

## Symposium Organic Thin Film Electronics: From Molecular Contacts to Devices (SYOE)

jointly organized by  
Section Thin Films (DS),  
Section Chemical and Polymer Physics (CPP),  
Section Surface Physics (O), and  
Section Semiconductor Physics (HL)

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### Overview of Invited Talks and Sessions

(lecture rooms H1 and H32,

Poster B: the posters should be in place at 17:30; kernel time of the poster session is 18:00-20:00)

#### Invited Talks

SYOE 4.1	Tue	9:30–10:15	H1	<b>Vapor and Solution Deposited Small Molecule Organic Thin Film Transistors</b> — •THOMAS JACKSON
SYOE 5.1	Tue	11:15–12:00	H1	<b>Organic electronic devices and their applications</b> — •PAUL HEREMANS
SYOE 6.1	Tue	14:30–15:15	H32	<b>Theory of polymer devices: OFETs and OLEDs</b> — •REINDER CO- EHOORN
SYOE 7.1	Tue	16:30–17:15	H32	<b>Electronic spectrum and spin states of a single organic molecule</b> — •HERRE VAN DER ZANT
SYOE 10.1	Wed	16:45–17:30	H32	<b>Single grain contacts</b> — •GREGOR WITTE

#### Sessions

SYOE 1.1–1.5	Mon	14:30–16:00	H32	<b>Organic Interfaces (abstracts see DS 5.1-5)</b>
SYOE 2.1–2.7	Mon	16:00–18:00	H32	<b>Organic Photovoltaics (abstracts see DS 6.1-7)</b>
SYOE 3.1–3.4	Mon	18:00–19:15	H32	<b>Organic Film Aging (abstracts see DS 7.1-4)</b>
SYOE 4.1–4.5	Tue	9:30–11:15	H1	<b>Organic Transistors</b>
SYOE 5.1–5.4	Tue	11:15–12:45	H1	<b>Organic Devices</b>
SYOE 6.1–6.5	Tue	14:30–16:15	H32	<b>Transport in Organics Materials</b>
SYOE 7.1–7.4	Tue	16:30–18:00	H32	<b>Single Molecule Contacts</b>
SYOE 8.1–8.108	Tue	18:00–20:00	Poster B	<b>Poster Session SYOE</b>
SYOE 9.1–9.8	Wed	14:30–16:45	H32	<b>Organic Light Emitting Diodes (abstracts see DS 16.1-8)</b>
SYOE 10.1–10.6	Wed	16:45–18:45	H32	<b>Contact Properties (further abstracts see DS 17.2-6)</b>

The organizers gratefully acknowledge FV DS for providing the additional room and timeslots for the symposium SYOE. Especially the joined sessions SYOE 1, SYOE 2, SYOE 3, SYOE 9, and SYOE 10 (on Monday and Wednesday afternoon) wouldn't have been possible otherwise.

**SYOE 1: Organic Interfaces (abstracts see DS 5.1-5)**

Time: Monday 14:30–15:45

Location: H32

Joined session with DS: The abstracts are listed under DS 5.1-5.

**SYOE 2: Organic Photovoltaics (abstracts see DS 6.1-7)**

Time: Monday 16:00–17:45

Location: H32

Joined session with DS: The abstracts are listed under DS 6.1-7.

**SYOE 3: Organic Film Aging (abstracts see DS 7.1-4)**

Time: Monday 18:00–19:15

Location: H32

Joined session with DS: The abstracts are listed under DS 7.1-4

**SYOE 4: Organic Transistors**

Time: Tuesday 9:30–11:15

Location: H1

**Invited Talk**

SYOE 4.1 Tue 9:30 H1

**Vapor and Solution Deposited Small Molecule Organic Thin Film Transistors** — •THOMAS JACKSON — Center for Thin Film Devices and Materials Research Institute, Department of Electrical Engineering, Penn State University, University Park, PA, USA, 16802

Organic thin film transistor (OTFT) device performance rivals or exceeds that of a-Si:H devices, and low OTFT processing temperature allows fabrication on a variety of surfaces including cloth, paper, or polymeric substrates. For device and system use, OTFTs must demonstrate the uniformity, reproducibility, reliability, and integration with other devices needed for practical applications. As an application demonstration we have integrated vapor-deposited OTFTs with organic light emitting diodes (OLEDs) and have fabricated small test displays on polyester substrates to investigate device characteristics and passivation and isolation requirements.

Many organic device applications are likely to be cost sensitive and solution-deposited organic semiconductors offer important advantages for low-cost processing. However, solution processed semiconductors typically lack the molecular-level order which may be necessary for good carrier transport and large field-effect transistor mobility. Working with J. Anthony (University of Kentucky) we have investigated functionalized pentacenes and pentacene derivatives. Surprisingly, solution-deposited films of some of these materials show good molecular ordering and, using these materials, we have fabricated simple circuits, including ring oscillators, and OTFTs with mobility  $> 2 \text{ cm}^2/\text{V}\cdot\text{s}$ .

SYOE 4.2 Tue 10:15 H1

**Dielectric Interface Modification by UV irradiation: A Novel Method to control OFET charge carrier transport properties** — •NIELS BENSON, MARTIN SCHIDLEJA, CHRISTIAN MELZER, and HEINZ VON SEGGERN — University of Technology Darmstadt, Institute of Material Science, Petersenstr. 23, 64287 Darmstadt, Germany

In the present talk a novel concept is introduced, which allows for a change in OFET polarity by polymer dielectric interface modification. This concept is based on the irradiation of the gate dielectric by ultra violet radiation prior to the organic semiconductor deposition. As a result balanced unipolar charge carrier transport properties of n- and p-type pentacene based OFETs were obtained. The change in OFET polarity manifests itself in a large positive threshold voltage shift of approximately 60V for both charge carrier types. On the basis of detailed studies using contact angle and x-ray photo electron spectroscopy measurements, a possible cause for the threshold voltage shift is discussed. We could show that during the UV treatment step, polar groups such as C=O and according to literature -COH, recently identified as electron traps by Chua et al., are formed in the polymeric gate dielectric, influencing the OFET charge carrier properties. In line with this idea, negative charge carriers are localized within the PMMA dielectric once the UV modified OFET is driven in electron accumulation mode. This results in a positive threshold voltage shift inhibiting the electron- and promoting the hole-transport. The area density of trapped electrons necessary for the observed threshold voltage shift is estimated to be  $\geq 3.9 \cdot 10^{12} \text{ cm}^{-2}$ .

SYOE 4.3 Tue 10:30 H1

**Electric field induced gap states in pentacene** — •DIETMAR KNIPP<sup>1</sup>, AMARE BENOR<sup>1</sup>, ARNE HOPPE<sup>1</sup>, VEIT WAGNER<sup>1</sup>, and ARMIN VÖLKE<sup>2</sup> — <sup>1</sup>International University Bremen, School of Engineering and Science, 28759 Bremen, Germany — <sup>2</sup>Palo Alto Research Center, Electronic Materials and Device Laboratory, Palo Alto, California, USA

Despite the realization of pentacene transistors with high mobility the electronic transport is not fully understood. In particular the creation of gap states and the influence of gap states on the charge transport are still under investigation. To study the creation of electronic defects electrical in-situ measurements of pentacene TFTs were carried out. The devices with hole mobilities ranging from  $0.2\text{-}0.5 \text{ cm}^2/\text{Vs}$  were exposed to oxygen and moisture to study the influence on the device characteristic. Exposing the transistor to oxygen does not lead to a change of the transistor characteristic. Only if an electric field is applied while exposing the devices to oxygen a change of the device characteristic is observed. Applying voltages to the device leads to a shift of the onset of the drain current towards positive gate voltages. As a consequence the subthreshold slope is distinctly increased. The threshold voltage and the mobility are not affected by the oxygen contamination. Numerical simulations of the device characteristic reveal that the onset of the drain current is caused by acceptor-like defect states deep in the bandgap. A good agreement between the simulation and the experiment was observed by using a Gaussian distribution of defect states.

SYOE 4.4 Tue 10:45 H1

**Spatially-Resolved Photoresponse Measurements on Pentacene Thin-Film Transistors** — MATTHIAS FIEBIG<sup>1</sup>, CHRISTOPH ERLÉN<sup>2</sup>, PAOLO LUGLI<sup>2</sup>, UDO BEIERLEIN<sup>1</sup>, and •BERT NICKEL<sup>1</sup> — <sup>1</sup>Dep. für Physik und CeNS, Ludwig-Maximilians-Universität, München — <sup>2</sup>Institute for Nanoelectronics, Technische Universität München

Spatially resolved photoresponse has been measured on pentacene thin film transistors. The technique allows for the investigation of the response to illumination with a spatial resolution in the submicron regime. Enhanced photoresponse was observed close to the negatively biased electrode. We have modelled the experiment using drift-diffusion simulations and a photo doping mechanism. In this model holes in pentaene can drift, while electrons remain almost fixed at their site of generation until they recombine. The electron lifetime extracted from this model is in the order of 10 ps.

SYOE 4.5 Tue 11:00 H1

**Reduced contact and sheet resistance in bottom-contact pentacene field-effect transistors using palladium electrodes** — •D. V. PHAM<sup>1</sup>, G. DECK<sup>1</sup>, C. BOCK<sup>1</sup>, U. KUNZE<sup>1</sup>, D. KÄFER<sup>2</sup>, G. WITTE<sup>2</sup>, and CH. WÖLL<sup>2</sup> — <sup>1</sup>Lehrstuhl für Werkstoffe und und Nanoelektronik, Ruhr-Universität Bochum, D-44780 — <sup>2</sup>Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, D-44780

The influence of the source and drain contact metals (Au, Pd, and Pt) on the morphology and on the OFET performance was investigated.

The devices consisted of metal source and drain electrodes contacting a 110-nm-thick pentacene film thermally deposited on SiO<sub>2</sub> dielectrics ( $d = 40$  nm) with an n<sup>+</sup>-doped Si substrate serving as the gate electrode. Transistors with channel lengths from  $L = 3$   $\mu\text{m}$  to 100  $\mu\text{m}$  at a constant channel width  $w = 2$   $\mu\text{m}$  are prepared in order to separate the sheet resistance from the parasitic resistance of the contacts and leads. The contact resistance of transistors with Pd electrodes is four times smaller and the sheet resistance is eight times smaller than those of transistors with Pt or Au electrodes. The reduced sheet resistance is

also reflected by a reduced trap density. Although Pt has a higher work function than Au and Pd the transistors with Au and Pt electrodes have similarly electrical characteristics. This can be explained by the film morphology. In order to study the nucleation of the pentacene on the OFET substrate further samples are prepared with an 8-nm-thick pentacene film. While the growth on the Au and Pt electrodes is completely different to the film morphology on silicon dioxide the growth on Pd is similar to that on the insulator.

## SYOE 5: Organic Devices

Time: Tuesday 11:15–12:45

Location: H1

### Invited Talk

SYOE 5.1 Tue 11:15 H1

**Organic electronic devices and their applications** — ●PAUL HEREMANS — IMEC, Leuven, Belgium

Organic electronics will be enabled not only by thin film transistors, but also by such devices as memory and diodes.

In this presentation, we will focus on devices that can enable RFID applications or other autonomous sensor tags. Such applications require in particular transistor circuits operating at low voltage. Several strategies could be followed to achieve this, and we will provide a comparison between the performance and limitations that can be expected by complementary logic versus ambipolar logic. A second device needed for RFID applications is a diode for high frequency rectification. We will start by outlining the specifications required for these diodes. Then, we will show the state of the art of the performance that has been achieved to this date by diodes made using, on the one hand, transistors with the drain shorted to the gate, and, on the other hand, “Schottky” diodes with a rectifying metal contact. Finally, results of practical organic RFID tags using Schottky diodes will be shown.

SYOE 5.2 Tue 12:00 H1

**Ambipolar transport and light emission in polymer field-effect transistors in top gate geometry** — ●JANA ZAUMSEIL, CARRIE DONLEY, JI-SEON KIM, CHRISTOPHER MCNEILL, RICHARD FRIEND, and HENNING SIRRINGHAUS — Cavendish Laboratory, Cambridge University, JJ Thomson Avenue, Cambridge CB3 0HE, United Kingdom

We have recently demonstrated that ambipolar charge transport is a generic feature of a wide range of polymer field-effect transistors (FETs) when appropriate injecting electrodes and trap-free dielectrics are used. An intriguing feature of ambipolar FETs with simultaneous hole and electron accumulation is the radiative recombination of opposite charge carriers within the channel, and thus light emission. Here we demonstrate ambipolar light-emitting FETs based on electroluminescent conjugated polymers in bottom contact/top gate geometry using gold electrodes and polymer gate dielectrics. We observe light emission from a narrow recombination zone whose position is controlled by the applied gate and source-drain voltages and depends on the ratio of hole to electron mobility and contact resistance. The light output is proportional to the drain current with quantum efficiencies comparable to those of polymer LEDs despite very high current densities. Width and intensity distribution of the emission zone were found to depend strongly on the microstructure of the polymer film. Light-emitting FETs thus allow insight into the transport properties of organic field-effect transistors that are not obvious from current-voltage characteristics alone.

SYOE 5.3 Tue 12:15 H1

**Electrical characteristics of Ferroelectric Field Effect Transistors (FeFETs) incorporating Langmuir-Blodgett films** — ●HERMANN KOHLSTEDT<sup>1</sup>, ANDERAS GERBER<sup>4</sup>, RAINER WASER<sup>1</sup>, TIMOTHY REECE<sup>2</sup>, STEPHEN DUCHARME<sup>2</sup>, EDUARD RIJE<sup>3</sup>, MARTIN ROECKERRATH<sup>3</sup>, and JÜRGEN SCHUBERT<sup>3</sup> — <sup>1</sup>Institute of Solid State Research (IFF), and CNI \* Center of Nanoelectronic Systems for Information Technology, 52425 Jülich, Research Center Jülich, Germany — <sup>2</sup>Nebraska Center for Materials and Nanoscience, — <sup>3</sup>Institute for Bio and Nanosystems (IBN1), and CNI \* Center of Nanoelectronic Systems for Information Technology, 52425 Jülich, Research Center Jülich, Germany — <sup>4</sup>Smart Materials, Caesar Research Center, 53175 Bonn, Germany

We report the electrical characteristics of a kind of non-volatile memory device consisting of a field-effect transistor where the gate insulator includes a thin ferroelectric polymer film, producing a Ferroelectric-FET, or FeFET. Each device consisted of a p-type silicon substrate, with diffusion-doped source and drain contacts, SiO<sub>2</sub>, HfO<sub>2</sub>, CeO<sub>2</sub> or DyScO<sub>3</sub> as dielectric buffer layer, a ferroelectric Langmuir-Blodgett film of a 70% vinylidene fluoride-30% trifluoroethylene copolymer, and a gold gate electrode. Details of the fabrication procedure will be presented. The source-drain conductance showed hysteresis due to polarization reversal in the ferroelectric film as the gate bias voltage was cycled. State retention was approximately several minutes. The FeFET is a promising low-voltage and nonvolatile memory element that affords fast non-destructive readout.

SYOE 5.4 Tue 12:30 H1

**Current injection and contacts to Cu(TCNQ)** — ●ARTUR HEFCZYC, LARS BECKMANN, EIKE BECKER, HANS-HERMANN JOHANNES, and WOLFGANG KOWALSKY — Institut für Hochfrequenztechnik, Technische Universität Braunschweig, Braunschweig, Germany

The development of organic electronics has caused increasing interest in non-volatile organic memories. Although many groups have reported memory effects in a wide range of material systems, the details of the switching mechanism are still not known. We have investigated the influence of contacts in devices based on the Cu(TCNQ) charge transfer complex by using combinations of different metals as well as metals and oxides. Our results show that the configuration of the contacts as well as the details of current injection have a crucial influence on device properties, e.g. on the polarity of the voltages required for switching. We report on the experimental results and the conclusions that can be drawn for the physics of the switching mechanism.

## SYOE 6: Transport in Organics Materials

Time: Tuesday 14:30–16:15

Location: H32

### Invited Talk

SYOE 6.1 Tue 14:30 H32

**Theory of polymer devices: OFETs and OLEDs** — ●REINDER COEHOORN — Philips Research Laboratories, High Tech Campus 4, 5656 AE, Eindhoven, The Netherlands

The main challenge in the development of microscopic transport models and device models for polymer organic field effect transistors (OFETs) and organic light emitting diodes (OLEDs) is to properly

include the effects of structural and energetic disorder of the materials used. In this talk, first an overview is given of the various methods for modelling the mobility in disordered organic materials on a microscopic scale, using numerical Monte Carlo, Master Equation (ME), and analytical percolation models. From ME modelling, it is shown that disorder leads to a carrier concentration dependence of the effective steady state, and has important consequences for the frequency

dependence of the complex impedance. Furthermore, it leads to a filamentary, rather than uniform current density, as quasi-3D-visualized in the talk. This is expected to affect the device efficiency and (potentially) the lifetime. Subsequently, recent experimental evidence will be presented that proves the important role of disorder in polymer LEDs and FETs, including recent results on dual gate and ambipolar light emitting OFETs, and on blue polymer OLEDs. In the final part of the talk, an overview will be given of the various challenging questions to be solved, including the question below which (sub)layer thickness the "mobility" concept is no longer meaningful.

The results presented in this talk have been obtained in collaboration with D.M. de Leeuw (Philips Research), S.L.M. van Mensfoort, B. Ramachandhran and P.A. Bobbert (Eindhoven University of Technology) and E.C.P. Smits (University of Groningen).

SYOE 6.2 Tue 15:15 H32

**Trapped-Space-Charge-Limited Currents in Organics** — ●GERNOT PAASCH<sup>1</sup>, PAUL BLOM<sup>2</sup>, MAGDA MANDOC<sup>2</sup>, and BERT DE BOER<sup>2</sup> — <sup>1</sup>IFW Dresden, Germany — <sup>2</sup>University of Groningen, The Netherlands

The Mott-Gurney law for space charge limited current (SCLC) has been modified early [1] to account for the presence of exponentially distributed traps. This expression has been widely used to analyse transport in organic light emitting diodes. However, the theory fails to describe the rather weak temperature dependence observed for electron transport, for instance in PPV derivatives [2]. There we have shown that the trap-limited SCLC law is essentially modified if the density of transport states is of Gaussian type. Here, we discuss the origin of this modification and present a detailed analysis of the modified law. In addition, we derive further modifications for different combinations of densities of states of both the transport states and the trap distribution. As a result, rather different dependencies of the current on voltage, layer thickness and temperature are possible. Consequently, one has to exercise care in order to obtain reliable trap parameters from SCLC.

[1] P. Mark and W. Helfrich, *J. Appl. Phys.* 33, 205 (1962).

[2] M. M. Mandoc, B. de Boer, G. Paasch, P. W. M. Blom, submitted.

SYOE 6.3 Tue 15:30 H32

**Macroscopic and Microscopic Simulations of the Charge Transport in Conjugated Polymers** — ●CARSTEN DEIBEL<sup>1</sup>, MARIA HAMMER<sup>1</sup>, ANDREAS BAUMANN<sup>1</sup>, INGO RIEDEL<sup>2</sup>, and VLADIMIR DYAKONOV<sup>1,2</sup> — <sup>1</sup>Experimental Physics VI, Physical Institute, Julius-Maximilians- — <sup>2</sup>Div. Functional Materials for Energy Technology, ZAE Bayern e.V., Am Hubland, 97074 Würzburg, Germany

The charge carrier mobility is a key characteristic for describing charge transport in disordered organic semiconductors. Its multiple dependencies, e.g. on temperature and electric field, can be understood by considering hopping transport in a gaussian density of states. Microscopically, the hopping process can be looked at by Monte Carlo simulations, with the density of states distribution as input, and the mobility as output parameter. Macroscopically, the numerical solu-

tion of the Poisson equation can be utilised. Despite their different approaches, both models are able to give insight into charge transport in conjugated polymers. The application of the simulation results of these two models to experimentally observed transient photoconductivity and space charge limited current experiments of polymer devices will be discussed.

SYOE 6.4 Tue 15:45 H32

**Charge mobility of discotic mesophases of hexabenzocoronene derivatives: a multiscale quantum/classical study of the effects of side chain substitution and temperature** — ●DENIS ANDRIENKO<sup>1</sup>, VALENTINA MARCON<sup>1</sup>, KURT KREMER<sup>1</sup>, JAMES KIRKPATRICK<sup>2</sup>, and JENNY NELSON<sup>2</sup> — <sup>1</sup>Max Planck Institute for Polymer Research, Ackermannweg 10, Mainz — <sup>2</sup>Department of Physics, Imperial College London, Prince Consort Road, London SW7 2BW, United Kingdom

Discotic liquid crystals form columnar phases, where the molecules stack on top of each other and the columns arrange in a regular lattice. The self-organization into stacks results in the one-dimensional charge transport along the columns. Using atomistic molecular dynamics (MD) simulations we study the solid and liquid crystalline columnar discotic phases formed by the alkyl-substituted hexabenzocoronene mesogens. Correlations between the molecular structure, packing, and dynamical properties of these materials are established. Combining Kinetic Monte Carlo and MD trajectories a correlation between the material morphology and charge mobility is then obtained. We are able to reproduce the trends and magnitudes of mobilities as measured by pulse-radiolysis time-resolved microwave conductivity technique.

SYOE 6.5 Tue 16:00 H32

**Trap-Controlled Hole Transport in a Small Molecule Organic Semiconductor** — ●ARNE FLEISSNER, HANNA SCHMID, ROLAND SCHMECHEL, CHRISTIAN MELZER, and HEINZ VON SEGGERN — TU Darmstadt, Institute of Materials Science, Electronic Materials Department, Petersenstr. 23, 64287 Darmstadt, Germany

The transport of charge carriers through organic semiconductors is strongly affected by trap states in the energy gap. In this work, a well defined concentration of hole traps is deliberately introduced into a small molecule hole transporter in order to control the mode of charge carrier transport and mobility. For that purpose, the host material N,N'-di(1-naphthyl)-N,N'-diphenylbenzidine ( $\alpha$ -NPD) is molecularly doped by thermal co-evaporation with 4,4',4''-tris-[N-(1-naphthyl)-N-(phenylamino)]-triphenylamine (1-NaphDATA), which is known to create 0.4eV-deep neutral hole traps. Using a mechanical chopper to control the mass flow of the dopant, doping concentrations as low as 100ppm were achieved. The influence of the trap concentration on charge transport and mobility is studied on diode-like structures by an optical time-of-flight method. Non-dispersive hole transport is observed for undoped  $\alpha$ -NPD. The introduction of 100ppm hole traps results in non-dispersive but trap-controlled transport and reduces the mobility by orders of magnitude. For increasing the trap concentration to over 1000ppm, the transition to dispersive transport is observed.

## SYOE 7: Single Molecule Contacts

Time: Tuesday 16:30–18:00

Location: H32

### Invited Talk

SYOE 7.1 Tue 16:30 H32

**Electronic spectrum and spin states of a single organic molecule** — ●HERRE VAN DER ZANT — Kavli Institute of Nanoscience, Delft, The Netherlands

With electromigration nanogaps on an aluminum gate electrode have been made and single molecules have been trapped between the electrode pairs. Three-terminal measurements on samples with the same molecule (OPV-5, Co4L4 grid molecule, Mn-12, single-metal atom complexes) share common features showing Coulomb blockade and Kondo physics at low temperature. Of crucial importance is the observation of molecule-specific properties as deduced for example from the interaction between electronic transport and vibrational modes or spin states in the molecule. Transport through an individual thiol end-capped oligophenylenevinylene molecule with five benzene rings (OPV-5) has been studied in great detail and displays more than fifteen excitations in the differential low-temperature conductance map.

