

## DS 39: Poster Session II

Time: Thursday 16:00–18:30

Location: Poster F

DS 39.1 Thu 16:00 Poster F

**Charge transfer effects in binary mixtures of organic semiconductors: DIP:F6-TCNNQ as a case study** — ●GIULIANO DUVA<sup>1</sup>, VALENTINA BELOVA<sup>1</sup>, ALEXANDER HINDERHOFER<sup>1</sup>, ALEXANDER GERLACH<sup>1</sup>, ANDREAS OPITZ<sup>2</sup>, PAUL BEYER<sup>2</sup>, and FRANK SCHREIBER<sup>1</sup> — <sup>1</sup>Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen (Germany) — <sup>2</sup>Humboldt-Universität zu Berlin, Department of Physics, Brook-Taylor-Str. 6, 12489 Berlin (Germany)

Binary mixtures of organic semiconductors have been studied in planar and bulk heterojunction architectures [1], and a correlation between the structural and optical properties has been found [2]. The orientation of the molecular components of donor-acceptor type binary mixtures has been recently shown to have a dramatic impact on charge-transfer efficiency [3]. However, charge transfer effects in donor-acceptor organic systems have not been fully understood yet. We use several experimental techniques to characterize the structure and molecular orientation and identify charge-transfer effects within systems of DIP as the donor and F6-TCNNQ as the acceptor, namely in bulk heterojunction architecture. Remarkably, charge transfer effects studied by means of IR spectroscopy, UV-vis and spectroscopic ellipsometry, and PL are related to structural properties of the films obtained by means of XRR and GIXD together with morphological characterization by means of AFM. [1]A. Hinderhofer and F. Schreiber, Chem. Phys. Chem. 13 (2012); [2]K. Broch et al., J. Chem. Phys. 139 (2013); [3]G. Aghamohammadi et al., J. Phys. Chem. C 118 (2014).

DS 39.2 Thu 16:00 Poster F

**Orientation controlled growth of metal phthalocyanines and their optical characterization** — JAN KUHNERT, ●MICHAEL KOTHE, WOLFRAM HEIMBRODT, and GREGOR WITTE — Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany

Phthalocyanines in combination with metal oxides are promising materials for future electronic devices such as organic solar cells (OPV). Despite their technological importance a microscopic understanding of optoelectronic excitations in such hybrid systems has yet not been achieved. To gain deeper insight ordered model systems with well-defined interfaces are mandatory. In this contribution we have studied the interrelation of structural and optical properties of Phthalocyanine thin films that were grown onto various substrates. Their structure were studied by means of XRD, AFM while the optical properties were analyzed by continuous wave and time-resolved photoluminescence spectroscopy and absorption measurements.

DS 39.3 Thu 16:00 Poster F

**Preparation and Characterisation of Crystalline C<sub>60</sub> and Pentacene Interfaces** — ●ANDREA KARTHÄUSER, TOBIAS BREUER, and GREGOR WITTE — Molekulare Festkörperphysik, Philipps-Universität Marburg, Renthof 7, D-35032 Marburg, Germany

Their tunable electronic properties as well as their high photon cross-sections have resulted in increased research efforts in organic semiconductors. However, the complex nature of their interface characteristics concerning the correlation between structural and electronic properties, has not yet been entirely elucidated, mostly due to the lack of appropriate model systems. Here we report on the preparation of such a model system of the donor-acceptor pair Pentacene (PEN, C<sub>22</sub>H<sub>14</sub>) and Buckminster-Fullerene (C<sub>60</sub>). Two strikingly different interfaces can be realised between these two compounds, due to their different molecular geometry, which have been theoretically predicted to strongly influence the stability of the interface formation [1] and the electronic properties [2]. Depositing C<sub>60</sub> on upright oriented PEN grown on SiO<sub>2</sub>, causes pronounced step decoration and yields non-crystalline C<sub>60</sub> adlayers [3]. Here we reserved the system and deposited PEN onto single crystalline C<sub>60</sub> films that were grown on NaCl(100). The resulting morphology and molecular orientation have been analysed by AFM, XRD and - after successfully transferring the films to conducting substrates - also by NEXAFS spectroscopy.

[1] Fu, Y. T. et al. Adv. Mater. (2013), 25, 878. [2] Yi, Y. P. et al. J. Am. Chem. Soc. (2009), 131, 15777. [3] Breuer, T. et al. ACS Appl. Mater. Interfaces (2013), 5, 9740.

DS 39.4 Thu 16:00 Poster F

**Reactive Metal/Organic Interfaces Studied with HAXPES and Nanojoule Calorimetry** — ●HAN ZHOU<sup>1</sup>, HANS-JÖRG DRESCHER<sup>1</sup>, MIN CHEN<sup>1</sup>, BENEDIKT KLEIN<sup>1</sup>, CLAUDIO KRUG<sup>1</sup>, MALTE ZUGERMEIER<sup>1</sup>, MALTE SACHS<sup>1</sup>, STEFAN KACHEL<sup>1</sup>, MIHAELA GORGOI<sup>2</sup>, and J. MICHAEL GOTTFRIED<sup>1</sup> — <sup>1</sup>Fachbereich Chemie, Philipps Universität Marburg, Hans-Meerwein-Straße 4, 35032 Marburg, Germany — <sup>2</sup>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Metal/organic interfaces are of the critical importance to the performance of modern organic semiconductor devices. Besides the idealized model systems with an atomically abrupt and chemically inert interface, more realistic systems with the formation of extended diffusion and reaction zones between metal and organic phase must be considered. These extended interfaces required bulk sensitive methods such as Hard X-ray Photoelectron Spectroscopy (HAXPES) and Nanojoule Calorimetry for investigation. Here, we report on the interfaces between (a) Ca and sexithiophene (6T) and (b) Co and tetraphenylporphyrin (2HTPP), two model systems in which interface reactions were observed. Ca in contact to 6T forms CaS, resulting in massive structural changes of the organic semiconductor. In contrast, the reaction of Co with 2HTPP is much more specific and leads to the formation of the complex CoTPP as a well-defined product. Depth profiling with HAXPES and complementary studies provide a comprehensive picture of the chemical and electronic structure of the interfaces.

DS 39.5 Thu 16:00 Poster F

**Investigation of organic thin films of DIP and C<sub>60</sub> mixtures using *in situ* X-ray diffraction techniques** — ●HEIKO FRANK, CHRISTOPHER LORCH, RUPAK BANERJEE, ALEXANDER HINDERHOFER, ALEXANDER GERLACH, and FRANK SCHREIBER — Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen

Mixtures of organic semiconductors offer a variety of applications, including devices such as photovoltaic cells [1]. The optical and electrical properties of such devices depend *inter alia* on the structure of these mixtures and therefore on the preparation conditions [2,3]. Thus, understanding the structure of organic thin films is a key point for the optimization of such systems.

