Symposium Tayloring Organic Interfaces: Molecular Structures and Applications (SYSA)

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

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Overview of Invited Talks and Sessions

(lecture rooms H 0105, H 2013, and H 2032;
Poster area Poster A: the posters should be in place at 14:30; kernel time of the poster session is 17:00-20:00)

Invited Talks

SYSA 1.1	Tue	9:30–10:00	H 0105	**Level alignment at metal/organic interfaces** — •Fernando Flores
SYSA 2.1	Tue	10:45–11:15	H 0105	**Organic film growth and organic-metal interfaces** — •Norbert Koch
SYSA 2.5	Tue	12:00–12:30	H 0105	**Molecular n-doping of organic semiconductors** — •Antoine Kahn, Calvin Chan
SYSA 3.1	Tue	14:30–15:00	H 2013	**Charge transport and contact effects in organic semiconductors** — •Alberto Salleo, Leslie Jimison, Jonathan Rivnay, Ludwig Goris, Michael Toney
SYSA 4.1	Tue	16:30–17:00	H 2013	**Polymer electronics - Charge transport at organic-organic heterointerfaces** — •Henning Sirringhaus
SYSA 6.1	Wed	14:30–15:00	H 2013	**Organometallic Nanojunctions Probed by Different Chemistries: Thermo-, Photo, and Mechanochemistry** — •I. Stich, M. Konopka, R. Turansky, J. Reichert, N. L. Doltsinis, H. Fuchs, D. Marx
SYSA 7.1	Wed	17:45–18:15	H 2013	**Designing the nanostructure of the organic polymer - metal interface** — •Stephan V. Roth
SYSA 8.1	Thu	17:00–17:30	H 2032	**Nanostructure and transport in regioregular polythiophenes and their block copolymers** — Rui Zhang, Bo Li, Jessica R. Cooper, Mihaela Iovu, Genevevie Sauve, David N. Lambeth, Detlef-M. Smilgies, Richard D. McCullough, •Tomasz Kowalewski

Sessions

SYSA 1.1–1.4	Tue	9:30–10:45	H 0105	**Bandalignment in Organic Materials**
SYSA 2.1–2.7	Tue	10:45–13:00	H 0105	**Organic Interface Structure and Growth**
SYSA 3.1–3.6	Tue	14:30–16:30	H 2013	**Organic Devices I**
SYSA 4.1–4.7	Tue	16:30–18:30	H 2013	**Organic Devices II**
SYSA 5.1–5.91	Tue	14:30–20:00	Poster A	**Poster Session SYSA**
SYSA 6.1–6.11	Wed	14:30–17:30	H 2013	**Organic Interfaces (further abstracts see DS 19.2-11)**
SYSA 7.1–7.6	Wed	17:45–19:30	H 2013	**Organic Polymer-Metal Interfaces (further abstracts see DS 20.2-6)**
SYSA 8.1–8.5	Thu	17:00–18:30	H 2032	**Nanostructured Block Copolymer Films (further abstracts see DS 35.2-5)**

The organizers gratefully acknowledge FV DS for providing the additional room and timeslots for the symposium SYSA. Especially the joined sessions SYSA 6, SYSA 7, and SYSA 8 (on Wednesday and Thursday afternoon) wouldn't have been

possible otherwise.

SYSA 1: Bandalignment in Organic Materials

Time: Tuesday 9:30–10:45 Location: H 0105

Invited Talk SYSA 1.1 Tue 9:30 H 0105

Level alignment at metal/organic interfaces — •Fernando Flores — Universidad Autónoma de Madrid, Madrid, Spain

A unified model, embodying the Induced Density of Interface States (IDIS), Pauli repulsion and intrinsic molecular dipoles is presented for describing the level alignment at a metal/organic interface. The IDIS model takes into account how charge is transferred between the metal and the organic material [1]: in particular, charge transfer is determined by the relative position of the metal workfunction and the organic Charge Neutrality Level (CNL), as well as by an interface parameter, S, which measures how this potential difference is screened. The Pauli repulsion dipole originates from the orthogonalization of the metal and organic wavefunctions; this dipole is calculated using a many-body LCAO hamiltonian [2], resulting in an effective reduction of the metal workfunction. Intrinsic molecular dipoles are also introduced in this unified model, in such a way that the level alignment at the metal/organic interface is obtained from a calculation that combines all these effects in a selfconsistent way. As a first example, organic materials with no intrinsic molecular dipole are considered (PTCDA, PTCBI, CBP and CuPc). For these cases it will be shown that the IDIS-dipole represents most of the realignment induced at the metal/organic interface, with the Pauli repulsion dipole yielding minor corrections to the IDIS model. In a second example, the Cu/benzenethiolate/pentacene heterostructure is analyzed including IDIS, Pauli repulsion and intrinsic molecular dipoles [3]. The Cu/benzenethiolate interface realignment can be understood in these terms as a function of the benzenethiolate coverage: this also enables us to determine, using the metal workfunction evolution, the molecule orientation as a function of coverage. An extension of this model to heterostructures allows us to analyze in similar terms the benzenethiolate/pentacene interface.

[1] H.Vazquez et al, Europhys. Lett. 65, 802 (2004) [2] H.Vazquez et al, J. Chem. Phys. 126, 144703 (2007) [3] M.G.Betti et al, Phys. Rev. Lett., in press.

SYSA 1.2 Tue 10:00 H 0105

Consistent experimental determination of the charge neutrality level and the pillow effect at metal/organic interfaces — •Mandy Grobosch[1], Olga V. Molodtsova[1], Victor Yu. Aristov[1,2], and Martin Knupfer[1] — [1]IFW Dresden, D-01069 Dresden, Germany — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow distr., 142432, Russia

Experimental results of combined X-ray and ultraviolet photoemission spectroscopy studies for the interface dipoles at metal/organic and organic/organic heterointerfaces have been analyzed on the basics of the induced density of interfaces states model(1,2). For the estimation of the interface dipole as well as the metal work function we have analyzed the following interfaces: Au/CuPc, Ag/CuPc, Au/CuPcF4, Ag/CuPcF4, and the respective heterointerfaces between copper phthalocyanine (CuPc) and its fluorinated relative (CuPcF4). We demonstrate that a consistent analysis of a selected set of interfaces is possible, which allows the determination off all microscopic parameters of the model, and moreover enables the prediction of the electronic properties of further, yet unknown interfaces. This additionally represents a starting point for the experimental determination of further important material dependent parameters such as the charge neutrality level of organic semiconductors.

1 H. Vazquez, F. Flores, and A. Kahn, Organic Electronics 8, 241 (2007).

2 H. Vazquez, Y.J. Dappe, J. Ortega, and F. Flores, J. Chem. Phys. 126, 144703 (2007).

SYSA 1.3 Tue 10:15 H 0105

Measuring the energy level alignment at all interfaces in a complete OLED — Selina Olthof, Rico Meerheim, Karsten Walzer, and •Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden, Germany

As the number of layers used for typical organic semiconductor devices is increasing in the course of optimization, interfaces between those layers become increasingly important for device performance. These interfaces are governed by the relative HOMO and LUMO positions as well as by interface dipoles originating from effects like polarization, chemical reactions and bond formation. As our charge injection layers are electrically doped, band bending and the resulting depletion layers play a significant role as well. To be able to perform simulations of the full device for further optimization it is necessary to measure the energy alignment at all metal/organic and organic/organic interfaces. This can be done by ultraviolet photoelectron spectroscopy (UPS) and x-ray photoelectron spectroscopy (XPS). We performed such interface resolved studies of a complete OLED by UPS and XPS. As an example, we chose the structure of a long living red OLED: ITO - MeO-TPD:F4-TCNQ - α-NPD - α-NPD:Ir(MDQ)2acac - BAlq - BPhen:Cs - Ag.[1] For photoelectron spectroscopy, the OLED was built stepwise measuring for each interface the thickness dependent photoelectron spectra. The measurements show that the doped layers strongly influence the energetic positions of the intrinsic layers, and that the commonly assumed vacuum level alignment is not fulfilled. [1] R. Meerheim et al., Appl. Phys. Lett. 89, 061111 (2006)

SYSA 1.4 Tue 10:30 H 0105

Intramolecular band structure and disorder effects in monolayers of linear molecules — •M. Häming[1], J. Ziroff[1], M. Wiessner[1], O. Seitz[2], E. Salomon[3], A. Kahn[3], D. Cahen[2], A. Schöll[1], F. Reinert[1], and E. Umbach[1] — [1]Universität Würzburg, Experimentelle Physik II, D-97074 Würzburg — [2]Weizmann Institute of Science, Department of Materials and Interfaces, Israel — [3]Princeton University, Department of Electrical Engineering, USA

For a detailed understanding of charge transport on a molecular level a comprehensive understanding of the molecular electronic structure is mandatory. Self assembled alkyl monolayers (SAM) are appropriate model systems due to interesting charge transport properties and their relatively simple molecular structure. We have investigated the intramolecular band structure of alkyl/Si(111) SAMs with high resolution photoemission spectroscopy (HR-PES) using variable photon energy. There are significant changes in the valence band spectra for photon energies between 30 eV and 190 eV indeed, but the electronic dispersion is blurred due to a strong DOS effect. This is very unlikely a property of the intramolecular band structure, but rather the consequence of disorder in the molecular layer. In reverse, this effect can provide structural information. A comparison between the PES data and projections of the total DOS onto the free electron final state for different distributions of alkyl orientations allows to estimate the spread in the molecular orientation angle and thus the degree of disorder. Consequently, this needs to be taken into account for a proper description of the intramolecular electronic structure.

SYSA 2: Organic Interface Structure and Growth

Time: Tuesday 10:45–13:00 Location: H 0105

Invited Talk SYSA 2.1 Tue 10:45 H 0105

Organic film growth and organic-metal interfaces — •Norbert Koch — Humboldt-Universität zu Berlin, Institut f. Physik, Berlin, Germany

The structure, morphology, and electronic properties of thin films formed by conjugated organic molecules are key factors determining the function and efficiency of organic (opto-) electronic devices. Molecules chemisorbed on metal surfaces can undergo significant conformation changes, often facilitated by a hybridization of molecular and metal electron wavefunctions. The resulting energy levels at such interfaces are determined by a complex interplay of molecular orientation, charge transfer, and conformation dependent dipoles, which will be exemplified for strong electron acceptor molecules on coinage metal surfaces. The modification of metal surfaces with electron acceptors can be used to control the energy level alignment of subsequently deposited organic layers. Thin organic films on insulating substrates are of interest for organic field effect transistors. Co-deposited rod-like conjugated molecules can form new crystalline intercalated structures with electronic properties significantly different from those of the pure materials. It will be shown that the appropriate combination of two different molecules facilitates (i) control over the energy levels, and (ii) widely tunable charge transport properties.

SYSA 2.2 Tue 11:15 H 0105

Growth analysis at the contacts of nanoscale oligothiophene field effect transistors — •Arne Hoppe, Torsten Balster, and Veit Wagner — Jacobs University Bremen, School of Engineering and Science 28725 Bremen

Decreasing the size of bottom contact organic field effect transistors (OFETs) to the nanoscale in order to achieve high performance devices with enhanced integration density leads to new challenges such as contact resistance and modified growth modes on nanostructured surfaces. The growth behavior of dihexyl-substituted oligothiophenes is investigated by in-situ electrical characterisation and by AFM topography analysis. DH4T, DH5T, and DH6T show oscillations in the charge carrier mobility with layer thickness reflecting the length of the individual molecules. Downscaling of the channel length to the sub-micrometer region allows the direct analysis of the contact resistance and reveals that oscillations occur not only in the mobility, but in the contact resistance as well. Typical mobility values for micrometer devices are as high as 6 x 10-2 cm2/Vs despite contact resistance. With further shrinking of the channel length we find the suppression of the oscillations observed before. By a growth analysis by AFM, we attribute this behaviour to the disturbed growth close to the contacts due to lateral material diffusion, i. e. due to a step-flow growth mode. Due to this diffusion we find excess organic material in the channel for channel lengths below 500 nm. These findings indicate that nanoscale transistors below a critical channel length can exploit the step-flow growth mode to suppress the mobility drops caused by fractional monolayers.

SYSA 2.3 Tue 11:30 H 0105

Growth and Electronic Structure of Pentacene on Pd & Pt Surfaces — •Daniel Käfer and Gregor Witte — Physikalische Chemie I, Ruhr-Universität Bochum, Germany

Due to its high charge carrier mobility pentacene is a promising molecular semiconductor for the fabrication of organic field effect transistors (OFETs). While gold has been commonly used as electrode material in pentacene based thin film transistors recent studies have shown improved device characteristics for Pd electrodes.

In this study the growth and structures of pentacene films on single-crystalline and polycrystalline Pd and Pt surfaces has been investigated by means of SEM and NEXAFS spectroscopy. Significant differences were found for the molecular orientation in multilayer films grown on both substrates, which is important for the realization of OFETs in view of the large anisotropy of charge carrier mobility in crystalline pentacene. In addition a rather different film morphology was observed for the various substrates ranging from a quasi layer-by-layer fashion to extreme dewetting. The interaction strength of pentacene with both metal surfaces was further characterized by TDS measurements. Moreover, by using UPS the electronic structure of pentacene thin films on Pd and Pt has been analyzed in detail. These results reveal a different electronic coupling between the metal substrate and the first monolayer on the one hand, and between the first layer and pentacene multilayers on the other hand, which has to be taken into consideration for an understanding and optimization of charge injection in such devices.

SYSA 2.4 Tue 11:45 H 0105

X-ray standing wave study of pentacene and perfluorinated pentacene on Cu(111) — •A. Gerlach[1], F. Schreiber[1], S. Duhm[2], N. Koch[2], A. Vollmer[3], T. Suzuki[4], and J. Zegenhagen[5] — [1]Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — [3]Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung, Albert-Einstein-Str. 15, 12489 Berlin, Germany — [4]Institute for Molecular Science, Myodaiji, Okazaki 444-8787, Japan — [5]European Synchrotron Radiation Facility, 6 Rue Jules Horowitz, BP 220, 38043 Grenoble Cedex 9, France

The adsorption geometry of pentacene (PEN) and perfluorinated pentacene (PFP) on Cu(111) is studied using the X-ray standing wave technique. The element specific structural information derived from the C(1s)and F(1s) photoelectron signals demonstrate the different bonding mechanism of both molecules.

While PEN interacts strongly with the copper substrate and adsorbs with an average bonding distance of only 2.34±0.02 Å, the carbon core of the PFP molecule is located at 2.98 ± 0.07 Å. Despite the relatively weak interaction of PFP with the substrate the molecules experience a mild distortion upon adsorption with the fluorine atoms being slightly above the molecular plane at 3.08 ± 0.04 Å. Based on the XSW results we discuss the influence of the intramolecular dipole on the charge transfer across the interface.

Invited Talk SYSA 2.5 Tue 12:00 H 0105

Molecular n-doping of organic semiconductors — •Antoine Kahn and Calvin Chan — Princeton University, Princeton, NJ, USA

Chemical doping of organic molecular films is a powerful way to improve charge injection and transport in organic devices, and to enhance device functionality. However, n-type doping is challenging, often hindered by the energetic requirements of transferring an electron from the dopant HOMO to the host low lying LUMO. We recently demonstrated efficient n-doping of the electron transport material tris{2,5-bis(3,5-bis-trifluoromethyl-phenyhl)-thieno}[3,4-b,h,n]-1,4,5,8,9,12-hexaazatriphenylene (THAP), which has a 4.59 eV electron affinity (EA), with cobaltocene (CoCp, IE = 4.07 eV). We now introduce a stronger n-dopant, i.e. decamethylcobaltocene (CoCp*2), and demonstrate n-doping of copper phthalocyanine (CuPc, EA = 3.25 eV). CoCp*2 is found to have a remarkably low IE of 3.30 eV. N-doping is evidenced by a large upward swing of the Fermi-level in the gap of CuPc, and confirmed by current-voltage (I-V) measurements. A 10$ˆ{4}$- to 10$ˆ{7}$-fold increase in current density of the interface-doped device as compared to the undoped CuPc device is due to enhanced injection. An additional 10$ˆ{3}$-fold increase in current density is observed for the uniformly doped device and is attributed to enhanced conductivity of the bulk film. The application of p- and n-doping of CuPc to an organic homojunction p-i-n diode with a 1.47 eV built-in potential is demonstrated.