Their energies agree with the ones from optical measurements and are attributed to vibrational modes of the molecule. A consistent set of measurements shows that the spin states, the charging energies and the electronic spectrum are completely renormalized by the presence of the gold electrodes. In case of the doubly charged molecule the data indicate delocalized orbitals with an antiferromagnetic ground state and an exchange of 1.7 meV.

Molecules are provided by Thomas Bjørnholm (OPV-5, single-metal atom complexes), M. Ruben and J.-M. Lehn (Co4L4 grid molecules) and A. Cornia (Mn-12).

SYOE 7.2 Tue 17:15 H32

**Ultrathin contacts for single molecules: Ag nanostructures on Si(100)** — ●GERNOT GARDINOWSKI, JENDRZEJ SCHMEIDEL, HERBERT PFNÜR, JÖRG MEYER, and CHRISTOPH TEGENKAMP — Institut für Festkörperphysik, Leibniz-Universität Hannover, 30167 Hannover,

Germany

The fabrication and characterization of metallic nanometer-sized (nm) gaps suitable for conductivity measurements of single molecules has been investigated systematically. First results of conductivity measurements of single molecules and of their direct observation by STM are presented. Epitaxially grown Ag structures with a thickness down to 10 monolayers on Si(100) were used for a controlled gap formation by electromigration (EM). The gaps obtained range from several nm down to sub-nm, as revealed by lateral conductivity measurements and by scanning tunneling microscopy done under ultra high vacuum conditions. Annealing to 300 K closes the gap by surface diffusion of Ag and a new cycle of opening by EM at low temperature (77K) can be performed. The functionality of the contacts is demonstrated by adsorption of single ferrocenedithiol molecules. The zero bias resistance is around 40kOhm. In addition, the  $dI/dV$  curve shows clearly molecular contributions in the range of 50meV and 150meV, which can be attributed to ferrocene induced states near the Fermi edge, as revealed by DFT calculations.

SYOE 7.3 Tue 17:30 H32

**High-Aspect Ratio Nanogap Electrodes for Averaging Molecular Conductance Measurements** — SEBASTIAN MARKUS LUBER<sup>1</sup>, FAN ZHANG<sup>1</sup>, SIMONE LINGITZ<sup>1</sup>, ALLAN GLARGAARD HANSEN<sup>1</sup>, FELIX SCHELIGA<sup>2</sup>, EMMA THORN-CSÁNYI<sup>2</sup>, MAX BICHLER<sup>1</sup>, and ●MARC TORNOW<sup>3,1</sup> — <sup>1</sup>Walter Schottky Institut, TU München, Germany — <sup>2</sup>Technische und Makromolekulare Chemie, Universität Hamburg, Germany — <sup>3</sup>Institut für Halbleitertechnik, TU Braunschweig, Germany

We present a method to fabricate a pair of closely spaced metal electrodes on the cleaved plane of a GaAs/AlGaAs heterostructure grown

by Molecular Beam Epitaxy (MBE). These smooth, co-planar electrodes oppose each other in a predetermined distance of a few nanometers, continuously over their entire width of tens of microns. We propose this structure for the determination of the average electrical conductance of molecules. As test system, we measured the current-voltage characteristics of 8.5 nm long Oligo-(p-phenylenevinylene) molecules assembled across electrode pairs of separation  $8 \pm 2$  nm and width 30  $\mu\text{m}$ . The observed non-linear I-V characteristics are in good qualitative agreement with model calculations.

SYOE 7.4 Tue 17:45 H32

**Kondo effect by controlled cleavage of a single molecule contact** — ●RUSLAN TEMIROV and STEFAN TAUTZ — International University Bremen, Bremen, Germany (Jacobs University Bremen as of spring 2007)

Contact properties are one of the unresolved challenges in the rapidly growing field of molecular electronics. Here we present a single molecule transport experiment with optimum control over contacts, carried out in an STM in a symmetric configuration, i.e. with a molecule between two chemical contacts. We start with a geometrically and spectroscopically well-characterized chemical bond between a  $\pi$ -conjugated molecule and a single crystalline metal surface and vary this contact by a controllable and gradual structural modification, until the metal-molecule bond is cleaved. In this way, the molecular wire is tuned smoothly from the mixed-valence strong-coupling to the intermediate-coupling Kondo regime, in which electron transport is highly correlated, and beyond, up to the point when the contact is cleaved. This tuning is achieved by a gradual de-hybridisation of a molecular orbital from the metallic states due to mechanical stress [1].

[1] R. Temirov and S. Tautz. cond-mat/0612036.

## SYOE 8: Poster Session SYOE

Time: Tuesday 18:00–20:00

Location: Poster B

SYOE 8.1 Tue 18:00 Poster B

**Controlling the shape of Nanogaps for single molecular contacts manufactured by directed Electromigration** — ●VICTOR MARINOV, ARNE HOPPE, and VEIT WAGNER — School of Engineering and Science, International University Bremen, Campus Ring 8, 28759 Bremen, Germany

Controlled fabrication of nanogaps separating two metal electrodes are of crucial importance for single molecule electronics. Among others, electromigration is a well-known technique to form such nanogaps with the inherent advantage to allow for an additional gate electrode. We report on a study to control the shape and the geometry of nanogaps in gold nano-wires on silicon oxide, which also serves as an insulator to the third electrode. We present a new approach, which allows forming of well-defined self-centered nanogaps by using an AC current source as well as asymmetric gap-formation in case a DC current source is applied. Combining both techniques with an intelligent active feedback loop for the applied voltage in dependence of the measured conductivity allows to get control over a wide range of different shapes of the junction as well as on the height profile of the resulting pair of electrodes. This approach has proven to be extremely robust against initial wire width and yields nanogaps of very well defined mesoscopic shape at room temperature.

SYOE 8.2 Tue 18:00 Poster B

**Chemical Bonding and Charge Distribution at Metallic and Molecular Nanocontacts** — ●COSIMA SCHUSTER and UDO SCHWINGENSCHLÖGL — Institut für Physik, Universität Augsburg, 86135 Augsburg

Electrical properties of metallic nanocontacts or molecular devices are addressed by the transport through a central atom or a molecule sandwiched between metallic electrodes. The resulting transport characteristics reflects both the metal-molecule contact and the molecule itself. The features of a nanocontact device strongly depend on the local electronic structure at the different molecular sites. Details of the chemical bonding, such as hybridization or charge transfer hence play a key role for understanding the device, and structural relaxation due to the metal-molecule contact has to be taken into consideration. We investigate the local electronic structure for various aluminium nanocontact geometries and the gold-dithiolbenzene transport interface. Our in-

vestigations result in two characteristic features: the suppression of hybridization and the violation of charge neutrality at the neck of the contact. Since both features trace back to the spacial restriction of the crystal structure due to the contact, they are typical of metallic nanocontacts in general. The influence of the particular shape of the nanocontact and the experimental setup is discussed. Especially, for the gold-dithiolbenzene transport interface we find that the local DOS at carbon sites without sulfur bonding almost vanishes at the Fermi energy, which explains the experimental observation of an insulating state.

SYOE 8.3 Tue 18:00 Poster B

**Electrostatic trapping of individual polymer molecules between microfabricated electrodes** — ●ALEKSANDAR IVANOV, ARNE HOPPE, JÜRGEN FRITZ, and VEIT WAGNER — International University Bremen, D-28759, Bremen, Germany (Jacobs University Bremen, as of Spring 2007)

Reliable deposition of single molecules between electrodes is a crucial step in the fabrication of molecular electronic devices. We report on an approach for deposition and electrostatic trapping of conducting polymers in solution followed by electrical measurements. Here we used regioregular poly(3-hexylthiophene) (P3HT), a polymer with an average chain length of 250 nm. Microfabricated interdigitated Au electrodes on silicon oxide (channel length of 200 nm, 100 nm) fabricated by e-beam lithography are dipped in a highly diluted polymer solution. During dipping a moderate DC voltage (0 ... 3 V) was applied. The dipping was followed by electrical measurements performed in air. Low current levels (< 50 pA) were recorded without an applied field during dipping. A significant increase of the current across the electrodes up to several 100 nA upon application of external DC fields in solution revealed the trapping of a low number of conducting polymers. Surprisingly the current level kept changing for several minutes before it stabilized. These changes depended strongly on the polarity of the applied voltage during dipping and are interpreted as rearrangement of polymer chains under applied voltage. The effect of field strength and polarity on trapping efficiency as well as the dependence of current on the number of molecules and channel length will be discussed.

SYOE 8.4 Tue 18:00 Poster B

**Measurement of charge transport through a polymer in a molecular junction at a solid-liquid interface** — ●STEFAN EILERS<sup>1</sup>, FRANK DIERSCHKE<sup>2</sup>, KLAUS MÜLLEN<sup>2</sup>, and JÜRGEN RABE<sup>1</sup> — <sup>1</sup>Humboldt-Universität zu Berlin, Germany — <sup>2</sup>Max Planck Institute for Polymer Research Mainz, Germany

The charge transport in molecules is essential for future applications in molecular electronics. Here, charge transport measurements on a metal-polymer-metal-system are presented. For the measurement gold electrodes, which are produced by electron beam lithography with a gap of 50 nm, are applied. Chains of polycarbazole, longer than 100 nm, are used to bridge the gap. The polymer is adsorbed from solution partly onto the electrodes and onto the substrate between the electrodes. I-V-characteristics are measured. Asymmetric characteristics are obtained potentially due to non-symmetric arrangement and adsorption of the polymer between the electrodes. The characteristics can be described by a model which treats the polymer as a resistor with a voltage dependent conductance and which takes into account the particular interfaces of the junction as barriers

SYOE 8.5 Tue 18:00 Poster B

**Two-Photon Photoemission Spectra of Heterogeneous Electron Transfer** — ●DMITRY TSIVLIN<sup>1</sup>, LARS GUNDLACH<sup>2</sup>, FRANK WILLIG<sup>3</sup>, and VOLKHARD MAY<sup>1</sup> — <sup>1</sup>Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Germany — <sup>2</sup>Dynamik von Grenzflächenreaktionen, Hahn-Meitner-Institut Berlin, Glienicker Straße 100, 14109 Berlin, Germany — <sup>3</sup>Department TH, Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin

Heterogeneous electron transfer from dye molecules into the conduction band continuum of TiO<sub>2</sub> has received considerable interest recently. It has been suggested that signatures of vibrational dynamics related to the dye can be distinguished in the photoelectron emission spectra measured shortly after the charge transfer process [1].

In the present study we simulate the time- and energy-resolved spectra of electrons emitted from the TiO<sub>2</sub> rutile surface with attached perylene derivatives. The interplay of the molecule and crystal contributions to the spectrum is discussed within a simple tight-binding model. Taking into account the finite escape depth and phonon-induced dephasing of the electrons inside the crystal an interpretation of the experimentally observed non-exponential photoemission signal decay on the femtosecond time-scale is proposed [2].

[1] L. Wang, V. May, R. Ernstorfer, L. Gundlach and F. Willig, Springer Series in Chemical Physics Vol.87 (Springer-Verlag, submitted). [2] L. Gundlach, R. Ernstorfer, and F. Willig, Phys. Rev. B 74, 035324 (2006).

SYOE 8.6 Tue 18:00 Poster B

**Quantum chemical calculations of PTCDA and NTCDA adsorbates on Ag(110)** — ●A. ABBASI<sup>1,2</sup>, R. SCHOLZ<sup>1</sup>, and M. SCHREIBER<sup>2</sup> — <sup>1</sup>Walter Schottky Institut, Technische Universität München — <sup>2</sup>Institut für Physik, Technische Universität Chemnitz

The interactions between small Ag(110) clusters and a single NTCDA or PTCDA molecule are investigated with different *ab initio* techniques. As both Hartree-Fock (HF) theory and density functional theory (DFT) with a gradient-corrected density functional do not contain any correlation energy reproducing the van-der-Waals interaction, we compare these approaches with the fastest numerical technique where the leading term of the van-der-Waals interaction is included, i.e. second order Møller-Plesset theory (MP2). Both HF and DFT result in bended optimized geometries where the adsorbate is interacting mainly via the oxygen atoms, with the core of the molecule repelled from the substrate. Only at the MP2 level, the inclusion of the major part of the attractive van-der-Waals interaction brings the adsorbate back to an arrangement close to parallel to the substrate. With respect to experimental data obtained on Ag(111), the calculated distance between adsorbate and substrate is somewhat smaller, indicating that the open Ag(110) surface interacts more strongly with the organic compounds. This is consistent with the fact that only Ag(110) induces a brickwall unit cell of the adsorbate, a clear sign for a particularly large adsorption energy. The resulting model geometries are analysed in terms of cohesive energy, Mulliken charges, core level shifts, and vibrational properties.

SYOE 8.7 Tue 18:00 Poster B

**Structural properties and scanning tunneling data of a monolayer of PTCDA on the Ag(111) surface** — ●MICHAEL ROHLFING — Fachbereich Physik, Universität Osnabrück

The adsorption of a monolayer of 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) on the Ag(111) surface constitutes one of the best studied adsorption systems of organic molecules on metals [1]. Here we present density-functional calculations of this prototypical systems, yielding detailed insight into its structural properties. Using the local-density approximation as the best choice for the exchange-correlation functional, we discuss the bond lengths inside the molecules, their distortion due to adsorption, and their position and orientation relative to the substrate and to each other. Based on the obtained geometric and electronic structure we calculate scanning-tunneling microscopy and spectroscopy data within the Tersoff-Hamann framework. To this end, two-dimensional Fourier transform methods and spatial extrapolation techniques are employed to evaluate the sample wave functions at the tip position. We obtain constant-current images and spectral data that reveal detailed information about the electronic structure of the system.

[1] A. Kraft, R. Temirov, S. K. M. Henze, S. Soubatch, M. Rohlfing, and F. S. Tautz, Phys. Rev. B 74, 041402(R) (2006).

SYOE 8.8 Tue 18:00 Poster B

**X-ray studies of structure and crystallinity of Poly(3-hexylthiophene)** — ●SIDDHARTH JOSHI<sup>1</sup>, SOUREN GRIGORIAN<sup>1</sup>, ULLRICH PIETSCH<sup>1</sup>, ACHMAD ZEN<sup>2</sup>, and DIETER NEHER<sup>2</sup> — <sup>1</sup>Festkörperphysik, Universität Siegen, Siegen, Germany — <sup>2</sup>Institut für Physik, Universität Potsdam, Potsdam, Germany

Poly (3-hexylthiophene) P3HT is one of the most promising  $\pi$ -conjugated polymers used in polymer-electronics and exhibits relatively high charge carrier mobility. Our studies are focussed on the investigation of the structural order and the degree of crystallinity of semi-crystalline films with thickness  $\sim$  50 nm of low-and high-molecular weights materials. Various x-ray scattering geometries have been used in order to determine the vertical and lateral crystalline structures of P3HT films. Based on additional investigations using AFM and TEM we concluded that the thin film of low molecular weight fraction samples consist of highly ordered crystallites with ribbon- or whiskers-like structures embedded in an amorphous matrix. Further, the small charge-carrier mobility in low-Mw films is mainly due to the charge-carriers scattering in the amorphous region. In contrast, the higher mobility in high-Mw fraction can be explained by the fact that this fraction consists of small partially-ordered domains where the chains either folded back into the disordered phase, or interconnect into neighbouring domains creating an efficient inter-chain transport. Also, we have determined the degree of crystallinity for low-and- high molecular weight fractions utilising Ruland's method indicating an increase of crystallinity with increasing the concentration of polymer samples.

SYOE 8.9 Tue 18:00 Poster B

**Electrical Conduction in Semiconducting Thin Films of (Partially) Fluorinated Phthalocyanines** — ●HARRY BRINKMANN<sup>1</sup>, CHRISTIAN KELTING<sup>1</sup>, OLGA TSARYOVA<sup>2</sup>, DIETER WÖHRLE<sup>2</sup>, and DERCK SCHLETTWEIN<sup>1</sup> — <sup>1</sup>Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, 35392 Gießen — <sup>2</sup>Institut für Organische und Makromolekulare Chemie, Universität Bremen, 28334 Bremen

Partially fluorinated phthalocyanines with two fluorine atoms in each benzene ring of the ligand (F8Pc) or phthalocyanines with one fluorine atom in each benzene ring (F4Pc) represent molecules with interesting intermediate characteristics between the p-type unsubstituted phthalocyanines F0Pc and the n-type perfluorinated F16Pc as seen in, e.g. semiempirical quantum chemical calculations and also in photoelectron spectroscopy experiments. We report here about the growth of zinc and copper complexes of F16Pc, F8Pc, F4Pc and F0Pc on organic and inorganic insulating substrates suitable for OFET applications. The development of the electrical conduction was studied in-situ during film growth and the results are discussed with respect to the growth mode of films. In a number of cases the formation of an ultrathin conductive layer in the monolayer range could be established, typically followed by a reorganization towards island growth (Stranski-Krastanov growth mechanism).

SYOE 8.10 Tue 18:00 Poster B

**Structural and electronic properties of highly ordered CuPc thin films on differently passivated vicinal silicon surfaces** — ●GIANINA GAVRILA<sup>1</sup>, TEODOR TOADER<sup>1</sup>, STEFAN SEIFFERT<sup>1</sup>, WALTER BRAUN<sup>2</sup>, and DIETRICH ZAHN<sup>1</sup> — <sup>1</sup>Chemnitz University of Technology, Semiconductors Physics Department, D-09107 Chemnitz — <sup>2</sup>BESSY GmbH, Albert-Einstein-Straße15, D-12489, Berlin

One intriguing way of controlling the orientation of organic molecules on inorganic substrates is by designing the geometric structure of the substrate surface, e.g. by the steps and terraces of vicinal surfaces. Near Edge X-ray Absorption Fine Structure investigations of Copper Phthalocyanine (CuPc) deposition on differently passivated vicinal Si(111)-7x7 surfaces revealed that the molecular orientation of CuPc molecules can be controlled by different substrate pretreatment. On hydrogen passivated vicinal Si(111)-7x7 the individual CuPc molecules adopt a standing upright geometry and form structures aligned parallel to the step edges on the substrate. In contrast, on antimony (Sb)-passivated vicinal Si(111) surfaces columns of CuPc are again predominantly parallel to the step edge direction but the individual molecules are lying flat on the terraces. The electronic properties of such highly ordered CuPc thin films is revealed by means of photoemission spectroscopy (PES). Photon energy dependent measurements performed on thin CuPc films deposited onto Sb passivated vicinal silicon surfaces revealed an intermolecular energy band dispersion of about 0.25 eV for the highest occupied molecular orbitals. The NEXAFS and PES results are correlated with scanning tunnelling microscopy images.

SYOE 8.11 Tue 18:00 Poster B

**Ballistic Electron Transport through titanylphthalocyanine films** — ●SONER ÖZCAN<sup>1</sup>, JÜRGEN SMOLINER<sup>1</sup>, MAX ANDREWS<sup>1</sup>, GOTTFRIED STRASSER<sup>1</sup>, THOMAS DIENEL<sup>2</sup>, ROBERT FRANKE<sup>2</sup>, and TORSTEN FRITZ<sup>2</sup> — <sup>1</sup>Inst. für Festkörperelektronik, TU-Wien, Austria — <sup>2</sup>Inst. für angewandte Photophysik, TU-Dresden, Germany

In this article, Au/titanylphthalocyanine/GaAs diodes incorporating ultra smooth thin films of the archetypal organic semiconductor Titanylphthalocyanine were investigated by Ballistic Electron Emission Microscopy/Spectroscopy (BEEM/S). To guarantee good internal sample resistance and optimized BEEM signals, molecular beam epitaxial (MBE) grown GaAs samples were used as substrates. On these substrates, TiOPc-films were grown with organic MBE. Finally, a 7 nm Au layer was evaporated on the samples. Our BEEM images indicate that the molecular beam epitaxial grown organic films have a very homogeneous transmission compared to simple evaporated films organic films. Analyzing the BEEM spectra we find that the TiOPc increases the BEEM threshold voltage compared to reference Au/GaAs diodes. The Schottky barrier heights were measured for various temperatures and show an approximately linear increase from 1.2 eV at room temperature to 1.5 eV at T=10K

SYOE 8.12 Tue 18:00 Poster B

**Experimental measurements and calculations of electronic structure of organic semiconductor copper phthalocyanine** — ●OLGA MOLODTSOVA<sup>1</sup>, VICTOR ARISTOV<sup>1,2</sup>, VOLODYMYR MASLYUK<sup>3</sup>, DENIS VYALIKH<sup>4</sup>, VICTOR ZHILIN<sup>2</sup>, YURI OSSIPIYAN<sup>2</sup>, THOMAS BREDOW<sup>5</sup>, INGRID MERTIG<sup>3</sup>, and MARTIN KNUPFER<sup>1</sup> — <sup>1</sup>IFW Dresden, D-01069 Dresden, Germany — <sup>2</sup>Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow distr., 142432, Russia — <sup>3</sup>Martin-Luther-Universität at Halle-Wittenberg, Fachbereich Physik, Germany — <sup>4</sup>Institute of Solid State Physics, TU Dresden, D-01069 Dresden, Germany — <sup>5</sup>Institute for Physical and Theoretical Chemistry, Bonn University, D-53115 Bonn, Germany

The filled and unoccupied electronic states of the organic semiconductor copper phthalocyanine (CuPc) have been determined using a combination of experimental and theoretical techniques, by means of direct and resonant photoemission, near-edge x-ray absorption fine structure and quantum-chemical calculations at density-functional level. The experimentally obtained electronic states of CuPc are in excellent agreement with the results of ab initio density of states, allowing to derive the detailed site specific information. Our results are of general importance for understanding and tailoring of novel electronic properties, which may be achieved by, e.g. functionalisation or doping of phthalocyanines. The proposed approach to establish the site, element, and angular-momentum character specific electronic structure, especially of empty states, may readily be applied to other organic semiconductors.

SYOE 8.13 Tue 18:00 Poster B

**Chemistry and electronic properties of metal-organic semiconductor interfaces: Fe and Co on CuPc** — ●VICTOR ARISTOV<sup>1,2</sup>, OLGA MOLODTSOVA<sup>1</sup>, YURI OSSIPIYAN<sup>2</sup>, BRYAN DOYLE<sup>3</sup>, STEFANO NANNARONE<sup>3,4</sup>, and MARTIN KNUPFER<sup>1</sup> — <sup>1</sup>IFW Dresden, D-01069 Dresden, Germany — <sup>2</sup>Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow distr., 142432, Russia — <sup>3</sup>TASC-INFM Laboratory, Area Science Park, Basovizza, I-

34012 Trieste, Italy — <sup>4</sup>Dipartimento di Ingegneria dei Materiali ed Amb., Università di Modena e Reggio Emilia

The creation of a spin transistor based on a semiconductor was proposed in 1990 by Datta and Das [1]. Nowadays the attractive idea to create a spin-transistor based on an organic semiconductor thin film (OMTF) has been proposed. The main problem in the development of such a device is to produce ferromagnetic metallic contacts as an injector of spin-polarized electrons into OMTF and as a drain of these spin-polarized electrons from the channel. This problem could be solved by fabrication and investigation of contacts such as Fe (Co, Ni) thin films to an OMTF. In this contribution we present the results of extensive investigations of chemistry and electronic properties of the interface formation between Fe(Co) and the archetypal organic semiconductor copper phthalocyanine (CuPc). The studies were performed by means of core-level and valence-band high-resolution photoemission electron spectroscopy as well as by near-edge x-ray absorption fine structure and using the synchrotron radiation facility ELETTRA (Italy). [1] S. Datta and B. Das, Appl. Phys. Lett. 56, 665 (1990).