In this work, we investigate organic thin films consisting of mixtures of DIP and C<sub>60</sub> with a molecular ratio of 1:1 on SiOx substrates. The films are prepared using organic molecular beam deposition (OMBD) and characterized *in situ* and in real-time [4] using X-ray reflectivity (XRR) and grazing incidence X-ray diffraction (GIXD). Our results indicate that the structural ordering of the mixed films has a strong dependence on the kinetics of the growth, which can be influenced by parameters like the temperature of the substrate, the total deposition rate and the growth type (continuous vs. interrupted growth).

[1] J. Wagner *et al.*, Adv. Funct. Mater. **20**, 4295 (2010) [2] A. Hinderhofer and F. Schreiber, ChemPhysChem **13**, 628 (2012) [3] R. Banerjee *et al.*, Phys. Rev. Lett. **110**, 185506 (2013) [4] S. Kowarik *et al.*, Europ. Phys. J. - Special Topics **167**, 11 (2009)

DS 39.6 Thu 16:00 Poster F

**Electron-impact induced HF elimination in fluorinated PAHs: Molecular building blocks for new carbon nanostructures** — ●JÜRGEN WEIPPERT<sup>1</sup>, SEYITHAN ULAS<sup>1</sup>, PATRICK WEIS<sup>1</sup>, JEAN-FRANCOIS GREISCH<sup>2</sup>, KONSTANTIN Y. AMSHAROV<sup>3</sup>, ARTUR BÖTTCHER<sup>1</sup>, and MANFRED M. KAPPES<sup>1,2</sup> — <sup>1</sup>Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany — <sup>2</sup>Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — <sup>3</sup>University Erlangen-Nürnberg, Institut für Organische Chemie, Henkestr. 42, 91054, Germany

Electron-impact induced HF-elimination (EIIHF) from fluorinated PAHs (F-PAHs) has been used to create curved molecular carbon structures which cannot be accessed synthetically. We have studied this process using three F-PAHs: C<sub>26</sub>H<sub>14</sub>F<sub>2</sub>, C<sub>36</sub>H<sub>15</sub>F<sub>3</sub> and C<sub>60</sub>H<sub>21</sub>F<sub>9</sub>. The products of the sequential EIIHF (C<sub>26</sub>H<sub>12</sub><sup>+</sup>, C<sub>36</sub>H<sub>12</sub><sup>+</sup> and C<sub>60</sub>H<sub>12</sub><sup>+</sup>) have been deposited mass-selectively onto HOPG substrate and their electronic, thermodynamic and vibrational properties

analysed by means of UPS, XPS, AFM, TDS and Raman spectroscopy. For all studied molecules HF-elimination is the major fragmentation channel. In contrast to large planar  $C_{60}H_{21}F_9$  molecules, the smaller precursors were found to be entirely dehydrofluorinated upon  $70\text{eV } e^-$  impact. The hydrodefluorination of  $C_{60}H_{21}F_9$  molecules stops after the sixth EIIHF-step and the resulting products exhibit molecular structures (caps) of relevance for further (n,m)-selective growth of SWCNT.

DS 39.7 Thu 16:00 Poster F

**CHARGE TRANSFER IN ORGANIC MIXED FILMS OF DIINDENOPERYLENE AND PDIR-CN2** — ●VALENTINA BELOVA<sup>1</sup>, GIULIANO DUVA<sup>1</sup>, PAUL BEYER<sup>2</sup>, ALEXANDER HINDERHOFER<sup>1</sup>, ALEXANDER GERLACH<sup>1</sup>, FRANK SCHREIBER<sup>1</sup>, and ANDREAS OPITZ<sup>2</sup> — <sup>1</sup>Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — <sup>2</sup>Department of Physics, Humboldt-Universität zu Berlin, Brook-Taylor-Straße 6, 12489 Berlin, Germany

Interface doping by molecular charge transfer is a promising approach to tune the electronic properties of organic semiconductors without changing their molecular arrangement [1]. DIP (diindenoperylene) was chosen as a prototypical donor with good charge transport properties and optical contrast [2]. Since DIP ( $C_{32}H_{14}$ ) possesses relatively high ionization energy (5.35 eV) it requires strong acceptor like PDIR-CN2 ( $C_xH_yO_4N_4$ ) with electron affinity 4.3 eV. We studied thin blended (co-evaporated) films by structural and optical methods in order to investigate charge transfer effect between the HOMO of DIP and the LUMO of PDIR-CN2. Optical studies involved FTIR spectroscopy, spectroscopic ellipsometry, UV-VIS absorption, as well as photoluminescence (temperature dependent) and Raman spectroscopy. Structural and morphological characterisation of the mixed films was carried out by X-ray diffraction and atomic force microscopy. Signatures of intermolecular interaction in DIP:PDIR-CN2 mixtures are discussed.

[1] A. Hinderhofer/F. Schreiber, ChemPhysChem, 13, 628 (2012) [2] J. Wagner et al., Adv. Funct. Mater. 20, 4295 (2010)

DS 39.8 Thu 16:00 Poster F

**Epitaxial TTF-TCNQ Thin Films on KCl(100): New Preparation Methods and Observation of Interface-Mediated Thin Film Polymorph** — ●ALEXANDER MÄNZ, TOBIAS BREUER, and GREGOR WITTE — Molekulare Festkörperphysik, Fachbereich Physik, Philipps-Universität Marburg, Renthof 7, 35032 Marburg

Though the bulk properties of the prototypical organic charge-transfer complex Tetrathiafulvalene-Tetracyanoquinodimethane (TTF-TCNQ) have been studied in detail, the influence of defects and crystallite size on resulting electronic properties as well as an integration of these materials in organic thin film devices is barely explored. One important requirement for such a comprehension is the precise control over crystallite size and quality. In this study, we report on different strategies to prepare crystalline TTF-TCNQ thin films and compare their structural quality. While conventional organic molecular beam deposition of TTF-TCNQ onto KCl(100) substrates enables the growth of epitaxial thin films with grain dimensions of up to  $2\ \mu\text{m}$ , further enhancement of the crystallite dimensions by raising the growth temperature is thermally limited by vanishing sticking and onset of vaporization. Using more sophisticated methods like hot wall evaporation, however, allows to overcome these limitations and yields crystalline islands with extensions enhanced by two orders of magnitude. Furthermore, we identify and provide a full structure solution of a yet unknown interface-mediated thin film polymorph of TTF-TCNQ, which is adopted in films of thicknesses below  $1\ \mu\text{m}$ .