SYSA 2.6 Tue 12:30 H 0105

Electronic structure of the CuPc/BPE-PTCDI donor/acceptor hetero interface of organic solar cells for varied O2 and TCNQ doping concentrations — Corinna Hein, •Eric Mankel, Johanna Härter, Thomas Mayer, and Wolfram Jaegermann — Technische Universität Darmstadt, Materials Science Institute, Surface Science Division, Petersenstr. 23, 64287 Darmstadt

The bilayer hetero junction model solar cell of Copper phthalocyanine (CuPc) / BPE-PTCDI, a perylene derivative, shows a low efficiency of 0.8% only. With synchrotron induced photoemission (SXPS) in the course of interface formation we find the development of potential barriers due to band bending, hindering charge collection. To overcome the formation of the barrier we test p-doping of the CuPc layer by oxygen or by TCNQ, which are strong electron acceptors. Oxygen doping of CuPc was performed by evaporation in O2 atmosphere at pressures in the range from 10-8mbar to 10-3mbar which leads to oxygen concentrations less than 1%. A shift of the CuPc Fermi level by 200meV was achieved. TCNQ doping was performed by coevaporation. With increasing TCNQ content in the percent region, a shift of the CuPc Fermi level up to 450meV has been achieved. The doping mechanism has been analyzed by performing SXPS on the TCNQ/CuPc interface. In the course of CuPc deposition we find a shift of the CuPc HOMO by 450 meV indicating electron transfer. In addition an interface dipole of 320 meV is formed.

SYSA 2.7 Tue 12:45 H 0105

Ambipolar organic semiconductor blendsfor photovoltaic cells — •Andreas Opitz, Markus Bronner, Julia Wagner, Marcel Götzenbrugger, and Wolfgang Brütting — Institute of Physics, University of Augsburg,Germany

Blends of organic semiconducting materials, so-called bulk-heterojunctions, are widely used in ambipolar field-effect transistors and as photoactive films in solar cells. One particularly interesting material system is a mixture of n-conducting fullerene (C_{60}) and p-conducting copper-phthalocyanine (CuPc) prepared by co-evaporation.

The electronic properties of these blends were analysed by X-ray and ultraviolet photoelectron spectroscopy in dependence on the mixing ratio [1]. A common vacuum level is observed suggesting that a phase separation of the two materials in the blends occurs only on the nanometer scale. The HOMO and the core level spectra show no evidence for a charge transfer or a chemical reaction among the materials in the ground state. These results also indicate a reduced energy offset between the HOMO of the donor and the LUMO of the acceptor in bulk heterojunctions in comparison to planar heterojunctions. As a consequence photovoltaic cells reveal higher built-in and open circuit voltage for the bilayered system. Nevertheless, photovoltaic cells using mixtures yield higher photocurrents due to the presence of donor/acceptor interface in the whole active film [2].

[1] A. Opitz et al., *Appl. Phys. Lett.* **90** (2007) 212112.
[2] W. Brütting et al., *Macromol. Symp.* (2007), accepted.

SYSA 3: Organic Devices I

Time: Tuesday 14:30–16:15 Location: H 2013

Invited Talk SYSA 3.1 Tue 14:30 H 2013

Charge transport and contact effects in organic semiconductors — •Alberto Salleo[1], Leslie Jimison[1], Jonathan Rivnay[1], Ludwig Goris[1], and Michael Toney[2] — [1]Materials Science Department, Stanford University, Stanford CA 94305 — [2]Stanford Synchrotron Radiation Laboratory, Menlo Park CA

The long-standing promise of organic electronics, i.e. the ability to design molecular materials at will, is complicated by the fact that one needs to predict the microstructure of the semiconductor from the molecular structure. Thus, in order to truly design novel semiconductors, one must understand how microstructure and transport are related. In polymeric semicrystalline semiconductors, mobility is well described by a multiple trapping and release model. The beneficial effect of annealing in poly(thiophenes) for instance can be understood as a tightening of the trap energy distribution. Regio-regularity on the other hand does not affect crystalline texture (i.e. intergrain coupling) or tail state distributions but only the crystalline mobility. Finally, the microstructure of the polymeric semiconductor plays a role in other device non-idealities. For instance, we will show that tailoring the microstructure of the polymer allows to eliminate a well-known non-ideality of short-channel TFTs (L<10 um) due to ambipolar injection at the drain contact.

SYSA 3.2 Tue 15:00 H 2013

Integrated circuits based on low cost polymer electronics — •Klaus Schmidt, Andreas Ullmann, Markus Böhm, Jürgen Krumm, Robert Blache, Alexander Knobloch, Dietmar Zipperer, and Walter Fix — PolyIC GmbH & Co. KG, Fürth, Germany

It is expected that low-cost organic electronics will open a new mass market besides the already existing market for conventional and more expensive Si-based technology. We have fabricated different multi-bit RFID-Transponder based on polymer electronics. Polymer rectifiers working at 13.56 MHz and fast integrated organic circuits up to 0.6 MHz are demonstrated. A 64-bit transponder operating at a supply voltage of about 14V was realized based on poly-(3-hexylthiophene) as p-type semiconductor material with charge carrier mobility of about 0.02 cm2/Vs. The polymeric devices are very stable and exhibit high electrical performance and lifetime. Since the polymeric materials used for our devices are all soluble, it is possible to fabricate our electronic circuits by a cost efficient roll to roll printing process. Thus, completely high speed printed and low cost polymer electronics can be realized.

SYSA 3.3 Tue 15:15 H 2013

Peculiarities of OFET performance due to hopping transport near the gate insulator interface — •Susanne Scheinert[1] and Gernot Paasch[2] — [1]TU Ilmenau — [2]IFW Dresden

The operation of thin film field-effect transistors is determined by the channel at the interface to the gate oxide. There the carrier concentration can be changed from depletion to accumulation and the electric field increases from source to drain. For variable range hopping in disordered organic semiconductors as the active layer, the mobility depends on both the carrier concentration and the field. Our numerical simulation study shows that besides the known dependency of the field-effect mobility on the gate voltage there occur in addition (i) a strong modification of the saturation current, (ii) a shift of the threshold voltage, and (iii) an increase of the inverse threshold slope. In addition, (iv) the influence of the dependency on the mobility is critically determined by the transistor channel length. The origin of all these peculiarities is clarified by analyzing the internal profiles of concentrations and fields. Conclusions are drawn on the possibilities of parameter extraction from measured current characteristics.

SYSA 3.4 Tue 15:30 H 2013

High resolution mapping of the electrostatic potential in organic thin film transistors by phase electrostatic force microscopy — •Paolo Annibale, Cristiano Albonetti, Pablo Stoliar, and Fabio Biscarini — CNR-Institute for the Study of Nanostructured Materials (ISMN), Bologna, Italy

We investigate by a scanning probe technique termed phase-electrostatic force microscopy the local electrostatic potential and its correlation to the morphology of the organic semiconductor layer in operating ultra-thin film pentacene field effect transistors.

In order to address experimentally the role of defects in the device performance it is necessary to map the local electrostatic potential in the semiconductor layer with a resolution comparable with that of the morphological features associated to them.

This technique yields a lateral resolution of about 60 nm, allowing us to visualize that the voltage drop across the transistor channel is stepwise. Spatially localized voltage drops, adding up to about $\frac{3}{4}$ of the potential difference between source and drain, are clearly correlated to the morphological domain boundaries in the pentacene film.

This strongly supports and gives a direct evidence that in pentacene ultra-thin film transistors charge transport inside the channel is ultimately governed by domain boundaries.

SYSA 3.5 Tue 15:45 H 2013

Observation of charge injection and trapping in depleted channels of organic field effect transistors — •Christopher Siol, Christian Melzer, and Heinz von Seggern — Electronic Materials Division, Institute of Materials Science, Technische Universität Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany

The measurement of I-V characteristics is the standard means of transistor investigation. However, it gives limited information about the electronic processes that determine the transistor operation. Kelvin probe force microscopy (KPFM), however, gives the opportunity to resolve the surface potential locally. This allows one to separate the injection phenomena from the charge transport in the channel.

Here the surface potential in the channel of n- and p-type pentacene OFETs with poly(methyl methacrylate) dielectrics has been measured during operation. In the on state the conducting accumulation layer links surface potential of the channels to the contact electrodes. However, driving the device into the off state causes depletion of the channel from mobile charge carriers. Then, the surface potential depends on the gate potential but might be altered due to the presence of trapped charges in the channel. Depending on the device history, such trapped charges are observed. Additionally, by applying high gate fields to the already depleted transistor an injection of complementary charge carriers has been observed even for high injection barriers.

SYSA 3.6 Tue 16:00 H 2013

Influence of gap states on the electrical stability of pentacene Thin Film Transistors — •Amare Benor, Arne Hoppe, Veit Wagner, Rahul Dewan, and Dietmar Knipp — Jacobs University Bremen, School of Engineering and Science, 28759 Bremen, Germany

Despite the realization of polycrystalline pentacene transistors with high mobility, the creation of gap states and the influence of gap states on the charge transport and the device stability is still under investigation. In order to study the creation of electronic defects and the influence of these defects on the device stability electrical in-situ measurements of pentacene TFTs were carried out. The TFTs were prepared by Organic Molecular Beam Deposition with hole mobilities ranging from $0.2-0.5 cm^2/Vs$. The devices were exposed to oxygen to study the influence on the device characteristics. Unexposed devices are stable, whereas devices exposed to dry oxygen exhibit a shift of the threshold voltage upon prolonged device operation. Stressing the transistor in the on-state (negative bias) leads to a shift of the threshold voltage towards negative gate voltages, whereas prolonged bias stress in the off-state causes a shift of the threshold voltage in the opposite direction. The gap states are formed 0.18 eV (acceptor-like states) and 0.62 eV (donor-like states) above the valence band maxima. The shift of the threshold voltage due to bias stress is determined by the ratio of acceptor-like and donor-like states in the pentacene film. The charge carrier mobility and the on/off ratio of the transistor are not affected by the gap states. A simple density-of-states model will be presented, which allows for the explanation of the experimental results.

SYSA 4: Organic Devices II

Time: Tuesday 16:30–18:30 Location: H 2013

Invited Talk SYSA 4.1 Tue 16:30 H 2013

Polymer electronics - Charge transport at organic-organic heterointerfaces — •Henning Sirringhaus — Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom

Conjugated polymer semiconductors offer new opportunities for the controlled manufacturing of active electronic circuits by a combination of solution processing and direct printing. We will review current understanding of their device physics with a particular emphasis on understanding the electronic structure of polymer heterointerfaces and charge injection at metal-semiconductor interfaces governing the device performance. Recent advances towards realizing ambipolar organic transistors through control of interface electronic structure will be presented. We will also review recent progress towards manufacturing of organic transistor circuits by high-resolution printing techniques for applications in displays and low-cost intelligent labels.

SYSA 4.2 Tue 17:00 H 2013

How to adjust or avoid hysteresis in poly(vinyl alcohol) based organic field effect transistors — •Martin Egginger[1], Mihai Irimia-Vladu[2], Reinhard Schwödiauer[2], Andreas Tanda[3], Siegfried Bauer[2], and Serdar Sariciftci[1] — [1]LIOS, JK University Linz, Altenbergerstr. 69, 4040 Linz, Austria — [2]SOMAP, Soft Matter Physics, JK University Linz, Altenbergerstr. 69, 4040 Linz, Austria — [3]plastic electronic, Rappetsederweg 28, 4040 Linz, Austria

Poly(vinyl alcohol) (PVA) is an interesting water soluble gate insulator material in organic field effect transistors. Transistors with and without hysteresis in the transfer characteristic can be produced, depending on the process conditions of the PVA dielectric. Sodium acetate, an ionic salt that is needed in the production of PVA, is not completely removed during the industrial purification process. Such ionic impurities cause the hysteresis in PVA based organic field effect transistors [1]. While a hysteresis is desirable in memory elements it is unwanted in transistors for electronic circuits. Ways to prepare transistors with a desired transfer characteristic are described. Furthermore the influence of different ions on the size of the hysteresis is investigated. Finally we discuss that varying measurement conditions (temperature, sweep frequency and amplitude) also influence the size of the hysteresis.

[1] Martin Egginger, Mihai Irimia-Vladu, Reinhard Schwödiauer, Andreas Tanda, Irene Frischauf, Siegfried Bauer and Niyazi Serdar Sariciftci, Adv. Mat. 2007 (accepted), DOI: 10.1002/adma.200701479

SYSA 4.3 Tue 17:15 H 2013

Advanced modelling of optoelectronic characteristics of OLEDs — •Robert Nitsche[1], Matthias Kurpiers-Günther[1], Michael Thomschke[2], Matthias Schober[2], and Karl Leo[2] — [1]sim4tec GmbH, Schönfelder Landstr. 8, 01328 Dresden — [2]Insitut für Angewandte Photophysik, TU Dresden, George-Bähr-Str. 1, 01069 Dresden

A rapid development of highly efficient OLED devices could be observed during the last years. The main work was carried out using experimental trial and error methods which are cost intensive and time consuming. A better approach is to conduct numerical simulations for device design and optimization beforehand, thus reducing the experimental work significantly and gaining a deep understanding of the underlying device physics.

Here, we report on simulation results of multilayer single carrier devices and multilayer fluorescent and phosphorescent OLEDs including doped transport and emitter layers, using the integral OLED device simulator SimOLED. We first give an overview on optical and electrical modelling of OLEDs and discuss methodologies to obtain correct input parameters from fitting experimental results. Special focus is paid to the ambiguity of the extracted parameters to be used for further device modelling. The simulation results are compared to experimental data and conclusions are drawn concerning the distribution of electric field, recombination rates and exciton densities as well as charge carrier balance in the devices. Finally, we propose a generalized scheme for performing OLED simulations with predictive character.

SYSA 4.4 Tue 17:30 H 2013

Charge carriers dynamic and radiative recombination processes in organic light emitting devices studied by a sub-microsecond pulsed electroluminescence technique — •Eugenio Lunedei, Paolo Annibale, Yiqiang Zhan, and Carlo Taliani — ISMN-CNR, Bologna, Italy

Despite the realization of OLEDs with high performances and organic transistors with high mobility, the dynamic of charge carriers within a working device its is not always fully understood. The transport of charge through organic semiconductors is strongly affected by trap states in the energy gap, presence of interfaces, structural disorder and injection barriers at contacts. The transport properties are sometimes not obvious from I/V curves alone: the correlation between radiative emission and a pulsed charge injection allows to characterize both transport and optical properties of device. By making use of our time-resolved electroluminescence correlator capable of sub-μs voltage pulsewidth and time-resolution down to ns scale, we were able to follow the recombination processes in multilayer devices based on small molecules (as $\mathrm{Alq_3}$ and $\mathrm{T_6}$), blend of polymers, in inverted OLEDs with TCOs anode and in light emitting OFETs of $\mathrm{T_6}$ and Pentacene. The charge carriers mobility is directly obtained by ToF measurements as well as its dependance on the applied voltage and on the trap-site density within the organic layers; furthermore, the possibility to record complete electroluminescence spectra during the application of the electric pulse and in successive time windows gives a new insight on the fate of injected charges and on the nature of trapping sites.