SYOE 8.14 Tue 18:00 Poster B

**Engineering of the energy level alignment in silicon/organic and silicon/metal heterostructures by methyl-termination of Si(111)** — ●RALF HUNGER<sup>1</sup>, BENGT JÄCKEL<sup>1</sup>, TAEK LIM<sup>1</sup>, TETSUYA OSAKA<sup>2</sup>, DAISUKE NIWA<sup>2</sup>, LAUREN WEBB<sup>3</sup>, NATHAN LEWIS<sup>3</sup>, and WOLFRAM JAEGERMANN<sup>1</sup> — <sup>1</sup>Institut für Materialwissenschaften, TU Darmstadt — <sup>2</sup>Waseda University, Tokyo — <sup>3</sup>CalTech, Pasadena

For optimizing the charge transport across inorganic / organic phase boundaries in hybrid devices, the control over the relative position of the respective electron energy levels is of utmost importance. We have studied the effect of the methyl-termination on the energy level alignment of Si(111)-CH<sub>3</sub>/ZnPc and Si(111)-CH<sub>3</sub>/Ag, Cu, and Au interfaces. The methyl-terminated Si(111) surface is an interesting model system as it allows for chemical and electronic surface passivation with 100% organic coverage and a high degree of ordering [Hunger et al., Phys. Rev. B 72, 045317 (2005)].

The interfaces were prepared by stepwise evaporation in vacuum and subsequent characterization by synchrotron photoelectron spectroscopy at BESSY 2. We observed a modification of the energy level alignment for Si / ZnPc and Si / Ag interfaces by the methyl-termination by about +0.3 eV and -0.2 eV, respectively. These modifications can be understood by an interface dipole in case of the silicon/methyl/organic dye contact, and a lowering of the metal work function effect for the silicon/methyl/Ag junction.

SYOE 8.15 Tue 18:00 Poster B

**Investigation of interlayers at the organic-metal interface by laser desorption/ionization time-of-flight mass spectrometry** — ●SEBASTIAN SCHOLZ, QIANG HUANG, KARSTEN WALZER, and KARL LEO — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

Since Tang and VanSlyke invented the first efficient OLED, much work was done to improve organic semiconductor device characteristics. Hereby, the behavior of the interfaces between the organics and the metals used as anode and cathode is still an open question. We investigate these metal/organic and organic/metal interfaces with laser desorption/ionization time-of-flight mass spectrometry (LDI-TOF-MS) and discuss differences between them. The main advantages of this technique are the possibilities to analyze undestroyed molecules, to trace impurities, degradation products, and photo-chemical reaction products as well as metal-organic adducts on organic semiconductor thin films. We study commonly used metals like Ag and Al as bottom and top contacts and different hole and electron transport materials like MeO-TPD and BPhen. We find that organic materials evaporated onto previously deposited metals create a sharp interface without further reactions, while the evaporation of "hot" metal onto organic films may cause chemical reactions within the underlying organic material. This leads to improved electron injection into gap states of electron transport materials from the top metal contact, while for the injection of holes, a sharp interface without chemically modified interlayers is beneficial.

SYOE 8.16 Tue 18:00 Poster B

**The effect of fluorination on pentacene/Au interface energetics and charge reorganization energy** — ●ANTJE VOLLMER<sup>1</sup>, STEFFEN DUHM<sup>2</sup>, YUICHI SAKAMOTO<sup>3</sup>, TOSHIYASU SUZUKI<sup>3</sup>, and NORBERT KOCH<sup>2</sup> — <sup>1</sup>BESSY GmbH, Berlin, Germany — <sup>2</sup>Humboldt-Universität zu Berlin, Inst. f. Physik, Berlin, Germany — <sup>3</sup>Inst. f.

Molecular Science, Okazaki, Japan

The energy level alignment between conjugated organic semiconductors and metals is a key factor determining the performance of organic-based electronic devices. Hole injection barriers (HIB) at organic/metal interfaces can be directly determined by ultraviolet photoelectron spectroscopy (UPS), while angle-resolved UPS allows to assess molecular orientations at surfaces. Using these methods we investigated interfaces between two prototypical organic semiconductors, pentacene (PEN) and perfluoropentacene (PFP), and Au(111). PEN and PFP are used in organic field-effect transistors with high hole (PEN) and electron (PFP) mobility. The present AR-UPS study highlights with unprecedented accuracy the effects of perfluorination (of PEN) on the interface energy levels, and of molecular layer thickness on interface energetics. The HIB for the monolayer of each organic material on Au was almost identical, despite the very different ionization energy of PEN and PFP. We also found distinctly different molecular level energies against layer thicknesses, attributed to different polarization energies. UPS for monolayers of the two organic materials corroborated that the charge reorganization energy of PEN/Au(111) is larger than for PEN in the gas phase, and even larger for PFP/Au(111).

SYOE 8.17 Tue 18:00 Poster B

**Electronic structure of the organic semiconductor blend C<sub>60</sub>/CuPc** — ●ANDREAS OPITZ<sup>1</sup>, MARKUS BRONNER<sup>1</sup>, WOLFGANG BRÜTTING<sup>1</sup>, MARCEL HIMMERLICH<sup>2</sup>, JUERGEN A. SCHAEFER<sup>2</sup>, and STEFAN KRISCHOK<sup>2</sup> — <sup>1</sup>Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany — <sup>2</sup>Institut für Physik und Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany

Mixed organic materials are widely used for ambipolar organic field-effect transistors (OFETs) and photovoltaic cells (OPVCs). One particular material system used in both device types is a blend of n-conducting fullerene (C<sub>60</sub>) and p-conducting copper-phthalocyanine (CuPc) prepared by co-evaporation.

The electronic properties of these blends deposited on a gold electrode were analysed by X-ray and ultraviolet photoelectron spectroscopy in dependence on the mixing ratio. The energies of the highest occupied molecular orbitals (HOMO), the core levels and the vacuum level are found to vary with the mixing ratio. This energy shift is related to the common work function in the molecular blend which varies linearly with the mixing ratio between the values of the neat materials. As reported in the literature for layered systems there is no evidence for a chemical reaction of these two materials in blend systems.

SYOE 8.18 Tue 18:00 Poster B

**Study of reactions at the interface P(VDF-TrFE)/Al and P(VDF-TrFE)/PEDOT:PSS** — ●DIPANKAR MANDAL, KLAUS MUELLER, OLAF SEIFARTH, PATRICK HOFFMAN, KARSTEN HENKEL, and DIETER SCHMEISSER — Brandenburgische Technische Universität Cottbus, Angewandte Physik/Sensorik, 03046 Cottbus

Due to potential use in non volatile memory application, Poly(vinylidene fluoride/trifluoroethylene) (P(VDF-TrFE)) is a great deal of interest, especially to produce organic field effect transistors (OFET). Right now it was found that Aluminum is one of the cost-effective inorganic electrode candidate. On the other hand, poly(3,4-ethylenedioxythiophene):poly(4-styrenesulfonate) (PEDOT:PSS) shows promising behavior for the application as organic electrode. In part of our investigations we have systematically studied surface interactions of organic ferroelectric thin films (P(VDF-TrFE)) with inorganic (Al) and organic layers (PEDOT:PSS). By X-ray photoelectron spectroscopy (XPS) it has been found that there is an interfacial reaction with Al and the copolymer. In contrast, for electrodes made of PEDOT:PSS, we found not such kind of behavior. In this case, we found no evidence for any surface reaction. Furthermore, we present our results concerning the orientation of permanent dipoles in the co-polymer (formed between hydrogen and fluorine atom). Here, we use Near-edge X-ray absorption fine structure (NEXAFS) analysis at the U 49/2 - PGM2 beam line of the BESSY-II Synchrotron. This work is supported by Deutsche Forschungsgemeinschaft (DFG) within priority program 1157 (DSCH 745/11-1).

SYOE 8.19 Tue 18:00 Poster B

**Ballistic Electron Transport through titanylphthalocyanine films** — ●SONER ÖZCAN<sup>1</sup>, JÜRGEN SMOLINER<sup>1</sup>, MAX ANDREWS<sup>1</sup>, GOTTFRIED STRASSER<sup>1</sup>, THOMAS DIENEL<sup>2</sup>, ROBERT FRANKE<sup>2</sup>, and TORSTEN FRITZ<sup>2</sup> — <sup>1</sup>Inst. für Festkörperelektronik, TU-Wien, Austria — <sup>2</sup>Inst. für angewandte Photophysik, TU-Dresden, Germany

In this poster, Au/titanylphthalocyanine/GaAs diodes incorporating ultra smooth thin films of the archetypal organic semiconductor Titanylphthalocyanine were investigated by Ballistic Electron Emission Microscopy/Spectroscopy (BEEM/S). To guarantee good internal sample resistance and optimized BEEM signals, molecular beam epitaxial (MBE) grown GaAs samples were used as substrates. On these substrates, TiOPc-films were grown with organic MBE. Finally, a 7 nm Au layer was evaporated on the samples. Our BEEM images indicate that the molecular beam epitaxial grown organic films have a very homogeneous transmission compared to simple evaporated films of organic films. Analyzing the BEEM spectra we find that the TiOPc increases the BEEM threshold voltage compared to reference Au/GaAs diodes. The Schottky barrier heights were measured for various temperatures and show an approximately linear increase from 1.2 eV at room temperature to 1.5 eV at T=10K

SYOE 8.20 Tue 18:00 Poster B

**Investigation of the charge carrier injection in pentacene transistors with modified contacts** — ●PETER NILL<sup>1</sup>, NORBERT KOCH<sup>2</sup>, and JENS PFLAUM<sup>1</sup> — <sup>1</sup>Universität Stuttgart, 3. Phys. Institut, 70550 Stuttgart, Germany — <sup>2</sup>HU Berlin, Institut für Physik, 12489 Berlin, Germany

A crucial aspect concerning the performance of thin-film field-effect transistors (TFTs) is the charge carrier injection across the interface between the metal contacts and the molecular layer. Recently, we [1] pointed out that the position of electronic states contributing to charge injection depends on the respective molecular orientation as well as on possible molecular overlayers on the metal surface. Based on this observation we present our current investigation on the possibility to exploit this effect in order to alter the injection characteristics in pentacene-based TFTs with bottom-contact geometry. In our approach, we prepare by thermal treatment an additional molecular monolayer on top of the Au contacts, whereas the SiO<sub>2</sub> channel region remains uncovered. A 30nm thick pentacene film is then thermally deposited onto this structure as the TFT's active transport layer. Electronic characterisation reveals a significant enhancement of the saturation current by up to one order of magnitude for TFTs with modified versus those with un-modified metal contacts. As the measured hole mobility remains the same for both transistor structures we will discuss the observation of an enhanced saturation current in the context of an effective lowering of the contact resistance.

[1] N. Koch, et al., Organic Electronics 7 (2006) 537.

SYOE 8.21 Tue 18:00 Poster B

**Improved sheet conductance in pentacene field-effect transistors using thiol and selenol modified electrodes** — ●CLAUDIA BOCK<sup>1</sup>, DUY VU PHAM<sup>1</sup>, ULRICH KUNZE<sup>1</sup>, DANIEL KÄFER<sup>2</sup>, GREGOR WITTE<sup>2</sup>, and CHRISTOF WÖLL<sup>2</sup> — <sup>1</sup>Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum, D-44780 Bochum — <sup>2</sup>Physikalische Chemie I, Ruhr-Universität Bochum, D-44780 Bochum

In this work we demonstrate that a thiol and selenol treatment of the metal electrodes in bottom-contact pentacene field-effect transistors leads to an improved film homogeneity in the channel region, to a reduced trap-density and an improved sheet conductance. The devices consist of Ti/Au (1 nm/20 nm) electrodes prepared on an SiO<sub>2</sub> dielectric ( $d = 40$  nm) which is thermally grown on a highly doped silicon substrate. The channel length was varied from  $L = 3 \mu\text{m}$  to  $L = 100 \mu\text{m}$ . The electrodes are modified by self-assembled monolayers of anthracene-2-thiol (AnT) and anthracene-2-selenol (AnS). Finally, a thin pentacene film is deposited in a molecular-beam deposition chamber ( $T = 65^\circ\text{C}$ ). An untreated transistor acts as a reference sample. Two-terminal measurements for transistors with different channel length are used to separate the channel from the contact resistance. The contact resistance of the treated transistors are comparable to those of the reference sample, whereas the sheet-resistance of the channel is reduced up to one order of magnitude. The effective mobility  $\mu_{eff}$  of the transistors treated in AnT (estimated from the linear region of the output characteristic) is corrected to  $\mu_{cor} = 0.25 \text{ cm}^2/\text{Vs}$  by considering the contact resistance.

SYOE 8.22 Tue 18:00 Poster B

**Contact resistances in organic field effect transistors** — ●NICOLAS SPETHMANN, ELIZABETH VON HAUFF, and JÜRGEN PARISI — Department of Physics, Energy and Semiconductor Research Laboratory, Carl von Ossietzky University of Oldenburg, 26111 Oldenburg, Germany



In this study organic Field-Effect-Transistors (oFETs) are used to investigate the transport properties of charge carriers in organic semiconductors. From the current-voltage characteristics material parameters such as the mobility  $\mu_{FET}$  can be extracted. The extracted parameters have to be corrected for contact resistances, as these can dominate the overall behavior of an oFET. It is also important to get an improved understanding of the physical mechanisms at a metal/organic semiconductor contact for applications such as organic photovoltaics. In this study we use two different approaches to isolate the contact resistance of an oFET from the channel resistance. Firstly, the channel length of the oFET was varied for different devices; while the contact resistance remains constant, the channel resistance scales according to the channel length. Thus it is possible to extract the contact resistance. However, the deviations from device to device can complicate this analysis. Furthermore one cannot differentiate between the contact resistance at source and drain. These disadvantages can be overcome by the second approach: A gated four-probe structure was used to directly measure the voltage drop at the source and the drain in an operating transistor. The organic semiconductors used were poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl-C61-butyric acid methyl ester (PCBM).

SYOE 8.23 Tue 18:00 Poster B

**Initial growth of evaporated copper phthalocyanine thin films** - — ●BISWAS INDRU<sup>1</sup>, PEISERT HEIKO<sup>1</sup>, NAGEL MATHIAS<sup>1</sup>, CASU MARIA BENEDETTA<sup>1</sup>, SCHUPPLER STEFAN<sup>2</sup>, NAGEL PETER<sup>2</sup>, PELLEGRIN ERIC<sup>2,3</sup>, and CHASSÉ THOMAS<sup>1</sup> — <sup>1</sup>Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Auf der Morgenstelle 8, 72076 Tübingen, Germany — <sup>2</sup>Forschungszentrum Karlsruhe, Institut für Festkörperphysik, P. O. Box 3640, 76021 Karlsruhe, Germany — <sup>3</sup>Consorcio para la Construcción, Equipamiento y Explotación del Laboratorio de Luz de Sincrotrón, P. O. Box 68, 08193 Bellaterra (Barcelona), Spain

The growth of copper phthalocyanine thin films evaporated on polycrystalline gold is examined in detail, using near-edge x-ray absorption fine structure (NEXAFS) spectroscopy and surface-sensitive x-ray photoemission spectroscopy (SXPS). Measurements were done at the Angstromquelle Karlsruhe ANKA (WERA beamline). The molecular orientation of thin-films between 0.2 to 3 nm thickness was examined, focussing on the layers directly at the interface. By utilising the different surface sensitivities of both methods, it was possible to distinguish between the uppermost layer and the layer directly at the interface to gold. It was found that about three layers at the interface grow parallel to the substrate surface, whereas subsequent molecules are perpendicular oriented. Thus, the buried interfacial layer(s) in thin film systems can be differently oriented compared to the majority of molecules.

SYOE 8.24 Tue 18:00 Poster B

**Conductivity of transparent Indium-Tin-Oxide-nanoparticle/polymer composite layers** — ●NORMAN MECHAU<sup>1</sup>, ANNA PRODI-SCHWAB<sup>2</sup>, and ROLAND SCHMECHEL<sup>1</sup> — <sup>1</sup>Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe, Germany — <sup>2</sup>Degussa AG, Science to Business Center, 45764 Marl, Germany

The conductivity and optical absorption behavior of transparent composite layers consisting of conductive polymer poly(3,4-ethylenedioxythiophene)/poly(4-styrene sulfonate) (PEDT:PSS) mixed with high conductive Indium Tin Oxide (ITO) nanoparticles was investigated. Below the percolation threshold of the ITO nanoparticles, at a volume fraction of the ITO  $\sim 0.16$ , the conductivity decreases with increase of the ITO content. The reason for this decrease is a compensation of charge carriers between the p-doped PEDT:PSS and the n-doped ITO. By applying a simple harmonic oscillator approximation, based on superposition of two phase system and a partial compensation of carriers the change in the optical characteristics can be explained. Furthermore, the reduction of the total numbers of charge carriers by compensation explains the decrease of conductivity.

SYOE 8.25 Tue 18:00 Poster B

**Growth of sexithiophene (6T) films studied by reflectance difference spectroscopy** — ●L.D. SUN<sup>1</sup>, S. BERKEBILE<sup>2</sup>, G. WEIDLINGER<sup>1</sup>, G. KOLLER<sup>2</sup>, F.P. NETZER<sup>2</sup>, M.G. RAMSEY<sup>2</sup>, M. HOHAGE<sup>1</sup>, and P. ZEPPEFELD<sup>1</sup> — <sup>1</sup>Institute of experimental physics, Johannes Kepler University Linz, Linz, Austria — <sup>2</sup>Institute of Physics, Karl-Franzens University Graz, Graz, Austria

As a linear differential optical method, reflectance difference spectroscopy (RDS) is extremely sensitive to any kind of optical transition

which is polarization dependent, from single molecule excitation to excitons of molecular aggregates. Here, we report our in-situ RDS investigation of 6T film growth on anisotropic substrates, namely Cu(110)-(2x1)O and TiO<sub>2</sub>(110). The orientation of 6T molecule and the optical property of 6T thin film have been monitored over the entire range of the film thickness up to several nm. At submonolayer coverage, the optical property of the film is close to that of single molecule. However, already when the thickness of the film approach to one completed monolayer, excitonic state represented by Davydov splitting sets in. Following the evolution of RD spectrum, the growth mode and the film morphology can be deduced. For 6T grows on Cu(110)-(2x1)O, all molecules in the film are uniaxially aligned with their long molecular axes parallel to the CuO rows and to the Cu substrate surface. Similar growth mode has also been observed for 6T growth on TiO<sub>2</sub>(110) at liquid nitrogen temperature. However the 6T growth on TiO<sub>2</sub>(110) at room temperature shows a different behavior.

SYOE 8.26 Tue 18:00 Poster B

**Para-sexiphenyl thin films grown on KCl(001) substrates** — ANDREI ANDREEV<sup>1</sup>, GERARDO SOSA<sup>2</sup>, THOMAS HABER<sup>3</sup>, ANDREY KADASHCHUK<sup>4</sup>, ●GREGOR HLAWACEK<sup>1</sup>, ROLAND RESEL<sup>3</sup>, HELMUT SITTER<sup>2</sup>, SERDAR SARICIFTCI<sup>5</sup>, and CHRISTIAN TEICHERT<sup>1</sup> — <sup>1</sup>Inst. of Physics, University of Leoben, Austria — <sup>2</sup>Inst. of Semiconductor and Solid State Physics, University Linz, Austria — <sup>3</sup>Inst. of Solid State Physics, Graz University of Technology, Austria — <sup>4</sup>Inst. of Physics, Natl. Acad. of Sci. of Ukraine, Kiev, Ukraine — <sup>5</sup>Inst. f. Organic Solar Cells (LIOS), University Linz, Austria

Para-sexiphenyl (6P) films grown on KCl(001) substrates are promising for optoelectronic devices. In this work we use Atomic Force Microscopy (AFM), x-Ray diffraction (XRD) and photoluminescence (PL) in order to find the parameters controlling film morphology, structure and quality. It is shown that the initial growth stage is characterized by the formation of long needles, generating a rectangular network in accordance with the substrate surface symmetry. With increasing coverage, terraced mounds composed of upright standing molecules developing between the needles. Both features are single crystalline as shown by XRD and TEM. PL studies have shown that the emission spectra contain two different components - a structured spectrum due to intrinsic excitons and a broad red-shifted band ascribed to some kind of defects. It was shown that the relative intensity of the defect band is much weaker in the films grown on KCl comparing to that on mica. This finding confirms the high quality of the films and supports an idea of structural origin of these defects.

SYOE 8.27 Tue 18:00 Poster B

**structural and electrical properties of poly(3-octylthiophene) films: a scanning probe microscopy study** — JOSE ABAD<sup>1</sup>, BEATRIZ PEREZ-GARCIA<sup>1</sup>, ELISA PALACIOS-LIDON<sup>1</sup>, ANTONIO URBINA<sup>2</sup>, and ●JAIME COLCHERO<sup>1</sup> — <sup>1</sup>cioy, departamento de fisica, universidad de murcia, murcia, spain — <sup>2</sup>departamento de electronica, universidad politecnica de cartagena, cartagena, spain

Poly-(3-octylthiophene) (P3OT) is one of the most promising materials for applications in organic solar cells. In the present work we find that P3OT thin films (50-500nm) present a very rich nanostructure which is studied by scanning force microscopy techniques. From a morphological point of view, self-assembled lamellar structures are formed on the surface of the films, their morphologies are very rich depending on the polymer films growth conditions (drop casting or spin coating).

Kelvin force microscopy (KFM) is applied to study the electrical properties of the films under different working conditions, in particular under light illumination and while an electrical current is passing through the thin film. We find that, on the lamellar structures, different surface potential domains are visualized by KFM.

SYOE 8.28 Tue 18:00 Poster B

**A flexible approach to the fabrication of chemical gradients using functional monomolecular films** — ●NIRMALYA BALLAV<sup>1</sup>, ANDREY SHAPORENKO<sup>1</sup>, ANDREAS TERFORT<sup>2</sup>, and MICHAEL ZHARNIKOV<sup>1</sup> — <sup>1</sup>Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany — <sup>2</sup>Anorganische und Angewandte Chemie, Universität Hamburg, 20146 Hamburg, Germany

We present a new approach for the fabrication of chemical gradients on different substrates. The key idea of the method is tuning the exchange-reaction between a self-assembled monolayer covering the substrate and a potential molecular substituent by electron irradiation. As test systems, we used alkanethiolate monolayers on gold, which are well-known to undergo an exchange-reaction with molecules

capable of building self-assembled monolayer on the same substrate upon the immersion in the respective solution. We show that the rate and extent of the exchange-reaction, which is very slow at normal conditions, can be significantly influenced and precisely tuned by electron irradiation. Based on the developed approach and using the exchange reaction between the non-substituted and carboxyl-substituted alkanethiols, we were able to fabricate a hydrophilicity gradient as a test example. Generally, the irradiation-exchange approach can be used for the preparation of any gradient (biocompatibility, etc.) by a choice of a proper molecular substituent. Another advantage of the approach lies in its flexibility, since a gradient of any form and size, down to several tens of nanometers, can be prewritten by electron beam and mediated by the subsequent exchange reaction.

