoltage spectroscopy (SPV). The exponential defect tails below the band gap of In₂S₃ were reduced for In₂S₃:Cl. The analysis of the SPV spectra allowed to distinguish different mechanisms of charge separation and to deduce the conduction band offsets (about 0.3 eV and 0.05 eV for np-TiO₂/In₂S₃:Cl and np-TiO₂/In₂S₃, respectively).

DS 32.54 Thu 17:00 Poster B2

Wire-based dye-sensitized solar cells using electrodeposited zinc oxide on passivated metals — ●TIM HELBIG, MELANIE RUDOLPH, and DERCK SCHLETTWEIN — Justus-Liebig-University Giessen, Institute of Applied Physics, Heinrich-Buff-Ring 16, D-35392 Giessen, Germany

Metal substrates provide good properties as electrode material in dye-sensitized solar cells (DSSC) such as good processability, high conductivity and mechanical flexibility. In order to be used in DSSC the metal has to be inert against the iodine-containing electrolyte used in DSSC. Passivated metals such as tungsten, stainless steel or aluminum are covered with a natural oxide layer providing protection against corrosion and are therefore of interest as electrode materials. Zinc oxide thin films were prepared as porous semiconductor on tungsten or aluminum wires by electrochemical deposition. The indoline dye D149 was adsorbed to the surface of the porous zinc oxide as a sensitizer. The films were studied as a photo anode of a DSSC.

DS 32.55 Thu 17:00 Poster B2

Laser processing for CIGS thin-film solar cells — ●XI WANG^{1,2}, DORENA FLEISCHER², PIERRE LORENZ², MARTIN EHRHARDT², XI-AOWU NI¹, and KLAUS ZIMMER² — ¹Nanjing University of Science & Technology, Xiaolingwei 200, 210094 Nanjing, China — ²Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstraße 15, 04318 Leipzig, Germany

The Cu(InGa)Se₂ (CIGS) thin-film solar cell attracts increasing attention because of its low cost, flexible character and high efficiency. Laser is an effective tool in performing the monolithic integrated interconnection and external integrated interconnection for the module fabrication. CIGS thin-film solar cells were scribed with picosecond

laser with a pulse length of 10 ps and a wavelength of 1064 nm. The material modification and the electrical properties were influenced by the laser parameters such as fluence, frequency, and scanning speed. In the present study, the interaction mechanisms of CIGS thin-film solar cell material with picosecond laser beam were investigated. The laser-induced material removal and the material morphology of the laser-scribed areas were analyzed by scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX). The electrical current voltage (I-V) curves with the open circuit voltage and parallel resistance were measured with an in situ measurement. Goal of the examination was the improvement of the generation of scribes in the CIGS material under attention to electrical properties in combination with surface characteristics for optimal preparation of further steps of production.

DS 32.56 Thu 17:00 Poster B2

Influence of surface treatments on the charge recombination characteristics in porous ZnO for dye-sensitized solar cells — ●CHRISTOPH RICHTER, MAX BEU, and DERCK SCHLETTWEIN — Institute of Applied Physics, Justus Liebig University of Giessen, Heinrich Buff-Ring 16, 35392 Giessen, Germany.

ZnO films to be used in dye-sensitized solar cells (DSC) can be grown by electrochemical deposition of a porous ZnO/EosinY hybrid material from an aqueous solution of ZnCl₂. In a subsequent step the EosinY has to be desorbed to provide a porous network of ZnO for the adsorption of a sensitizer. The step of EosinY desorption is performed in an aqueous solution of 10.5 pH KOH. This treatment can alter the surface of ZnO which typically leads to changes in the charge transfer characteristics (mainly recombination) at the semiconductor/electrolyte interface in the assembled DSC. In this work different methods of EosinY desorption and different post-treatment steps of the surface are studied. The consequences of the different treatment steps on the charge transfer from porous ZnO to an iodine-containing electrolyte are studied by IV-curves and electrochemical impedance spectroscopy. Appropriate strategies to compensate surface changes introduced by the desorption step of EosinY are presented.