DS 39.9 Thu 16:00 Poster F

**Influence of graphene interlayer on CoPc/Pt(111) interface** — ●MALGORZATA POLEK<sup>1</sup>, HILMAR ADLER<sup>1</sup>, ALEXANDER GENERALOV<sup>2</sup>, MATHIAS GLASER<sup>1</sup>, MILUTIN IVANOVIĆ<sup>1</sup>, ALEXEI PREOBRAJENSKI<sup>2</sup>, JOHANNES UIHLEIN<sup>1</sup>, HEIKO PEISERT<sup>1</sup>, and THOMAS CHASSÉ<sup>1</sup> — <sup>1</sup>University of Tübingen, Institute of Physical and Theoretical Chemistry, Auf der Morgenstelle 18, 72076 Tübingen, Germany — <sup>2</sup>MAX IV Laboratory, Ole Römers väg 1, 22363 Lund, Sweden

In optoelectronic devices based on organic semiconductors such as transition metal phthalocyanines (TMPcs), interactions at interfaces between organic molecules and metal substrates can significantly affect the device performance. The introduction of graphene as an additional buffer layer can help to tune these interactions and thus the electron transport across the interface as recently shown for TMPcs on graphene/Ni(111) [1]. Due to the interfacial doping effect, graphene

on Ni(111) is however a rather specific system. We compare therefore CoPc on graphene/Ni(111) to CoPc on graphene/Pt(111). The system was studied using synchrotron radiation based techniques: Photoemission and X-ray absorption spectroscopies (PES, XAS). Thin films of CoPc on Pt(111) and graphene/Pt(111) are composed of well-ordered, flat lying molecules on the substrate surface. Similar to Ni(111), a charge transfer to the central metal atom of CoPc was observed at the interface between CoPc and Pt(111). In contrast to Ni(111) however, the introduction of graphene as an interlayer prevents the charge transfer completely.

[1] J. Uihlein et al., J. Chem. Phys. 2013, 138, 081101.

DS 39.10 Thu 16:00 Poster F

**Strong Interaction of MnPc on Ni(111): Influence of Graphene Buffer Layer** — ●JOHANNES UIHLEIN<sup>1</sup>, HEIKO PEISERT<sup>1</sup>, HILMAR ADLER<sup>1</sup>, MATHIAS GLASER<sup>1</sup>, MALGORZATA POLEK<sup>1</sup>, RUSLAN OVSYANNIKOV<sup>2</sup>, MAXIMILIAN BAUER<sup>2</sup>, and THOMAS CHASSÉ<sup>1</sup> — <sup>1</sup>Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Tübingen, Germany. — <sup>2</sup>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany.

The interactions at interfaces of transition metal phthalocyanines (TMPcs) on metal substrates strongly influence the charge transport across these interfaces, which may become important for possible future organic electronic and spintronic devices. Molecule-substrate interactions may influence the local charge and thus the spin state of the central metal atom within the first molecular layer. This will be especially important for metal atoms possessing an open shell structure. For CoPc and FePc it was shown that with insertion of a graphene buffer-layer these interactions can be modified, depending on the central metal atom.[1][2] In contrast to CoPc and FePc, MnPc suffers serious damage to its molecular structure on Ni(111) with impact on the electronic structure. The insertion of graphene prevents the chemical reaction and an interfacial charge transfer is observed.[3] The studies were carried out using X-ray absorption and photoemission spectroscopies.

[1] J. Uihlein et al., J. Chem. Phys. 2013, 138, 081101.

[2] J. Uihlein et al., J. Phys. Chem. C 2014, 118, 10106.

[3] J. Uihlein et al., J. Phys. Chem. C 2014, accepted.

DS 39.11 Thu 16:00 Poster F

**The adsorption and DBD-plasma-polymerization of thiophene on titania** — ●SEBASTIAN DAHLE<sup>1,2</sup>, MARIA SONNENBERG<sup>2</sup>, MARCEL MARSCHEWSKI<sup>2</sup>, EIKE HÜBNER<sup>3</sup>, and WOLFGANG MAUS-FRIEDRICHS<sup>1,2</sup> — <sup>1</sup>Clausthaler Zentrum für Materialtechnik, Technische Universität Clausthal, Agricolastraße 2, D-38678 Clausthal-Zellerfeld, Germany — <sup>2</sup>Institut für Energieforschung und Physikalische Technologien, Technische Universität Clausthal, Leibnizstraße 4, D-38678 Clausthal-Zellerfeld, Germany — <sup>3</sup>Institut für Organische Chemie, Technische Universität Clausthal, Leibnizstraße 6, D-38678 Clausthal-Zellerfeld, Germany

The adsorption of thiophene from the gas phase onto clean and oxidized titanium foils as well as onto perchloric acid or bromine pre-treated titanium foils did not yield any chemical interaction or even stable adsorption. Especially the oxidative polymerization as classical approach for the synthesis and deposition of polythiophene cannot be employed for titania substrates. Using a dielectric barrier discharge plasma during the thiophene gas dosage results in the deposition of plasma-polymerized thiophene films at quite large deposition rates. The deposition mode, however, changes from a Frank-van-der-Merwe-type growth within the first seconds towards the deposition of two different classes of particles presumably originating from gas phase agglomeration.

DS 39.12 Thu 16:00 Poster F

**Real-time observation of superlattice formation in co-evaporated binary mixtures of Picene and Perfluoropen-tacene** — ●JOHANNES DIETERLE<sup>1</sup>, KATHARINA BROCH<sup>2</sup>, ALEXANDER HINDERHOFER<sup>1</sup>, HEIKO FRANK<sup>1</sup>, JIRI NOVAK<sup>3</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 — <sup>2</sup>Cavendish Laboratory, University of Cambridge, Cambridge, UK — <sup>3</sup>Central European Institute of Technology, Masaryk University, Kamenice 5, CZ-62500 Brno, Czech Republic

Studies of the mixing and ordering behaviour of binary organic semiconductor blends are not only relevant for applications, where blends are often used as the active layer, but also interesting for fundamental research, as new, mixing induced, ordering schemes may evolve [1,2].

For a detailed understanding of the mechanisms of structure formation during growth of binary blends, controlled growth and full structural characterization is crucial. For binary blends of Picene ( $C_{22}H_{14}$ ) ('high gap') and Perfluoropentacene ( $C_{22}F_{14}$ ) ('low gap') we observe the formation of a superlattice during co-evaporation. To study the dynamics of the superlattice formation and possible transient effects we perform real-time x-ray scattering and optical spectroscopy during growth of the blends.