SYOE 8.29 Tue 18:00 Poster B

**Why a switch doesn't switch - a case study on stilbene on Si(100)** — ●PHILIPP MARTIN SCHMIDT, KARSTEN HORN, and THORSTEN KAMPEN — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Stilbene is the monomer building block of phenylenevinylene-type oligomers and polymers. In gas-phase and solutions the molecule undergoes an interconversion around its central C=C double bond upon irradiation with UV-light of 250-320nm wavelength [1]. This cis-trans-isomerization of the free molecule follows an in-plane hula-twist mechanism [2] whose pathway can be assumed to work as well in constraint systems, that is on surfaces - thus assessing a "molecular switch". Stilbene-isomers on the Si(100)-surface have been investigated by UPS, XPS and NEXAFS thereby gaining information on the orientation of the molecules and their interaction with the surface. Especially NEXAFS-spectroscopy allows for an identification and differentiation of the two isomers in the adsorbed phase. Cis-Stilbene has been exposed to monochromatized UV-light of different wavelengths between 250 and 450nm. NEXAFS spectra reveal that the molecules are absolutely stable upon radiation and no conformational changes could be induced. A further analysis of NEXAFS spectra in combination with theoretical calculations gives an explanation of the inhibition of isomerization due to molecule-surface-interactions. 1. R.J. Sensen et al., J. Chem. Phys. 98, 6291 (1993) 2. W.Fuß, et al., Angew. Chem. Int. Ed. 43, 4178 (2004)

SYOE 8.30 Tue 18:00 Poster B

**Intermolecular interaction in PTCDA, NTCDA, and NDCA as determined by comparative gas phase and thin film photoemission spectroscopy** — ●JENS SAUTHER, JENS WÜSTEN, STEFAN LACH, and CHRISTIANE ZIEGLER — Department of Physics, University of Kaiserslautern, D-67663 Kaiserslautern

The interaction of pi-conjugated organic molecules among each other influences such important properties as their electronic structure and their thin film growth behavior. Both are of utmost interest for the development of organic semiconductor devices.

Here, ultraviolet photoemission spectra of pi-conjugated organic molecules in the gas phase are compared with ultraviolet photoemission spectra of those molecules in the condensed phase and with DFT calculations. This allows to obtain values for the effects of electron correlation, intra- and intermolecular polarization which cannot be determined by thin film spectra alone. Furthermore this analysis gives information about the character of intermolecular bonding. Such an analysis was performed on the related molecules 3,4,9,10-perylene-tetracarboxylic acid dianhydride (PTCDA), 1,4,5,8-naphthalene-tetracarboxylic acid dianhydride (NTCDA) and 1,8-naphthalene dicarboxylic acid anhydride (NDCA). All three systems show intermolecular hydrogen bridge bonding involving the anhydride group(s).

SYOE 8.31 Tue 18:00 Poster B

**Morphology and OFET properties of poly(3,3''-didodecyl-[2,2':5',2'':5'',2'']-quaterthiophene) (PQT-12) with different molecular weights** — ●PATRICK PINGEL<sup>1</sup>, ACHMAD ZEN<sup>1</sup>, BURKHARD STILLER<sup>1</sup>, DIETER NEHER<sup>1</sup>, SYBILLE ALLARD<sup>2</sup>, and ULLRICH SCHERF<sup>2</sup> — <sup>1</sup>Institute of Physics, University of Potsdam, Am Neuen Palais 10, 14469 Potsdam — <sup>2</sup>Macromolecular Chemistry, University of Wuppertal, Gauß-Str. 20, 42097 Wuppertal

It is well-known that molecular packing in thin-film organic field-effect transistors plays a crucial role in determining their field-effect mobilities. Here, we used PQT-12, which tend to adopt a better planar conformation compared to well-known poly(3-hexylthiophene) (P3HT). Since it is well established for P3HT that the average chain

length largely determines the OFET-properties, we investigated different molecular weight fractions of PQT-12 ( $M_w = 1,700$  to  $12,000$  g/mol) regarding to morphology and transport. In contrast to findings on P3HT, the OFET mobilities were above  $10^{-3}$  cm<sup>2</sup>/Vs also for the lowest molecular weight fraction and the smallest mobility ( $10^{-5}$  cm<sup>2</sup>/Vs) was found in the intermediate- $M_w$ . Studies of the optical, thermal and structural properties of PQT-12 solid samples suggest that the fraction with the shortest chains forms highly-crystalline layers. We attribute this behaviour to the very narrow molecular weight distribution of this low molecular weight fraction. Apparently, the OFET properties of both PQT-12 and P3HT are similar in that the OFET mobility depends largely on the overall crystallinity of the semi-conducting layer.

SYOE 8.32 Tue 18:00 Poster B

**Structure and Morphology of Highly Ordered Organic Films of PTCDI-C<sub>8</sub> on SiO<sub>2</sub>** — ●TOBIAS KRAUSS<sup>1</sup>, ESTHER BARRENA<sup>1,2</sup>, DIMAS GARCIA DE OTEYZA<sup>1</sup>, XUE NA ZHANG<sup>1</sup>, JÁNOS MAJOR<sup>1</sup>, VOLKER DEHM<sup>3</sup>, FRANK WÜRTHNER<sup>3</sup>, and HELMUT DOSCH<sup>1,2</sup> — <sup>1</sup>Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, 70569 Stuttgart, Germany — <sup>2</sup>Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57 — <sup>3</sup>Institut für Organische Chemie, Universität Würzburg, Am Hubland 97074, Würzburg

For organic electronics there is a particular need of molecules with n-type behavior in order to enable the fabrication of complimentary circuits and ambipolar transistors. A remarkable high electron carrier mobility of  $0.6$  cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup> was reported for OFETs based on PTCDI-C<sub>8</sub> (N,N\*-dioctyl-3,4,9,10-perylene tetracarboxylic diimide) films making this molecule a promising candidate for organic n-type semiconductors. In this work we present for the first time a complete characterization of the structure of PTCDI-C<sub>8</sub> films deposited on SiO<sub>2</sub> by means of specular x-ray diffraction and grazing incidence x-ray diffraction (GIXD). We provide the optimized conditions for growth of PTCDI-C<sub>8</sub> films with an outstanding degree of crystalline order and discuss the thermal behavior of their structural properties.

SYOE 8.33 Tue 18:00 Poster B

**Raman characterization of vacuum-deposited thin TiOPc films: influence of applied electric field and temperature on polymorphism and orientation** — ●BRITT-ELFRIEDE SCHUSTER, HEIKO PEISERT, and THOMAS CHASSÉ — Institute of Physical and Theoretical Chemistry, University of Tübingen, Auf der Morgenstelle 8, 72076 Tübingen, Germany

Titanyl(IV)phthalocyanine (TiOPc) is an attractive material and a promising candidate for various applications e.g. in optoelectronic devices. As the physical properties of thin organic films are affected by polymorphism and orientation, they are crucial to device efficiency and performance. Therefore, detailed studies of the influences of preparation parameters and effects of ambient conditions are necessary. In the present work we characterize thin TiOPc films prepared by vacuum deposition on various technically relevant model substrates like sapphire, quartz and HOPG. Deposition parameters during the growth (substrate temperature, electric field and film thickness) were systematically varied to study their influences on the growth of these organic films using laterally resolved (confocal) Raman scattering in combination with electronic absorption spectroscopy. In addition, after the growth in UHV, annealing in the temperature range from 298 K to 473 K and applying a DC electric field have been investigated. The Raman spectra are distinctly influenced by details of the growth and postgrowth conditions and they are discussed in terms of a factor group splitting. The results reveal a clear change in the composition of the polymorphic modifications and a variation in molecular arrangement.

SYOE 8.34 Tue 18:00 Poster B

**Tuning the molecular organization in organic heterostructures** — ●CLAUDIA WEIS<sup>1</sup>, ESTHER BARRENA<sup>1,2</sup>, DIMAS GARCIA DE OTEYZA<sup>1</sup>, XUE NA ZHANG<sup>1</sup>, and HELMUT DOSCH<sup>1,2</sup> — <sup>1</sup>Max-Planck-Institut für Metallforschung, — <sup>2</sup>Institut für Theoretische und Angewandte Physik,

Pentacene and fluorinated copper-phthalocyanines (F<sub>16</sub>CuPc) are among the most popular building blocks for prototype organic heterostructures in modern electronic devices. When deposited onto pentacene on SiO<sub>2</sub>, F<sub>16</sub>CuPc molecules assemble in a lying-down configuration along the pentacene step edges, whereas on top of the pentacene terraces, they arrange in the energetically preferred upright-standing configuration[1]. In the present work, we show by X-ray

diffraction measurements and atomic force microscopy that the lying-down configuration is suppressed if a small amount ( $\leq 2\text{ML}$ ) of an additional molecule, i.e. PTCDI- $\text{C}_8$  (N,N\*-dioctyl-3,4,9,10-perylene tetracarboxylic diimide), is deposited onto the pentacene prior to the  $\text{F}_{16}\text{CuPc}$  growth. Forcing the molecular arrangement exclusively to the upright-standing phase is essential for optimal charge carrier transport along the film plane as required in ambipolar transistors or the recently demonstrated organic light-emitting transistors (OLETs).

[1] D. G. de Oteyza *et al.*, Chem. Mater. **18**, 4212 (2006).

SYOE 8.35 Tue 18:00 Poster B

**Evolution of structure and morphology of perylene films with different thicknesses and deposition rates** — ●MARYAM BEIGMOHAMADI, PHENWISA NIYAMAKOM, AZADEH FARAHZADI, STEPHAN KREMER, CHRISTIAN EFFERTZ, PHILIP SCHULZ, THOMAS MICHELY, and MATTHIAS WUTTIG — Institute of Physics (IA), RWTH Aachen University of technology 52056 Aachen, Germany

A systematic study of the growth of highly ordered perylene films deposited on amorphous substrates is presented. The dependence of the structure and morphology of the films on thickness and deposition rate is characterized by Atomic Force Microscopy (AFM) and X-ray Diffraction (XRD). Atomic force microscopy reveals that every grain contains at least one screw dislocation. An analysis of the XRD peak profiles allowed us to determine the microstrain and vertical grain size. The changes of grain size and dislocation density with thickness and deposition rate have been analyzed.

SYOE 8.36 Tue 18:00 Poster B

**Highly ordered phthalocyanine films on polycrystalline gold foil - on the** — ●BISWAS INDRIO<sup>1</sup>, SCHUSTER BRITT-ELFRIEDE<sup>1</sup>, PEISERT HEIKO<sup>1</sup>, NAGEL MATHIAS<sup>1</sup>, CASU MARIA BENEDETTA<sup>1</sup>, SCHUPPLER STEFAN<sup>2</sup>, NAGEL PETER<sup>2</sup>, PELLEGRIN ERIC<sup>2,3</sup>, and CHASSÉ THOMAS<sup>1</sup> — <sup>1</sup>Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Auf der Morgenstelle 8, 72076 Tübingen, Germany — <sup>2</sup>Forschungszentrum Karlsruhe, Institut für Festkörperphysik, P. O. Box 3640, 76021 Karlsruhe, Germany — <sup>3</sup>Consortio para la Construcción, Equipamiento y Explotación del Laboratorio de Luz de Sincrotrón, P. O. Box 68, 08193 Bellaterra (Barcelona), Spain

The orientation of phthalocyanines in thin-films has been reported earlier to be determined by the possibility of "locking in" the growth mode to an orientation parallel to the substrate, and in the case of relatively rough substrates, no "lying" orientation has been observed at film thicknesses of more than a few nanometres. [1] The detailed preparation conditions however may significantly affect the substrate morphology. In particular, the parameters of the argon ion sputtering procedure may be varied, which can lead to various results. The orientation of evaporated copper phthalocyanine thin-films on differently prepared gold foils was examined by NEXAFS and Raman spectroscopy. Argon ion sputtering at higher energies leads to weakly ordered films with perpendicular orientation, while lower energies lead to highly ordered films of parallel molecules. Thus, the morphology of the substrate has to be viewed in detail for each preparation procedure.

[1] Peisert *et al.*, Surf. Sci. **600** (2006) 4024.

SYOE 8.37 Tue 18:00 Poster B

**Interface Morphology Snapshots of Vertically Segregated Thin Films of Semiconducting Polymer / Polystyrene Blends** — ●JAKOB HEIER<sup>1</sup>, FERNANDO CASTRO<sup>2</sup>, and ROLAND HANY<sup>1</sup> — <sup>1</sup>Empa, Swiss Federal Laboratories for Materials Testing and Research, Laboratory for Functional Polymers, Dübendorf, Switzerland — <sup>2</sup>Departamento de Física e Matemática, Universidade de São Paulo, Ribeirão Preto, Brazil

Significant progress has been made in the photovoltaic energy conversion using organic semiconducting materials. One of the focuses of attention is the morphology of the donor-acceptor heterojunction at the nanometer scale, to ensure efficient charge generation and loss-free charge transport at the same time. Here, we present a method for the controlled, sequential design of a bilayer polymer cell architecture that consists of a large interface area. We used surface-directed demixing of a donor conjugated/guest polymer blend during spincoating to produce a nanostructured interface, which can, after removal of the guest polymer with a selective solvent, be covered with an acceptor layer. Our experimental results indicate that length-scales of interface topographical features can be adjusted from the nanometer to micrometer range.

SYOE 8.38 Tue 18:00 Poster B

**Structure and unusual thermal behaviour of a prototype organic semiconductor (Diindenoperylene)** — ●BERND MAIER, JÖRG IHRINGER, and FRANK SCHREIBER — Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

A recently suggested model for the bulk structure is compared with X-ray powder data collected at  $18 < T < 298\text{ K}$  in steps of  $\Delta T = 10\text{ K}$  with a modified image plate Camera (Huber) and at room temperature with an automated X-ray powder diffractometer, both in Guinier-geometry. The unit cell agrees well with the suggested model. Refinement of lattice constants (program SIMPRO) yield  $b = 13.08$  (0.016),  $c = 15.09$  (0.008) at  $298\text{ K}$  and  $b = 12.97$  (0.020),  $c = 14.94$  (0.009) at  $18\text{ K}$ . The thermal dependence at  $18 < T < 298\text{ K}$  will be given. Due to pseudo symmetry the lattice constants (space group  $P\bar{1}$ ) correlate strongly with atomic coordinates. A profile refinement with the Rietveld Method would solve the problem, however, there is some more work needed to evaluate a first set of approximate atomic coordinates.

In addition, a highly irreversible phase transition to high temperature phase occurs. Upon heating with a rate of  $0.2\text{ K/min}$  the high temperature phase appears at around  $370\text{ K}$ . The high temperature phase remains stable when cooling to  $50\text{ K}$ . However, only part of material undergoes this transition, as both phases coexist in the whole temperature range.

SYOE 8.39 Tue 18:00 Poster B

**High charge carrier mobility in organic semiconductor diphenylanthracene (DPA)** — ●ASHUTOSH TRIPATHI and JENS PFLAUM — 3. Physikalisches Institut, Pfaffenwaldring 57, Universität Stuttgart, 70550 Stuttgart

In this work we focus on the growth and the electronic properties of the organic semiconductor 9,10-diphenylanthracene (DPA). DPA consists of two phenyl groups attached at the opposite (9,10)-positions of the anthracene backbone and may be considered similar to rubrene, which shows high field-effect mobility in its (ab)-plane crystal surface. Advantageously, DPA has a substantially low vapor pressure at RT, has a relatively high melting point ( $\approx 430\text{ K}$ ) and is thermally stable upon melting.

We have grown DPA single crystals from zone-refined material and analyzed their temperature dependent electronic transport behavior. These ultra-pure single crystals exhibit both electron and hole transport. The high charge carrier mobilities measured by Time-of-Flight (TOF) at RT for electrons ( $\approx 13\text{ cm}^2/\text{Vs}$ ) and holes ( $\approx 3.7\text{ cm}^2/\text{Vs}$ ) make this material a prominent candidate for ambipolar device applications if one overcomes the barrier for charge carrier injection occurring at the metal-DPA-interface. The mobility behavior of holes follows a band-like transport in the high temperature regime (200K - 400K). Assuming a pure band-like conduction in the low temperature regime, the saturation of the mobility yields a valence bandwidth of the order of 2 meV, which demands for a more sophisticated approach to describe the electronic behavior of DPA.

SYOE 8.40 Tue 18:00 Poster B

**Tunneling in organic thin films** — ●KERSTIN KELLER, FLORIAN ROTH, and MICHAEL HUTH — Physikalisches Institut, University Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt am Main

BEDT-TTF (ET)- and Cu-phthalocyanine (CuPc)-based organic thin films are prepared by organic molecular beam deposition (OMBD). Using an in-situ shadow mask technique planar tunnel junctions in cross-junction geometry are fabricated. This device structure is used to investigate the electronic properties of the organic thin film at low temperatures employing tunneling spectroscopy.

SYOE 8.41 Tue 18:00 Poster B

**Investigation on thin films of new substituted quarterthiophene** — ●KINGA ZELENETSKAYA<sup>1</sup>, EVELIN JÄHNE<sup>1</sup>, HANS-JÜRGEN ADLER<sup>1</sup>, CHRISTIAN LOPPACHER<sup>2</sup>, LUKAS ENG<sup>2</sup>, JÖRG GRENZER<sup>3</sup>, and ANDREA SCHOLZ<sup>3</sup> — <sup>1</sup>Professur für Makromolekulare Chemie und Textilchemie, Fachrichtung Chemie und Lebensmittelchemie, Technische Universität Dresden, Mommsenstrasse 4, D-01062 Dresden, Germany — <sup>2</sup>Institut für Angewandte Photophysik, Fachrichtung Physik, Technische Universität Dresden, George-Bähr-Strasse 1, D-01062 Dresden, Germany — <sup>3</sup>Institut für Ionenstrahlphysik und Materialforschung, Forschungszentrum Rossendorf, Bautzner Landstrasse 128, D-01328 Dresden, Germany

$\alpha,\omega$ -dicyano substituted  $\beta,\beta^*$ -dibutylquarterthiophene (DCND-ButQT) was synthesized and fully characterized by  $^1\text{H-NMR}$  and  $^{13}\text{C-NMR}$ , elemental analysis, UV-visible spectroscopy, DSC, TGA

and cyclic voltammetry. The band gap energy ( $\Delta E_g$ ) calculated from cyclic voltammetry data was found to be 1.97 eV, which is in the range of semiconductor materials ( $\Delta E_g < 3.0$  eV).

DCNDButQT was deposited on different substrates (Al<sub>2</sub>O<sub>3</sub>, SiO<sub>2</sub>, TiO<sub>2</sub>) by vacuum deposition and solution-cast methods. The structure of the thin films analysed by AFM and XRD showed different morphology depending on cast method. The spin-coating and drop-casting films showed amorphous structure, whereas the vacuum-deposition films exhibit a fine crystalline structure. AFM of vacuum-deposition film revealed the formation of well-ordered terrace structures, the step between adjacent terraces is about 1.5 nm.

SYOE 8.42 Tue 18:00 Poster B

**Skew crystal optics: Optical properties of pentacene probed by generalized spectroscopic ellipsometry** — •DANIEL FALTERMEIER<sup>1</sup>, BRUNO GOMPF<sup>1</sup>, MARTIN DRESSEL<sup>1</sup>, MATHIAS SCHUBERT<sup>2</sup>, ASHUTOSH TRIPATHI<sup>1</sup>, and JENS PFLAUM<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, D-70550 Stuttgart — <sup>2</sup>Department of Electrical Engineering, University of Nebraska-Lincoln, P.O. Box 880511, Lincoln, U.S.A.

There exist an increasing number of band structure calculations for organic semiconductors. For verification of these theories reliable optical data from single crystals are required. In principle, with traditional spectroscopic tools the anisotropic complex dielectric properties of a crystal can be determined. Problems arise for absorbing crystals, and in general for those with symmetries lower than orthorhombic. We demonstrate that generalized spectroscopic ellipsometry measures the complex dielectric polarization response functions along major polarization axes in triclinic systems. For the example of the organic semiconductor pentacene we demonstrate, that this can be achieved on a single crystal plane, when measuring under multiple azimuth angles, distinct angles of incidence and different incoming polarization states. We obtain, in addition to the major dielectric polarization response functions, that the optically determined major polarization axes directions are almost in perfect agreement with the crystallographic x-ray data, showing that these directions are in fact equivalent, for which so far no proof or indication existed. The results are compared with band structure calculations along the main symmetry directions.

SYOE 8.43 Tue 18:00 Poster B

**Interplay of chain geometry and quantum coherence in a conjugated polymer** — •E. DA COMO<sup>1</sup>, K. BECKER<sup>1</sup>, J. M. LUPTON<sup>2</sup>, and J. FELDMANN<sup>1</sup> — <sup>1</sup>Photonics and Optoelectronics Group, LMU, Munich, Germany — <sup>2</sup>University of Utah, Salt Lake City, USA

The performance of optoelectronic devices based on conjugated polymers depends on the influence of morphology on the electronic structure. Within this context, we correlate the photophysics and the chain morphology of a model fluorene polymer, poly-(9,9-dioctylfluorene) (PFO), at the single molecule level. PFO shows different phases that can be identified by photoluminescence spectroscopy. Well resolved and red-shifted emission bands are observed for the planarized beta-phase while a less structured blue emission is characteristic of the glassy phase. The identification of these features, at the single molecule level [1], raises the question of how chain geometry influences the electronic properties. Using low temperature single molecule excitation polarization anisotropy measurements we probe the conformation of isolated chains in both phases. The results demonstrate that beta-phase molecules show higher polarization values than the twisted glassy phase molecules, reflecting an elongated character of these chains. Most importantly, a strong correlation exists between the zero phonon linewidth and the emission polarisation anisotropy of the beta-phase molecules. Extremely narrow lines (0.5 meV) are observed for fully polarized emission. This indicates that the beta phase constitutes a 1D crystalline polymer where the exciton can reach quantum coherence times of ~3 ps. [1] K. Becker et al. JACS, 127, 7306 (2005).

SYOE 8.44 Tue 18:00 Poster B

**Correlation between the topography and the optical properties of rubrene single crystals** — •RAINER STÖHR<sup>1</sup>, GARETH BEIRNE<sup>2</sup>, PETER MICHLER<sup>2</sup>, JÖRG WRACHTRUP<sup>2</sup>, and JENS PFLAUM<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Univ. Stuttgart, 70550 Stuttgart, Germany — <sup>2</sup>Institut für Strahlenphysik, Univ. Stuttgart, 70550 Stuttgart, Germany

On the surface of rubrene single crystals high hole mobilities on the order of 15 cm<sup>2</sup>/Vs have been observed, making this molecule interesting for organic device applications. However, the influence of surface de-

fects on the transport behavior as well as on the optical characteristics is not yet understood in detail.

We present our first studies of the time- and locally-resolved micro-photoluminescence ( $\mu$ -PL) investigations performed on the (001) surface of rubrene single crystals grown by sublimation. After the growth, the (001) crystal surfaces were investigated by optical microscopy and AFM. Various topologies were found which can be related to different conditions at the respective position in the oven during growth.

Measuring the optical response of numerous rubrene crystals by  $\mu$ -PL at various positions on the respective (001) surface, four peaks could be identified. These peaks show different intensity and decay-time behaviors upon changes in both temperature (varied from 4 K to 100 K) and applied laser power (varied from 200 nW to 2 mW).

We will carefully discuss the assignment of these peaks to various excitons with respect to studies currently reported in literature [1].

[1] H. Najafov *et al.*, PRL **96**, 056604 (2006).

SYOE 8.45 Tue 18:00 Poster B

**Optical characterization of pentacene thin films by variable angle spectroscopic ellipsometry** — •ALEXANDER HINDERHOFER, UTE HEINEMEYER, STEFAN KOWARIK, ALEXANDER GERLACH, and FRANK SCHREIBER — Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen

Pentacene has been found to be a promising candidate for both field-effect transistors and photovoltaic diodes due to its high mobilities. Pentacene thin films grow in single-crystal grains and show high optical anisotropy with uniaxial symmetry. We use variable angle ellipsometry in transmission as well as in reflection on different substrates to determine the optical constants of the in-plane and the out-of-plane axes. The data analysis of such anisotropic systems is presented and the resulting optical constants are shown. Spectral features related to the vibronic progression and the different transitions (between 1.5-3eV) involved will be discussed. Furthermore, it is possible to take the spectra sufficiently fast to follow organic molecular beam deposition in real time at one fixed angle of incidence. Based on the post-growth results we analyze the real-time data and detect changes in the optical properties during growth.