SYSA 4.5 Tue 17:45 H 2013

Magnetic field effects on the triplet-polaron quenching in Ir(III)-complexes — Alex Thiessen, •Dirk Hertel, and Klaus Meerholz — Institute of Physical Chemistry, University of Cologne, Luxemburger Str. 116, 50939 Cologne, Germany

Recently [1], we reported a study of phosphorescence quenching in polyspirobifluorene doped with the phosphorescent emitter platinum-porphyrin (PtOEP). It was shown that the phosphorescence reduction is due to the interaction of triplet excitons with charges (polarons) in a unipolar diode structure. The rate constant for triplet-polaron interaction has been evaluated to be 10-13 cm3/s leading to an interaction radius of 0.2 nm. In our current work we have used the methodology [1] to elucidate the role of this process in materials relevant to phosphorescent OLEDs. We have studied a red-emitting Ir(III)-complex doped into low molecular weight materials and in polymers. It will be shown, that the efficiency of triplet-polaron annihilation depends mostly on the nature of the matrix and not on the structure of the heavy-metal complex. The results give insight to a possible origin of the magneto-resistance effects in organic materials [2]. Recently [3], it has been proposed that triplet-polaron annihilation might play a crucial role. We will discuss the influence of magnetic fields on the triplet-polaron annihilation for our model system.

References [1] Hertel, D.; et al. J. Phys. Chem. B 2007, 111, 12075. [2] Mermer, O.; et al. Phys. Rev. B 2005, 72, 202202. [3] Desai, P.; et al. Phys. Rev. B 2007, 75, 094423.

SYSA 4.6 Tue 18:00 H 2013

Hysteresis effects and non-volatile memory behaviour of organic heterostructure devices. — •Frank Lindner, Karsten Walzer, and Karl Leo — Institut für Angewandte Photophysik, TU Dresden, D-01062 Dresden

Within the last few years, organic memory devices have attracted considerable attention. During such experiments, we observed a hysteretic current-voltage behaviour of organic heterostructure devices. We report reproducible bistable electrical switching and memory phenomena in an organic multilayer heterostructure, consisting of materials which are well characterized from organic light emitting device investigations. Similar to OLEDs, the organic layers were embedded between a ITO and a metal contact. In contrast to other organic memory concepts we reached a high reproducibility and stability. The measured current-voltage characteristics shows two states of different conductivity at the same applied voltage. We could achieve more then 1000 Write-Read-Erase cycles without degradation. It was found that the ratio of the ON/OFF current depends on the writing and erasing voltage, respectively. The two states were yet retained for several days before reading the devices. Both states are stable at room temperature and can be measured reproducibly. We discuss the device operation mechanism. Device performance tests show that the heterostructure devices are a promising candidate for high-density, low-cost electrically addressable data storage applications.

SYSA 4.7 Tue 18:15 H 2013

C(V) and C(t) measurements on MFIS structures consisting P[VDF/TrFE] as ferroelectric layer — •Karsten Henkel, Bernd Seime, Ioanna Paloumpa, Klaus Müller, and Dieter Schmeisser — Brandenburgische Technische Universität Cottbus, Angewandte Physik - Sensorik, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany

Ferroelectric Field Effect Transistors (FeFETs) are considered as a candidate for future non volatile and non destructive readout memory cells. A possible low cost solution is the use of poly[vinylidene fluoride trifluoroethylene] (P[VDF/TrFE]). Using P[VDF/TrFE] we focus on metal ferroelectric insulator semiconductor (MFIS) capacitor structures. In this contribution we will summarize our investigations related to capacitance measurements in dependence of applied bias (C(V)) and time (C(t)). The thickness of the ferroelectric layer as well as the thickness and the material of the buffer layer have been investigated for optimization of the write voltage. CV measurements at higher temperatures deliver decreased flatband voltage shifts within one CV loop resulting in lower memory windows. At temperatures around 100°C the hysteresis totally vanished, pointing out the ferroelectric behavior of the system. C(t) measurements at a constant bias have been performed for retention analysis of the MFIS stack. After applying a writing pulse we could distinguish between a higher and a lower capacitance state for more than 5 days. This work is supported by Deutsche Forschungsgemeinschaft within priority program 1157 (SCHM 745/11-2).

SYSA 5: Poster Session SYSA

Time: Tuesday 14:30–20:00 Location: Poster A

SYSA 5.1 Tue 14:30 Poster A

Structure and Morphology of conducting Polymerfilms for Photovoltaic Applications — •Matthias Ruderer[1], Ezzeldin Metwalli[1], Weinan Wang[1], Gunar Kaune[1], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS E13, James-Franck-Str. 1, 85747 Garching, Germany — [2]HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

Conducting polymers have shown to be interesting candidates for photovoltaics due to their high absorption coefficient, low costs etc. Nevertheless there are stringent constraints in device fabrication due to the short exciton diffusion length. Therefore the structure of the polymerfilm is crucial. It was shown that a blended structure compared to a layered structure increases the efficiency [1].

In the presented work we focus on such blend films. Two conducting polymers of different classes, of poly(phenylene vinylene) (PPV) and polythiophene (PT) derivatives, are blended with different ratios. Films are prepared by using spin coating. With optical spectroscopy (UV/Vis and FT-IR) the absorbed part of the optical spectrum and the stability under ambient conditions is detected. The structure and morphology of the films are investigated with scattering methods (GI(U)SAXS) [2] and the critical blending ratio for the bicontinuous structure is determined.

[1] S. V. Chasteen, J. O. Härter, G. Rumbles, J. C. Scott, Y. Nakazawa, M. Jones, H.-H. Hörhold, H. Tillman, and S. A. Carter. J. Appl. Phys., 99:033709, 2006. [2] P. Müller-Buschbaum. Anal.Bioanal.Chem., 376:3, 2003.

SYSA 5.2 Tue 14:30 Poster A

Influence of water on the work function of conducting Poly(3,4-ethylenedioxythiophen)/poly(styrenesulfonate) — •Antje Vollmer[1], Andreas Elschner[2], and Norbert Koch[3] — [1]Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung m.b.H.,BESSY, Berlin, Germany — [2]H. C. Starck GmbH, Leverkusen, Germany — [3]Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany

The use of intrinsic conducting polymers ICPs as electrodes and hole injection layers in optoelectronic devices based on conjugated organic materials is a key for the successful implementation of organic electronics. Most ICPs today are based on aqueous dispersions of poly(3,4-ethylene-dioxythiophene) and poly(styrenesulfonate)PEDT:PSS. One of the reasons for this success is the high work function of PEDT:PSS, leading to low hole injection barriers at interfaces between the ICP and the active organic layers. However, reported values for the work function of PEDT:PSS exhibit a significant spread from 4.8 to 5.2 eV. This inconsistency makes it diffcult to predict hole injection barriers in actual devices. Residual water in the film was found to alter the films work function significantly.

N. Koch, A. Vollmer, A. Elschner, Appl. Phys. Lett. 90 (2007) 043512

SYSA 5.3 Tue 14:30 Poster A

Crystallization of Ferroelectric PVDF-TrFE in Cylindrical Nanopores — •Nitin Shingne[1,2], Markus Geuss[2], Ulrich Gösele[2], Martin Steinhart[2], and Thomas Thurn-Albrecht[1] — [1]Department of Physics, Martin Luther University, Hoher Weg 8, D-06120, Halle — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120, Halle

Using differential scanning calorimetry and wide angle X-ray scattering we studied the crystallization and melting as well as the paraelectric to ferroelectric phase transition in templated 1D nanostructures of Polyvinylidenefluoride-co-trifluroethylene P(VDF-TrFE). Self-ordered porous alumina membranes served as templates. Previous studies on poly(vinylidenefluoride) have shown that the crystal orientation in the nanostructures is controlled by the kinetics of crystallization and can lead to strong orientation phenomena. Similar texture effects are observed for the copolymer studied here which can be understood in detail by taking into account that crystal growth occurs in the high temperature hexagonal phase. In all cases studied it was observed that the molecular chain axis, i.e. the c-axis, is oriented perpendicular to the long axis of the nanopores. In particular, for the copolymer the (110) lattice planes are oriented parallel to the template surface. At room temperature, the dipoles in the ferroelectric phase are preferentially oriented at an angle of 30° with respect to the long axis of the pores. Therefore, strong longitudinal polarization is present in the native nanofibers or is accessible by poling.

SYSA 5.4 Tue 14:30 Poster A

Pentacene film growth on HOPG — •Jan Götzen, Daniel Käfer, Christof Wöll, and Gregor Witte — Physikalische Chemie I, Ruhr-Universität Bochum, 44780 Bochum

Recent studies have shown that the structure and molecular orientation in organic thin films depends sensitively on the interaction with the substrate which is of vital interest for an understanding and optimization of organic thin film electronic devices. Here we report a characterization of the microstructure, morphology and thermal stability of pentacene films grown by OMBD onto freshly cleaved HOPG by employing STM, AFM, NEXAFS, XRD and TDS. Despite a rather weak, essentially van-der Waals-type substrate interaction pentacene molecules adsorb with their planes oriented parallel to the surface and form a commensurate monolayer due to the close match of the molecular carbon frame and the underlying graphite lattice. This packing motive, however, is not maintained in multilayer films where instead molecules in subsequent layers are tilted around their long axis. The mutlilayer growth is further characterized by the formation of individual, elongated crystalline islands exhibiting the Siegrist bulk polymorphism and thus parallels the growth scenario observed previously for pentacene on Au(111). Identical structures were observed for rather different growth conditions (rate and temperature) and therefore indicate the presence of equilibrium film structures. In contrast films with upright oriented molecules were obtained if the graphite had been briefly sputtered to roughen the substrate surface and thus emphasizes the importance of micro-roughness on the resulting film growth.

SYSA 5.5 Tue 14:30 Poster A

Investigations of contact resistances in polythiophene organic field effect transistors via a gated four-probe method — •Fabian Johnen, Elizabeth von Hauff, and Jürgen Parisi — *Institute of Physics, Energy and Semiconductor Research Laboratory, Carl von Ossietzky Univerität of Oldenburg, 26111 Oldenburg, Germany*

In this study the effect of contact resistances on device behaviour in polythiophene (P3HT) organic field effect transistors (OFETs) was investigated. The transistors consist of a contact geometry with Au source and drain electrodes and two additional Au channel electrodes between the source and drain contacts. The contact geometry is patterned using photolithography. High impedance electrometers are used to measure the potentials at each of the channel electrodes. The voltage drop in the source and drain contact regions can then be determined. This allows for direct investigation of the temperature and field dependence of the contact resistance. The thickness of the PH3T layer was varied to investigate the influence of the thickness on the accuracy of the four-probe method.

SYSA 5.6 Tue 14:30 Poster A

Self-Assembled Monolayers of Anthraceneselenol on Au(111): simulations and experiments — •Anna Track[1,2], Georg Heimel[4], Daniel Käfer[4], Asif Bashir[4], Gregor Witte[3], and Egbert Zojer[1] — [1]Institute für Festkörperphysik, Technische Universität Graz, Petersgasse 16, A-8010 Graz, Austria. — [2]Institut für Physik, Karl-Franzes Universität Graz, Universitätsplatz 5, 8010 Graz, Austria. — [3]Department of Material Science and Engineering, Massachusetts Institute of Technology, 77 Massachusetts Ave., Cambridge, MA.,USA. — [4]Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, 44780 Bochum, Germany.

Molecular and organic electronics interfaces between organic films and metal substrates are of particular interest because they dictate charge injection properties. Self-assembled monolayers (SAMs) of fully conjugated molecules (characterized by a considerable conductivity) provide ideal model systems for an in depth study of such interfaces on a molecular level. Here, we combine various experimental techniques (including STM, LEED and UPS) with density functional theory based slab-type band-structure calculations to derive structural and electronic properties for the case of anthracene-2-selenol SAMs on Au(111). From these calculations valuable details about the charge rearrangements at the surface, binding energy, work function modification upon SAM formation, as well as the alignment between molecular levels and metallic states can be derived. Of prime importance is a detailed microstructural characterisation, where we use the calculations to highlight potential pitfalls in the interpretation of STM pictures of aromatic SAMs.

SYSA 5.7 Tue 14:30 Poster A

PTCDA on Au(111), Ag(111) and Cu(111): Correlation of interface charge transfer to bonding distance — •Steffen Duhm[1], Alexander Gerlach[2], Ingo Salzmann[1], Benjamin Bröker[1], Robert L. Johnson[3], Frank Schreiber[2], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin — [2]Universität Hamburg — [3]Universität Tübingen

The electronic structure at the interfaces of 3,4,9,10-perylene tetracarboxyilic dianhydride (PTCDA) and the metal surfaces Au(111), Ag(111) and Cu(111) was investigated using ultraviolet photoelectron spectroscopy (UPS). By combining these results with recent x-ray standing wave data from PTCDA on the same substrates clear correlation between the electronic properties and the interface geometry is found. The charge transfer between the molecule and the metal increases with decreasing average bonding distance along the sequence Au - Ag - Cu. Clear signatures of charge-transfer-induced occupied molecular states were found for PTCDA on Ag(111) and Cu(111). As reported previously by Zou et al. [1] a new hybrid state was found at the Fermi-level (E_F) for PTCDA/Ag(111), rendering the monolayer metallic. In contrast, the hybrid state for PTCDA/Cu(111) was observed well below E_F, indicating even stronger charge transfer and thus a semiconducting chemisorbed molecular monolayer. The hybridisation of molecular and Au electronic states could not be evidenced by UPS.

[1] Y. Zou, L. Kilian, A. Schöll, Th. Schmidt, R. Fink and E. Umbach, Surf. Sci. **600**, 1240 (2006)

SYSA 5.8 Tue 14:30 Poster A

Photoluminescence degradation of blue OLED emitters — •Stephan Winter, Sebastian Reineke, Karsten Walzer, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden

Organic light-emitting diodes (OLEDs) based on small molecule materials are currently developed for applications in flat panel displays and general lighting sources. Key parameters of such devices are high efficiency, long lifetime, and appropriate colour properties. Most of the efficient deep blue emitters still suffer from rather fast degradation and, thus, require further improvement.

The aim of the present work is to gain a fundamental understanding of the intrinsic degradation processes causing the low stability of blue OLED emitters. For this purpose, we study the photoluminescence (PL) degradation instead of the most often investigated electroluminescence degradation to separate electrically and optically caused effects.

We show a newly developed PL lifetime measurement system which allows the study of degradation processes under the influence of either electron or hole currents. First, we demonstrate the importance of a proper encapsulation for PL lifetime. Next, using this set-up, we demonstrate the very high PL stability of the highly efficient blue singlet emitter 2,2',7,7'-tetrakis(2,2-diphenylvinyl)spiro-9,9'-bifluorene (Spiro-DPVBi) under electron and hole currents and make a comparison to the lifetime of OLEDs using the same emitter.

SYSA 5.9 Tue 14:30 Poster A

Investigation of the Schottky Barrier in Ag/CuPc/H-Si(111) Structures — •Iulia Genoveva Korodi, Jan Ivanco, and Dietrich R.T. Zahn — Chemnitz University of Technology, Semiconductor Physics, D-09107 Chemnitz, Germany

In this work molecular layers of copper phthalocyanine (CuPc) with thicknesses ranging from 1ML to 4ML were deposited on hydrogen passivated n-type silicon (111) substrate by Organic Molecular Beam Epitaxy (OMBE) under high vacuum (HV) conditions. Metal contacts of silver (Ag) were formed on top using thermal evaporation under the same HV conditions. In situ current-voltage (I-V) measurements were performed on these organic modified systems in order to investigate the influence of the CuPc interlayers on the barrier height of Ag/H-Si(111) Schottky contacts. The Schottky barrier height (0.665 ± 0.005 eV for the Ag/H-Si reference sample) tends to decrease (i.e. by approximately 0.15 eV for 4ML) with increasing organic interlayer thickness. The I-V curves under forward bias were simulated in order to extract the Schottky barrier and the results were compared with experimental ones.