- [1] A. Hinderhofer and F. Schreiber, *ChemPhysChem* 13, 628 (2012)  
 [2] A. Aufderheide et al., *Phys. Rev. Lett.* 109, 156102 (2012)

DS 39.13 Thu 16:00 Poster F

**Indium-Tin-Oxide (ITO) Surface Functionalization with Organic Self-Assembled-Monolayers** — ●JULIA RITTICH, SEBASTIAN MÄDER, BEATE SCHULZ, and MATTHIAS WUTTIG — I. Institute of Physics (IA), RWTH Aachen University, Germany

In recent years optoelectronic devices based on organic thin-films have gained considerable interest. The performance of devices such as organic light emitting diodes (OLED) or organic solar cells (OSC) depends critically on the interfaces between the different layers, e.g. the organic layer and the transparent conductive oxide (TCO) electrode. The most common material for such a transparent anode is Tin doped Indium-Oxide (ITO). In order to improve the device functionality the electronic alignment at the interface between the anode and the organic layer became the focus of interest. One way to change the electronic properties of the contact is given by the application of self-assembled monolayers (SAM).

In this study, self-assembled monolayers with high nano-dipoles were used to tailor the work function of the ITO anode. The used molecules are based on functional groups of phosphonic and carboxylic acid to anchor to the surface. In order to investigate the change in work function alignment to the organic layer and the coverage and arrangement of the surface dipoles, ultraviolet and X-ray photoelectron spectroscopy (UPS/XPS) measurements were performed.

DS 39.14 Thu 16:00 Poster F

**Recombination of charge carriers on nano-interfaces** — ●JĘDRZEJ SZMYTKOWSKI — Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Gdańsk, Poland

It is well known that the recombination of charge carriers plays a key role in the decreasing of efficiency for photovoltaic cells. The interfaces between nanostructures can be considered as the recombination centers. In this work, the role of tail and deep states on the process of interface recombination has been demonstrated. In order to analyze this effect, the disordered materials described by the double-exponential density of states (DOS) have been assumed. The studies of concentration effect on the time of recombination have been performed. Additionally, we report on the influence of temperature on the increasing of recombination order.

DS 39.15 Thu 16:00 Poster F

**Tailoring Surface Properties of Metals and Metal-Oxides Using Self-Assembled-Monolayers** — ●SEBASTIAN MÄDER, JULIA RITTICH, DOMINIK MEYER, and MATTHIAS WUTTIG — I. Physikalisches Institut IA, RWTH Aachen

Due to the high demand of power and of efficient lighting, the field of optoelectronic devices based on organic thin-films has gained considerable interest. Organic films offer a way of producing lightweight, flexible, inexpensive and eco-friendly light emitting diodes (OLED) and solar cells (OSC). Since the device functionality depends critically on the interface between the active organic layer and the cathode or the anode, an alignment of the electronic charge transport levels is a crucial step towards efficient charge transfer at this interface. One way to achieve this aim is given by the application of self-assembled monolayers (SAM).

In this work, we present a method to achieve a universal work function for noble metals using self-assembled monolayers with high interface-dipoles. Furthermore, we transferred the concepts and methods learned from the metal surfaces in order to achieve a tailored work function of transparent conductive oxides (TCOs) suited as an anode to contact organic active layers. The alignment of the work function as well as the surface coverage was examined using ultraviolet and X-ray photoelectron spectroscopy (UPS/XPS).

DS 39.16 Thu 16:00 Poster F

**Investigation of the metallization of P(VDF-TrFE) with gold by RF-sputter deposition** — ●ALEXANDER HINZ<sup>1</sup>, OLEKSANDR

POLONSKY<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>2</sup>, GONZALO SANTORO<sup>2</sup>, EZZELDIN METWALLI<sup>3</sup>, YUAN YAO<sup>3</sup>, THOMAS STRUNSKUS<sup>1</sup>, FRANZ FAUPEL<sup>1</sup>, STEPHAN V. ROTH<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>3</sup> — <sup>1</sup>CAU zu Kiel, Kaiserstr. 2, 24143 Kiel — <sup>2</sup>DESY, Notkestr. 85, 22607 Hamburg — <sup>3</sup>TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching

Although it is well established in industry and important for many applications the sputter deposition of metals onto organic surfaces is yet to be completely understood. Due to the inherent complexity (e.g. bombardment of the organic surfaces by energetic ions) of the sputtering process the basic mechanisms determining the final microstructure are still to be identified. The complexity of sputter deposition and the post-deposition changes which are to be expected necessitate the use of in-situ methods. In-situ grazing incidence small angle scattering (GISAXS) has been used to extract structural information with high spatial and temporal resolution from a growing Au-film deposited via RF-sputter deposition onto a P(VDF-TrFE)-film. The Au-P(VDF-TrFE) system has been chosen as a model system of a relatively inert metal-polymer pair. Analysis of the GISAXS data yields information about the morphology of the growing Au-film. Comparing these results to simulated scattering data provides further information about the basic growth mechanisms acting at different stages of the growth of the metal film.

DS 39.17 Thu 16:00 Poster F

**Copper Phthalocyanine as Contact Primer for Organic Semiconductor Films on Metal Substrates** — ●ALEXANDER MÄNZ and GREGOR WITTE — Molekulare Festkörperphysik, Fachbereich Physik, Philipps-Universität Marburg, Renthof 7, 35032 Marburg

Organic self assembled monolayers can be utilized as contact primer for the growth of organic semiconductors on metal surfaces. In order to avoid involved charge transport limitations of SAMs, flat lying PAHs such as Phthalocyanines can be used alternatively. In our study we exemplarily used Copper Phthalocyanine (CuPc) as contact primer for the growth of the organic semiconductor Pentacene (PEN) on coinage metals. The initial stage of growth was investigated by means of AFM and NEXAFS, which give insight into the morphology and the molecular orientation of submonolayer coverages. Additionally, films with thicknesses up to 30 nm were analyzed by means of XRD. In all cases we observed PEN to grow in upright orientation, adopting the thin film polymorph as known for PEN on inert substrates. This observation is in contrast to the thin film growth of other planar PAHs like PTCDA on CuPc monolayers.

DS 39.18 Thu 16:00 Poster F

**Temperature Induced Phase Transition in Pentacene Thin Films** — ●LEONARD VON HELDEN, TOBIAS BREUER, and GREGOR WITTE — Molekulare Festkörperphysik, Philipps Universität Marburg, Renthof 7, D-35032 Marburg, Germany

Pentacene( $C_{22}H_{14}$ ) is a widely investigated organic semiconductor and serves as model system for organic thin film growth. It is known to form crystalline thin films in two slightly different, consecutively growing polymorphs on SiO<sub>2</sub>: the "thin film phase" (TFP) and the "Campbell phase" (CP), i.e. bulk phase.<sup>1</sup> Here we report a study on high temperature dynamics, which was realized by mounting a metal cap on top of the sample under vacuum conditions, providing an unmodified surface of the organic thin film. XRD and AFM measurements prove a phase transition of the TFP into the energetically favored CP, when heated about 40 K beyond its usual desorption point. Moreover we found, that sample contact to ambient air has a tremendous influence on the desorption and transition process.