SYOE 8.46 Tue 18:00 Poster B

**Optical Properties of Pentacene and Tetracene Thin-Films and Single Crystals** — •DANIEL FALTERMEIER<sup>1</sup>, BRUNO GOMPF<sup>1</sup>, MARTIN DRESSEL<sup>1</sup>, ASHUTOSH TRIPATHI<sup>2</sup>, and JENS PFLAUM<sup>2</sup> — <sup>1</sup>Physikalisches Institut, Universität Stuttgart, D-70550 Stuttgart — <sup>2</sup>Physikalisches Institut, Universität Stuttgart, D-70550 Stuttgart

Pentacene and tetracene are among the most promising organic semiconductors for future device applications due to their high hole mobilities at room temperature. But unlike their electrical properties, their optical behaviour is not well characterized and even the fundamental optical constants and their spatial anisotropy are not investigated to a sufficient degree. We present a systematic study by spectroscopic ellipsometry, AFM and x-ray diffraction on purified and highly ordered pentacene and tetracene films prepared under different conditions on Si/SiO<sub>2</sub>. The optical data are compared with measurements on single crystals grown by gas-phase sublimation technique. The results clearly show the influence of different structural polymorphs and of photo-oxidation processes on the optical properties. By comparison with the respective quinone-derivatives of pentacene and tetracene the reaction products can be identified by their optical response. Additionally the optical and structural results are correlated to temperature dependent mobility measurements.

SYOE 8.47 Tue 18:00 Poster B

**Novel Fullerene Derivatives for Polymer Solar Cells** — •JOACHIM A. RENZ<sup>1</sup>, JULIA M. MAYOROVA<sup>2</sup>, PAVEL A. TROSHIN<sup>2</sup>, SVETLANA M. PEREGUDOVA<sup>3</sup>, ALEXANDER S. PEREGUDOV<sup>3</sup>, RIMMA N. LYUBOVSKAYA<sup>2</sup>, GERHARD GOBSCH<sup>1</sup>, and HARALD HOPPE<sup>1</sup> — <sup>1</sup>Institute of Physics, Ilmenau Technical University, Weimarer Str. 32, 98693 Ilmenau, Germany — <sup>2</sup>Institute of Problems of Chemical Physics of RAS, Semenov pr. 1, Chernogolovka, Moscow Region, 142432, Russia — <sup>3</sup>A. N. Nesmeyanov Institute of Organoelement Compounds of RAS, Vavilova St. 28, B-334, Moscow, 119991, Russia

Several novel methanofullerenes have been synthesized. The molecular structures of these new C<sub>60</sub> derivatives resemble closely the structure of the up to date most successful fullerene, [6,6]-phenyl C<sub>61</sub>-butyric acid methyl ester (PCBM), which is applied in organic solar cells for more than 10 years. Polymer solar cells were produced by blending these novel fullerenes or PCBM with poly[3-hexylthiophene] (P3HT)

in bulk heterojunctions and characterized by standard methods like current-voltage characteristics and spectral photocurrent.

SYOE 8.48 Tue 18:00 Poster B

**Formation of metallic indium-phase from indium tin oxide-nanoparticles under reducing conditions and its influence on the electrical properties** — ●GERRIT GÜNTHER<sup>1</sup>, GABI SCHIERNING<sup>1</sup>, RALF THEISSMANN<sup>1</sup>, ROBERT KRUK<sup>1</sup>, CHARSTEN BÄHTZ<sup>2</sup>, and ROLAND SCHMECHEL<sup>1</sup> — <sup>1</sup>Institute of Nanotechnology, Forschungszentrum Karlsruhe, D-76021 Karlsruhe — <sup>2</sup>HASYLAB at DESY, D-22603 Hamburg

Tin doped indium oxide (ITO) acts as a transparent electrode in numerous organic electro-optical devices. Thin films of ITO-nanoparticles were heat-treated under reducing atmosphere. A significant improvement in conductivity of three orders of magnitude was hereby observed in the range between 350°C to 650°C, where no sintering took place, yet. This is a well known but little discussed fact for this electrode material thus motivating the investigation of ITO-nanoparticles in different gaseous atmospheres. In situ synchrotron-XRD experiments were conducted in argon-, oxygen- and hydrogen-gas at temperatures between 25°C and 450°C. Complementary ex situ susceptibility measurements were carried out with reduced samples which were kept under inert conditions after preparation. The results revealed the formation of a metallic indium-tin-phase even under weakly reducing conditions. This metallic phase is expected to have a crucial influence on the thin films electrical and optical properties. It most likely explains the drastic increase of conductivity in the temperature region between 350°C and 650°C.

SYOE 8.49 Tue 18:00 Poster B

**Influence of chamber pressure and deposition rate on structural properties and surface morphology of amorphous OVPD processed films** — ●PHENWISA NIYAMAKOM<sup>1</sup>, MARYAM BEIGMOHAMADI<sup>1</sup>, AZADEH FARAHZADI<sup>1</sup>, FRANK JESSEN<sup>2</sup>, HOLGER KALISCH<sup>2</sup>, ROLF JANSEN<sup>2</sup>, NICO MEYER<sup>3</sup>, DIETMAR KEIPER<sup>3</sup>, MARTIN KUNAT<sup>3</sup>, MICHAEL HEUKEN<sup>2,3</sup>, CHRISTIAN EFFERTZ<sup>1</sup>, PHILIP SCHULZ<sup>1</sup>, HOLGER SCHWAB<sup>4</sup>, THOMAS MICHELY<sup>1</sup>, and MATTHIAS WUTTIG<sup>1</sup> — <sup>1</sup>Institute of Physics (IA), RWTH Aachen University of Technology, 52056 Aachen, Germany — <sup>2</sup>Institute of Electromagnetic Theory, RWTH Aachen University of Technology, Kopernikusstr. 16, 52074 Aachen, Germany — <sup>3</sup>AIXTRON AG, Kackertstr. 15-17, 52072 Aachen, Germany — <sup>4</sup>Philips Technologie GmbH, Philipsstr. 8, 52066 Aachen, Germany

For Organic Light Emitting Devices (OLEDs), the absence of long-range order in amorphous films results in smooth surfaces and efficient radiative recombination, allowing for the realization of high performance organic optoelectronic devices. To tailor structure and morphology of these organic films, an understanding of the influence of deposition parameters, controlling film properties, is necessary. In this study, the Organic Vapor Phase Deposition (OVPD) was selected as the deposition technique. The influence of chamber pressure and deposition rate on  $\alpha$ -NPD films on Si substrates has been investigated by Atomic Force Microscopy and X-Ray Reflectometry. A remarkable dependence of film roughness on these parameters has been observed. Models to account for this behavior will be presented.

SYOE 8.50 Tue 18:00 Poster B

**Systematic studies on the morphology of OVPD processed films upon substrate temperature and deposition rate** — ●AZADEH FARAHZADI<sup>1</sup>, PHENWISA NIYAMAKOM<sup>1</sup>, MARYAM BEIGMOHAMADI<sup>1</sup>, CHRISTIAN EFFERTZ<sup>1</sup>, NICO MEYER<sup>2</sup>, DIETMAR KEIPER<sup>2</sup>, MICHAEL HEUKEN<sup>2,4</sup>, HOLGER SCHWAB<sup>3</sup>, MOHAMMAD REZA RAHIMI TABAR<sup>5,6</sup>, THOMAS MICHELY<sup>1</sup>, and MATTHIAS WUTTIG<sup>1</sup> — <sup>1</sup>Institute of Physics (IA), RWTH Aachen University of Technology, 52056 Aachen, Germany — <sup>2</sup>AIXTRON AG, Kackertstr. 15-17, 52072 Aachen, Germany — <sup>3</sup>Philips Technologie GmbH, Philipsstr. 8, 52066 Aachen, Germany — <sup>4</sup>Institute of Electromagnetic Theory, RWTH Aachen University of Technology, Kopernikusstr. 16, 52074 Aachen, Germany — <sup>5</sup>CNRS UMR 6529, Observatoire de la Côte d'Azur, BP 4229, 06304 Nice Cedex 4, France — <sup>6</sup>Department of physics, Sharif University of Technology, 11365-9161 Tehran, Iran

In order to tailor and modify thin film properties to be suitable for organic light emitting devices (OLED) it is necessary to study and understand the influence of deposition parameters on thin film growth. The chosen material is  $\alpha$ -NPD processed by organic vapor-phase deposition (OVPD). Film growth in OVPD is controlled by three independent parameters which are deposition rate, substrate temperature and

chamber pressure. Our study is focused on the influence of deposition rate and substrate temperature on the film morphology. A remarkable dependence of the film morphology upon deposition parameters has been observed. A detailed quantitative morphology analysis provides excellent description of the growth mechanism of OLED films.

SYOE 8.51 Tue 18:00 Poster B

**Phase separation in vacuum co-deposited pentacene/6,13-pentacenequinone thin films** — ●INGO SALZMANN<sup>1</sup>, RICARDA OPITZ<sup>1</sup>, SIEGFRIED ROGASCHESKI<sup>1</sup>, JÜRGEN RABE<sup>1</sup>, NORBERT KOCH<sup>1</sup>, and BERT NICKEL<sup>2</sup> — <sup>1</sup>Humboldt-Universität zu Berlin, Institut für Physik, Newtonstraße 15, D-12489 Berlin, Germany — <sup>2</sup>Ludwig-Maximilians-Universität, Department für Physik und CeNS, Geschwister-Scholl-Platz 1, D-80539 München, Germany

Pentacene (P) and 6,13-pentacenequinone (PQ) have been vacuum co-deposited onto SiO<sub>2</sub> in order to control phase separation in thin films for the application as bulk heterojunctions in organic photovoltaic devices. Structural investigations by means of scanning electron microscopy (SEM) and atomic force microscopy (AFM) revealed pronounced phase separation of the two materials at length scales that turned out to be tuneable by the variation of the deposition rate. X-ray diffraction (XRD) provided evidence for polymorphism in pure films of P and PQ on SiO<sub>2</sub>. While pure films exhibited both the bulk and thin film phase, the bulk phase is mainly suppressed within the co-deposited films (P+PQ). This was corroborated by Fourier-transform infrared spectroscopy (FT-IR) results. SEM investigations of pure and co-deposited films indicated that PQ bulk crystallites of up to 200nm height form continuous paths to the substrate and grow within a matrix formed of P and PQ thin film phases. The obtained heterojunction morphologies thus appear interesting for the application in organic-based photovoltaic cells.

SYOE 8.52 Tue 18:00 Poster B

**Utilization of pentacene as a photoactivator and an exciton transporter in organic solar cells** — ●ZIRUO HONG, BERT MAENIG, MARTIN PFEIFFER, and KARL LEO — Institut für Angewandte Photophysik, Technische Universität Dresden, Dresden, Germany

Power conversion efficiency ( $\eta_E$ ) of organic solar cells based on pentacene/C60 heterojunctions is mainly limited by open circuit voltage ( $V_{oc}$ ), although the extremely long exciton diffusion length (LD) of pentacene among organics is of advantage for solar cell applications.

In this work, pentacene/zinc phthalocyanine (ZnPc)/C60 multi-heterojunctions were introduced to increase  $V_{oc}$ . Here,  $V_{oc}$  is dominated by ZnPc/C60 interface. Excitons in pentacene layer diffuse into ZnPc layer via energy transfer, and contribute to photocurrent. Thus  $\eta_E$  was improved. According to quenching effect of ZnPc on luminescence from pentacene, exciton diffusion from pentacene to ZnPc was determined by efficiency of pentacene-to-ZnPc energy transfer, not LD.

Currently, we are seeking possibility of taking advantage of long LD and high hole mobility in pentacene films, to overcome two of critical shortcomings of organic solar cell materials, namely short LD and low charge carrier mobilities, by imbedding organic nanoclusters in pentacene films. The only role that the nanoclusters play pentacene matrix is as a sensitizer, i.e. transferring photon energy they absorb to pentacene, and the rest part of the photovoltaics is as same as pentacene based heterojunctions. Therefore, the limitation of short LD and low hole mobilities of some organic absorbers can be removed. The related experiment is being carried out.

SYOE 8.53 Tue 18:00 Poster B

**Efficient Platform for Characterisation and Data Analysis of Organic Solar Cells** — ●MORITZ K. RIEDE<sup>1,2</sup>, MARKUS GLATTHAAR<sup>1</sup>, MICHAEL NIGGEMANN<sup>1,2</sup>, KRISTIAN O. SYLVESTER-HVID<sup>2</sup>, TOBIAS ZIEGLER<sup>1</sup>, BIRGER ZIMMERMANN<sup>2</sup>, ANDREAS W. LIEHR<sup>2</sup>, ANDREAS GOMBERT<sup>1</sup>, and GERHARD WILLEKE<sup>1</sup> — <sup>1</sup>Fraunhofer Institute for Solar Energy Systems, Heidenhofstr. 2, 79110 Freiburg, Germany — <sup>2</sup>Material Research Center Freiburg, Stefan-Meier-Str. 21, 79104 Freiburg, Germany

Organic Solar Cells (OSCs) present a new and interesting approach to photovoltaic energy conversion with the prospects of low cost fabrication. Efficient dissociation of the photo-generated excitons and consequent charge collection is achieved by blending electron donor and acceptor materials. The resulting composite, called a „bulk-heterojunction“, acts as photovoltaic absorber. The currently most investigated donor:acceptor composite consists of the conjugated polymer poly(3-hexylthiophene) (P3HT) and the fullerene derivative 1-(3-methoxycarbonyl)-propyl-1-1-phenyl-(6,6)C<sub>61</sub> (PCBM).

The making of OSCs is a simple process but with many possible parameter variations, even for a fixed choice of donor:acceptor composite. To allow for a systematic and efficient analysis of how such production parameters influence the OSC performance, a robust and extensible platform for OSC fabrication and characterisation was developed. This platform enables both reliable data acquisition and efficient data management as well as mining of OSC data.

SYOE 8.54 Tue 18:00 Poster B

**Anticorrelation between exciplex emission and photovoltaic efficiency in PPV polymer based solar cells** — ●CHUNHONG YIN<sup>1</sup>, THOMAS KIETZKE<sup>1,2</sup>, DIETER NEHER<sup>1</sup>, and HANS-HEINRICH HÖRHOLD<sup>3</sup> — <sup>1</sup>University of Potsdam, Institute of Physics, Am Neuen Palais 10, 14469 Potsdam, Germany — <sup>2</sup>Institute of Materials Research and Engineering (IMRE), Research Link 3, 117602 Singapore — <sup>3</sup>University of Jena, Institute of Organic Chemistry and Macromolecular Chemistry, Humboldtstr. 10, 07743 Jena, Germany

By studying the photoluminescence emission and photovoltaic properties of blends of PPV-based electron donating and accepting polymers, we observed a strict anticorrelation between the relative exciplex emission in the solid state and the photovoltaic efficiency of corresponding blend devices. Thermal annealing led to a decrease in exciplex emission accompanied by an increase in photovoltaic efficiency. Comparative studies on defined bi-layer geometries bilayer devices did not show any influence on the annealing step. Consequently, we conclude that the photocurrent is mainly determined by the efficiency to form free carriers rather than by the transport and free carrier recombination.

SYOE 8.55 Tue 18:00 Poster B

**Electronic transport properties of self-assembled thin films of inorganic nanoparticles and polymers** — ●ROLF KNIPRATH and STEFAN KIRSTEIN — Institut für Physik, Humboldt Universität zu Berlin

We report on the electronic transport properties and the photovoltaic effect observed in composite thin films of nanoporous TiO<sub>2</sub> and hole-conducting polymers. These organic-inorganic heterojunction structures represent a hybrid of all-organic and inorganic dye-sensitized solar cell concepts. The nanoporous films of TiO<sub>2</sub> were grown on transparent conducting oxide substrates with a layer-by-layer self-assembly process using TiO<sub>2</sub> nanoparticles and served as electron conductors. By drop-casting polymer solutions on top we fabricated two types of heterojunction devices: For the first type, we applied a water-soluble thiophene polymer that acted as both a light absorber and a hole transport layer (HTL). For the second type we sensitized TiO<sub>2</sub> with strongly light absorbing CdTe nanoparticles and used the transparent polymer TFB as a HTL. I-V-measurements through Au back contacts under white light and in the dark yielded a diode characteristic with photovoltages of up to 0.8 V for both setups and photocurrent densities on the order of 1  $\mu\text{A}/\text{cm}^2$ .

SYOE 8.56 Tue 18:00 Poster B

**Serial Interconnection of Polymer Solar Cells: Design Rules towards Photovoltaic Modules** — ●BURHAN MUHSIN, JOACHIM RENZ, GERHARD GOBSCH, and HARALD HOPPE — Institute of Physics, Ilmenau Technical University, Weimarer Str. 32, 98693 Ilmenau, Germany

We have prepared relatively large area polymer solar cells and modules based on thin film blends of poly[3-hexylthiophene] / [6,6]-phenyl C61-butyric acid methyl ester (P3HT/PCBM). The size of each solar cell exceeds 5 cm<sup>2</sup>. By serial interconnection of the individual solar cells, we achieve multiples of the single cell open circuit voltage. Design rules for efficient serial interconnection are discussed.

SYOE 8.57 Tue 18:00 Poster B

**Hybrid Solar Cells based on Crystalline TiO<sub>2</sub> Nanoparticles** — ●BEATE REINHOLD<sup>1,2</sup>, MARKUS NIEDERBERGER<sup>1</sup>, DIETER NEHER<sup>2</sup>, and MARKUS ANTONIETTI<sup>1</sup> — <sup>1</sup>Max Planck Institute of Colloids and Interfaces, Colloid Department, Am Mühlenberg 1, 14476 Potsdam-Golm — <sup>2</sup>University of Potsdam, Institute of Physics, Am Neuen Palais 10, 14469 Potsdam, Germany

Using a nonaqueous route, crystalline TiO<sub>2</sub> nanoparticles with a diameter of ca. 5 nm were synthesized [1]. These nanoparticles were used as electron-transporting components in hybrid solar cells. Two device concepts were tested. In one case, the TiO<sub>2</sub> particles were blended together with the electron accepting polymer poly(p-phenylene vinylene). In the second case, the nanoparticles were coated on top of the

pure polymer to form a dense electron-transporting layer. The photovoltaic properties of the layers prepared with different TiO<sub>2</sub> content, layer thickness and annealing temperature are presented and discussed in relation to the optical properties.

[1] M. Niederberger, G. Garnweitner, F. Krumeich, R. Nesper, H. Cölfen, M. Antonietti, Chem. Mater. 16 (2004) 1202.

SYOE 8.58 Tue 18:00 Poster B

**Anticorrelation between exciplex emission and photovoltaic efficiency in PPV polymer based solar cells** — ●CHUNHONG YIN<sup>1</sup>, THOMAS KIETZKE<sup>1,2</sup>, DIETER NEHER<sup>1</sup>, and HANS-HEINRICH HÖRHOLD<sup>3</sup> — <sup>1</sup>University of Potsdam, Institute of Physics, Am Neuen Palais 10, 14469 Potsdam, Germany — <sup>2</sup>Institute of Materials Research and Engineering (IMRE), Research Link 3, 117602 Singapore — <sup>3</sup>University of Jena, Institute of Organic Chemistry and Macromolecular Chemistry, Humboldtstr. 10, 07743 Jena, Germany

By studying the photoluminescence emission and photovoltaic properties of blends of PPV-based electron donating and accepting polymers, we observed a strict anticorrelation between the relative exciplex emission in the solid state and the photovoltaic efficiency of corresponding blend devices. Thermal annealing led to a decrease in exciplex emission accompanied by an increase in photovoltaic efficiency. Comparative studies on defined bi-layer geometries bilayer devices did not show any influence on the annealing step. Consequently, we conclude that the photocurrent is mainly determined by the efficiency to form free carriers rather than by the transport and free carrier recombination.

SYOE 8.59 Tue 18:00 Poster B

**Dye sensitized solar cells based on novel bipolar spiro compounds** — CHERUBIN NOUMISSING SAO, KRISTIAN ONKEN, TOBAT P. I. SARAGI, and ●JOSEF SALBECK — Macromolecular Chemistry and Molecular Materials (mmCmm), Department of Science and Center for Interdisciplinary Nanostructure Science and Technology (CINSA<sup>T</sup>), University of Kassel, Heinrich-Plett-Strasse 40, 34109 Kassel, Germany

We report dye sensitized solar cells (DSSC) based on novel bipolar spiro compounds containing perylene and diphenylamino moiety. The corresponding compound has high extinction coefficient ( $\sim 10^5 \text{ M}^{-1} \text{ cm}^{-1}$ ) and, therefore, is a potential compound for DSSCs applications. After an ultraviolet treatment of the device, the short circuit current density increases from 0.04 mA cm<sup>-2</sup> to 0.10 mA cm<sup>-2</sup> especially with t-butyl ammonium ion containing cell. In contrast, no noticeable change in current density in device containing Lithium ion has been observed.

SYOE 8.60 Tue 18:00 Poster B

**Transparent conducting oxides deposited on plastic substrates and organic semiconductors** — ●PETR NOZAR<sup>1</sup>, LUCA MILANA<sup>2</sup>, RICCARDO LOTTI<sup>2</sup>, EUGENIO LUNEDI<sup>1</sup>, and CARLO TALIANI<sup>1,2</sup> — <sup>1</sup>Istituto per lo Studio dei Materiali Nanostrutturati, CNR, Via P. Gobetti, 101, 40129 Bologna, Italy — <sup>2</sup>Organic Spintronics, Srl, Via P. Gobetti, 101, 40129 Bologna, Italy

Transparent conducting oxides have been deposited successfully on plastic substrates and organic semiconductors by brand-new Pulsed Plasma Deposition (PPD) technique. This deposition method has been developed by Organic Spintronics, Srl. The deposition process is based on an ablation of an oxide target by pulsed electron and plasma beams. The physical and chemical properties of oxide layers deposited by PPD are superior to those obtained by PLD.

SYOE 8.61 Tue 18:00 Poster B

**Optical Simulation of Organic Solar Cells With ZnO:Al Optical Spacers** — ●VOLKER LORRMANN<sup>1,2</sup>, DANIEL RAUH<sup>1,2</sup>, CARSTEN DEIBEL<sup>2</sup>, VLADIMIR DYAKONOV<sup>1,2</sup>, and INGO RIEDEL<sup>1</sup> — <sup>1</sup>Div. Functional Materials for Energy Technology, ZAE Bayern e.V., Am Hubland, D97074 Würzburg, Germany — <sup>2</sup>Experimental Physics VI, Faculty of Physics and Astronomy, Julius-Maximilians University of Würzburg, Am Hubland, D97074 Würzburg, Germany

Organic bulk heterojunction solar cells are thin-film systems with reflecting metal electrode on the back. This configuration inhibits interference of incident and reflected light within the device causing a non-ideal absorption profile within the active layer. To adjust the intensity distribution to maximum absorption in the absorber film a new functional layer, so called optical spacer (OS), is included between the active layer and the metal electrode. For this approach, wide-gap materials like TiO<sub>x</sub> or ZnO:Al represent promising candidates because they are electron conducting, match the wanted positions of energy

bands and could be solution processed. Devices with nanoparticulate ZnO:Al optical spacer have been investigated by simulation of the electric field distribution throughout the device. We found optimized photocurrents for OS layer thicknesses < 120 nm, while being strongly depending on the active layer thickness. However, the maximum gain in absorption due to the OS is only small as compared to experimental results reported in the literature.