SYSA 5.10 Tue 14:30 Poster A

Investigation of buried metal-organic interface with Photoelectron spectros-copy (PES) — •Pavo Vrdoljak[1], Achim Schöll[1], Friedrich Reinert[1], and Eberhard Umbach[2] — [1]Universität Würzburg, Experimentelle Physik II, 97074 Würzburg — [2]Forschungszentrum Karlsruhe, 76021 Karlsruhe

Metal-organic interfaces are of crucial importance for electronic devices since they influence the layer morphology, the electronic structure at contacts, and the charge carrier transport. Various investigations have addressed this issue from the viewpoint of surface science, applying model systems with thin organic films on flat (single crystalline or amorphous) metal substrates. The contacts in electronic devices, however, can be very different. This is mainly due to the morphological roughness of the interface in case of a metal top contact deposited on an organic layer and the possible influence on the electronic structure. In case of real contacts also interdiffusion has to be taken into account. However, surface sensitive techniques such as photoelectron spectroscopy (PES) and atomic force microscopy (AFM) can not immediately access the buried interface. To tackle this problem we have applied and optimised a lift-off technique which allows the removal of the metal top-contact in the UHV and analyse the interface between the contact and the organic film. We will present first PES and AFM results of Au contacts deposited on PTCDA layers.

SYSA 5.11 Tue 14:30 Poster A

Morphology, electronic and crystal structure of Pentacene/Fullerene layered and co-deposited thin films on PEDOT:PSS — •Ingo Salzmann, Steffen Duhm, Ricarda Opitz, Jian Zhang, Jürgen P. Rabe, and Norbert Koch — Humboldt-Universität zu Berlin, Institut für Physik, D-12489 Berlin, Germany

The electronic structure of bilayer and co-deposited thin films of pentacene (P) and fullerene (C60) on the conducting polymer poly(ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) has been investigated by ultraviolet photoelectron spectroscopy. For a film of C60 on P covered PEDOT:PSS an energy offset between the highest occupied molecular orbital (HOMO) levels of C60 and P of 1.7 eV was found. The P-HOMO was Fermi-level pinned with the HOMO-onset at 0.35 eV binding energy and charge transfer between P and PEDOT:PSS lowered the sample work function by 0.7 eV. The C60 energy levels were vacuum level aligned relative to P. Reversing the deposition sequence leads to an onset of the P-HOMO at 0.3 eV above the Fermi level indicating a lack of thermodynamic equilibrium between PEDOT:PSS and P. Co-deposited films (ratio 1:1) exhibited an offset between the P and C60 HOMO levels of 1.1 eV, which increased to the initial value of 1.7 eV by pre-covering PEDOT:PSS with a thin P layer. Atomic force microscopy and x-ray diffraction investigations revealed phase separation of P and C60 in the co-deposited films as well as crystalline growth of P in all cases, whereas C60 was crystalline only if grown on P. Organic photovoltaic device characteristics could be correlated with the results above.

SYSA 5.12 Tue 14:30 Poster A

Transport properties and morphology of solution processed pentacene transistors — •Markus Kasper, Claudia Bock, and Ulrich Kunze — Werkstoffe und Nanoelektronik, Ruhr Universität Bochum, D-44780 Bochum, Germany

Recent developments have shown that precursors enabling solution deposition of pentacene thin films begin to rival vacuum deposited pentacene for organic field-effect transistor (OFET) applications. In this contribution 13,6-N-Sulfinylacetamidopentacene (NSFAAP) is used to fabricate and characterise bottom-contact OFETs with SiO_2 dielectric. We study the influence of source and drain contact metals and the effect of a supplemental HMDS pretreatment of the gate oxide on the transport properties and the pentacene film morphology. In order to separate the sheet resistance from the parasitic series resistance of the contacts and leads different transistors with a channel length between $L = 3$ and 100 μm are prepared. All transistors have a constant channel width of $W = 2$ mm. The pentacene thin films are deposited by spin coating NSFAAP from a $CHCl_3$ solution in air and thermally converting the precursor to pentacene in a nitrogen environment. In order to achieve a homogenous film morphology and an improved coupling of the organic film to the electrodes the process parameters like spinning speed and conversion temperature are optimised.

SYSA 5.13 Tue 14:30 Poster A

Phosphorescence Quenching in Ir(III)-complexes — •Alex Thiessen, Dirk Hertel, and Klaus Meerholz — Institute of Physical Chemistry, University of Cologne, Luxemburger Str. 116, 50939 Cologne, Germany

Recently [1], we reported a study of phosphorescence quenching in polyspirobifluorene doped with the phosphorescent emitter platinum-porphyrin (PtOEP). It was shown that the phosphorescence reduction is due to the interaction of triplet excitons with charges (polarons) in a unipolar diode structure. The rate constant for triplet-polaron interaction has been evaluated to be 10-13 cm3/s leading to an interaction radius of 0.2 nm. In our current work we have used the methodology [1] to elucidate the role of this process in materials relevant to phosphorescent OLEDs. We have studied a red-emitting Ir(III)-complex doped into low molecular weight materials and in polymers. It will be shown, that the efficiency of triplet-polaron annihilation depends mostly on the nature of the matrix and not on the structure of the heavy-metal complex. The results give insight to a possible origin of the magneto-resistance effects in organic materials [2]. Recently [3], it has been proposed that triplet-polaron annihilation might play a crucial role. We will discuss the influence of magnetic fields on the triplet-polaron annihilation for our model system.

References [1] Hertel, D.; et al. J. Phys. Chem. B 2007, 111, 12075. [2] Mermer, O.; et al. Phys. Rev. B 2005, 72, 202202. [3] Desai, P.; et al. Phys. Rev. B 2007, 75, 094423.

SYSA 5.14 Tue 14:30 Poster A

Investigation of the influence of substrate temperature on growth, structure and morphology of VTE processed perylene thin films on SiO_2 substrates — •Philip Schulz, Phenwisa Niyamakom, Azadeh Farahzadi, Christian Effertz, Maryam Beigmohamadi, and Matthias Wuttig — Institute of Physics (IA), RWTH Aachen University, 52074 Aachen, Germany

It has been shown recently, that perylene based Organic Thin Film Transistors (OTFTs) are capable to yield high field effect mobilities. The substrate temperature during deposition has a pronounced influence on the growth of perylene thin films processed by Vacuum Thermal Evaporation (VTE). By adjusting this parameter the structure of the film, and in turn its electronic and optical properties, can be controlled in order to tailor the film to suit the specific application.

In this work, perylene thin films have been evaporated on SiO_2 layers held at temperatures between 235 K and 340 K. Subsequently, the structural and optical properties have been determined ex-situ by a set of complementary characterisation techniques.

The morphology of the films is investigated by Atomic Force Microscopy (AFM) yielding the roughness and lateral correlation length. Density and film thickness have been determined from X-ray Reflectometry (XRR). The vertical grain size, microstrain and d-spacing have been extracted from X-ray Diffraction experiments (XRD). The optical constants and anisotropy were analysed by ellipsometry measurements. All results have been correlated to the film adhesion on substrates modified with different surface treatments.

SYSA 5.15 Tue 14:30 Poster A

Luminescence line shifts of ultrathin rubrene layers on epitaxial aluminium oxide — •Mathias Müller, Olga Krylova, and Moritz Sokolowski — Institut für physikalische und theoretische Physik, Universität Bonn, Wegelerstraße 12, 53111 Bonn

We have investigated the photoluminescence properties of rubrene films on an ultrathin layer of aluminium oxide under UHV-conditions. The ultrathin alumina layer was grown epitaxially on $Ni_3Al(111)$ by heating of the sample under low oxygen pressure. Afterwards rubrene films of varying thickness (d) were evaporated onto the alumina. The photoluminescence (PL) was measured at 40 K using an argon-ion-laser for excitation and an N_2 cooled CCD-Spectrometer for detection. PL-Spectra could be detected from d=0,6 Å upwards. Both the positions and the intensities of the transitions show strong changes depending on the nominal film thickness. With increasing film thickness the intensity decreases by three orders of magnitude whereas the entire spectrum shifts continuously to smaller wavenumbers ($1200\,cm^{-1}$ for d=0,6 Å to 79 Å). These changes are tentatively interpreted as an emission from the center of small clusters, that have been formed on the surface. Funding by DFG research unit 557 is gratefully acknowledged.

SYSA 5.16 Tue 14:30 Poster A

Interface reactions of ferroelectric copolymer layers with different electrode materials — •Klaus Müller, Dipankar Mandal, Karsten Henkel, Ioanna Paloumpa, and Dieter Schmeisser — Brandenburgische Technische Universität Cottbus, Angewandte Physik - Sensorik, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany

The ferroelectric copolymer poly(vinylidene fluoride trifluoroethylene) (P(VDF-TrFE)) is a possible material for low cost applications as organic nonvolatile memory element. We present an XPS interface investigation of the copolymer/electrode interface. Below 100nm film thickness, interface phenomena becomes important. Possible interface reactions could lead to a reduction of the ferroelectric functionality.We present a comparative study of the two interfaces Al/P(VDF-TrFE) and PEDOT:PSS/P(VDF-TrFE). The result is a clear indication of a surface reaction in between the Aluminum-electrodes. In contrast, for PEDOT:PSS the measurements shows a layer by layer formation of the interface PEDOT:PSS/PVDF without any reaction. Second, we present a study of remanent polarization of ultrathin spincoated films of the copolymer, in a thickness range from 5 to 100mn, with organic electrodes like PEDOT:PSS. The measurements are carried out by using the flatband shift of a capacitance-voltage (CV) characteristic. This shift of flatband voltage is used as value for the electric polarization of the polymer.

SYSA 5.17 Tue 14:30 Poster A

Temperature dependent growth and morphology of perylene thin films on gold substrates — •Phenwisa Niyamakom, Philip Schulz, Azadeh Farahzadi, Li Ding, Maryam Beigmohamadi, and Matthias Wuttig — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

In this study, the influence of substrate temperature on the growth and morphology of thin perylene films deposited on gold substrates us studied. The films have been deposited at different substrate temperatures and film thicknesses by vacuum thermal evaporation (VTE), have been investigated. Atomic force microscopy (AFM) has been performed to study film morphology as the surface roughness and evolution of perylene film growth. The structural properties and molecular vibrations of perylene thin films have been studied by X-ray diffractometry (XRD) and Fourier transform infrared spectroscopy (FTIR). Finally, a model for the perylene thin film growth is presented.

SYSA 5.18 Tue 14:30 Poster A

Strong screening in photoemission at interfaces between organic semiconductors and gold: polarization effects versus charge transfer — •Daniel Kolacyak[1], Heiko Peisert[1], André Petershans[2], and Thomas Chassé[1] — [1]Universität Tübingen, Institut für Physikalische Chemie — [2]Forschungszentrum Karlsruhe, Institut für Technische Chemie

We studied electronic polarization effects at organic/metal interfaces using combined photoemission spectroscopy (PES) and x-ray excited Auger electron spectroscopy (XAES) as a function of the organic layer thickness. As a model system, sandwich structures of metallphthalocyanines (e.g consisting of PcMg and PcZn) were deposited on gold. It was found, that the screening of the photohole is remarkably increased for molecules directly at the interface whereas further layers are affected weakly. This may be caused by a fast charge transfer across the interface as a result of the photoionization due to the overlap organic/metal wave functions. Furthermore, differences in the screening were found for buried molecules and molecules on the surface of the organic film ascribed to different polarization energies. The influence of the morphology and orientation was studied by comparing different substrates: polycrystalline gold foil and single crystalline Au(100).

SYSA 5.19 Tue 14:30 Poster A

An Infrared Spectroscopy and X-ray Diffraction Study of the medium length *n*-Hexadecanol solidified in mesoporous silicon — Anke Henschel, •René Berwanger, Rolf Pelster, Klaus Knorr, and Patrick Huber — Saarland University, Saarbruecken, Germany

The conformation and arrangement of the *n*-alcohol $C_{16}H_{33}OH$ confined in tubular pores of porous silicon (mean pore diameter 10nm, pore length 70 μm) is investigated by combined Infrared Spectroscopy and X-Ray Diffraction measurements. The phase behaviour is reminiscent of the one found for the linear n-alkanes confined in mesoporous silicon[1]: the long axes of the molecules are oriented perpendicular to the pore axes. About the long axes of the pores we find a four-fold symmetry of the diffraction pattern, coinciding with the symmetry of the silicon matrix. The confined alcohol exhibits six dominant domains.

We find distinct changes in the vibration characteristics, in the structure factor as well as the phase transition temperatures of the confined alcohol as compared to the bulk phase. The phase sequence in the pores is liquid, Rotator and crystalline. The melting and freezing transitions are reduced by 20 K.

[1] A. Henschel, T. Hofmann, P. Huber, K. Knorr, Phys. Rev. E 75, 021607 (2007)

SYSA 5.20 Tue 14:30 Poster A

NTCDA as transparent electron transport material in organic p-i-n solar cells — •Christiane Falkenberg[1], Christian Uhrich[1], Selina Olthof[1], Bert Männig[1,2], Moritz Riede[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01069 Dresden, Germany, http://www.iapp.de — [2]Now at Heliatek GmbH, Liebigstr. 26, 01187 Dresden, Germany

In organic p-i-n-solar cells, the active layer where light is absorbed and free charge carriers are generated is sandwiched between two doped charge carrier transport layers which are preferentially electron or hole conducting. In order to increase the efficiency of organic photovoltaic devices, the properties of those doped layers play a crucial role: high conductivities and charge carrier mobilities, thermal and morphological stability, and a good energy level alignment relative to the neighboring active layers are required. We investigate here the electron transport materials and successfully substitute the standard system consisting of n-C_{60} by the wide-gap material NTCDA (naphthalenetetracarboxylic dianhydride). Unlike C_{60}, it does not absorb in the visible range and therefore blocks the excitons which were created in the active layer. Combined photoelectron spectroscopy (PES) and absorption determine HOMO and LUMO energies of -8.01eV and approximately -4.5...-4.0eV, respectively. Furthermore, the electronic structure of the aluminum/NTCDA-contact and the morphology of thin evaporated layers are analyzed via PES and AFM, respectively. The power conversion efficiency of simple p-i-n-cell structures is improved by 10% upon substitution of C_{60} in electron transport layers by NTCDA.

SYSA 5.21 Tue 14:30 Poster A

Surface modification for improved charge injection in copper electrode/ organic semiconductor interfaces of p-type OFET applications — •Johannes Frisch[1], Norbert Koch[1], and Silvia Janietz[2] — [1]Humboldt-Universität zu Berlin, Department of Physics, Newtonstrasse 15, D-12489 Berlin, Germany — [2]Fraunhofer-Institute of Applied Polymer Research, Department Polymer Elektronics, Geiselbergstr. 69 D-14476 Potsdam, Germany

Very important for the development of practical applications in organic field effect transistors (OFETs) are high On-current and ON/Off ratio. The On-current in p-type OFET devices is limited by the hole injection density. One way to modify charge injection properties is to introduce a monolayer of the strong electron acceptor tetrafluorotetracyanoquinodimathane (F4-TCNQ) at the Cu-electrode/ organic hole transport layer (OHTL) interface. The adsorbed monolayer of F4-TCNQ results in an increase in work function and consequently in a reduction of the hole injection barrier. XPS analysis showed a significant difference between untreated and modified surfaces. Top gate structure OFETs with bottom contact and flexible substrates were produced to evaluate the influence of the modified Cu-electrode/ OHTL interface. The OFET-performance was evaluated in comparison to the conventional device structure without F4-TCNQ. The results of the Transfer-measurements and Output-characteristics corroborate the advantages of the modification with respect to high On-current, lower threshold voltage and operational stability.