- [1] C. Ambrosch-Draxl et al., *New Journal of Physics*, 11, 125010, (2009)

DS 39.19 Thu 16:00 Poster F

**Spectroscopic and transport properties of a novel charge transfer salts** — ●TORSTEN HAHN<sup>1</sup>, FLORIAN RÜCKERL<sup>2</sup>, and SIMON LIEBING<sup>1</sup> — <sup>1</sup>Institut für Theoretische Physik, Leipziger Str. 23, TU Freiberg, D-09599 Freiberg — <sup>2</sup>IFW Dresden, Helmholtzstraße 20, D-01069 Dresden

The recently synthesized Picene/F4TCNQ charge transfer salt [1] shows promising physical properties for the application in molecular electronics. Based on theoretical calculation within the density functional theory framework we predict the material to act as a molecular diode with high rectification ratio [2]. We further conclude that the hybrid states formed by the donor / acceptor system are playing the

key role to determine the spectroscopic and quantum transport properties. Additionally we extend our investigation to other novel charge transfer salts like Chrysene/F4TCNQ or Tetracene/F4TCNQ. We will show that the tuning of spectroscopic and transport properties through intramolecular charge transfer is a general concept which opens a new route towards functional materials for molecular electronics.

[1] Mahns, B. et. al., *Cryst. Growth and Design* 14, 1338-1346 (2014). [2] T. Hahn, S. Liebing, and J. Kortus, *Nanoscale* 6, 14508 (2014).

DS 39.20 Thu 16:00 Poster F

**The Role of Chemical Defects for Charge Injection Barriers at Metal / Organic Semiconductor Interfaces** — ●HERMANN EDLBAUER, SHASHANK S. HARIVYASI, EGBERT ZOJER, and OLIVER T. HOFMANN — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, 8010 Graz, Austria

The efficiency of organic electronic devices is strongly determined by the contact resistance caused by the interface of the organic semiconductor and the metal electrode. One approach for its reduction is modifying the work function of the metal contact by adsorbing a monolayer of deliberately chosen molecules onto the metal surface. Our density functional theory (DFT) calculations for instance show that a monolayer of the electron acceptor tetrafluoro-benzoquinone adsorbed on Cu(111) causes a work function increase of about 0.5 eV. However, imperfections and chemical defects, e.g., through hydrogen adsorption, can mitigate this effect. Within this work, we investigate how sensitively the injection barrier depends on the formation of chemical defects. In particular, the corrugation of the electrostatic potential above the surface and the implications for the formation of “hot spots” are discussed. This is studied by a gradual hydrogenation of parts of the molecules in a supercell. Using ab initio thermodynamics, further we show how the number of chemical defects and hence the work function change can be linked to the partial pressures of the participating molecules in a surrounding gas phase.

DS 39.21 Thu 16:00 Poster F

**Characterization of surface contaminants of medical devices by means of Synchrotron Radiation-based FTIR microspectroscopy and X-Ray spectrometry** — BEATRIX POLLAKOWSKI<sup>1</sup>, ●ANDREA HORNEEMANN<sup>1</sup>, BONNIE TYLER<sup>2</sup>, RORY STEVEN<sup>2</sup>, PEGGY EMMER<sup>1</sup>, and BURKHARD BECKHOFF<sup>1</sup> — <sup>1</sup>Physikalisch-Technische Bundesanstalt, Berlin, Germany — <sup>2</sup>National Physics Laboratory, London, United Kingdom

It is an emerging topic to develop metrology tools for a traceable characterization of advance biomaterials for the medical device industry. One aspect concerns the detection and identification of defect structures and contaminants, which may lead to delamination, cracking and spalling of the coating and ultimately lead to the device failure. This work deals with analysis of contaminants dedicatedly deposited on relevant substrates. Bis-steramide is a surface contamination originating from the production and packing process. Employing both vacuum-based and ambient techniques, represented here by X-ray fluorescence analysis under grazing incidence condition (GIXRF) and FTIR spectroscopic techniques, it allows for a traceable and reliable analysis of mass deposition and the chemical species of the contaminants. The combination of GIXRF and XAFS offers a non-destructive access to depth-resolving analysis with respect to both, the chemical speciation and the depth-dependent elemental composition. The results on different bis-steramide samples with varying layer thicknesses show that the combination of complementary methods substantially supports the development of a metrology for complex biomaterial for medical devices.

DS 39.22 Thu 16:00 Poster F

**Epitaxial Growth and Photoluminescence of  $\alpha$ -Sexithiophene on KCl- and Si/SiO<sub>2</sub>-Substrates** — ●FRIEDER LENNART MÜNTZE<sup>1,2</sup>, HISAO YANAGI<sup>2</sup>, and DERCK SCHLETTWEIN<sup>1</sup> — <sup>1</sup>Institute of Applied Physics, Justus-Liebig-University Gießen, D-35390 Giessen — <sup>2</sup>Graduate School of Materials Science, Nara Institute of Science and Technology, Nara 630-0192, Japan

$\alpha$ -Sexithiophene ( $\alpha - 6T$ ) is a well-known organic semiconductor with possible applications in organic electronics. Different crystalline phases of  $\alpha - 6T$  have been established. Either nanofibers or 3D islands can be formed. This has an influence on the photoluminescence(PL)-properties of the materials. In this work, three differently coloured domains of  $\alpha - 6T$  were obtained in sublimation studies. These samples were analysed with UV-vis, PL-spectroscopy and XRD to determine

the respective crystal phase. These films were studied which proved to be of the 1T-structure established in the literature for films grown on KCl(001) or onto Si/SiO<sub>2</sub> substrates for temperatures up to 150 °C. On the KCl, we found nanofibers while on the Si/SiO<sub>2</sub> substrates, islands were formed. When excited by UV the islands emitted in the green part of the spectrum while the needles on KCl emitted orange. For films grown on KCl at 180 °C, however, needles were formed that emitted in the green part of the spectrum. Based on these findings, based on the polarization dependence of the emission intensity and based on the orientation of the needles relative to the substrate the orientation of  $\alpha - 6T$  relative to the different substrate surfaces is discussed.