SYOE 8.62 Tue 18:00 Poster B

**Comparison of different anode materials in efficient small molecule organic solar cells** — ●KERSTIN SCHULZE<sup>1</sup>, BERT MÄNNIG<sup>1</sup>, MARTIN PFEIFFER<sup>1</sup>, KARL LEO<sup>1</sup>, YUTO TOMITA<sup>2</sup>, CHRISTIAN MAY<sup>2</sup>, EDUARD BRIER<sup>3</sup>, EGON REINOLD<sup>3</sup>, and PETER BÄUERLE<sup>3</sup> — <sup>1</sup>Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, 01069 Dresden, Germany, www.iapp.de — <sup>2</sup>Fraunhofer IPMS, Maria-Reiche-Straße 2, 01109 Dresden, Germany — <sup>3</sup>Abteilung Organische Chemie II, Universität Ulm, 89081 Ulm, Germany

We present efficient organic solar cells using two different transparent conductive oxides (TCOs) as anode material: Indium Tin Oxide (ITO) and Aluminium doped Zinc Oxide (ZAO). As shown by our group before photovoltaic devices using an oligothiophene derivative as donor and fullerene C60 as acceptor reach power efficiencies of up to 3.4 % [1]. In a similar way, organic solar cells using a new kind of this oligothiophene derivative and C60 with comparable power efficiencies will be presented in combination with different anode materials. The open-circuit voltage (Voc) of these heterojunction solar cells is defined by the Fermi-levels of the free charge carriers in the active materials. The influence of the workfunction of the TCO on the performance of the photovoltaic device will be presented. Additionally, the IV-curves of these solar cells depend on the kind of the oligothiophene derivative and this will be discussed on two oligothiophene types as well.

[1] K. Schulze, C. Urich, R. Schüppel, K. Leo, M. Pfeiffer, E. Brier, E. Reinold, P. Bäuerle, Adv. Mater. 18, 2872 (2006)

SYOE 8.63 Tue 18:00 Poster B

**Investigation of organic heterojunction solar cells by photo-induced absorption** — ●TONI MÜLLER, RICO SCHÜPPEL, BERT MÄNNIG, MICHAEL HOFFMANN, and KARL LEO — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden

Investigations on organic heterojunction solar cells have shown an increase of the open-circuit voltage when a spacer is inserted between the photoactive interface of an acceptor and a donor. To improve the understanding of these acceptor/spacer/donor-systems, we have investigated three of these systems. For all three systems, we find an increasing open-circuit voltage with increasing spacer thickness. As a first explanation this increase can be caused by an increased charge carrier density. To test this assumption the systems were analyzed by the means of photo-induced absorption spectroscopy (PIA).

N,N'-dimethylperylene-3,4:9,10-dicarboximide (MePTCDI) was used as absorbing acceptor material. For this material we found a charge carrier signal at a wavelength of 830nm of the probe light. With 4,4',4''-Tri(N-carbazolyl)triphenylamine (TCTA) as spacer material a decrease of the charge carrier density with increasing spacer thickness was found. We study and discuss a decrease of lifetimes and a decreased charge carrier generation due to smaller energy differences of the HOMO- and LUMO-levels as possible explanations for that behaviour.

SYOE 8.64 Tue 18:00 Poster B

**Infrared Light from organic light emitting diodes** — ●THOMAS ROSENOW, KARSTEN WALZER, and KARL LEO — Institut für Angewandte Photophysik, TU Dresden, D-01062 Dresden, Deutschland

Organic light emitting diodes for the visible part of the electromagnetic spectrum have recently achieved excellent performance and have stimulated work on devices emitting in the near infrared. We demonstrate such near-infrared organic light-emitting diodes (NIR-OLEDs) containing copper, palladium, and platinum phthalocyanine as emitting materials. These NIR-OLEDs exhibit electroluminescence at 1095 nm, 1025 nm and 966 nm. Low driving voltages are achieved by using electrically doped transport layers. A yellow singlet emitter serves as host for the emitting materials and improves the energy transfer to the emitter. Using this approach, the external quantum efficiency is increased up to 0.1 % at room-temperature. Furthermore, light-output at a voltage of 3 V and a current density of 20 mA/cm<sup>2</sup> are observed.

SYOE 8.65 Tue 18:00 Poster B

**Simulation of Phosphorescent Organic Light Emitting Diodes** — ●OLIVER WEISS<sup>1,2</sup>, FRYDERYK KOZŁOWSKI<sup>2</sup>, ARVID HUNZE<sup>2</sup>, and HEINZ VON SEGGERN<sup>1</sup> — <sup>1</sup>Department of Materials Science, Technical University of Darmstadt, Germany — <sup>2</sup>Siemens AG, CT MM 1, Günther-Scharowsky-Str. 1, 91058 Erlangen, Germany

Numerical Simulation has proven to be a valuable tool for the qualitative and quantitative description of fluorescent 3- and 4-layer OLED devices. Since actual high efficient SM-OLED stacks comprise of wide band gap host materials doped by phosphorescent guest molecules, the simulation model was extended to phosphorescence. The one-dimensional model differentiates between singlet and triplet states on host and guest molecules. Triplets on the host are formed by the recombination of free charges, triplets on the guest via transfer from the host, trap recombination and intersystem crossing from singlet states. Rate equations describe exciton diffusion as well as radiative decay, using different diffusion lengths and time constants for every guest material. Triplet-triplet annihilation and triplet-polaron quenching were implemented using rate equations published by M. Baldo. The results of simulating a simple high efficient phosphorescent OLED stack are presented in comparison to experimental data.

This work has been supported by the German Federal Ministry of Education and Research (BMBF) within the framework of the OPAL project.

SYOE 8.66 Tue 18:00 Poster B

**Materials and Structures for Future Organic Laser Diodes** — ●BODO WALLIKIEWITZ, MATTHIAS DE LA ROSA, DIRK HERTEL, and KLAUS MEERHOLZ — Universität zu Köln, Institut für Physikalische Chemie, Luxemburgerstr. 116, 50939 Köln

The performance of organic light emitting diodes (OLEDs) has made tremendous progress over the past decade, nevertheless the realization of organic laser diodes remains a challenge. To achieve lasing optical gain manifested by amplified spontaneous emission (ASE) is mandatory. We have investigated low ASE thresholds (5 uJ/cm<sup>2</sup>) and high gain (50 cm<sup>-1</sup>) of cross-linked conjugated copolymers. Crosslinkable materials can be structured to second order DFB gratings. Polymer lasers with the emitter and resonator made of the same material are investigated. The threshold of this polymer laser is 1.5 uJ/cm<sup>2</sup>. To realize an electrically driven laser it is necessary to confine the wave guided mode in the active layer in order to prevent losses induced by the metal contacts in the device. We obtained a low ASE threshold of 10 uJ/cm<sup>2</sup> in an electrical contactable device by using thick emitter, electron and hole transport layers (HTL). Film thickness and refractive index were optimized for each layer. OLEDs are characterized and the influence of thick multilayers on OLEDs performance is discussed. The efficiency decreases from 9 Cd/A for a standard 100nm OLED to 5 Cd/A for a 1 um multilayer OLED. The ratio of the edge to top emission intensity increases for a factor of 14 for the 1 um multilayer OLED. Current densities of 500 A/cm<sup>2</sup> are achieved for thick HTL and a mobility of 2x10<sup>-3</sup> cm<sup>2</sup>/Vs is extracted.

SYOE 8.67 Tue 18:00 Poster B

**Revealing the Dynamics in Polymer-based Optoelectronic Devices** — ●SEBASTIAN BANGE, ANDREW KUKSOV, and DIETER NEHER — Physik weicher Materie, Universität Potsdam, Am Neuen Palais 10, 14469 Potsdam, Germany

We report on measurements of charge carrier dynamics in polymer light-emitting diodes based on a new commercial blue polyfluorene-type copolymer. Investigations of charge carrier dynamics in thin-film devices face several difficulties due to experimental limitations when transit times reach the submicrosecond regime. For small-molecule devices, some elaborate methods have been reported to overcome limitations which heavily rely on multilayer structures.[1] Here, we report on the application of a new type of transient electroluminescence (TEL) method for the determination of electron dynamics relying on interlayer formation of spincoatable polymers. Detailed investigations show the relationship between our new method, standard TEL in thin film devices and time-of-flight (TOF) studies in thick layers. The role of injection barriers at the contacts is investigated, and the difference in trapping effects for TOF and TEL pointed out.

[1] R. A. Klenkler, G. Xu, H. Aziz et al., Appl Phys Lett 88 (24) (2006)

SYOE 8.68 Tue 18:00 Poster B

**Degradation of PVK-based electrophosphorescent devices** — ●ANDRIY KUKSOV, XIAOHUI YANG, and DIETER NEHER — University of Potsdam, Institute of Physics, Am Neuen Palais 10, 14469 Potsdam, Germany

Organic light-emitting diodes based on the hole-conducting polymer PVK blended with electron-transporting molecules and phosphorescent Iridium-complexes have recently been shown to exhibit high external quantum efficiencies and very good color stability [1]. Unfortunately, these diodes based on polymer blends degrade quite rapidly. Therefore, understanding the mechanisms of degradation is of high importance in the view of the commercialization of polymer-based OLEDs. It has been proposed that phase-separation of the individual components in the blend layers is the main origin of device degradation. By comparing the photoluminescence (PL) and electroluminescence (EL) of as-prepared and aged devices, we conclude that phase separation is not the determining factor. In contrast, the effect of ageing is clearly revealed in transient electroluminescence (TEL) experiments. This suggests that the rapid degradation of these blend devices is due to chemical rather than physical ageing.

SYOE 8.69 Tue 18:00 Poster B

**New electron acceptor material for organic hole transport materials** — ●RALF KRAUSE<sup>1,2</sup>, GÜNTER SCHMID<sup>2</sup>, STEFAN SEIDEL<sup>1,2</sup>, ARVID HUNZE<sup>2</sup>, and ALBRECHT WINNACKER<sup>1</sup> — <sup>1</sup>Department of Materials Science VI, University of Erlangen-Nuremberg, Germany — <sup>2</sup>Siemens AG, CT MM 1, Günther-Scharowsky-Str. 1, 91052 Erlangen, Germany

The injection and transport properties of organic materials are of fundamental interest to improve the understanding of small molecule OLEDs. In the past years it was shown that the use of electrically doped transport layers leads to devices with low driving voltages, which is essential to achieve high power efficiencies. We evaluated a p-doping material with an evaporation temperature lower than 300°C and investigated its properties in hole-only devices and OLEDs. N,N-di(naphthalen-2-yl)-N,N-diphenyl-benzidine (NPB), a commercial hole-transport material is used as matrix for this doping material. Both materials were coevaporated with different concentrations. The best possible concentration increases the conductivity more than 5 orders of magnitude compared with pure NPB. The transparency of the doped hole transport layer is much higher than for the commonly used organic dopants like 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ) due to its lower intensity charge transfer band.

SYOE 8.70 Tue 18:00 Poster B

**High efficient white Organic Light Emitting Diodes** — ●STEFAN SEIDEL<sup>1,2</sup>, RALF KRAUSE<sup>1,2</sup>, FRYDERYK KOZŁOWSKI<sup>2</sup>, GÜNTER SCHMID<sup>2</sup>, ARVID HUNZE<sup>2</sup>, and ALBRECHT WINNACKER<sup>1</sup> — <sup>1</sup>Department of Materials Science VI, University of Erlangen-Nuremberg, Germany — <sup>2</sup>Siemens AG, CT MM 1, Günther-Scharowsky-Str. 1, 91058 Erlangen, Germany

Due to the rapid progress in the last years the performance of organic light emitting diodes (OLEDs) has reached a level where general lighting presents a most interesting application target. We demonstrate, how the color coordinates of the emission spectrum can be adjusted using a combinatorial evaporation tool to lie on the desired black body curve representing cold and warm white, respectively. The evaluation includes phosphorescent and fluorescent dye approaches to optimize lifetime and efficiency, simultaneously. Detailed results are presented with respect to variation of layer thicknesses and dopant concentrations of each layer within the OLED stack. The most promising approach contains phosphorescent red and green dyes combined with a fluorescent blue one as blue phosphorescent dopants are not yet stable enough to achieve long lifetimes. This work has been supported by the German Federal Ministry of Education and Research (BMBF) within the framework of the OPAL project.

SYOE 8.71 Tue 18:00 Poster B

**Multimode spontaneous emission of optically confined organic photonic dots** — ●MAIK LANGNER, CLEMENS SCHRIEVER, ROBERT GEHLHAAR, HARTMUT FRÖB, VADIM G. LYSSENKO, and KARL LEO — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany, www.iapp.de

We report on the preparation and photoluminescence of photonic dots of the organic semiconductor tris-(8-hydroxyquinoline) aluminum (AlQ<sub>3</sub>). The organic material is thermally evaporated onto a distributed Bragg reflector (DBR) through a carbon film mask directly attached to the sample with micrometer sized holes. To obtain photonic dots with various lateral shapes and diameters between 1 and 5 μm, an additional DBR is grown on the top. The mirrors consisting of alternating SiO<sub>2</sub>- and TiO<sub>2</sub>-layers are produced by reactive electron-beam

evaporation and provide maximum reflectivities with  $R_{max} > 99.6\%$  enabling microcavities with high quality factors in vertical direction. Using a photoluminescence setup with micrometer lateral resolution, the spontaneous emission of the structured samples is studied after 407 nm cw laser excitation. This setup records the linear emission angle and polarization-dependent using a spectrometer-CCD combination. As a result of the three dimensional optical confinement, the emission spectra show a number of discrete modes with spectral separations dependent on the structural size. The experimental results are compared with different models based on numerical methods.

SYOE 8.72 Tue 18:00 Poster B

**Magneto-resistance in organic semiconductors** — ●ULRICH NIEDERMEIER<sup>1,2</sup>, MICHAEL VIETH<sup>1</sup>, WIEBKE SARFERT<sup>1</sup>, MANFRED RÜHRIG<sup>1</sup>, RALPH PÄTZOLD<sup>1</sup>, and HEINZ VON SEGGERN<sup>2</sup> — <sup>1</sup>Siemens AG, CT MM 1, Günther-Scharowsky-Str. 1, 91058 Erlangen, Germany — <sup>2</sup>TU Darmstadt, Department of Materials Science, Petersenstr. 23, 64287 Darmstadt, Germany

Organic semiconductors are promising materials for use in novel electronic devices such as organic light emitting diodes (OLEDs). Recently it has been demonstrated that the resistance of OLEDs changes in the presence of an external magnetic field [1]. The organic magneto-resistance (OMR) effect is isotropic regarding the direction of the magnetic field and can be observed at room temperature. Since the investigated structures do not contain any ferromagnetic materials the OMR is to be distinguished from the well-known giant magneto-resistance in spin-valve structures. We performed magneto-resistance measurements and electro-optical characterizations of various OLED structures. As a result we show the dependence of the OMR effect on both the magnitude of the magnetic field and the voltage applied to the OLEDs. Furthermore, we point out that the OMR effect can be influenced by varying the materials of the organic layers and the cathode.

[1] T. Francis, Ö. Mermer, G. Veeraraghavan, M. Wohlgenannt, New J. Phys. **6**, 185, 2004.

SYOE 8.73 Tue 18:00 Poster B

**Simulation of Light Extraction from OLEDs** — ●NILS A. REINKE, MICHAEL HUTZEL, CHRISTIAN BERGNER, STEFAN NOWY, and WOLFGANG BRÜTTING — University of Augsburg, Institute of Physics, Experimental Physics, Augsburg, Germany

Light extraction from organic light emitting devices is dominated by two optical effects, a) wide angle interference and b) multiple beam interference. In a) directly radiated light interferes with the reflection on the metallic electrode and leads to light emission, which is strongly dependent on the position of the emitting dipole layer. In b) light is reflected back and forth between two reflecting layers. In this study emission spectra were calculated by two different simulation techniques: a so-called dipole approach and an absorption model. For the former, radiant molecules are treated as oscillating dipole antennae. This classical approach allows calculating the far field radiation of these dipoles. The absorption model [1] presumes that the same pathway taken by the radiation from an external light source to couple into leaky modes is used by photons generated inside the organic multilayer structure to leave the device. The emission spectrum of an OLED is then given by the product of the spectral distribution of the generated photons times the probability of the photons to leave the device as leaky modes. The applicability of these two models was verified for two different types of OLEDs. The first type comprising one transparent electrode for which wide angle interference is dominant and the second including two reflective electrodes for which multiple beam interference is more important. [1] N. A. Reinke et. al, Opt. Comm, 2667 (2006) 191-197

SYOE 8.74 Tue 18:00 Poster B

**Charge transport and triplet quenching in conjugated polymers** — ●DIRK HERTEL and KLAUS MEERHOLZ — Institute of Physical Chemistry, University of Cologne, Luxemburger Str. 116, 50939 Cologne

According to spin statistics the formation of excited states in OLEDs from uncorrelated charge carriers yields 25% singlet and 75% triplet states, the latter do usually not contribute to electroluminescence. Little is known about triplet charge carrier (polaron) interaction in conjugated polymers. The quenching of triplets by polarons might play an important role for the degradation of OLEDs or for applications such as organic lasers, since triplets are accumulated in the device due to their long lifetime. The investigation of charge transport in a poly-



spirobifluorene with a hole transporting unit by current voltage characteristics as a function of temperature yields hole mobilities of 10-4 cm<sup>2</sup>/Vs for the SCLC regime. Comparison of the SCLC mobility with mobilities obtained by time of flight (ToF) measurements shows that in the SCLC regime the mobility is trap limited. The ToF mobility is temperature and electric field dependent. From combined experimental investigations of time resolved phosphorescence spectroscopy and charge transport studies we are able to show that triplet quenching is a significant loss mechanism. The test system is PtOEP doped the poly-spirobifluorene copolymer. The triplet polaron quenching constant is about 10-13 cm<sup>3</sup>/s. The influence of PtOEP concentration and film thickness on the quenching efficiency is discussed.

SYOE 8.75 Tue 18:00 Poster B

**Hole transport in solution processed multi layer devices** — ●ANGELES PITARCH, DIRK HERTEL, and KLAUS MEERHOLZ — Institut für Physikalische Chemie, Universität zu Köln, Luxemburgerstr. 116, 50939 Köln

Luminescent conjugated polymers are increasingly used as active components in optoelectronic devices such as light emitting diodes (LEDs). The most promising approach to achieve multiple layers for purely solution processed devices is the crosslinking of small molecules after deposition, which leads to insoluble layers. We have studied charge transport in unipolar devices by current voltage measurements and transient current experiments. Our hole transport layers (HTL) consist of triphenylene-diamine derivatives with different oxidation potential. This allows tuning of the energy level offset between the anode (ITO/PEDOT) work function and the highest occupied molecular orbital (HOMO) of the hole transport materials. The current voltage characteristics show a transition from injection limited conduction to space charge limited conduction (SCLC) for decreasing energy level offset. The occurrence of SCLC depends as well on temperature. We have carried out investigations of doping, induced upon crosslinking and processing conditions on current voltage characteristics of crosslinked HTLs. The results are indicative of charge transport governed by bulk effects. The hole mobility reaches values of 10<sup>-3</sup> cm<sup>2</sup>/Vs. Experimental data were fitted according to recent charge transport models taking into account trapping and a charge density dependent mobility, respectively.

SYOE 8.76 Tue 18:00 Poster B

**Thick Multilayer Devices for Potential Organic Laser Diodes** — ●BODO WALLIKIEWITZ, MATTHIAS DE LA ROSA, DIRK HERTEL, and KLAUS MEERHOLZ — Universität zu Köln, Institut für Physikalische Chemie, Luxemburgerstr. 116, 50939 Köln

The performance of organic light emitting diodes (OLEDs) has made tremendous progress over the past decade, nevertheless the realization of organic laser diodes remains a challenge. To achieve lasing optical gain manifested by amplified spontaneous emission (ASE) is mandatory. We have investigated low ASE thresholds (5 uJ/cm<sup>2</sup>) and high gain (50 cm<sup>-1</sup>) of cross-linked conjugated copolymers. Crosslinkable materials can be structured to second order DFB gratings. Polymer lasers with the emitter and resonator made of the same material are investigated. The threshold of this polymer laser is 1.5 uJ/cm<sup>2</sup>. To realize an electrically driven laser it is necessary to confine the wave guided mode in the active layer in order to prevent losses induced by the metal contacts in the device. We obtained a low ASE threshold of 10 uJ/cm<sup>2</sup> in an electrical contactable device by using thick emitter, 3electron and hole transport layers (HTL). Film thickness and refractive index were optimized for each layer. OLEDs are characterized and the influence of thick multilayers on OLEDs performance is discussed. The efficiency decreases from 9 Cd/A for a standard 100nm OLED to 5 Cd/A for a 1 um multilayer OLED. The ratio of the edge to top emission intensity increases for a factor of 14 for the 1 um multilayer OLED. Current densities of 500 A/cm<sup>2</sup> are achieved for thick HTL and a mobility of 2x10<sup>-3</sup> cm<sup>2</sup>/Vs is extracted.

SYOE 8.77 Tue 18:00 Poster B

**Inverted OLED based on RT Pulsed Plasma Deposition of IMO top-anode** — ●EUGENIO LUNEDI<sup>1</sup>, YIQIANG ZHAN<sup>1</sup>, VALENTIN DEDIU<sup>1</sup>, PETER NOZAR<sup>1</sup>, and CARLO TALIANI<sup>1,2</sup> — <sup>1</sup>ISMN - CNR — <sup>2</sup>Organic Spintronics s.r.l., Via Gobetti 101, 40129 Bologna, Italy

The advent of a new Room Temperature Pulsed Plasma Deposition (RT PPD) technique opens the possibility to integrate the use of Transparent Conducting Oxides (TCO) with soft materials (1). We applied PPD to create transparent and conducting electrodes on organic light emitting devices. Aim of the research is to develop inverted

(i.e. with reversed layer ordering) *top*-emitting diode structure with a transparent anode; traditional OLEDs use a transparent *bottom* electrode made of Indium Tin Oxide (ITO) on glass to let the emitted light exit from the device. Nevertheless, such a structure is not suitable to be directly integrated on the n-type FET-driven backplanes used as circuit in active-matrix OLED displays. The deposition of TCOs as top layer on sandwich of organics is crucial to fabricate efficient inverted OLEDs. Radio-frequency sputtering, up to now the process mostly used to create the top electrode, causes serious degradation of organics. We used RT PPD to deposit TCOs as IMO (Indium Molybdenum Oxide) and ZnO on vacuum-sublimed inverted devices (Al/AlQ3/NPB/IMO). These new materials offer flat surface, very high transparency (exceeding 90%) in VIS-IR and good hole injection properties (sheet resistance 40Ω/□). Experimental results show no damage of underlying organics arising from PPD and low turn-on voltages of devices.

(1) Organic Spintronics: Patent Pending (2006).