DS 32.57 Thu 17:00 Poster B2

Thin magnesium silicide semiconducting films for photo-voltaics — ●CARINA EHRIG^{1,2}, RALF KRAUSE¹, GÜNTER SCHMID¹, and CHRISTOPH BRABEC² — ¹Siemens AG, CT RTC MAT MPV-DE, Erlangen — ²Lehrstuhl für Werkstoffe der Elektronik- und Energietechnik, FAU Erlangen-Nürnberg, Erlangen

The semiconducting magnesium silicide (Mg₂Si) is a promising candidate for a low-cost and efficient absorber layer for solar cells. Its main application so far is as a high-performance thermoelectric material due to its high figure of merit. Little is known, however, about its applicability as a photoactive material. The metal-rich semiconducting Mg₂Si is the only stable phase in the Mg-Si system. It has a narrow indirect band gap of 0.78 eV. Its absorption coefficient of $\alpha = 3.5 \times 10^5 \text{ cm}^{-1}$ at 2.5 eV is about 40 times higher than that of c-Si, which makes it an interesting material for producing thin solar cells.

In the present work, Mg₂Si thin films were produced by thermal evaporation of Mg on Si substrates and subsequent annealing. This results in the formation of flat and homogeneous Mg₂Si layers, which can be adjusted in thickness by varying the annealing temperature and time as well as the amount of Mg deposited. The Mg₂Si films are characterized in terms of morphological, electrical and optical properties. Furthermore, measurements on the photoactivity of these layers will be discussed as well as several ideas for the usage of this material in solar cell devices. For example, the formation of a pn-junction consisting of a p-type silicon wafer and an n-type Mg₂Si thin layer as well as other solar cell designs are proposed.

DS 32.58 Thu 17:00 Poster B2

Electrical and structural characterization of CdTe thin film solar cells with In₂S₃ buffer layer — ●FELIX LIND¹, JOHANNA KRAMMER², CHRISTOPH HEISLER¹, CHRISTIAN KRAFT¹, CHRISTIAN-HERBERT FISCHER², and WERNER WESCH¹ — ¹Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 3, 07743 Jena — ²Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin

As an alternative to the commonly used toxic CdS, in this work In₂S₃ is used as n-type buffer layer in CdTe thin film solar cells. In contrast to CdS, In₂S₃ can be deposited in a non-vacuum process at low temperatures without producing toxic waste. The In₂S₃ buffer layers with varied chlorine concentrations and thicknesses were fabricated with the

"ion layer gas reaction" (ILGAR) process. Subsequently the CdTe layers were deposited by the physical vapour deposition (PVD) method. The electrical properties of the complete solar cells were investigated by means of current-voltage measurements (I-V) and external quantum efficiency (EQE). The results show that the conversion efficiencies and quantum efficiencies are significantly lower for the CdTe thin film solar cells with In₂S₃ buffer layer compared to solar cells with CdS buffer layer. Scanning transmission electron microscopy (STEM) was used to investigate the structural properties. It was found that the post deposition CdCl₂-treatment leads to a non-uniform and lower thickness of the In₂S₃ layer. Altogether CdTe solar cells with In₂S₃ buffer layer are producible in principle at the used process parameters, but show no improvement compared to CdS buffer layer.

DS 32.59 Thu 17:00 Poster B2

Composition-dependent atomic-scale structure of Cu(In,Ga)S₂ — ●STEFANIE ECKNER¹, HELENA KÄMMER¹, TOBIAS STEINBACH¹, MARTIN GNAUCK¹, ANDREAS JOHANNES¹, CHRISTIANE STEPHAN², SUSAN SCHORR², and CLAUDIA SARAH SCHNOHR¹ — ¹Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — ²Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