DS 39.23 Thu 16:00 Poster F

**Organic light emitting diode (OLED) on Silicon for Biomedical Sensor Applications** — ●MATTHIAS JAHNEL<sup>1</sup>, MICHAEL THOMSCHKE<sup>1</sup>, BEATRICE BEYER<sup>1</sup>, KARSTEN FEHSE<sup>1</sup>, KARL LEO<sup>2</sup>, and VOLKER KIRCHHOFF<sup>1</sup> — <sup>1</sup>Fraunhofer Institute for Organic Electronics, Electron Beam and Plasma Technology FEP, Maria-Reiche-Strasse 2, 01109 Dresden, Germany — <sup>2</sup>Institut für Angewandte Photophysik, Technische Universität Dresden (TUD), 01062 Dresden, Germany

Organic thin film devices like light emitting diodes (OLED) or organic photo diodes (OPD) integrated on silicon backplanes could be one promising way to achieve low cost sensors. We present two types of top emitting OLED devices that are suitable for lab-on-a-chip applications. Both include optically filtered green light emission, 1st case by a single titanium dioxide (TiO<sub>2</sub>) layer in 2nd case using a distributed-Bragg-reflector (DBR) based on TiO<sub>2</sub> and silicon oxide (SiO<sub>2</sub>). These OLED devices are covered with a thin film encapsulation. We investigated the influence of the substrate surface temperature during the deposition on the performance of the devices and compared them to reference devices without TiO<sub>2</sub> layers. Further, we achieved a narrow emission spectrum with a Full Width at Half Maximum (FWHM) of 20 nm and additionally a minimized angular dependency of the electroluminescence peak. Both device architectures can be used for large area deposition as well as integration onto Silicon-CMOS backplanes and resultingly, a combination of optical functional dielectric layers with organic electronic devices in bio and medical sensor applications.

DS 39.24 Thu 16:00 Poster F

**Investigation of Stearates as Solution-Processable Electron Injection Layers in Organic Light-Emitting Diodes** — ●FLORIAN ULLRICH<sup>1,2,3</sup>, SEBASTIAN STOLZ<sup>1,3</sup>, NORMAN MECHAU<sup>1,3,4</sup>, GERARDO HERNANDEZ-SOSA<sup>1,3,4</sup>, MALTE JESPER<sup>5</sup>, MANUEL HAMBURGER<sup>1,5</sup>, and ERIC MANKEL<sup>1,6</sup> — <sup>1</sup>InnovationLab GmbH, Heidelberg, Germany — <sup>2</sup>University of Heidelberg, Kirchhoff-Institute for Physics, Germany — <sup>3</sup>Karlsruhe Institute of Technology, Light Technology Institute, Germany — <sup>4</sup>Karlsruhe Institute of Technology, Institute of Microstructure Technology, Germany — <sup>5</sup>University of Heidelberg, Organisch-Chemisches Institut, Germany — <sup>6</sup>TU Darmstadt, Material-Wissenschaft, Surface Science, Germany

One crucial obstacle which has to be overcome for the production of efficient organic light-emitting diodes (OLEDs) by high-throughput printing techniques is the injection of electrons into the device, since typical cathode layers with low work-functions like calcium or barium are highly reactive and cannot be solution-processed.

In this work, we investigate alkalimetal stearates as solution processable electron injection layers in OLEDs. Therefore yellow emitting OLEDs with different concentrations of Cs, Rb, K and Na stearate were fabricated and the influence on device performance, such as efficiency, efficacy and operational lifetime, was studied. For the various stearates, significantly different current efficiencies were observed with a maximum value of about 9 cd/A which equals that of reference devices. Photoelectron spectroscopy in comparison to Kelvin probe measurements as well as layer thickness characterization are in progress.

DS 39.25 Thu 16:00 Poster F

**Enhanced Infrared Spectroscopy of Organic Field Effect Transistor (OFET) Materials for an In-Line Production Control** — ●MICHAEL SENDNER<sup>1,2</sup>, ANTON HASENKAMPF<sup>1</sup>, and AN-NEMARIE PUCCI<sup>1,2,3</sup> — <sup>1</sup>Kirchhoff-Institut für Physik, Universität Heidelberg — <sup>2</sup>InnovationLab GmbH, Heidelberg — <sup>3</sup>Centre for Advanced Materials, Universität Heidelberg

For a mass production of flexible organic devices, such as Organic Field Effect Transistors (OFETs), printing in a roll-to-roll-process becomes of increasing importance. For the realization of an in-line produc-

tion control a fast characterization of the organic semiconductors is needed. Infrared spectroscopy enables the possibility of controlling contaminations of the organic semiconductors and at the same time the determination of film thickness of the used materials. A reduction of the measurement time is possible if one uses metal nanostructures which enhance the vibrational signals of the materials due to collectively excited conduction electrons (plasmons). We show that metal nanostructures are a possible tool for in-line control of organic semiconductors on a flexible organic substrate by means of enhancement and measurement time.

DS 39.26 Thu 16:00 Poster F

**Nanospectroscopic studies in organic thin film devices** — ●XIAOYAN DU<sup>1</sup>, BENEDIKT RÖSNER<sup>1</sup>, PETER WARNICKE<sup>2</sup>, XUECHEN JIAO<sup>3</sup>, TAYEBEH AMERI<sup>4</sup>, and RAINER FINK<sup>1</sup> — <sup>1</sup>Physikalische Chemie II, FAU Erlangen-Nürnberg, 91058 Erlangen, Germany — <sup>2</sup>Paul-Scherrer-Institut, Villigen, Schweiz — <sup>3</sup>Department of Physics, NCSU, Raleigh, North Carolina 27695-8202, USA — <sup>4</sup>FAU Erlangen-Nürnberg, Institute of Materials for Electronics and Energy Technology (I-MEET), Germany

The performance of organic thin film devices are greatly dependent on the morphology of the active layer. Combining Atomic Force Microscopy (AFM), Transmission Electron Microscopy (TEM) and chemical sensitive methods like Scanning Transmission X-ray Microscopy (STXM) and Resonant Soft X-ray Scattering (RSOXS) can enable us to gain a better understanding of the structure-performance relationship on the nanometer scale. Combining these techniques, we were able to correlate the organic field effect transistor properties of thin films of 6,13-Dihydro-6,13-diazapentacene (DHDAP) with the film morphology which is influenced by the deposition temperature. While STXM is particularly suited to monitor the molecular orientations locally, AFM indicates crystallinity smaller than the oriented domains. STXM, RSOXS and TEM were combined to study active layer morphology of ternary organic solar cells. Our results clearly showed that the miscibility between polymers and fullerenes is a key factor in determining the functionality of ternary solar cells. The structure findings correlate with the device performance.

DS 39.27 Thu 16:00 Poster F

**Accurate measurement of the exciton diffusion length based on a single solar cell** — ●BERNHARD SIEGMUND, JOHANNES BENDUHN, KOEN VANDEWAL, CHRISTIAN KÖRNER, and KARL LEO — Institut für Angewandte Photophysik, Dresden, Germany

The photo-current of organic solar cells is the result of a multi-step process. It includes the generation and diffusion of excitons as well as their separation into free charge carriers, their transport to the electrodes, and their final extraction.