SYOE 8.78 Tue 18:00 Poster B

**Characterization of Large Area Organic Photodetectors on Flexible Substrates** — ●SANDRO TEDDE<sup>1</sup>, EDGAR ZAUS<sup>1</sup>, TOBIAS RAUCH<sup>1</sup>, JENS FÜRST<sup>1</sup>, and PAOLO LUGLI<sup>2</sup> — <sup>1</sup>Siemens AG, CT MM 1, Günther-Scharowsky-Str. 1, 91052 Erlangen — <sup>2</sup>TU München, Lehrstuhl für Nanoelektronik, Arcisstraße 21, 80333 München

Photodetectors realized by solution processable organic semiconductors offer the possibility to realize large area and low weight devices on flexible substrates with low cost production processes. We report on organic photodetectors, with areas up to 40mm<sup>2</sup>, processed on flexible multibarrier coated PET foils. A poly-3-hexyl-thiophene (P3HT):[6,6]-phenyl C61 butyric acid methyl ester (PCBM) blend, forming a bulk heterojunction represents the active light absorbing layer for visible light. A thin film encapsulation ensures protection of the device against oxygen and moisture and the maintenance of a good flexibility. Accelerated lifetime tests using a climatic chamber under different temperature and humidity conditions have been performed. By the use of ITO as bottom electrode and a semitransparent metallic top electrode it is possible to realize semitransparent devices for the visible spectral range. The effects on the current-voltage curves while curving the substrates will be additionally presented. For demonstration purpose a linear array of 14 large area photodetectors (40mm<sup>2</sup>) was produced, indicating the light response of each detector by an LED.

SYOE 8.79 Tue 18:00 Poster B

**Annealing Studies on Organic Photodetectors using Impedance Spectroscopy** — ●EDGAR ZAUS<sup>1</sup>, SANDRO TEDDE<sup>1</sup>, TOBIAS RAUCH<sup>1</sup>, JENS FÜRST<sup>1</sup>, and GOTTFRIED DÖHLER<sup>2</sup> — <sup>1</sup>Siemens AG, CT MM 1, Günther-Scharowsky-Str. 1, 91050 Erlangen — <sup>2</sup>Max Planck Research Group for Optics, Information and Photonics, University of Erlangen-Nürnberg, Günther-Scharowsky-Str. 1, 91052 Erlangen

Organic photo detectors offer various advantages over inorganic devices, e.g. large area imaging at low fabrication costs and the realization of the devices on flexible substrates. A poly-3-hexyl-thiophene (P3HT):[6,6]-phenyl C61 butyric acid methyl ester (PCBM) blend, forming a bulk heterojunction, is a widely used absorbing material due to its good exciton dissociation properties. Annealing of the device leads to a significant improvement of bulk heterojunction organic solar cells as reported in literature. We show that also the performance of organic photodetectors is influenced positively by thermal treatment. Results obtained from impedance spectroscopy measurements in addition to current-voltage characteristics and charge extraction by linearly increasing voltage (CELIV) measurements give insight into the annealing effects.

SYOE 8.80 Tue 18:00 Poster B

**Determination of charge carrier mobility in poly(3-hexylthiophene) with different current transient measurement techniques** — ●ANDREAS BAUMANN, CARSTEN DEIBEL, and VLADIMIR DYAKONOV — Experimental Physics VI, Physical Institute, Julius-Maximilians University of Würzburg, Am Hubland, D-97074 Würzburg, Germany

The carrier mobility in organic disordered materials, such as conjugated polymers, plays an important role in understanding the behaviour of organic electronic devices. We investigated the mobility of charge carriers in poly(3-hexylthiophene) (P3HT) using different current transient measurement methods. Besides the conventional transient photoconductivity experiment, time-of-flight (TOF), we used ex-

traction current transient techniques, such as charge carrier extraction by linearly increasing voltage (CELIV), probing equilibrium carriers instead. The field and temperature dependence of the mobility will be discussed in view of hopping transport in a Gaussian density of states distribution.

SYOE 8.81 Tue 18:00 Poster B

**Investigation of the non-linearity in Output Characteristics of Organic Field-Effect Transistors** — ●ANDREI HERASIMOVICH, SUSANNE SCHEINERT, and INGO HÖRSELMANN — TU Ilmenau, PF, 98684 Ilmenau, Germany

Organic field effect transistors (OFETs) have shown a promising potential for applications as active matrix displays and RFID. For such applications they must have good electrical characteristics, which not always can be reached. For instance, a nonlinearity takes place in output characteristics of OFETs at the small drain/source voltages. This non linearity was attributed in literature to contact problems or field dependent mobility [1,2].

We have prepared OFETs in top contact (TOC) and bottom contact (BOC) design with channel lengths more than  $25\mu\text{m}$ . The measured output characteristics show only a nonlinearity for the TOC-transistors. From our 2D-simulations result, the field dependence of the mobility is not the reason for such long channel devices. However, bulk traps in the polymer layer can cause the nonlinearity in the TOC-structure whereas in the BOC design only the drain current is strongly reduced.

[1] D.J. Gundlach, L. Zhou, J.A. Nichols, T.N. Jackson, P.V. Neclidov, M.S. Shur, *J. Appl. Phys.* 100, 024509 (2006).

[2] S. Cherian, C. Donley, D. Mathine, L. LaRussa, W. Xia, N. Armstrong, *J. Appl. Phys.* 96, 5638 (2004).

SYOE 8.82 Tue 18:00 Poster B

**Bipolaron Mechanism for Hysteresis in Organic Field-Effect Devices** — ●GERNOT PAASCH<sup>1</sup> and SUSANNE SCHEINERT<sup>2</sup> — <sup>1</sup>IFW Dresden, Germany — <sup>2</sup>TU Ilmenau, Germany

Hysteresis effects occur usually in organic field-effect transistors or MOS capacitors. The capacitance-voltage curves for the two sweep directions of the gate voltage differ essentially by different flat band voltages, or equivalently different interface charges. In contrast to statements in the literature, trap recharging does not lead to this type of hysteresis [1]. We show that formation and dissociation of bipolarons (BP) or polaron pairs (PP) can cause this hysteresis in MOS capacitors with conjugated polymers as organic semiconductor. For energetically favored BPs (PPs) sufficient amount of the accumulation charge can be transformed into BPs (PPs) during the sweep from depletion to accumulation and the subsequent waiting time. At the beginning of the reverse sweep, the dissociation is retarded and the BPs (PPs) remain for some time at the interface leading to the shifted flat band voltage. For a quantitative estimate of the relevant relaxation times we made use of the reaction rate for BP formation determined recently from bias stress experiments [2].

[1] Th. Lindner, G. Paasch, S. Scheinert, *J. Appl. Phys.* 98, 114505 (2005).

[2] A. Salleo, R. A. Street, *Phys. Rev. B* 70, 235324 (2004).

SYOE 8.83 Tue 18:00 Poster B

**Current Transport Mechanism in a Pentacene Diode with a Tunneling Contact revealed by Numerical Simulation** — ●THOMAS LINDNER<sup>1</sup>, GERNOT PAASCH<sup>1</sup>, CHRISTOF WÖLL<sup>2</sup>, LARS RUPPEL<sup>2</sup>, ALEXANDER BIRKNER<sup>2</sup>, GREGOR WITTE<sup>2</sup>, and CARSTEN BUSSE<sup>2</sup> — <sup>1</sup>IFW Dresden, Germany — <sup>2</sup>Ruhr-Universität Bochum

A diode-like device has been fabricated [1] by deposition of pentacene on a surface-modified, single-crystalline Au-substrate. The tip of an STM is used as a tunneling electrode. The current-voltage characteristics of this device reveal an asymmetry with respect to the polarity, depending on film thickness [1]. Numerical simulations allow to relate the onset of the current at positive sample bias (depending on pentacene film thickness) to n-conduction, in contrast to the commonly observed p-type for poly-crystalline pentacene. The origin of this peculiarity is that for low positive voltage the hole current injected from the substrate limits the electron tunneling from the tip to the pentacene layer. This small hole current results in an increasing voltage drop between tip and layer. Once this voltage drop compensates the electron barrier, direct tunneling of electrons into the pentacene LUMO leads to a steeply increasing electron current, which shifts with the pentacene layer thickness. In contrast, at negative sample bias direct tunneling of electrons into the LUMO does not occur. A steeply increasing hole

current is observed that is independent on pentacene film thickness.

[1] L. Ruppel, A. Birkner, G. Witte, C. Busse, T. Lindner, G. Paasch, Ch. Wöll, submitted.

SYOE 8.84 Tue 18:00 Poster B

**Localized charge transfer between a molecular acceptor and polymer donors** — KUE SURK PARK<sup>1</sup>, ●JÖRN-OLIVER VOGEL<sup>1</sup>, DESSISLAVA SAINOVA<sup>2</sup>, SILVIA JANIETZ<sup>2</sup>, JÜRGEN RABE<sup>1</sup>, and NORBERT KOCH<sup>1</sup> — <sup>1</sup>Institut für Physik, Humboldt Universität zu Berlin, Berlin — <sup>2</sup>Fraunhofer-Institute of Applied Polymer Research, Golm, Germany

The environmental stability of poly(3-hexylthiophene) (P3HT) can be significantly improved by incorporation of (1,4-dithienyl-2,3,5,6-tetrafluorobenzene) (TFT) units in the main chain, which leads to an increase of the average polymer ionization energy in thin films as measured by photoemission spectroscopy. P3HT and P3HT-TFT copolymers can be rendered highly conductive by "doping" with the electron acceptor tetrafluoro-tetracyanoquinodimethane (TCNQF4), i.e., the formation of molecule-polymer charge transfer complexes. As the average ionization energy of P3HT-TFT increases for increasing TFT concentration, a decrease in the charge transfer efficiency with TCNQF4 could be expected. However, our infrared absorption spectroscopy investigations on such charge transfer systems indicate that the charge transfer is independent of the TFT concentration within copolymers. This suggests that the molecule-polymer charge transfer is due to a highly localized interaction between TCNQF4 and conjugated thiophene units.

SYOE 8.85 Tue 18:00 Poster B

**Influence of contact effects on the performance of printed pentacene Thin Film Transistors** — ●AMARE BENOR and DIETMAR KNIPP — International University Bremen, School of Engineering and Science, 28759 Bremen, Germany

Micro Contact Printing ( $\mu\text{CP}$ ) of self-assembled monolayer (SAMs) in combination with selective surface wetting was used to realize pentacene thin film transistors (TFTs). The combination of  $\mu\text{CP}$  and selective wetting/dewetting provides a universal route to pattern a variety of different materials including polymers and metal films. In our study we used the SAMs of octadecyltrichlorosilane (OTS),  $\text{CH}_3(\text{CH}_2)_{17}\text{SiCl}_3$ , which was printed on cleaned silicon or glass substrate. The printed monolayer leads to the formation of hydrophilic and hydrophobic regions, which facilitates the selective deposition of polymers or resists like Poly (methyl methacrylate), PMMA, on the hydrophilic regions. Following the selective deposition of a resist, a lift-off process was used to pattern gold and titanium metal thin films. This technique was applied to realize radio frequency (RF) coils and electrodes for pentacene TFTs. The techniques allows for patterning of electrodes down to  $2\mu\text{m}$ . Transistors fabricated by this approach exhibit charge carrier mobilities of  $0.2\text{-}0.4\text{ cm}^2/\text{Vs}$  and on/off ratios of  $10^6$ . The influence of the printed process on contact resistance of the TFTs, charge carrier mobility and the threshold voltage will be discussed. Finally, the electrical characteristic of pentacene TFTs prepared by printing will be compared with transistors prepared by conventional optical lithography.

SYOE 8.86 Tue 18:00 Poster B

**Frequency response of transconductance on OFETs with different source/drain contacts** — ●INGO HÖRSELMANN, ANDREI HERASIMOVICH, and SUSANNE SCHEINERT — TU Ilmenau, PF, 98684 Ilmenau, Germany

We prepared organic field effect transistors with spin coated TPD(4M)-MEH-PPV as semiconductor material. Silanized silicon dioxide was used as gate insulator. The source and drain contacts were implemented in bottom contact (BOC) and top contact (TOC) design with different contact materials evaporated through a shadow mask.

The two transistor designs were investigated by static measurements. Only TOC structure transistors show a nonlinearity in the output characteristic at low drain voltages. Additional we measured the frequency response of the transconductance at different gate voltages in linear and saturation regime. In case of top contact structures the transconductance shows in the linear transistor regime an additional phase shift above the cut-off frequency. This phase shift was caused by the frequency dependency of gate-drain capacitance.

We compare the measurement results with two dimensional device simulations. The nonlinearity in the output characteristic and the phase shift in the transconductance can be caused by trap states and anisotropic mobility.

SYOE 8.87 Tue 18:00 Poster B

**Nanoscale Organic Field-effect Transistors based on P3HT with switching frequencies above one Megahertz** — ●ARNE HOPPE<sup>1</sup>, PAUL WÖBKENBERG<sup>2</sup>, JÖRG SEEKAMP<sup>1</sup>, and VEIT WAGNER<sup>1</sup> — <sup>1</sup>School of Engineering and Science, International University Bremen, Campus Ring 8, 28759 Bremen, Germany — <sup>2</sup>present address: Imperial College London, UK

Switching speed is crucial for many applications in organic electronics. Therefore the improvement of the dynamic properties of organic field effect transistors (OFETs) is a mayor demand. The possibility to achieve higher frequency regimes will enable new fields of applications. We demonstrate high frequency organic thin film transistors based on high-mobility regio-regular poly(3-hexylthiophene) (r,r'-P3HT) as active material and silicon oxide as gate dielectric. Transistors built by e-beam lithography with sub-micron channel lengths and gold contacts in bottom configuration show unity-gain bandwidth beyond 1 MHz in air at low supply voltages of 10 V. For channel lengths L below 500 nm deviations from ideal L scaling law are observed experimentally, which are attributed to contact effects. We present a model beyond the ideal scaling law to predict the maximum operational frequency which is based on transistor parameters, geometry and contact resistance. Further deviations of measured transfer frequencies with respect to the expected values are discussed in terms of the organic material properties and interfaces to the gate isolator and electrodes.

SYOE 8.88 Tue 18:00 Poster B

**Organic field effect transistors with rubrene** — ●THOMAS DIEKMANN, SORAJA BONDI-FERNANDEZ, and ULRICH HILLERINGMANN — University of Paderborn, Department of Electrical Engineering EIM-E, 33098 Paderborn

While much research work is focused on the deposition of organic materials like *small molecules* by thermal evaporation in high vacuum this work shows results of a deposition process at backing pressure in inert gas atmosphere. First transistors are built on a silicon substrate which serves at the same time as common gate electrode. For gate dielectric thermally grown silicon dioxide is used with a layer thickness of 138 nm. Drain and source electrodes of gold are structured by UV-lithography and lift-off. At backing pressure in inert gas atmosphere small crystals of rubrene could be introduced into the transistor channel. In this way organic field effect transistors are fabricated that can drive a drain source current of about  $-44\mu\text{A}$  @  $V_{GS} = V_{DS} = -40\text{ V}$ .

SYOE 8.89 Tue 18:00 Poster B

**Temperature and Gate-Voltage Dependent Field Effect Mobility of the Conjugated Polymer Poly(3-Hexyl Thiophene)** — ●MARIA HAMMER<sup>1</sup>, JULIA SCHAFFERHANS<sup>1</sup>, INGO RIEDEL<sup>2</sup>, CARSTEN DEIBEL<sup>1</sup>, and VLADIMIR DYAKONOV<sup>1,2</sup> — <sup>1</sup>Experimental Physics VI, Physical Institute, Julius-Maximilians- — <sup>2</sup>Div. Functional Materials for Energy Technology, ZAE Bayern e.V., Am Hubland, 97074 Würzburg, Germany

We investigated the field effect mobility of regio-regular poly(3-hexyl thiophene), in dependence of temperature and charge carrier concentration in field effect transistors. The influence of the contact resistance at room temperature is studied: Only for channels above 80 micron length does the contact resistance become negligible, therefore showing the intrinsic field-effect mobility. Consequently, we present temperature dependent measurements for a long channel transistor. The data will be discussed in view of models for charge carrier mobility in disordered organic materials, in particular the parametric description by Pasveer et al [1].

[1] W. F. Pasveer et al., Phys. Rev. Lett. 94 (2005) 206601.

SYOE 8.90 Tue 18:00 Poster B

**Tuning the threshold voltage of organic field-effect transistors by an electret encapsulating layer** — MICHAEL SCHARNBERG<sup>1</sup>, VLADIMIR ZAPOROJTCHEKOV<sup>1</sup>, ●RAINER ADELUNG<sup>1</sup>, FRANZ FAUPEL<sup>1</sup>, CHRISTOPH PANNEMANN<sup>2</sup>, THOMAS DIEKMANN<sup>2</sup>, and ULRICH HILLERINGMANN<sup>2</sup> — <sup>1</sup>for Multicomponent Materials, Technical Faculty, University of Kiel, Germany — <sup>2</sup>Department EIM-E, Sensor Technology, University of Paderborn, Germany

High threshold voltages are a major problem for the realization of organic field effect transistors (OFETs). It was shown, that dual-gate FET structures allow to shift the threshold voltage. Here, we present a technique to adjust the threshold voltage of an OFET using a design similar to a dual-gate structure with an insulating Teflon-based electret layer as a second gate. The threshold voltage of a pentacene

bottom gate OFET was shifted from +13.1 V to -2.3 V by deposition of a 1.7  $\mu\text{m}$  thick electret layer proving the principal feasibility of this approach [1].

[1] M. Scharnberg, V.Zaporojtchenko, R. Adelung, F. Faupel, T. Diekmann, C. Pannemann, and U. Hilleringmann, Appl. Phys. Lett. 90 (2007) in press

SYOE 8.91 Tue 18:00 Poster B

**Organische Feldeffekttransistoren auf flexiblen Substraten** — ●STEFAN RICHTER<sup>1</sup>, MATTHIAS PLÖTNER<sup>1</sup>, WOLF-JOACHIM FISCHER<sup>1</sup>, XUAN-DUNG DANG<sup>2</sup> und WALDFRIED PLIETH<sup>2</sup> — <sup>1</sup>Technische Universität Dresden, Institut für Halbleiter- und Mikrosystemtechnik, 01062 Dresden — <sup>2</sup>Technische Universität Dresden, Institut für Physikalische Chemie und Elektrochemie, 01062 Dresden

Ziel der Arbeiten ist der Aufbau organischer Feldeffekttransistoren (OFETs) auf flexiblen Unterlagen mit kostengünstigen Techniken. Schwerpunkte sind die Entwicklung und Präparation geeigneter Referenzsubstrate zur Charakterisierung der organischen Halbleiter, ihre Strukturierung und Kontaktierung sowie die Gesamttechnologieentwicklung auf flexiblen Substraten. Im Ergebnis werden OFETs vorgestellt, die in Gate-unten-Anordnung auf Polymerfolien mit Al-Metallisierung aufgebaut werden. Diese dient als Gate-Elektrode und wird an der Oberfläche anodisch zu einem dünnen hoch-DK-Dielektrikum ( $\epsilon_r = 8..12$ ) oxidiert. Aus der großen Gatekapazität resultieren kleine Steuerspannungen. Das Oxid zeichnet sich zudem durch einen hohen spezifischen Widerstand ( $\rho = 1..2 * 10^{14} \Omega\text{cm}$ ) und große Durchbruchfestigkeit aus ( $E_{BD} = 6..8\text{ MV/cm}$ ). Als Source- und Drain-Elektroden dienen Goldstrukturen. Organische Halbleiterfilme aus Thiophenderivaten werden aus Lösung entweder ganzflächig durch Schleudern oder strukturiert durch Tintenstrahl Druck aufgebracht. Die mit Tintenstrahl Druck erzeugten Bauelemente weisen gegenüber den ganzflächig beschichteten deutlich verringerte Leckströme auf und erreichen Feldeffektbeweglichkeiten von bis zu  $2 * 10^{-3} \text{ cm}^2/\text{Vs}$ .

SYOE 8.92 Tue 18:00 Poster B

**Organic Thin Film Transistor Based Sensors with Chemically Reactive Interfacial Layers** — ●PETER PACHER<sup>1</sup>, A. LEX<sup>2</sup>, V. PROSCHEK<sup>1</sup>, O. WERZER<sup>1</sup>, P. FRANK<sup>1</sup>, S. TEMMEL<sup>2</sup>, E. TCHERNYCHOVA<sup>3</sup>, M. SZEZEN<sup>3</sup>, G. HLAWACEK<sup>4</sup>, Q. SHEN<sup>4</sup>, C. TEICHERT<sup>4</sup>, W. GROGGER<sup>3</sup>, R. RESEL<sup>1</sup>, R. SCHENNACH<sup>1</sup>, A. WINKLER<sup>1</sup>, C. SLUGOVIC<sup>2</sup>, G. TRIMMEL<sup>2</sup>, and E. ZOJER<sup>1</sup> — <sup>1</sup>Institute of Solid State Physics, TU Graz, 8010 Graz, Austria — <sup>2</sup>Institute for Chemistry and Technology of Organic Materials, TU Graz — <sup>3</sup>FELMI-ZFE, TU Graz — <sup>4</sup>Institute of Physics, MU Leoben, 8700 Leoben, Austria

We discuss the influence of reactive thin layers on the device performance of P3HT based organic thin film transistors (OTFTs). The CSTS layer (2-(4-Chlorosulfonylphenyl)-ethyltrichlorosilane) is characterized by XRR thickness measurements. Reflection absorption infrared spectroscopy (RAIRS) is used to study the chemical reaction of CSTS with ammonia gas (NH<sub>3</sub>). Density functional theory calculations are presented to explain the origin of the observed peaks and peak shifts of the RAIRS spectra and are in good agreement with our experimental data. XPS studies on samples before and after NH<sub>3</sub> exposure are a further proof for the proposed reaction to happen.

Particular attention is paid to how such thin films can be used as sensitizers. We find that the turn on voltage shifts from large positive values to negative values.

We believe that this novel sensor concept can open new routes for the design and the optimization in the field of organic sensors.

SYOE 8.93 Tue 18:00 Poster B

**Hysteresis in Bio-Organic Field-Effect Transistors** — ●STADLER PHILIPP<sup>1</sup>, BIRENDRA SINGH<sup>1</sup>, REINHARD SCHWOEDIAUER<sup>2</sup>, SIEGFRIED BAUER<sup>2</sup>, JAMES GROTE<sup>3</sup>, and SERDAR SARICITCI<sup>1</sup> — <sup>1</sup>LIOS Altenbergerstr. 69., 4040 Linz, Austria — <sup>2</sup>SOMAP Altenbergerstr. 69., 4040 Linz, Austria — <sup>3</sup>AFRL/MLPS, Wright-Patterson Air Force Base, Ohio USA

In organic field effect transistors (OFETs) the gate dielectric plays a crucial role - highly insulating thin film polymer layers are key-components in state of the art organic transistor devices. When replacing the polymer layer by introducing solution-processed thin film surfactant-modified biopolymer Desoxyribonucleic Acid (DNA) as gate dielectric [1], transistor-characteristics are changed towards remanence-like hysteresis behaviours. The hysteresis-loops probed in bio-organic field effect transistors (BiOFETs) derived from DNA and fullerene derivatives form bistable states which can be used for

memory devices at low operating voltage regime compared to similar organic thin film transistors using polymers as gate insulator. Bulk-interface interactions have been reported in various space-charge electrets without ferroelectric-like properties and - in the case of DNA - are probed with sandwich devices of pristine biopolymer (Metal-Insulator-Metal) as well as sandwich devices with biopolymer and semiconducting fullerene derivative (Metal-Insulator-Semiconductor-Metal) and bottom gate top electrode OFET devices itself. [1] T. B. Singh et al., Appl. Phys. Lett. 85, 5409 (2004).