SYSA 5.22 Tue 14:30 Poster A

Effect of blending ratio and internal order on the optical properties of P3HT:PCBM bulk heterojunction films — •Thomas Madena, Martin Knipper, Ingo Riedel, and Jürgen Parisi — Energy- and Semiconductor Research Laboratory, Department of Physics, University of Oldenburg, Carl-von-Ossietzky-Strasse 9-11, D-26111 Oldenburg

Organic solar cells represent thin film devices comprising a multilayer system of planar semiconductor films finished with a metal electrode. Internal reflections of the incident light and the resulting coherent superposition of electromagnetic waves travelling in opposite directions cause a spatially nonuniform light intensity distribution. Calculation of the intensity pattern along the cross section of the device is an essential step for optimizing the photocurrent in single junction and in particular multispectral tandem devices. Provided that thickness and optical constants of individual layers of the device are known optical simulation of the light propagation can be carried out via the transfer matrix formalism. In this work we investigated the absorber of solution-processed organic solar cells based on conjugated polymer-fullerene (P3HT: PCBM) bulk heterojunctions. Variation of the blending ratio and thermal annealing of the films have strong impact on the device performance. Ellipsometry was applied together with structural analysis of P3HT: PCBM films in order to relate their optical response to the film composition and thermally induced internal ordering. The results are correlated with the measured photocurrent and spectral response of solar cells with respective active layer composition.

SYSA 5.23 Tue 14:30 Poster A

Monitoring the growth of thin metal phthalocyanine films via Raman scattering — •Britt-Elfriede Schuster[1], Cameliu Himcinschi[2], Marius Toader[2], Heiko Peisert[1], Thomas Chassé[1], and Dietrich R. T. Zahn[2] — [1]Institute of Physical and Theoretical Chemistry, University of Tübingen; Auf der Morgenstelle 8, 72076 Tübingen, Germany. — [2]Semiconductor Physics, Chemnitz University of Technology; Reichenhainer Straße 70, 09126 Chemnitz, Germany.

Due to their unique properties, (metal) phthalocyanines (MPc) are highly attractive materials and promising candidates for various applications e.g. in fields of organic light emitting diodes or organic field effect transistors. Since device efficiency and performance are significantly influenced by the physical properties of the thin organic films, intensive studies of the growth and the influence of preparation parameters are very important for thin film technology. In this work the growth of copper(II)phthalocyanine (CuPc) and titanyl(IV)phthalocyanine (TiOPc) on the technically relevant substrate silicon is assessed by in situ monitoring of the Raman scattering of internal vibrational modes to study e.g. the evolution of the polymorphic modifications during the growth and/or the molecular arrangement within the organic layers. The thermal evaporation of metals like silver on the organic films under ultra-high vacuum conditions provides further information about the interface formation. In this regard the occurrence of new Raman modes, normally being infrared active, suggest the interaction of the metal with the phthalocyanine film via a charge transfer.

SYSA 5.24 Tue 14:30 Poster A

Improving electron injection in organic light emitting diodes using a thin Li3PO4 layer — •Andrea Gassmann, Christian Melzer, and Heinz von Seggern — Technische Universität Darmstadt, Institute for Materials Science, Electronic Materials Division, Petersenstr. 23, 64287 Darmstadt

In this contribution a novel cathode material is introduced allowing for device performances comparable to the benchmark cathode LiF / Al. A thin layer of the metal salt lithium phosphate Li3PO4 is deposited between the organic semiconductor and an Al cathode. In normal OLED structures it will be disclosed that both the current density and the luminance increase similarly to the characteristics of reference devices fabricated with LiF / Al cathodes. This increase can be ascribed to an enhanced electron injection.

Regarding the origin of the observed device characteristic improvement through Li3PO4 / Al, a field enhanced injection due to piled - up holes at the cathode side can be excluded since the improvement of device characteristics holds also true in electron-only devices. Moreover, it was observed that Li3PO4 is most beneficial to the device performance at a thickness of 7 Å. Concerning the doping ability of Li3PO4, devices with co-evaporated organic semiconductor were prepared revealing a deterioration of device characteristics. Furthermore, in capacitance/ voltage measurements no evidence of doping was found. Therefore, the focal point of Li3PO4 / Al research is attributed to interface properties what is the subject of current and future investigations.

SYSA 5.25 Tue 14:30 Poster A

Charge transfer doping of organic diodes: A theoretical study — •Oliver Ottinger, Christian Melzer, and Heinz von Seggern — Electronic Materials Division, Institute of Materials Science, Technische Universität Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany

Charge transfer doping is a promising concept for improving charge injection from metals into organic semiconductors. A self-consistent model of an unipolar electron-only metal/insulator/metal (MIM) diode based on drift diffusion theory was applied. It allows for the description of injection as well as space charge limited currents. The model was extended by charge transfer doping with arbitrary doping profiles. Besides modelling the steady state current density-voltage characteristics and the respective electric field- and charge carrier distributions, the response on an ac disturbance has been considered in order to model impedance measurements. Simulations were done for bulk doped and near-interface doped diodes.

It will be shown, that doping in the vicinity of the cathode results in an improved device performance. This stems from an electric field induced inherent barrier lowering promoting the electron injection. A bulk doped MIM system can be well understood as two Schottky diodes in series while one is forward and the other is reverse biased. Simulating CV characteristics it was shown that both resulting depletion capacitances determine the time dependent characteristics of the device.

SYSA 5.26 Tue 14:30 Poster A

Charge injection in light emitting organic field effect transistors — •Martin Schidleja, Christian Melzer, and Heinz von Seggern — Electronic Materials Division, Institute of Materials Science, Technische Universität Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany

Light emitting organic field effect transistors with different metals used as source and drain contacts are investigated. The transistors are built in a top-gate, bottom-contact configuration with poly(9,9-di-n-octyl-fluorene-alt-benzothidiazole) (F8BT) as organic semiconductor and poly(methyl methacrylate) (PMMA) as gate-dielectric. For the drain and source electrodes either gold or silver is used. While gold results in balanced injection barriers for hole and electron injection of about 1 eV, the use of silver disturbs this essential balance in the injection properties.

The drain current and the position of the recombination zone in the transistor channel at different voltages are measured for the respective transistors. It is found that the experimental data cannot be explained by the standard equations for ambipolar transistors, most probably due to large injection barriers and hence, high contact resistances. In order to evaluate the results, a numerical model is introduced, taking into account the influence of different injection-barriers on the ambipolar behaviour of organic field effect transistors by separate calculation of the injection currents at the source and drain contacts, respectively. Our results stress the importance of contact phenomena in light emitting organic field effect transistors.

SYSA 5.27 Tue 14:30 Poster A

Vacuum deposited films of dicyanovinylene-capped oligothiophenes for use in organic solar cells — •Marieta Levichkova[1], David Wynands[1], Moritz Riede[1], Martin Pfeiffer[2], Eduard Brier[3], Egon Reinold[3], Peter Bäuerle[3], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, TU Dresden, 01062 Dresden — [2]Heliatek GmbH, 01187 Dresden — [3]Institut für Organische Chemie II und Neue Materialien, Universität Ulm, 89081 Ulm

Solar cells based on oligothiophene derivatives comprising electron-accepting dicyanovinyl groups have shown high power efficiencies (up to 3.4%). Here, we study the effect of substrate temperature on the morphology and photopysical properties of DCV6T (α,ω-bis-(dicyanovenylen)-sexithiophene) films with the aim to optimize the active layer structure. The films are prepared by vapor deposition on quartz substrates covered with amorphous hole transport layer. During the evaporation of DCV6T, the substrates are kept at constant temperatures between 20°C and 100°C. AFM images show increased grain size and surface roughness of the samples grown at higher T_{sub}. The alteration of surface topography is accompanied by an enhanced and red-shifted absorption which we attribute to a more ordered molecular arrangement leading to a co-planarization of the thiophene rings within the oligomers. Also, for the samples grown at $T_{sub} \geq 80$°C, the overlap between absorption and luminescence increases which suggests an increase in exciton diffusion length. Finally, we will discuss the effect of the various DCV6T morphologies on the performance of solar cells.

SYSA 5.28 Tue 14:30 Poster A

Initial growth of evaporated copper phthalocyanine thin-films - Comparison of metal and oxide substrates — •Indro Biswas[1], Heiko Peisert[1], Mathias Nagel[1], Maria Benedetta Casu[1], Britt-Elfriede Schuster[1], Stefan Schuppler[2], Peter Nagel[2], Michael Merz[2], and Thomas Chassé[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Auf der Morgenstelle 8, 72076 Tübingen — [2]Institut für Festkörperphysik, Forschungszentrum Karlsruhe, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen

The growth of copper phthalocyanine thin films evaporated on various substrates has been examined in detail, using near-edge x-ray absorption fine structure (NEXAFS) spectroscopy and surface-sensitive x-ray photoemission spectroscopy (SXPS). The focus is on interfaces relevant for technical applications, i.e. metals and oxide conductors as contact electrodes in OLEDs and solar cells, and insulators as dielectric materials in OFETs. The molecular orientation of thin-films in the range of 0.2 to 3.0 nm thickness was examined, with a special focus on the layers directly at the interface. Metal substrates generally lead to an interfacial layer of flat lying molecules, even on rough polycrystalline substrates. On the used oxide substrates (SiO_2) and indium tin oxide) the initial molecular orientation is not lying on rough surfaces, with the exception of a single crystalline substrate (TiO_2). The growth mode is discussed in terms of interfacial and intermolecular interactions and of preparation parameters.

SYSA 5.29 Tue 14:30 Poster A

Transparent Contacting Materials for Organic Solar Cells — •Jan Meiss, Moritz K. Riede, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden

Organic solar cells are emerging as a possible inexpensive alternative to inorganic photovoltaics. A current cost issue of organic solar cells is the high price of indium tin oxide (ITO), the most commonly used transparent contacting material. We are exploring alternatives to replace the scarce and expensive indium. Promising candidates are ZnO:Al or the highly conductive polymer PEDOT:PSS.

Here, we present the first small-molecule organic solar cells employing only PEDOT:PSS as transparent anode. Both cells on glass and on flexible PET foil were made, using thermally evaporated ZnPc/C60 as donor-acceptor heterojunction and metal contacts as back electrode. Different methods to structure the PEDOT:PSS electrodes were investigated and are presented, e.g. by dip-coating in a solution of polystyrene in toluene or by using pre-patterned plastic foil.

Resulting prototype cells with open-circuit voltages of up to 0.48 V, currents of 5 mA/cmˆ2 and fill factors > 50% were obtained with efficiencies of up to 0.99% (on flexible plastic foil) and 0.7% (on glass) for non-optimized experimental cells.

SYSA 5.30 Tue 14:30 Poster A

Photo and electric-field induced absorption in organic materials for solar cell use — •Martin Knipper, Janet Neerken, and Jürgen Parisi — Energy and Semiconductor Research Laboratory, Department of Physics, University of Oldenburg, 26111 Oldenburg

Photo induced absorption (PIA) measurements are done at poly[2-metoxy-5-(3-,7-dimethyloctyloxy)-p-phenylene vinylene (MDMO-PPV) and at MDMO-PPV blended with [6,6]-phenyl-C61-butyric acid methyl ester (PCBM). This material combination is used for organic solar cells. The results from this optical measurement show us a charge transfer in the blended material. The aim of the new work is to do the absorption measurement electric-field induced. Therefore we sandwich the absorber layer between a transparent indium tin oxide (ITO) front electrode covered with a polymer buffer layer (PEDOT:PSS) and an aluminum back electrode. The aluminum electrode is semitransparent for this experiment. The electric-field induced absorption measurements show us signals at characteristic energies. From the peaks of the signal we can draw conclusions about absorption and charge transfer in the active layer of the organic solar cell in a real solar cell structure.

SYSA 5.31 Tue 14:30 Poster A

Light incoupling in small molecule organic solar cells — •Nikola Allinger[1], Jan Meiss[1], Moritz Riede[1], Karl Leo[1], and Wolf-Michael Gnehr[2] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01069 Dresden (Germany) — [2]Heliatek GmbH, Liebigstraße 26, 01187 Dresden (Germany)

Light incoupling is an essential topic for optimization of organic solar cells. In our group, we examine light incoupling of different kinds of transparent contacting materials as well as external dielectric coatings, using optical simulation of thin film systems and experimental methods. Thin films of small molecules are prepared by thermal evaporation in a multi-chamber UHV system. Complex refraction indices of various materials are calculated from reflection and transmission measurements of monolayers. For modelling of optical properties of thin film systems, we developed a numerical simulation program based on the transfer matrix method. The cell structures investigated consist of nanolayers of small molecules, using ZnPc/C60 as an acceptor-donor heterojunction. As contact materials, we compare the expensive standard material indium tin oxide (ITO) with more cost-efficient alternatives like thin Ag layers or spin-coated layers of the polymer PEDOT:PSS, and discuss the resulting cell properties. Additional dielectric layers of varying materials, like tris(8-hydroxy-quinolinate)-aluminum (Alq3) or N,N'-tetrakis(4-methoxyphenyl)-benzidine (MeO-TPD), are deposited on top of the stack and their influence on cell efficiencies is investigated.

SYSA 5.32 Tue 14:30 Poster A

Switching behaviour of organic field effect transistors — •Ingo Hörselmann, Andrei Herasimovich, and Susanne Scheinert — TU Ilmenau, Germany

We prepared an organic field effect transistor with source/drain electrodes self-alligned to the bottom gate contact, resulting in a low parasitic gate-drain capacitance of 6 pF/cm. As gate insulator we used a 200 nm silicon nitride layer grown by chemical vapor deposition (CVD). The active semiconductor material is spincoated Poly(3-hexylthiophene) P3HT. The channel length is 2 μm, the measured transconductance cut-off frequency is 2.4 kHz at V_{GS}=V_{DS}=-20 V.

To investigate the transient behavior of the transistor, we switched the drain and gate potential with rectangle pulses and recorded the transient response of the source and drain currents. Because of the low parasitic capacitance it is possible to record the delay between switching the potential and the current flow through the transistor channel. Hysterese effects were investigated by variation the duty factor of gate potential pulses, resulting in different on-currents.

We compare the measured switching behaviour with two dimensional device simulations. The simulation describes the tendency of the measurement. During switch on by decreasing the gate potential, the source current is greater than the drain current because the carriers are mostly injected from the soure contact to build up the channel. During switch off the currents at source and drain are similar, because the holes flow from the accumulation channel to both contacts.

SYSA 5.33 Tue 14:30 Poster A

Temperature dependant resonant photoemission and NEXAFS study of zinc(II)phthalocyanine on poly- and single crystalline gold — •Britt-Elfriede Schuster[1], Indro Biswas[1], Maria Benedetta Casu[1], David Batchelor[2], Martin Knupfer[3], Heiko Peisert[1], and Thomas Chassé[1] — [1]Institute of Physical and Theoretical Chemistry, University of Tübingen, 72076 Tübingen. — [2]BESSY GmbH, 12489 Berlin. — [3]Leibniz Institute for Solid State and Materials Research Dresden, P.O. Box 270116, 01171 Dresden.