Cascade structures of neat absorber layers have recently proven to be a convincing concept for efficient exciton harvesting with power conversion efficiencies comparable to those of tandem devices. Enhanced diffusion lengths of excitons would provide further improvements in terms of higher short-circuit currents. Bulk heterojunction devices would also profit from a longer diffusion length, since this would require less interface area for charge generation, which in turn inhibits free carrier recombination, improving both fill factor and open-circuit voltage.

In this work, we introduce an accurate as well as elegant way to determine the diffusion length of organic thin films based on the evaluation of the photo-current produced by an organic bilayer solar cell. In this context, a non-unity conversion probability of interfacial excitons into extracted charge carriers might complicate data analysis. Applying varying gradients of optical fields, we demonstrate how to determine both this conversion probability and the diffusion length independently by means of a single device measurement.

DS 39.28 Thu 16:00 Poster F

**Electrodeposited Al-doped ZnO used in Hybrid Organic-Inorganic Solar Cells** — ●NADINE DANNEHL<sup>1,2</sup>, JENNIFER T. DAMASCO TY<sup>1</sup>, HISAO YANAGI<sup>1</sup>, and DERCK SCHLETTWEIN<sup>2</sup> — <sup>1</sup>Graduate School of Materials Science, Nara Institute of Science and Technology, Nara 630-0192, Japan — <sup>2</sup>Institute of Applied Physics, Justus-Liebig-University Gießen, D-35390 Giessen

Hybrid organic-inorganic solar cells which use dyes as absorbers, polymers as donors and inorganic nanostructures as acceptors combine the advantages of organic and inorganic materials. In our study, we investigate hybrid solar cells fabricated with Al-doped zinc oxide (AZO) grown by electrochemical deposition using  $AlCl_3$  as aluminum source.

The AZO films with different Al : Zn molar ratios (0.5%, 2.5%, 5.0%) were grown on ZnO- and AZO-seeded Indium-Tin-Oxide (ITO) substrates. The seed layers were deposited by spin-coating methanolic precursor solutions of the respective metal salts onto ITO-substrates followed by annealing. To fabricate the cells a solution of 1:1 poly(3-hexylthiophen) (P3HT) and [6,6]-Phenyl C61 butyric acid methyl ester (PCBM) in 1:1 chlorobenzene and trichlorobenzene was spin-coated onto the electrodeposited AZO layer. A  $MoO_3$  electron-blocking layer and a Au electrode were vapor-deposited on top of the organic layer to complete the cells. Nanorods with diameters of about 40 nm and high vertical orientation were obtained from electrolyte solutions with 0.5% Al : Zn molar ratios. The solar cells fabricated from these nanorod array structures achieved efficiencies up to 1.1% showing the principle applicability of such layers.

DS 39.29 Thu 16:00 Poster F

**Analytical Transmission Electron Microscopy on Small Molecule Bulk Heterojunction Organic Solar Cells** — DIANA NANOVA<sup>1,2,4</sup>, ●LARS MÜLLER<sup>1,2,4</sup>, FELIX SCHELL<sup>2,4</sup>, MICHAEL SCHERER<sup>1,2,4</sup>, ANNE K. KAST<sup>3,4</sup>, PIRMIN KÜKELHAHN<sup>2,3</sup>, RASMUS R. SCHRÖDER<sup>3,4</sup>, ROBERT LOVRINCIC<sup>1,4</sup>, and WOLFGANG KOWALSKY<sup>1,4</sup> — <sup>1</sup>Institute for High-Frequency Technology, TU Braunschweig, Germany — <sup>2</sup>Kirchhoff-Institute for Physics, Heidelberg University, Germany — <sup>3</sup>CellNetworks, BioQuant, Heidelberg University, Germany — <sup>4</sup>InnovationLab GmbH, Heidelberg, Germany

Understanding the interplay of morphology, material crystallinity and device performance in organic bulk heterojunction (BHJ) solar cells is crucial for the development of efficient devices. The application of electron energy loss spectroscopy (EELS), electron diffraction, and electron tomography in a transmission electron microscope (TEM) allows for a detailed analysis of the BHJ. Here, we investigate the influence of substrate composition and temperature during deposition on fluorinated zinc phthalocyanine / fullerene BHJs. Combined with device performance data, the influence of these two separately varied parameters is studied in terms of 3D-morphology and long range order within the materials. With additional EELS measurements that reveal electronic and even dielectric properties of the materials by application of the Kramers-Kronig relations, a diversified description of the investigated layer can be given.

DS 39.30 Thu 16:00 Poster F

**Highly conductive polythiophene brushes and its application for Organic Solar Cell** — ●RAVI-KUMAR DIVAKAR<sup>1,2</sup>, JI-LING HOU<sup>2</sup>, RENE SCHUBEL<sup>1</sup>, TAO ZHANG<sup>1</sup>, LARS MÜLLER-MESKAMP<sup>2</sup>, KARL LEO<sup>2,3</sup>, RAINER JORDAN<sup>1,3</sup>, and IHSAN AMIN<sup>1,3</sup> — <sup>1</sup>Makromolekulare Chemie, Technische Universität Dresden, 01069 Dresden, Germany — <sup>2</sup>Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — <sup>3</sup>Centre for Advancing Electronics Dresden, Technische Universität Dresden, George-Schumannstrasse 11, 01187 Dresden, Germany

Conductive polymers, especially polythiophene (PT) and its derivatives have attracted intensive interest both in research and industry due to its potential application for optoelectronic devices such as organic field effect transistors (OFETs), organic light emitting devices (OLEDs) and organic solar cells (OSCs). For most applications, PT is dissolved in a good solvent such as chlorobenzene, and then spin-coated onto dielectric substrates such as SiO<sub>2</sub>. However, the spin-coated PT film may form a wrongly oriented polymer chains which may result in a low conductivity of the film. Here, we report on fabrication of PT brushes via direct photografting on aminofunctionalized surfaces. The resulted polymer brush chains have “out of plane” orientations and thus show a high conductivity. We foresee the highly conductive polythiophene brushes would have potential applications in OLEDs, OFETs and OSCs.

DS 39.31 Thu 16:00 Poster F

**Growth of pinholes in metal electrodes of organic photovoltaic cells** — ●DANIEL FLUHR, ROLAND RÖSCH, BURHAN MUHSIN, MARCO SEELAND, and HARALD HOPPE — Institute of Physics, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Lifetime is still a major problem of organic photovoltaic (OPV) cells. There are many reasons for solar cell degradation varying from shunts induced by impurities or electromigration over photoinduced oxidation of active layer materials to corrosion and delamination of the metal contact both induced by oxygen or water ingress.