SYOE 8.94 Tue 18:00 Poster B

**Polyvinylalcohol Dielectrics in Metal-Insulator-Metal, Metal-Insulator-Semiconductor and Organic Field Effect Transistor Structures** — ●MARTIN EGGINGER<sup>1</sup>, MIHAI IRIMIA-VLADU<sup>2</sup>, REINHARD SCHWÖDIAUER<sup>2</sup>, ANDREAS TANDA<sup>3</sup>, SIEGFRIED BAUER<sup>2</sup>, and N. SERDAR SARICIFTCI<sup>1</sup> — <sup>1</sup>LIOS, JK University Linz, Altenbergerstr. 69, 4040 Linz, Austria — <sup>2</sup>Soft Matter Physics, JK University Linz, Altenbergerstr. 69, 4040 Linz, Austria — <sup>3</sup>plastic electronic GmbH, Rappesederweg 28, 4040 Linz, Austria

Hysteresis is a well known phenomenon in the electrical characteristics of organic field effect transistors (OFETs) using polyvinylalcohol (PVA) as dielectric material. It was already proposed that mobile ionic impurities in the PVA might be the reason for the observed hysteresis effect. A side-product of PVA is sodium acetate (NaAc). Further cleaning the received PVA by dialysis, significantly removed NaAc in the as received PVA. In order to study the influence of the NaAc ions on the properties of PVA, measurements were performed with metal-insulator-metal (MIM), metal-insulator-semiconductor (MIS) and OFET structures with C60 as semiconductor. Comparing the transfer characteristic curves of OFETs using the \*as received\* PVA with the dialysis grade PVA shows a dramatic decrease of the hysteresis. With intentionally added impurities of NaAc into the dialysis grade PVA the hysteresis is observed again and is even enlarged. Measurements on OFETs correlate well with dielectric spectroscopy results on MIM and MIS structures, thereby demonstrating that hysteresis in PVA based OFETs is caused by ionic impurities.

SYOE 8.95 Tue 18:00 Poster B

**Influence of dielectric surface modification on perylene thin-film properties and OTFT performance** — ●CHRISTIAN EFFERTZ, MARYAM BEIGMOHAMADI, PHENWISA NIYAMAKOM, AZADEH FARAHZADI, PHILIP SCHULZ, and MATTHIAS WUTTIG — Institute of Physics (IA), RWTH Aachen University of Technology, 52056 Aachen, Germany

Organic Thin-Film Transistors (OTFTs) are promising for electronic application, e.g. as an active matrix for flexible displays. It has been suggested that some organic materials, such as perylene, show a high field-effect mobility, comparable to hydrogenated amorphous silicon (a-Si:H). Since the properties of the organic thin film have a major influence on the field-effect mobility, an understanding of the influence of structural properties and morphology on device efficiency is necessary.

In this study, perylene-based OTFTs have been investigated employing two different dielectric layers,  $\text{SiO}_2$  and  $\text{Al}_2\text{O}_3$  on top of highly doped silicon substrates, which were used as the gate contact. Thermally evaporated gold pads acted as the contacts for the source and drain of the devices. Subsequently the influence of surface modification of the dielectric layer, e.g. surface treatment by UV-ozone or self-assembled monolayers of octadecyltrichlorosilane (OTS), on film properties and device efficiency has been studied. Different characterization techniques, including the atomic force microscopy (AFM) for surface morphology, x-ray diffractometry (XRD) for structural analysis and drop shape analysis for determination of surface free energy, have been employed in this investigation.

SYOE 8.96 Tue 18:00 Poster B

**Charge transport in C<sub>60</sub>/CuPc donor-acceptor blends** — MARKUS BRONNER, ●ANDREAS OPITZ, and WOLFGANG BRÜTTING — Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

In recent years, large progress has been made in the realization of electronic circuits based on organic field-effect transistors (OFETs). However, these circuits as being built-up of unipolar (mostly p-type) OFETs only, have a number of drawbacks. To overcome them, recently, ambipolar OFETs have been suggested as a first step towards complementary organic circuits.

In this work we are analysing the ambipolar charge transport in blend systems of small organic molecules. These mixed layers are prepared by co-evaporation of n-conducting fullerene (C<sub>60</sub>) and

p-conducting copper-phthalocyanine (CuPc) on pre-structured TFT-substrates. It was found that the electrical characteristics (e.g. mobilities of holes and electrons and threshold voltages) depend strongly on the composition of the blend and on the preparation conditions like substrate treatment and substrate temperature during evaporation. The film structure and the morphology were analysed by X-ray diffraction and scanning force microscopy.

SYOE 8.97 Tue 18:00 Poster B

**Electrical and morphological characterization of sub-micrometer organic transistors** — ●F. ANTE<sup>1</sup>, S. ISSING<sup>1</sup>, J. GEURTS<sup>1</sup>, G. SCHMIDT<sup>1</sup>, L.W. MOLENKAMP<sup>1</sup>, N.S. OXTOBY<sup>2</sup>, M. MAS-TORRENT<sup>2</sup>, N. CRIVILLERS<sup>2</sup>, J. VECIANA<sup>2</sup>, and C. ROVIRA<sup>2</sup> — <sup>1</sup>Universität Würzburg, Physikalisches Institut (EP3), Am Hubland, D-97074 Würzburg, Germany — <sup>2</sup>Institut de Ciencia de Materials de Barcelona (CSIC), Campus UAB, 08193 Cerdanyola, Spain

We report on electrical and morphological characterization studies of tetrathiafulvalene (TTF) derivatives for sub-micron organic thin film transistors (OTFTs). The electrical properties of the vacuum deposited materials on highly n-doped silicon wafers with thermally grown  $\text{SiO}_2$  were measured in bottom contact geometry with e-gun evaporated metal contacts. The channel length was varied from 20  $\mu\text{m}$  to 0.5  $\mu\text{m}$  for 50 nm thick oxide using optical lithography. Smaller devices with channel length from 1000 nm to 80 nm were fabricated on 10 nm thick oxide with electron beam lithography. We present typical output and transfer characteristics for long and short channel devices and analyzed their scaling behaviour. Charge carrier mobilities above  $10^{-2} \text{ cm}^2/\text{Vs}$  were extracted. In situ studies during growth indicate an increase of mobility with thickness over the investigated range. From this result and from an AFM analysis we conclude 3D crystalline growth. Furthermore we give a correlation between grain sizes and device performance. We acknowledge support by the EU Integrated Project NAIMO (No NMP4-CT-2004-500355), DGI Spain (CTQ2006-06333/BQU) and CIRIT (2005SGR-005951).

SYOE 8.98 Tue 18:00 Poster B

**Organic field effect transistors for spin polarised transport - concept and recent advances** — ●MARKUS MICHELFEIT, JEAN GEURTS, GEORG SCHMIDT, and LAURENS W. MOLENKAMP — Uni Würzburg, Experimentelle Physik III, Am Hubland, 97074 Würzburg

The investigations of spin electronics and organic electronics have been constantly increasing in the last years. Our concept of an organic field-effect transistor (OFET) for spin-polarised transport combines the goals of these two fields of research. Thus the possibility of spin polarised transport would add a new degree of freedom to the conventional charge based transistor. Due to long spin relaxation times ( $\approx 1\mu\text{s}$ ) organic semiconductors are promising as active materials in such devices. We designed interdigitated source and drain stripe contacts made of CoFeB on a highly doped silicon wafer with a thermally grown  $\text{SiO}_2$ -layer, serving as gate electrode and isolator, respectively. The channel resistance should strongly depend on the state of magnetisation of the source and drain stripes: low resistance for parallel and high resistance for antiparallel magnetisation. For stripe widths of 0.5 and 2  $\mu\text{m}$ , respectively, stable states of parallel or antiparallel magnetisation were achieved by varying the external B-field, exploiting the width-dependence of their coercive field  $H_c$ . At 300K SQUID results show  $H_c = 2.4$  and 12 kA/m respectively. The next challenge is the tuning of contact impedance, which is a crucial factor for an ideal spin injection from the ferromagnetic contacts into the organic semiconductor. This work is funded by the DFG Schwerpunktprogramm 1121 on OFETs.

SYOE 8.99 Tue 18:00 Poster B

**Instabilities and Dynamic Behavior of the Potential Distribution in Organic FETs** — ●CHRISTOPHER SIOL, NIELS BENSON, CHRISTIAN MELZER, and HEINZ VON SEGGERN — Electronic Materials Department, Institute of Materials Science, Darmstadt University of Technology, Petersenstr. 23, 64287 Darmstadt, Germany

Kelvin probe force microscopy (KPFM) has recently been used to investigate lateral surface potential distributions in the channel of organic field effect transistors (OFETs). This methodology offers a microscopic view on electronic mechanisms in the transistor beyond the macroscopic information of output and transfer characteristics. In this work, frequency modulated KPFM under ultra high vacuum conditions is used to measure the surface potential distributions between source and drain of top and bottom contact pentacene OFETs. The electric force is detected by measuring the frequency modulation of the can-

tilever oscillation, allowing high lateral resolution. In particular, the instabilities of OFET characteristics during constant electrical stress are compared to the changes in the potential distribution. Additionally, the dynamic response of the surface potential on a time-dependent operation will be correlated with the overall temporal change in the current.

SYOE 8.100 Tue 18:00 Poster B

**Photodegradation of P3HT thin films under various ambient conditions** — ●RAPHAEL GUTBROD<sup>1</sup>, HANS-JOACHIM EGELHAAF<sup>1,2</sup>, HEIKO PEISERT<sup>1</sup>, and THOMAS CHASSÉ<sup>1</sup> — <sup>1</sup>University of Tübingen, IPTC, Auf der Morgenstelle 8, D-72076 Tübingen, Germany — <sup>2</sup>Christian-Doppler-Lab for Surface-Optical Methods, Konarka Austria GmbH, Altenberger Str. 69, A-4040 Linz, Austria

Poly-3-hexylthiophene (P3HT) is one of the most promising semiconducting materials for applications in organic field effect transistors (OFET). To improve the device performance, it is necessary to control the film morphology, its structure and the interface between insulator and active layer. An important parameter in terms of commercial use is the device lifetime. It is known, that photodegradation of P3HT in air reduces its semiconducting properties and thus the lifetime. Therefore, exact understanding of this process is important for further device optimization. The photooxidation of spin-coated P3HT thin films under various ambient conditions was studied using UV/Vis spectroscopy and the resulting oxidation products were characterized by X-ray photoelectron spectroscopy (XPS). We observed an increased oxidation time in presence of water. Furthermore, an influence of different substrates on the phenomenon was noticed. An insulator as top coating layer increases the oxidation time of the P3HT thin film as it works as diffusion barrier for oxygen and water. To understand the process on a molecular point of view, a possible reaction mechanism for the photodegradation is discussed.

SYOE 8.101 Tue 18:00 Poster B

**Organic FETs with high- $\kappa$  dielectric** — ●FLORIAN ROTH, KERSTIN KELLER, and MICHAEL HUTH — University Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt am Main

Organic thin films of small molecules such as CuPc or BEDT-TTF (ET) were grown by organic molecular beam deposition. Using an in-situ shadow mask technique field effect transistors in the inverted MISFET structure were prepared. To investigate their electronic properties for charge carrier densities up to  $10^{13} \text{ cm}^{-2}$  in the active layer a high- $\kappa$  dielectric layer was employed. In this context  $\text{SrTiO}_3$  layers were grown by rf-sputtering and characterized by x-ray diffraction. Furthermore, their temperature dependent dielectric properties were determined.

SYOE 8.102 Tue 18:00 Poster B

**Effects of capping on the thermal and long-term stability of organic thin film transistors** — ●STEPHAN MEYER<sup>1</sup>, STEFAN SELLNER<sup>2</sup>, GERHARD ULBRICHT<sup>2</sup>, FRANK SCHREIBER<sup>2</sup>, HELMUT DOSCH<sup>2</sup>, MATTHIAS FISCHER<sup>1</sup>, BRUNO GOMPF<sup>1</sup>, and JENS PFLAUM<sup>1</sup> — <sup>1</sup>Physikalische Institute, Universität Stuttgart — <sup>2</sup>MPI Stuttgart

The thermal robustness of organic semiconducting layers and their long-term performance determine their applicability in organic electronics. To address these issues we have performed studies on pentacene thin film transistors (TFTs) with and without encapsulation. The capping layer is realized by a  $\sim 100 \text{ nm}$  thick sputtered layer of aluminum oxide or by a  $\sim 3 \mu\text{m}$  polymer layer of poly-para-xylylene. A field-effect can be demonstrated for both capping materials up to temperatures of  $\sim 140^\circ\text{C}$ , which is about  $50^\circ\text{C}$  above the desorption point of uncapped pentacene thin films on  $\text{SiO}_2$ . A complex behavior of the temperature dependent hole mobility can be deduced from the TFT characteristics, indicating that the device operation at elevated temperatures is predominantly limited by the transistor structure and not by the organic material. Comparative studies on the long-term stability of the electronic TFT properties will be discussed for both capping materials. The microscopic mechanisms resulting in the structural breakdown of the pentacene layer have been analyzed by thermal desorption spectroscopy and temperature dependent x-ray diffraction. The thermally induced breakdown will be discussed also for other materials such as diindenoperylene [1].

[1] S. Sellner, et al., J. Mater. Res. 21, 455 (2006).

SYOE 8.103 Tue 18:00 Poster B

**Influence of the end cap chain length of Dn6T on OFET characteristics** — ●BENEDIKT GBUREK, TORSTEN BALSTER, and VEIT

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Comparative in- and ex-situ studies have been performed on organic field-effect transistors (OFETs) with the oligomers dihexylsexithiophene (DH6T) and didecylsexithiophene (DD6T) as organic channel materials. These two end-substituted oligothiophenes with the same number of thiophene rings differ only by the length of their alkyl end-chains. While DH6T is one of the best-known materials in OFET research, the similar DD6T is a rather new and promising material due to the transition into a liquid crystal phase at  $108^\circ\text{C}$ . In this phase, DD6T is supposed to show larger crystals, thus offering better conduction properties.

The charge carrier mobility of DD6T shows a stronger increase with increasing temperature (49 % in  $45^\circ\text{C}$ ) for room temperature grown films than DH6T. In addition, the slope of the DD6T mobility vs. temperature curves increases around  $100^\circ\text{C}$ , which corresponds to the transition into the liquid crystal phase. After cooling down of the sample, the mobility has the same value as before the thermal treatment, indicating a reversible phase transition. For room temperature deposited DD6T films, a lower charge carrier mobility ( $0.02 \text{ cm}^2/(\text{Vs})$ ) has been measured than for DH6T films ( $0.033 \text{ cm}^2/(\text{Vs})$ ). On the other hand, DD6T transistor characteristics exhibited higher stability upon exposure to air than those of DH6T.

SYOE 8.104 Tue 18:00 Poster B

**Inversion of micro-patterned polymer surfaces based on bi-component polyelectrolyte layers** — ●ALLA SYNYSKA<sup>1</sup>, MANFRED STAMM<sup>1</sup>, STEFAN DIEZ<sup>2</sup>, and LEONID IONOV<sup>2</sup> — <sup>1</sup>Leibniz Institute of Polymer Research Dresden, 01069 Dresden, Hohe Strasse 6, Germany — <sup>2</sup>Max-Planck-Institute of Molecular Cell Biology and Genetics, Pfotenhauerstrasse 108, 01307 Dresden, Germany

Micropatterned surfaces are of considerable importance for microelectronics, printing technology, microfluidic and microanalytical devices, information storage, biosensors, etc. However, once a pattern is generated it cannot be easily changed on the fly. Therefore, it is desirable to develop methods for fabrication of structured surfaces with switchable and rewritable patterns.

In the present study, we report on the fabrication of micropatterned surfaces which allow the switching of topography, wettability, and charge in an inverse manner. The concept of these stimuli-responsive surfaces, which are made by a combination of photolithography, lift-off and grafting to techniques, is based on the site-selective grafting of two oppositely charged polyelectrolytes. Depending on the pH of the surrounding one kind of the polymer chains is swollen (charged and hydrophilic) while the other is collapsed (uncharged and hydrophobic). The main advantage of such surfaces is their capability of inverse switching, for example hydrophilic patterns can be reversibly converted into hydrophobic ones and vice versa, via external stimuli.

SYOE 8.105 Tue 18:00 Poster B

**Nonlinear I-V Characteristics of Nanoparticle Compacts and Nanocomposites** — ●SIMONE HERTH<sup>1,2</sup>, XIAOPING WANG<sup>1</sup>, TERESA HUGENER<sup>1</sup>, HENRIK HILLBORG<sup>3</sup>, TOMMASO AULETTA<sup>3</sup>, LINDA SCHADLER<sup>1</sup>, and RICHARD SIEGEL<sup>1</sup> — <sup>1</sup>Rensselaer Polytechnic Institute, Troy, NY, USA — <sup>2</sup>Bielefeld University, Bielefeld, Germany — <sup>3</sup>ABB AB, Corporate Research, Schweden

Materials with nonlinear I - V characteristics are commonly used as field grading materials. In many cases, the non-linearity is achieved through the addition of equiaxed fillers to a polymer matrix. These composite field grading materials are optimized in terms of non-linearity, conductivity, and breakdown strength. One limitation in designing new field grading materials is a robust understanding of the relationship between powder morphology, composition and electrical characteristics of the powder, as well as a robust understanding of the relationship between powder conductivity and non-linearity and composite non-linearity. In this work, treatment of ZnO powder with a  $\text{SnF}_2$  solution resulted in a powder that yielded highly non-linear behavior. The highest non-linearity was achieved for powders with at least two different phases and a rough surface, as indicated by transmission electron micrographs. In contrast, the non-linearity of the nanocomposite conductivity is mainly determined by the conductivity of the nanofiller. The electrical behavior of the non-linear powder can be understood by a polarization of the nanoparticles at the interfaces, whereas the nonlinearity of the nanocomposites can be explained by a tunnelling mechanism between two particles.

SYOE 8.106 Tue 18:00 Poster B

**Conformational disorder of conjugated polymers** — SEBASTIAN WESTENHOFF<sup>2</sup>, WICHARD BEENKEN<sup>1</sup>, ARKADY YARTSEV<sup>3</sup>, and NEIL GREENHAM<sup>2</sup> — <sup>1</sup>Technische Universität Ilmenau, FG Theoretische Physik I, Postfach 100565, 98684 Ilmenau, Deutschland — <sup>2</sup>Cavendish Laboratory, University of Cambridge, Madingley Road, Cambridge CH3 0HE, United Kingdom — <sup>3</sup>Lunds Universitet, Kemisk Fysik, Box 124, 22100 Lund, Schweden

Conformational disorder of conjugated polymers is an important issue to be understood and quantified. In this paper we present a new method to assess the chain conformation of conjugated polymers based on measurements of intrachain energy transfer. The chain conformation is modeled on the basis of monomer-monomer interactions, such as torsion, bending, and stretching of the connecting bond. The latter two potentials are assumed to be harmonic, while the torsional potential was calculated by density functional theory using B3-LYP functional with the SVP basis set. The energy transfer dynamics of excitons on these chains are quantitatively simulated using Förster-type line-dipole energy transfer. This allows us to compare the simulated ground state conformation of single polymer chains to ultrafast depolarization experiments of poly [3-(2,5-dioctylphenyl)thiophene] in solution. We identify torsional rotation as the main contributor to conformational disorder and find that this disorder is mainly controlled by the energy difference between syn and anti bonds. [J. Chem. Phys. 125, 154903 (2006)]

SYOE 8.107 Tue 18:00 Poster B

**Vertically and relaxed excited state properties of neutral and charged oligofluorenes with and without keto-defect** — MENGTAO SUN<sup>2</sup>, WICHARD J.D. BEENKEN<sup>1</sup>, TÖNU PULLERITS<sup>3</sup>, and GUANGJIU ZHAO<sup>4</sup> — <sup>1</sup>Technische Universität Ilmenau, FG Theoretische Physik I, Postfach 100565, 98684 Ilmenau, Germany — <sup>2</sup>Chinese Academy of Sciences, Institute of Physics, Beijing, 100080, P. R. China — <sup>3</sup>Lunds Universitet, Kemisk Fysik, Box 124, 22100 Lund, Sweden — <sup>4</sup>Dalian Institute of Chemical Physics, State Key Laboratory of Molecular Reaction Dynamics, Dalian, 116023, P. R. China

Oxidation is one of the main degradation problems in conjugated poly-

mers. Stimulated from the recent experimental report of optical properties of charged oligofluorenes [Fratiloiu, S; et al. J. Phys. Chem. B 2006, 110, 5984-5993], we studied the electronic structure and optical properties of neutral and charged oligofluorenes with and without the keto-defect by time-dependent density functional theory (TD-DFT). Using 2D site and 3D cube representations of the density matrix, we found the vertically and relaxed excited states (i.e. absorption and emission) for the neutral species being like Frenkel-excitons. For both charged species, however, the first excited states represent spatial oscillations of the electron-hole pair over the whole oligomer chain. A single keto-defect forming a central fluorene-9-on monomer strongly affects the excited states of the neutral and anionic oligo-fluorenes by getting strong charge-transfer character, while those of the cation are nearly unchanged.

SYOE 8.108 Tue 18:00 Poster B

**Adsorption of CdTe nanoparticles on Poly(acrylic acid) brushes** — SMRATI GUPTA<sup>1</sup>, PETRA UHLMANN<sup>1</sup>, NIKOLAI GAPONIK<sup>2</sup>, and MANFRED STAMM<sup>1</sup> — <sup>1</sup>Leibniz-Institut für Polymerforschung Dresden, 01069 Dresden, Germany — <sup>2</sup>Technische Universität Dresden, Institut für Physikalische Chemie und Elektrochemie, 01062 Dresden, Germany

We report on the adsorption of amino functionalized CdTe nanoparticles on Poly(acrylic-acid) (PAA) polymer chains, tethered by one end to an underlying substrate in a polymer brush configuration. PAA brushes were prepared on silica substrate via \*grafting to\* method and 2-aminoethanethiol stabilized CdTe nanoparticles (2-4 nm) were prepared using the reaction between Cd<sup>2+</sup> and NaHTe under specific reaction conditions. Functionalized particles were found to get adsorbed on the brushes by the physical interaction between carboxylic groups of PAA polymer chains and amino groups of CdTe nanoparticles. Presence of CdTe nanoparticles on the polymer brushes was confirmed by the Atomic Force Microscopy (AFM), X-ray photoelectron spectroscopy (XPS) and Photoluminescence (PL) spectroscopy. Switching of the modified PAA brushes by changing the pH of surrounding media, explore the use of this system in the fabrication of the sensors.

## SYOE 9: Organic Light Emitting Diodes (abstracts see DS 16.1-8)

Time: Wednesday 14:30–16:30

Location: H32

Joined session with DS: The abstracts are listed under DS 16.1-8

## SYOE 10: Contact Properties (further abstracts see DS 17.2-6)

Time: Wednesday 16:45–18:45

Location: H32

### Invited Talk

SYOE 10.1 Wed 16:45 H32

**Single grain contacts** — GREGOR WITTE — Physikalische Chemie I, Ruhr-Universität Bochum, 44801 Bochum

Because of attractive features such as low-temperature processing and flexibility organic electronics is presently attracting significant attention. Of particular interest of current research is a detailed understanding and optimization of intrinsic charge transport mechanism present in these materials. Besides their technological relevance organic thin film transistors (OFETs) are frequently used to characterize the electronic properties of such organic semiconductors. However, due to structural imperfections like grain or domain boundaries within the films as well as contact related problems the intrinsic transport prop-

erties are masked and typically only effective parameters are obtained. While these problems can be avoided by investigating organic single crystals they are difficult to grow and frequently are not available in the required purity and perfection. An alternative strategy is based upon investigation of films containing large single crystalline grains as compared to the channel length of the used OFET device thus allowing single grain studies. In this talk I will give an overview of experimental approaches to realize single grain devices and to deal with proper contacts.

Joined session with DS: Further abstracts are listed under DS 17.2-6