The arrangement and the orientation of organic molecules are crucial for charge transport properties and thus essential for the efficiency of devices based on these materials. Mechanisms for the charge transport in organic materials depend significantly on the temperature. As an example, the localisation energy based on electron-phonon coupling decreases significantly at low temperature, as a consequence different transport channels (band-like or hopping) are possible. In this work we investigate whether such phenomena are accompanied by changes of the intermolecular interaction and the orientation of the molecules. We observe an increase of the molecular ordering of zinc(II)phthalocyanine at low temperatures (liquid He) in particular on polycrystalline Au using polarisation dependent near edge X-ray absorption spectroscopy (NEXAFS). This can be understood by an increase of the intermolecular interaction and by a decrease of the electron-phonon coupling. Resonant photoemission data for C1s show a weaker participator resonance intensity at low temperature, which is discussed in terms of different de-excitation channels.

SYSA 5.34 Tue 14:30 Poster A

Solution-processed OFET with pentacene layer — •Andrei Herasimovich, Carsten Geigengack, Ingo Hörselmann, and Susanne Scheinert — TU Ilmenau, Germany

The solubility is one important property of organic semiconductors for the low cost preparation of the polymer layers from solution. However, many organic materials with high charge carrier mobility such as pentacene are insoluble in organic solvents at room temperature. Our goal was to investigate electrical properties of organic field effect transistors (OFET) based on a pentacene semiconductor film obtained from soluble precursor (N -Acethyl -6,13 -epithioimino -6 -13 -aihydropentacene -S -Oxide). Pentacene films were fabricated by spin-coating from 1-2%(m/m) precursor in a chloroform solution followed by annealing at 130-200°C under a nitrogen atmosphere to convert the precursor to pentacene. The conversion was confirmed by XPS and GDOES (glow discharge optical emission spectroscopy) element analysis and by UV-VIS optical measurements. We have found that the annealing conditions influence strongly the electrical properties of the OFETs. However, transistors with optimized annealing conditions have a good inverse subthreshold slope of 0.2 V/dec, an on/off ratio of 10^6 and high charge carrier mobilities of 0.01-0.1 cm^2/Vs. We demonstrate also that OFET characteristics depend on insulator and contact properties.

SYSA 5.35 Tue 14:30 Poster A

Thin-Film Properties of DNA und RNA Bases: A Combined Experimental and Theoretical Study — •Andrea Haug, Sabine Schweizer, Florian Latteyer, Maria Benedetta Casu, Heiko Peisert, Christian Ochsenfeld, and Thomas Chassé — Institut für Physik. und Theoret. Chemie, Universität Tübingen

In recent years significant progress has been made in the use of organic materials as building blocks of organic electronics. The research has also been expanded in the field of bioorganic materials like DNA/RNA bases and their derivatives. The bases show interesting electronic properties that make possible the use of these molecules, e.g. as organic layers in OFET [1]. The structures of the DNA/RNA bases cytosine, uracil, and thymine in thin films with a nominal film thickness of >20 nm were studied using photoemission (XPS, UPS) and FTIR spectroscopy. The bases were evaporated in situ from powder on gold foil. The experimental results indicate that cytosine is composed of two energetically close tautomeric forms, whereas uracil and thymine exist only in one tautomeric form. For complementing the results, relative energies of tautomeric forms of cytosine, uracil, and thymine were calculated using Hartree-Fock (HF), density functional theory, and post-HF methods. Furthermore, the assignment of XPS spectra is supported by simple model considerations employing Koopmans ionization energies and Mulliken net atomic charges. The bases were also investigated in various film thicknesses (0.1-10 nm) focussing on the interface properties base-gold. [1] G. Maruccio et al. Nano Lett. 2003, 3, 479

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SYSA 5.36 Tue 14:30 Poster A

External Quantum Efficiency of p-i-n Solar Cells incorporating Oligothiophene:Fullerene Heterojunctions — •Holger Seifert[1], Rico Schueppel[1], Eduard Brier[2], Egon Reinold[2], Peter Baeuerle[2], Moritz K. Riede[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden — [2]Institut für Organische Chemie II und Neue Materialien, Universität Ulm

We investigate organic p-i-n solar cells with an oligothiophene derivative as donor and Fullerene C_{60} as acceptor materials. This donor-acceptor heterojunction leads to solar cells with an open circuit voltage as high as 1.0V and a reasonable power conversion efficiency of up to 3.4% [1].

Measuring current-voltage characteristics under monochromatic illumination of low intensity (non-standard reporting conditions), we find a wavelength dependent fill factor of these photovoltaic devices.

Furthermore, we determine the external quantum efficiency (EQE) from the photoresponse of these devices using a modulated monochromatic illumination on top of a white light bias as well as an external voltage bias. The EQE spectrum can be attributed to the spectrally different absorption of donor and acceptor. We discuss the dependence of the EQE spectrum from the applied external voltage with respect to the charge generation mechanism.

[1] K. Schulze et al., Adv. Mater. 18, 2872 (2006).

SYSA 5.37 Tue 14:30 Poster A

Electronic and optical properties of evaporated organic bulk heterojunctions — •Robin Knecht[1], Günther Schnurpfeil[2], and Derck Schlettwein[1] — [1]Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, D-35392 Gießen, Germany — [2]Institut für Organische und Makromolekulare Chemie, Universität Bremen, Leobener Strasse NW 2, D-28334 Bremen, Germany

The formation of evaporated blends of organic donor and acceptor molecules has gained interest recently for active interlayers in organic photovoltaic cells and organic field effect structures.

In this contribution we report about the combination of one component of high aggregation probability towards crystalline pathways (e.g. phthalocyaninato zinc II, *PcZn*) with another component of low aggregation probability towards a widely amorphous matrix (e.g. $Cl_4MePTCDI$, a chlorinated perylene imid).

Mixed films were created by simultaneous physical vapour deposition of both substances to create an evaporated organic bulk heterojunction and studied for their potential as materials for organic photovoltaic devices. Using transmission spectroscopy, structure analysis and photovoltaic test measurements electronic and optical properties were investigated and compared with the properties of the single films and solution spectra.

SYSA 5.38 Tue 14:30 Poster A

Comparison of high mobility P3HT and pBTTT semiconducting polymers — •Silviu Botnaras[1], Arne Hoppe[1], Benedikt Gburek[1], Martin Heeney[2], and Veit Wagner[1] — [1]Jacobs University Bremen, School of Engineering and Science, 28725 Bremen, Germany — [2]Centre for Materials Research, Queen Mary University of London, London E1 4NS, UK

Polythiophenes are well known for their semiconducting properties and for their application in organic electronic devices such as thin film transistors or organic solar cells. Due to the possibility of low-temperature solution-processing and high charge carrier mobility these polymers are possible candidates for large area commercial applications. Regioregular poly(3-hexylthiophene) (rr-P3HT) with reported charge carrier mobilities larger than 0.1 cm2/Vs has been well established as a polymeric model system in the last years. One disadvantage of P3HT, however, is the low stability under ambient conditions. Within the last two years a new class of polymers emerged with even higher mobilities and increased air stability: Polythienothiophenes. We report on a study of poly(2,5-bis(3-alkylthiophen-2yl)thieno[3,2-b]thiophene) (pBTTT) with reported charge carrier mobilities up to 0.6 cm2/Vs. We found charge carrier mobilities larger than 0.1 cm2/Vs for solution processed devices on silicon dioxide as insulating layer. A comparison of the pBTTT and P3HT devices is presented with respect to air stability, contact properties and functionality on silicon and polymeric substrates. The analysis demonstrates the superior properties for pBTTT.

SYSA 5.39 Tue 14:30 Poster A

Threshold voltage shift in OFETs due to charges stored in a polymer dielectric — •Niels Benson, Christian Melzer, and Heinz von Seggern — Technische Universität Darmstadt, Institute of Materials Science, Division: Electronic Materials, Petersenstraße 23, D-64287 Darmstadt, Germany

Considering organic field effect transistors (OFETs), we recently demonstrated that a significant positive threshold voltage shift of ΔVth $\approx$ 60V can be obtained when negative charges are trapped in a near surface layer of a polymer gate dielectric. This charge leads to an effective field enhancement at the contacts and allows for an effective hole injection from Ca electrodes into pentacene.

Here we present the complementary experiment, were a negative ΔVth is obtained as the result of positive charges stored in the OFET dielectric. The utilized pentacene OFET comprises Au drain/source electrodes, as well as a Polymethylmethacrylat (PMMA) insulator. The positive charge is stored in the PMMA dielectric by exposing the OFET to different electric field strengths at a forming temperature of T = 108°C. For an electric field strength of 2MV/cm between the transistor channel and the gate electrode, during the forming step, a negative threshold voltage shift of ΔVth $\approx$ -29V was obtained. In addition, to the observed threshold voltage shift an electron current is measured in the pentacene OFET, comprising Au source/drain electrodes. This current occurred despite an injection barrier of $\approx$ 2.2eV.

SYSA 5.40 Tue 14:30 Poster A

Visualizing the Frontier Orbitals of a Conformationally Adapted Metalloporphyrin — •Joachim Reichert[1], Alexander Weber-Bargioni[2], Willi Auwärter[1], Florian Klappenberger[1], Agustin Schiffrin[2], Yan Pennec[2], and Johannes Barth[1] — [1]Physik Department E20, TU München, Munich, Germany — [2]Departments of Chemistry and Physics & Astronomy, University of British Columbia, Vancouver, Canada

We present a molecular level study of the geometric and electronic properties of Co-tetraphenyl-porphyrin molecules adsorbed on the Cu(111) surface. Combined low-temperature scanning tunneling microscopy and near-edge X-ray absorption fine structure observations reveal how the metal substrate induces a conformational adaptation into a distorted saddle-shape geometry. By scanning tunneling spectroscopy we identify the molecules discrete energy levels and map their spatial electron density distributions. These results, along with a simple theoretical description, provide a direct correlation between the shape of frontier molecular orbitals and intramolecular structural features. In addition, it is demonstrated that the same concepts can be applied to address the interaction of cerium with surface anchored porphyrin host molecules.

SYSA 5.41 Tue 14:30 Poster A

Photoelectrochemical characterization of the role of organic sensitizers adsorbed on nanostructured ZnO — •Andreas Hastall, Thomas Loewenstein, and Derck Schlettwein — Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, D-35392 Gießen, Germany

Porous sensitized ZnO is a promising material for application as electrode in dye-sensitized solar cells (DSSC) to utilize the intense absorption of organic sensitizers in the visible spectral range [1]. Electrochemical deposition of ZnO from aqueous solutions is a low temperature process (<150°C) which allows the use of various substrates. The process can be performed at low energy input and cost and is therefore promising short pay-back times and high net energy gains. The role of the adsorbed sensitizer dye and resulting charge carrier generation, collection, but also recombination in the interface of ZnO/sensitizer/electrolyte of DSSC were analyzed in detail by transient photocurrent measurements, intensity modulated photocurrent and photovoltage spectroscopy (IMPS / IMVS) [2], photovoltage decay and charge-extraction [3]. Results will be discussed for different sensitizers adsorbed to the ZnO surface and for ZnO prepared on various substrates and optimized in structure and morphology.

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SYSA 5.42 Tue 14:30 Poster A

Co and Fe Adatoms in Biomolecular Nanotrenches: Control of Diffusion at the Atomic Scale and 1-D Nanotemplating — •Joachim Reichert[1], Agustin Schiffrin[2], Willi Auwärter[1], Alexander Weber-Bargioni[2], Agustin Schiffrin[2], Yan Pennec[2], Dean Cvetko[3], Albano Cossaro[3], Alberto Morgante[3], Larissa Niebergall[4], Valeri Stepanyuk[4], and Johannes Barth[1] — [1]Physik Department E20, TU München, Munich, Germany — [2]Departments of Chemistry and Physics & Astronomy, University of British Columbia, Vancouver, Canada — [3]INFM/TASC, Trieste, Italy — [4]MPI für Mikrostrukturphysik, Halle, Germany

We studied the self-assembly of the L-methionine amino acid on the noble metal Ag(111) surface under ultra-high vacuum conditions, by the means of low-temperature scanning tunneling microscopy and photoelectron spectroscopy (XPS). Molecular dimerization and self-assembly in 1-D nanostructures parallel to the <110> crystallographic orientations of the substrate atomic lattice is observed. Commensurate chains arrange into tunable and regular biomolecular gratings. An XPS analysis evidences zwitterionic self-assembly. The confinement of the surface state electrons was used to steer the positioning of single magnetic adatoms like Fe and Co in the molecular trenches at low temperatures. Also, the thermal motion of the transition metal atoms in the trenches was monitored in order to probe the influence of the adatom restriction on their diffusion characteristics and compared to 2-D particle movement.

SYSA 5.43 Tue 14:30 Poster A

Nanostructured organic photodiode with adaptable sensitivity — •Steve Pittner and Veit Wagner — Jacobs University Bremen, Germany

Organic materials show promising properties for cheap and high volume manufacturing of electronic devices. For light detection a drawback of those materials is the short electron-hole pair (exciton) diffusion length of usually far less than 100 nm. Thus, in order to built an effective organic photodiode the geometrical dimensions have to be small, so that all excitons can dissociate in the strong fields at the contacts or internally built-in interfaces. Subsequently the separated e$^-$ and h$^+$ will drift to their appropriate contact. The approach of using a nanoscale lateral finger structure compared to the commonly used stacked layer geometry shows two advantages. An now possible additional gate electrode offers the option to tune the sensitivity of such an organic photodiode. Furthermore, no transparent and electrical conductive encapsulation is required so that a transparent insulating polymer can be used here. This approach is shown for devices made of dihexyl-sexithiophene (DH6T) or the polymer P3HT as photosensitive organic semiconductor on Si/SiO$_2$ substrate.

SYSA 5.44 Tue 14:30 Poster A

The temperature dependence of amorphous thin film growth: the case of α-NPD — •Phenwisa Niyamakom, Philip Schulz, Azadeh Farahzadi, Tobias Lau, and Matthias Wuttig — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Both the substrate temperature during deposition and the deposition rate are important parameters, which have a pronounced influence on the morphology and related properties of an amorphous organic layer, including subsequently the device performance of OLEDs. We have studied the morphology and structural properties of N,N'-diphenyl-N,N'-bis(1-naphthyl)-1-1'biphenyl-4-4" diamine (α-NPD) films on silicon substrates by atomic force microscopy (AFM), X-ray reflectometry (XRR) and contact angle measurements. The α-NPD thin films have been deposited by vacuum thermal evaporation (VTE). A quantitative analysis of the AFM images has been performed to derive the surface morphology, surface roughness and correlation length. The film density and the surface roughness have been analyzed from XRR spectra. In addition, the surface free energy of α-NPD has been calculated from the contact angle in order to understand the wetting behavior of α-NPD on the silicon surface. From the data obtained, the evolution of α-NPD thin film growth with temperature dependence will be explained.

SYSA 5.45 Tue 14:30 Poster A

Contact resistance effects of P3HT field-effect transistors produced by Maskless Mesoscale Material Deposition (M3D) — •D. Belaineh[1], B. Gburek[1], V. Zöllmer[2], V. Ruttkowski[2], M. Busse[2], and V. Wagner[1] — [1]Jacobs University Bremen, School of Engineering and Science, Campus Ring 8, 28759 Bremen, Germany — [2]Fraunhofer Institut für Fertigungstechnik und angewandte Materialforschung (IFAM), Wiener Straße 12, 28359 Bremen, Germany

In search for improved contact properties of organic field-effect transistors (OFETs), conventional lithographic patterning of the source and drain electrodes is compared to manufacturing by the M3D technique. M3D is a direct-write method used for depositing silver particles as source and drain electrodes on Si/SiO2 substrates from an aerosolized functional ink. This method yields electrodes with a very rough surface structure which should give rise to very high local fields. The contact properties were determined by the transmission line method, i.e. by analyzing the channel conductance in dependence of the channel length L=10 to 50 μm. The results are compared to those from OFETs with smooth silver electrodes prepared by optical lithography, where the silver layer was either deposited by e-beam metallization or by sputtering. The investigations show that M3D allows to produce samples with similar contact properties as by using lithographic techniques. However, ongoing improvements of deposition process are expected to yield superior contact properties. Especially due to fast and gentle processing of the electrodes M3D is an interesting alternative of electrode structuring with potential for improved injection properties.