In order to exploit the full potential of Cu(In,Ga)S₂-based thin film solar cells, a deeper understanding of the composition-dependent atomic-scale structure along with its influence on electrical properties such as the band gap is necessary. In this study, element-specific first nearest neighbour distances of Cu(In,Ga)S₂ were determined as a function of the In/(In+Ga) ratio using extended X-ray absorption fine structure spectroscopy. All three bond lengths, namely Cu-S, Ga-S and In-S, are found to differ from each other and to remain nearly constant over the whole compositional range of $0 \leq \text{In}/(\text{In}+\text{Ga}) \leq 1$ despite the significant change of the lattice constants. Structural parameters have also been simulated with a valence force field model for all possible first nearest neighbour configurations surrounding the S anions. Excellent agreement between the calculated average bond lengths and the experimental values is obtained for a non-random distribution of In and Ga atoms that favours a mixed Cu-In-Ga configuration over the pure Cu-In or Cu-Ga first nearest neighbour shells.

DS 32.60 Thu 17:00 Poster B2

Photoluminescence study of polycrystalline silicon thin films prepared by liquid and solid phase crystallization — ●STEFFI SCHÖNAU, JÖRG RAPPICH, MOSHE WEIZMAN, DANIEL AMKREUTZ, and BERND RECH — Kekuléstr. 5, 12489 Berlin

Polycrystalline silicon thin films were prepared by depositing amorphous or microcrystalline silicon layers onto glass substrates and subsequent crystallization via solid or liquid phase crystallization approaches. Differences in layer morphology and quality were charac-

terized using low temperature photoluminescence (PL) spectroscopy and electron backscatter diffraction spectroscopy. The analysis of spectrally and spatially resolved photoluminescence from poly-Si thin films was shown to be a useful tool for a fast characterization of the sample recombination behavior of light induced charge carriers.

DS 32.61 Thu 17:00 Poster B2

A study of compensation in CZTSSe absorber layers by Photoluminescence spectroscopy and Capacitance-Voltage profiling — ●STEFFEN KRETZSCHMAR, SERGEJ LEVCENKO, JUSTUS JUST, and THOMAS UNOLD — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Technologie, Hahn-Meitner-Platz 1, D-14109 Berlin

With the demonstration of a conversion efficiency of 11.1% the potential of Cu₂ZnSn(S,Se)₄ (CZTSSe) as an alternative absorber material for thin film photovoltaics has been confirmed. Nevertheless only little knowledge exists on the electronic properties in the bandgap. Especially a thorough understanding of beneficial electronic properties and their dependence on the chemical composition of the material is needed to improve the CZTS solar cell performance further.

Here a study by Photoluminescence (PL) spectroscopy of absorber layers in a wide range of composition is presented. Excitation and temperature dependent PL-measurements are carried out and are related to the findings from Capacitance-Voltage (CV) profiling on solar cells made of absorber layers from the same growth process. The results exhibit a beneficial influence of compensation by donors on the conversion efficiency of CZTSSe solar cells.

DS 32.62 Thu 17:00 Poster B2

Development of a Laser based Zinc oxide treatment for the systematic variation of electro-optical properties — ●ERIK SCHUMANN^{1,2}, STEFAN HAAS², and JÜRGEN HÜPKES² — ¹Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany — ²IEK5 - Photovoltaik, Forschungszentrum Juelich GmbH, D-52425 Juelich, Germany

Zinc oxide is a widely used transparent conductive oxide (TCO), e.g. as front contact for thin film solar cells. Though already having a low absorption in the visible spectral range and a good conductivity, magnetron sputtered zinc oxide can be improved to increase the performance of thin film solar cells [1,2]. A laser treatment was developed to improve the electrical and optical properties of this material. The influence of the different process parameters were investigated. In addition, the effect of the ambient atmosphere, i.e. oxygen and nitrogen, were analysed. Different schemes to prevent exposure of zinc oxide to ambient atmosphere during laser treatment will be presented. This work is part of the LIST project (BMU: 0325299). [1] M. Berginski, PhD thesis, RWTH Aachen, FZ Juelich (2007) [2] M. Wimmer et. al., Thin Solid Films 520, 4203 (2012)