One issue concerns so-called pinholes through the metal back electrode of the device. These pinholes offer pathways for ingress of water

and oxygen which may attack the metal-organic interface by introducing delamination through formation of insulating metal oxides or hydrogen evolution. As charge injection and extraction is suppressed at delaminated areas, the active area taking part in power conversion - and hence the overall efficiency - becomes reduced.

We investigated the influence of different environmental conditions on the reduction of the active area of the OPV cell. Spatially resolved measurements give information on location and size of insulated areas induced by pinholes in the metal back contact. Time resolved measurements during degradation of the devices revealed the dynamics and rate of growth of these individual defects. Looking at different device structures provides conclusions for increasing the lifetime of organic photovoltaic cells.

DS 39.32 Thu 16:00 Poster F

**Identification of the weakest mechanical point in OPV devices** — ●AURÉLIEN TOURNEBIZE<sup>1</sup>, ALBERTO GREGORI<sup>2</sup>, STEFAN SCHUMANN<sup>3</sup>, ANDREAS ELSCHNER<sup>3</sup>, CHRISTINE DAGRON-LARTIGAU<sup>2</sup>, ROGER C. HIORNS<sup>4</sup>, AHMED ALLAL<sup>2</sup>, HEIKO PEISERT<sup>1</sup>, and THOMAS CHASSÉ<sup>1</sup> — <sup>1</sup>Institut für Physikalische und Theoretische Chemie, Tübingen, Germany — <sup>2</sup>EPCP, IPREM (UMR-5254), Université de Pau et des Pays de l'Adour, France — <sup>3</sup>Heraeus Precious Metals GmbH & Co. KG, Electronic Materials Division, Leverkusen, Germany — <sup>4</sup>CNRS, EPCP, IPREM (UMR-5254), Pau, France

While the electrical failure mechanisms in organic photovoltaic (OPV) devices have been thoroughly investigated, little is known about their mechanical stability, which is as important and critical to ensure long term reliability. In this study, a new set-up has been developed for the so-called probe using an inverted structure glass/ITO/ZnO/P3HT:PCBM/PEDOT:PSS/Ag. The technique has been extended varying low bandgap polymers for the active layer in combination with two different PEDOT:PSS formulations. After mechanical tests, the upper and lower surfaces have been characterized by AFM and XPS to locate the fracture point. A difference in the stress at break for devices made with different combinations of active and hole transporting layers is visible, suggesting different fracture paths. Acknowledgments The research leading to these results has received funding from the European Union Seventh Framework Programme (FP7/2011 under grant agreement ESTABLIS n° 290022).

DS 39.33 Thu 16:00 Poster F

**Multilayer Aluminum Thin Films as Effective Encapsulation for Flexible Organic Devices** — ●FELIX DOLLINGER, FREDERIK NEHM, KARL LEO, and LARS MÜLLER-MESKAMP — Institut für Angewandte Photophysik, Technische Universität Dresden, Deutschland

Thin film organic devices like organic solar cells require encapsulation against water vapor. Depending on the device, water vapor transmission rates (WVTR) in the range of  $10^{-5} \frac{g}{m^2 \cdot day}$  are needed for lifetimes of at least five years. In this work we aim at improving the encapsulation properties of opaque vacuum-evaporated aluminum back-electrodes to fulfill these barrier requirements.

Water diffusion through aluminum layers is defect-driven. To reduce defect densities, the growth behavior of the aluminum layer is modified by underlying metallic seed-layers which have shown improved performance in transparent metal thin-film electrodes.

Significant improvement of WVTR can be achieved with multilayer structures. Thin interlayers that decouple the defect positions in consecutive aluminum layers provide long and tortuous diffusion-paths for water-molecules. In our study, we use the electrical calcium-test to investigate stacks of aluminum layers with various interlayers with respect to steady-state WVTR and lag-time. The interlayers consist of different planarizing, diffusion-limiting, or getter materials that absorb water-molecules as they diffuse through the barrier.

These optimized aluminum multilayers are promising candidates for organic thin-film encapsulation.

DS 39.34 Thu 16:00 Poster F

**Calculation of hopping based electronic transport through donor-acceptor polymeric systems** — ●FLORIAN GÜNTHER<sup>1,2</sup>, SIBYLLE GEMMING<sup>1,3</sup>, and GOTTHARD SEIFERT<sup>2</sup> — <sup>1</sup>Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — <sup>2</sup>Physical Chemistry and Electrochemistry, TU Dresden, Germany — <sup>3</sup>Institute of Physics, TU Chemnitz, Germany

In order to design high performance organic transistors, semiconducting materials exhibiting high charge carrier mobility are needed. Current record hole as well as electron mobilities have been achieved by diketopyrrolopyrrole (DPP) based donor-acceptor polymers.

Our study addresses the influence of the molecular structure on the electronic transport properties of such systems. Thereby, we focus on intermolecular hopping since it plays the major role in the limitation of the charge transport. For this aim, we consider a model based on Marcus transfer theory. Here, we focus on the coupling matrix elements and their dependence on the stacking configuration. Using a Boltzmann-like approach for evaluating an average value of this quantity, we obtain good agreements to experimental trends. Especially the dominating transport type is nicely reproduced by our approach.

Our calculations are based on density functional based tight binding (DFTB), because it is a well appropriate method for our aim and computational most efficient compared to other first-principle approaches.

DS 39.35 Thu 16:00 Poster F

**Semitransparente leitfähige und flüssigprozessierbare Elektroden für die Optoelektronik** — ●PETER FISCHER, HARALD HOPPE und EDDA RÄDLEIN — TU Ilmenau

Diese Arbeit befasst sich mit der Lösung des Problems der Herstellung kostengünstiger leitfähiger semitransparenter flüssig-prozessierter Metalloxidschichten. Ein erster Ansatz hierzu in die Dotierung von Titandioxid mit Niob. In einem ersten Schritt wurde hierzu die Durchleitfähigkeit mit bestimmten Bauelementen getestet. Dabei galt es insbesondere homogene und engmaschig dichte Schichten zu erzeugen.

Das Thema ist für die kostengünstige Produktion von verschiedenen Optoelektronikbauteilen, wie z.B. Bildschirmen, Touch-Panels, organischen Solarzellen und Leuchtdioden bedeutend, aber auch in Bezug auf fundamentale physikalische Eigenschaften sehr interessant. Die zur Zeit als Standard verwendete Elektrode in der organischen Photovoltaik, Indiumzinnoxid (ITO), ist trotz ihrer hohen Leitfähigkeit und Transparenz für eine wirtschaftliche Verwendung auf Grund der hohen Kosten von Indium, die zur Zeit mehr als 50% des Preises einer organischen Solarzelle ausmachen, nicht geeignet.