SYSA 5.46 Tue 14:30 Poster A

Impedance analysis on organic ultrathin layers — •Sidhant Bom and Veit Wagner — Jacobs University Bremen, School of Engineering and Science, Campus Ring 8, 28759 Bremen, Germany

Impedance spectroscopy is a standard technique for thin film analysis to obtain important information as thicknesses, diffusion properties of mobile ions and leakage currents. The measured electrical impedance of a sample is modeled by a physical equivalent circuit of resistors and capacitors. In the present work this information is obtained as a function of frequency also for ultrathin organic layers in the monolayer regime.

A series of semiconducting and insulating polymers (regioregular poly-3-hexylthiophene (rr-P3HT), polymethylmethacrylate (PMMA)) and self assembled monolayers (octadecyltrichlorosilane (OTS), hexamethyldisilazane (HMDS), thiolated phospholipids) were deposited either on highly n-doped silicon wafers or on gold surfaces. E.g. ultrathin layers were obtained by dip coating a silicon wafer in rr-P3HT solution in chloroform. The thickness of 2 nm determined for this system by impedance measurement agrees well with the atomic force microscopy analysis and corresponds to a single layer of polymer chains. The leakage current is seen as an ohmic contribution at low frequencies and allows a systematic optimization of process parameters.

In summary, impedance spectroscopy allows very fast and convenient analysis of thin organic layers even down to the monolayer regime.

SYSA 5.47 Tue 14:30 Poster A

STM/NEXAFS INVESTIGATIONS OF METALLO-PHTHALOCYANINES GROWN ON FERROMAGNETIC Co(001) THIN FILMS — Kathrin Müller[1], Kathrin Heimer[2], Oleksiy Andreyev[2], Andreas Scheybal[1], Felix Schmitt[2], Jens Sauther[2], Rolf Bertschinger[1], Jan Peter Wüstenberg[2], Kim Timor[1], •Stefan Lach[2], Thomas Jung[1], Martin Aeschlimann[2], and Christiane Ziegler[2] — [1]Paul Scherrer Institut, Lab. for Micro&Nanostructures CH-5232 Villigen PSI — [2]TU Kaiserslautern Department of Physics D-67663 Kaiserslautern

Due to their chemical tunability and weak spin-orbit coupling organic semiconducting materials are promising candidates for future spintronic devices.

This motivates detailed investigations of the interface between organic-semiconductors like metallo-phthalocyanines and ferromagnetic metallic substrates. Here, a STM/NEXAFS study of the morphology of submonolayer up to multilayer CuPc and FePc thin films on epitaxially grown ferromagnetic Co(001) films will be presented. Cobalt was chosen for its high degree of spin polarization at the Fermi level. The STM data reveal that for monolayer coverages the morphology on smooth Co films is different for the two chosen metallo-phthalocyanines. This difference in morphology will be compared to data relevant for spintronic devices such as the spin polarization at the surface.

SYSA 5.48 Tue 14:30 Poster A

Optimization of organic thin film photovoltaic cells based on the oligothiophene derivative DCV6T — •David Wynands, Kerstin Schulze, Christian Uhrig, Moritz Riede, and Karl Leo — Institut für angewandte Photophysik, Technische Universität, 01096 Dresden, Germany

We have recently reported on a series of oligothiophene derivatives featuring dicyanovinylene end groups that can be used in combination with C$_{60}$ as acceptor material in organic thin film solar cells. The introduction of such electron-accepting groups provides a reduced bandgap and increased ionisation energy compared to the unsubstituted molecule. This allows solar cells with high photovoltages. DCV6T thin films absorb between 450nm and 680nm with an absorption coefficient of α=1.89*10^{5} cm^{-1} at the maximum (580nm). Using ITO coated glass as substrate and p-doped α-NPD as hole transport layer, we prepare solar cells with flat and bulk heterjunctions between DCV6T and C$_{60}$. A Voc of 0.9V is achieved in both cases. We show that by increasing the concentration of DCV6T in the bulk layers currents up to 10 mA/cm^{2} under 100mW/cm^{2} simulated sunlight can be reached. However, the fillfactor of 0.45 remains low and has to be improved further. To overcome restrictions of the single cells we also prepared tandem cells that reach efficiencies of 3.4% under 100mW/cm^{2} simulated sunlight.

SYSA 5.49 Tue 14:30 Poster A

Hole bandstructure and mobilities in guanine stacks — •Lars Matthes, Frank Ortmann, Karsten Hannewald, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Jena, Germany

DNA molecules are no longer regarded as passive molecules with the sole purpose to store genetic information. Nowadays nanowires derived from the DNA are also considered as possible candidates for molecular devices towards a further miniaturization of electronic technology. Therefore an investigation of intrinsic charge carrier mobilitites in such wires is needed. Moreover, the understanding of charge-transport processes in DNA is also highly relevant for biological phenomena such as radiation damage and repair.

Our model system is a stack of guanine molecules where we study the hole mobilities by means of a recently developed theory [1]. Thereby the interaction with phonons and hopping processes play a major role.

[1] Hannewald et al. PRB **69** , 075212 (2004)

SYSA 5.50 Tue 14:30 Poster A

Bundle Formation in Polyelectrolyte Brushes — •Jens-Uwe Günther, Heiko Ahrens, and Christiane A. Helm — Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17487 Greifswald, Germany

Theoretical predictions of bundling phenomena in semiflexible polyelectrolytes in the presence of monovalent and divalent counterions are tested with X-ray grazing incidence diffraction. We use amphiphilic diblock copolymers consisting of a hydrophobic anchor and a polyelectrolyte block (PEE-PSS, PBA-PAMPS, PIB-PMMA) grafted at the air-water interface to form polyelectrolyte brushes. The brush thickness determined by X-ray reflectivity amounts to 30-50% of the contour length. In-plane peaks are observed for different kind of counterions (monovalent Cs+ and Na+, divalent Ca2+ and Sr2+) and different ion concentrations in the subphase. Increased salt concentration in the polyelectrolyte brush leads to a decrease in bundle length, as well as to more chains per bundle hence larger bundle diameters. These observations are consistent with a decreased electrostatic repulsion between the chains, which lead to a decreased persistence length as well as a decreased repulsion between chains.

SYSA 5.51 Tue 14:30 Poster A

Chemical modification of GaAs surfaces with novel functional peptides — •Thomas Kaindl[1], Klaus Adlkofer[1], Tomoyuki Morita[2], Shunsaku Kimura[2], Michael Himmelhaus[1], and Motomu Tanaka[1] — [1]Physikalisch Chemisches Institut, INF 253, 69120 Heidelberg, Universität Heidelberg — [2]Department of Material Chemistry, Kyoto University Nishikyo-ku, 615-8510 Kyoto, Japan

The interconnection of biological molecules (peptides, enzymes, etc.) with solid based devices offers great advantages towards the creation of new functional hybrid materials. Molecular dipole engineering was achieved by deposition of helical peptides, carrying a large dipole moment, onto GaAs [100] surfaces. After optimization of the preparation protocols the formed monolayers were systematically studied by various surface sensitive methods. Ellipsometric film thickness measurements and topographic studies by AFM revealed a macroscopically uniform monolayer formation with few surface defects. The averaged tilt angle of the peptide helix axis was estimated by TM-FTIR, where all peptides showed nearly vertical orientation on the GaAs. To gain further information of the molecular level structure, radiation impeding grazing-incidence x-ray scattering out of specular plane experiments were carried out. The same functionalization protocol was successfully adapted to commercially available, high electron mobility transistors. Based on the preceding thorough structural characterization of the peptide layers on bulk GaAs, a significant influence of the molecular dipole moments on the transistors characteristics could be demonstrated.

SYSA 5.52 Tue 14:30 Poster A

Adhesion between alkyl chains determines head group conformation in phosphocholine monolayers — •Olaf Soltwedel[1], Christel Müller[2], Heiko Ahrens[1], Jens-Uwe Günther[1], and Christiane A. Helm[1] — [1]Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17487 Greifswald, Germany — [2]Institut für physikalische Chemie, Johannes-Gutenberg Universität, Jakob-Welder Weg 11, D-50055 Mainz, German

Phosphatidylcholine monolayers at the air-water interface with different alkyl chain lengths are investigated with isotherms, X-ray reflectivity and Grazing Incidence X-ray diffraction. The length and symmetry of the alkyl chains is varied, C14-C14, C16-C16, C18-C18, C14-C18, C18-C14, C16-C18 and C18-C16. Increasing the alkyl chain length by 2 CH$_2$-groups lowers the liquid-solid phase transition by about 15 mN/m. This is attributed to the increased adhesion between the ordered alkyl chains. The phase transition of C18-C14 and C14-C18 is between the one of C14-C14 and C16-C16, the analogue is observed for C16-C18 and C18-C16. To make it possible that the ordered part of the alkyl chains is the same for different chain lengths, the head group has to rearrange. In biological system, the bending of the glycerol occurs at the C2-atom, as it does in water-free choline crystals. But to maximize the thickness of the ordered alkyl chains, the headgroup conformation has to change. The thermodynamic observations are supported by X-ray measurements.

SYSA 5.53 Tue 14:30 Poster A

Isotope Effects in Partially Deuterated Polyelectrolyte Multilayers — •Oxana Ivanova[1], Manesh Gopinadhan[1], Olaf Soltwedel[1], Roland Steitz[2], and Christiane A. Helm[1] — [1]Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Straße 6, 17489 Greifswald, Germany — [2]Hahn-Meitner Institut, Glienicker Straße 100, D-14109 Berlin, Germany

Neutron reflectivity (spatial resolution 1nm) is a powerful tool for the investigation of thin polymeric layers. Deuteration is a labeling technique which monitors the internal order of the multilayers (superlattice structure by partial deuteration) as well as the water content, but the deuteration may affect structural and transport properties. Here we report data on the water uptake of selectively deuterated polyelectrolyte multilayers consisting of PSS, PSSd and PAH. A deuterated (PSSd/PAH)$_n$ layer keeps always one or two H$_2$O molecules per monomer pair more than a protonted (PSS/PAH)$_n$ layer, both at 0% r.h. and 100% H$_2$0 r.h. The film swells about 5% more in heavy water (100% r.h.) than in ordinary water, in heavy water the swelling of both the protonated and deuterated layers is pronounced and the same. After exposure to 100% r.h. D$_2$O, the drying is not fully reversible, the film thickness is the same, yet an increased scattering length density remains. After immersing the film into pure water, and subsequent drying (0% r.h.) the original scattering length density is obtained. This suggests an exchange of bound H$^+$ to bound D$^+$ due to exposure to D$_2$O within the polyelectrolyte multilayer.

SYSA 5.54 Tue 14:30 Poster A

Block-copolymer directed mesoporous TiO2 for solar cell applications — Mihaela Nedelcu[1], •Stefan Guldin[1,4], Sven Hüttner[1], Henry J. Snaith[2], Jinwoo Lee[3], Chris Orillal[3], Scott Warren[3], Ulrich Wiesner[3], and Ullrich Steiner[1] — [1]Department of Physics, Cavendish Laboratory, University of Cambridge, UK — [2]Department of Physics, University of Oxford, UK — [3]Materials Science Department, University of Cornell, Ithaca, USA — [4]4 Physik Department, Technische Universität München, Garching, D

Nanostructuring metal-oxides through polymer-assisted self-assembly has gained significant interest in the last 10 years for a wide range of applications. Dye-sensitized solar cells, for example, rely on a highly porous, polycrystalline metal-oxide electrode.

In our work we used a Poly(isoprene)-b-Poly(ethylenoxide) (PI-b-PEO) diblock-copolymer as a structure-directing agent for the formation of TiO_2. The block-copolymer phase separates into ordered domains, tens of nanometers in size. Titania precursors were incorporated through a non hydrolytic sol-gel route which swell only the hydrophilic PEO.

During temperature annealing the PI-block forms a carbon scaffold which enables high temperatures for the crystallisation of TiO_2 without loss of the mesostructure. This leads to a nanostructured material with improved crystallinity and a high surface area.

The benefits of these interesting material properties are presented in efficient dye-sensitized solar cells.

SYSA 5.55 Tue 14:30 Poster A

structural chances in thin block copolymer films during vapor treatment — •zhenyu di[1], christine papadakis[1], charles darko[1], dorthe posselt[2], and detlef-m smilgies[3] — [1]Physikdepartment E13, TU München — [2]Roskilde University, Denmark — [3]Cornell University, USA

The mesoscopic structures formed by self-assembly of diblock copolymers in thin film geometry are interesting for a variety of applications. However, spin coating leads to domain structures with defects. Vapor treatment has been shown to be an effective way to increase the long-range order.

We have studied the structural changes in thin films of poly(styrene-b-butadiene) diblock copolymers and their kinetics during vapor treatment. In this system, the initial lamellar orientation (parallel or perpendicular to the substrate) can be controlled by the block copolymer molar mass [1]. We have investigated both initial orientations as well as the influence of the initial film thickness, solvent selectivity, and the vapor pressure using grazing-incidence small-angle x-ray scattering with a time resolution of a few sec. The growth of the lamellar domains can be controlled by the degree of swelling.

[1] P. Busch, D. Posselt, D.-M. Smilgies, C.M. Papadakis et al. Macromolecules 36, 8717 (2003) and Macromolecules 40, 630 (2007).

SYSA 5.56 Tue 14:30 Poster A

Taylored Interfaces in PP-Glass Model Composites — •Hanna Brodowsky and Edith Mäder — Leibniz-Institut für Polymerforschung Dresden, Hohe Str. 6, D-01069

The interface between the reinforcing fiber and polymer matrix plays a crucial role for a composite's mechanical properties. In the vicinity of the fiber, a three dimensional "interphase" is formed on the fiber surface, in which the properties of the matrix differ from those in the bulk. This interphase can be taylored by using a suitable sizing (surface modification) of the fiber, e.g. suppressing or promoting heterogeneous nucleation of a thermoplastic matrix.

Polypropylene-glass fiber composites are prepared as single fiber model composites with varying sizings and different PP chain lengths. Static tests permit insights in the interfacial characteristics such as fracture energy release rate, shear strength and modulus. Cyclic tests on these model composites are used to study the nature of dissipative processes and the damage behaviour. An AFM characterisation of the fiber fracture surface provides supplementary information.

SYSA 5.57 Tue 14:30 Poster A

Simultaneous acquisition of rheological data and microscopic information — •Annette Fischer — Thermo Fisher Scientific, Dieselstr.4, 76227 Karlsruhe

Foams can be defined as composite materials characterized by a solid or liquid continuous matrix which surrounds a gaseous phase.The possibility of combining the properties of the continuous matrix and gas voids in a great variety of morphologies,is a powerful tool in the material industry to design materials with properties for nearly any kind of applications were performance and low weight are requested. The characterization of foam is very difficult.Numerous parameters have to be considered and controlled:foam quality,foam texture,size of the measurement apparatus compared to bubbles size,influence of foam production method, wall slip phenomena and foam compressibility. These numerous parameters do explain there is no general view concerning the behaviour of this kind of system. Rheological methods reveal information on macroscopic material properties.However,the mechanical material properties are strongly dependent on the underlying microstructure.Therefore information on the microstructure is often very helpful for a better understanding of a certain rheological behaviour. The new RheoScope module for the HAAKE Mars offers the possibility to record rheological properties and microscopic images simultaneously.The resulting measurements and pictures can be clearly correlated.

SYSA 5.58 Tue 14:30 Poster A

Structure of the top contact in photovoltaic devices: Au deposition on TiO2:PVK hybrid thin films — •Gunar Kaune[1], Mottakin M. Abul Kashem[1], Alexander Diethert[1], Weinan Wang[1], Sebastien Couet[2], Kai Schlage[2], Ralf Röhlsberger[2], Stephan V. Roth[2], Andreas Timmann[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department LS E13, James-Franck-Straße 1, 85747 Garching — [2]HASYLAB at DESY, Notkestraße 85, 22603 Hamburg

Photovoltaic energy conversion systems based on an inorganic semiconductor and a semi-conductive polymer, so called hybrid solar cells, promise to open new solar cell applications. In a common device, a thin metal film is deposited on top of the hybrid film in order to apply electrical contact. Since type and structure of this metal electrode influence the performance of the solar cell, the understanding of its structural growth and the interaction with the polymer layer is necessary.

In our study, we use a model system consisting of nanostructured titanium dioxide and poly-N-vinylcarbazole (PVK) blended with zinc phthalocyanine (ZnPc). On top of this, a thin gold film was deposited by rf-sputtering. In-situ to deposition, the growth of the gold film was probed with grazing incidence small angle scattering (GISAXS) with a very high time resolution of 1 second. Particular attention was paid to the initial stage of the growth, where the first gold particles form on the polymer surface. The results obtained from fitting the 2d scattering data are compared with information about the surface morphology obtained with atomic force microscopy.

SYSA 5.59 Tue 14:30 Poster A

Soft X-ray scanning transmission spectromicroscopy of diindenoperylene thin films — •Maria Benedetta Casu[1], Indro Biswas[1], George Tzvetkov[2,3], Jörg Raabe[3], and Thomas Chassé[1] — [1]Institute of Physical and Theoretical Chemistry, University of Tuebingen, 72076 Tübingen, Germany — [2]Physikalische Chemie II, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [3]Swiss Light Source, PSI, 5232 Villingen, Switzerland

Organic materials have been extensively investigated in the recent decades. They were considered very appealing not only because of a pure academic interest as a new class of materials but also because of their promising properties toward the electronic applications. Nowadays we can surely affirm that these materials kept their promise. Diindenoperylene is a perylene-based molecule that shows a very high hole mobility already in thin films, good film forming properties and thermal stability. Thus it may be promising as active layer in devices. In this work we present the results of scanning transmission X-ray microscopy (STXM) investigations on diindenoperylene thin films deposited on polycrystalline gold. STXM is a powerful technique that takes advantage from the use of synchrotron radiation, allowing the simultaneous investigation of structure, and electronic properties with excellent spatial resolution. Our STXM images together with nano near-edge X-ray absorption fine structure spectra (both taken at the C 1s edge) show that different electronic structure domains occur depending on different sample thicknesses. The implications of this finding will be discussed also in terms of growth of organic materials.

SYSA 5.60 Tue 14:30 Poster A

A new tool for gradual tuning the composition of binary self-assembled monolayers and chemical lithography: UV-promoted exchange reaction — •Nirmalya Ballav, Tobias Weidner, and Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

We demonstrate that exchange reaction between a primary self-assembled monolayer (SAM) and a potential molecular substituent, capable to form SAM on the same substrate can be promoted in a controlled way by preliminary exposure of the SAM to UV light with a suitable wavelength. Using a model system of a non-substituted alkanethiolate (AT) SAM as the primary film and COOH-substituted AT as the substituent, we showed that the composition of the binary mixed film formed by the UV promoted exchange reaction (UVPER) can be precisely varied and tuned over the entire concentration range by the selection of a proper UV exposure time. The reason for the promotion effect of the UV light treatment is the appearance of chemical and structural defects in the primary film, viz. photooxidation of the thiolate tailgroups and the structural and chemical defects in the aliphatic matrix. Since both these defects are stochastically distributed over the target film, no phase separation occurs, and the resulting mixed

SAM represents a true molecular mixture of both components. Apart from its usefulness for the preparation of mixed SAMs, the UVPER approach can be combined with lithography and applied for the fabrication of chemical patterns and molecular templates.

SYSA 5.61 Tue 14:30 Poster A

Interface energetics in highly ordered organic-organic heterosystems: Thermal induced layer swap in the system HBC on PTCDA — •Rainer Jacob, Christian Wagner, Thomas Dienel, and Torsten Fritz — Institut für Angewandte Photophysik, TU-Dresden, George Bähr Str. 1, 01069 Dresden

The structural and energetic properties of organic-organic and organic-inorganic interfaces play a crucial role in future devices based on ultra thin organic layers or single molecules. We will present results of a STM and LEED study of an organic-organic heterosystem consisting of two stacked highly ordered monolayers (ML) of hexa-peri-hexabenzocoronene (HBC) and perylene-3,4,9,10-tetracarboxylic-dianhydride (PTCDA) on Au(111). While the evaporation of one ML PTCDA onto a highly ordered HBC ML creates a stable organic-organic heterosystem [1], no such observation could be made for the reversed stack order, i.e., HBC on PTCDA on Au(111). Even light annealing at approx. 60°C of such a sample leads to a swap of the stack order and the creation of large sample areas where the consecutively evaporated HBC has displaced the PTCDA as first layer, with the PTCDA now forming an epitaxial layer on top of the ordered HBC. Force field calculations [2] revealed that interface energetics can be made responsible for the process observed, as there is a considerable energy gain per surface area when changing from HBC on PTCDA on Au(111) to PTCDA on HBC on Au(111).

[1] F. Sellam et al., Surf. Sci. 478, 113 (2001).

[2] S.C.B. Mannsfeld and T. Fritz, Mod. Phys. Lett. B 20, 585 (2006).

SYSA 5.62 Tue 14:30 Poster A

Improved efficiency of phosphorescent organic light emitting devices at high brightness — •Sebastian Reineke, Gregor Schwartz, Karsten Walzer, and Karl Leo — Institut für Angewandte Photophysik, 01062 Dresden, Germany

We present a novel emission layer (EML) structure for phosphorescent organic light emitting diodes (OLEDs) comprising mixed films of fac tris(2-phenylpyridine) iridium $[Ir(ppy)_3]$ dispersed in 4,4',4"-tris(N-carbazolyl)-triphenylamine (TCTA) which reduces the decrease of efficiency at high current densities. Based on results of photoluminescence experiments, we intermit the EML with thin neat layers of TCTA. Due to its high triplet energy, TCTA acts as an exciton blocking layer inside the EML which suppresses exciton migration on the dopant sites and, consequently, triplet-triplet annihilation. We show that this EML structure leads to a smaller efficiency decrease: Starting at initial external quantum efficiencies (IEQE) of 15.8 % and 14.4 % at low brightness for the reference and interlayer device, respectively, those structures yield critical current densities j_c of 140 mA/cm^2 and 270 mA/cm^2. Here, j_c defines the current density where the IEQE drops to half of its value.

SYSA 5.63 Tue 14:30 Poster A

Active layer thickness dependence in flexible P3HT field-effect transistors — •Benedikt Gburek and Veit Wagner — Jacobs University Bremen, School of Engineering and Science, Campus Ring 8, 28759 Bremen, Germany

Applications of organic electronics require cheap and fast production methods on e.g. flexible and transparent devices. Following these goals, organic field-effect transistors (OFETs) in top-gate architecture are produced on flexible and transparent plastic (PET) foils as device substrate. The organic semiconductor, regio-regular poly-(3-hexylthiophene) (rr-P3HT), and the gate insulator, polymethylmethacrylate (PMMA), are deposited wet-chemically under atmospheric conditions. Comparably high charge carrier mobility of 0.02 cmˆ2/(Vs) was determined at -40 V gate-source voltage in devices with 300 nm insulator thickness in the linear regime. Unlike the severe degradation of uncapped P3HT transistors, our device characteristics remain stable for several months due to the encapsulation with the PMMA gate insulator. Plastic devices fabricated in this way were used to analyze the dependence of the charge carrier mobility on the thickness of the P3HT layer. The mobility was found to be low for thin layers of several nm and to increase strongly with increasing layer thickness. For sufficiently large thickness, i.e. beyond 15 nm, the mobility remains constant. Thickness dependent charge transport properties were analyzed by fitting theoretical models. Beside gate voltage dependent mobility also contact resistance - a crucial point for further miniaturization of devices - was taken into account.

SYSA 5.64 Tue 14:30 Poster A

Real-Time Observation of PTCDA Growth on Ag(111) - a SMART Investigation — •Florian C. Maier[1], Pierre L. Levesque[2], Thomas Schmidt[1], Helder Marchetto[2], Ulrich Groh[1], Tomas Skala[2], Rainer Fink[3], Hans-Joachim Freund[2], and Eberhard Umbach[1,4] — [1]Universität Würzburg, Experimentelle Physik II, 97074 Würzburg — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14159 Berlin — [3]Univ. Erlangen-Nürnberg, Phys. Chemie II, 91058 Germany — [4]Forschungszentrum Karlsruhe, 76021 Karlsruhe

The spectro-microscope SMART, an aberration corrected high resolution LEEM/PEEM (Low Energy/Photo-Emission Electron Microscope) system, has been used to investigate the growth of thin organic films on metal substrates and their interaction. The growth of PTCDA (3,4,9,10 perylene-tetracarboxylic-acid dianhydrid) on a single-crystalline Ag(111) surface has been observed in-situ and in real-time at substrate temperatures between 220 and 390˜K. LEEM, PEEM and LEED studies reveal the dependence of the growth mode, the structure and the phase formation on both, the temperature and the substrate morphology. Whereas PTCDA grows in a mound like quasi layer-by-layer fashion at low temperatures, Stranski-Krastanov growth (i.e. a bi-layer followed by 3D islands) occurs above room temperature. Details of the real-time investigation like the dynamic behaviour of the growing layers, the metastability and desorption of single layers will be discussed. (Funded by BMBF, contract 05KS4WWB/4)

SYSA 5.65 Tue 14:30 Poster A

White top emitting OLED with angle independent emission characteristic — •Michael Thomschke, Patricia Freitag, Gregor Schwartz, Robert Nitsche, Karsten Walzer, and Karl Leo — Technische Universität Dresden, Institut für Angewandte Photophysik, Georg-Bähr-Straße 1, 01062 Dresden, Germany

The general device structure of a top emitting organic light emitting diode (OLED) consists of several organic layers sandwiched in between two metal contacts, with the top one being semitransparent for light outcoupling reasons. Due to the high reflectivity of the electrodes, strong microcavity effects occur which lead to a preferred emission of light of a certain wavelength with main outcoupling in forward direction. This creates rather narrow emission bands, accompanied by strong spectral shifts upon viewing angle variation [1].

By using an organic capping layer on top of the semitransparent metal contact, this unwanted effect can be reduced. This is important especially for white light emission for the use of OLEDs in future lighting applications. Our optical simulations show that the strong angular dependence of the emission color almost vanishes. To verify the simulations we study white top emitting OLEDs based on an approach of Schwartz [2] which are adapted to the top emitting case.

[1] Q. Huang, K. Walzer, M. Pfeiffer, K. Leo, M. Hofmann, T. Stübinger, J. Appl. Phys. 100 64507 (2006)

[2] G. Schwartz, K. Fehse, M. Pfeiffer, K. Walzer, K. Leo, Appl. Phys. Let. 89 083509 (2006)

SYSA 5.66 Tue 14:30 Poster A

Molecular Transport in Real-Space Density-Functional Calculations — •Paul Baumeister[1] and Tomoya Ono[1,2] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, 52428 Jülich, Germany — [2]Department of Precision Science and Technology, Osaka University, Suita, Osaka 565-0871, Japan

Real-space methods are very promising for large scale *ab initio* calculations of the electronic structure on systems with low symmetry. Especially the perfomance on massively parallel computers enables accurate first-principles calculations of large realistic setups. We have applied the transport formalism in real space [1] to π-conjugated organic molecules between copper surfaces. Focusing on the limit of zero bias voltage and applying a jellium model for the electrodes it becomes feasible to compute scattering wave functions and thus transport properties. Herein, the numerical results for the electronic structure of a molecule inside a junction are combined with analytical solutions of the jellium electrodes. Matching the incident and the outgoing wave function requires a Green-function method.

Support by the DFG-SPP 1243 and the Alexander von Humboldt foundation is gratefully acknowledged.

[1] K. Hirose, T.Ono, Y.Fujimoto, and S. Tsukamoto, *First-*

principles Calculations in Real-Space Formalism, Electronic Configurations and TransportProperties of Nanostructures (Imperial College Press, London, 2005).

SYSA 5.67 Tue 14:30 Poster A

Pentacene thin films on diamond surfaces: effect of surface termination — •W. Gajewski[1], F. Buth[1], M. Huth[2], B. Nickel[2], M. Stutzmann[1], and J.A. Garrido[1] — [1]Walter Schottky Institute, TU-Munich, Garching — [2]Physics Department, Ludwig-Maximilians University, Munich

We investigate the effect of diamond surface termination by oxygen or hydrogen on the structural and optoelectronic properties of pentacene thin films deposited on diamond. Pentacene films with thicknesses from 3 to 50 nm were deposited on O- and H-terminated diamond films, as well as on SiO2 surfaces for comparison. On O-terminated diamond surfaces, pentacene molecules are oriented almost perpendicular to the substrate, as revealed by X-ray diffraction and AFM. For H-terminated diamond surfaces the morphology of the pentacene films is much more complex, probably due to a Stransky-Krastanov like growth mode characterized by a first flat molecular layer followed by 3D island growth. Optical absorption as well as spectrally resolved photocurrent measurements in the energy range 0.5-6.0 eV performed at temperatures from 80 to 350K allow the detection of the excitonics and the HOMO-LUMO transition in the pentacene film, as well as specific charge transfer processes between diamond and pentacene. Current-voltage characteristics recorded for pentacene films with various thickness in the dark and under illumination reveal a complex temperature and electric field dependence of the electronic transport at the diamond/pentacene interface.

SYSA 5.68 Tue 14:30 Poster A

Vibrational and electronic properties of methylated silicon (111) surfaces in air — •Florent Yang[1], Ralf Hunger[2], Katy Roodenko[3], Karsten Hinrichs[3], Klaus Rademann[4], and Jörg Rappich[1] — [1]Hahn-Meitner-Institut Berlin, Dep. Si-Photovoltaics (SE1), Berlin, Germany — [2]Technische Universität Darmstadt, Institute of Materials Science, Darmstadt, Germany — [3]Institute of Analytical Sciences, Department Berlin, Germany — [4]Humboldt University Berlin, Department of Chemistry, Berlin, Germany

Controlling and monitoring the grafting of small organic molecule onto silicon (Si) surfaces is the centre of sustained efforts of many research groups. These investigations are widely motivated by the fabricating hybrid devices and sensors. The control of the work function, the creation of surface dipole, and the change in band bending obtained by an organic layer on Si is of great interest also for hetero-structure solar cells. Our work concerns the direct deposition of CH_3/CD_3 groups on flat hydrogenated p-Si(111) surfaces by anodisation in a Grignard reagent. The ultrathin films have been characterised by different techniques like IR-SE, AFM, XPS/UPS to obtain information about the thickness, the topography and the type of chemical bonds of the organic films on the surface. PL spectroscopy was used to investigate the recombination behaviour at such interfaces. Methylated Si surfaces show low surface recombination velocities and are not susceptible to rapid oxidation in ambient air. These modified surfaces passivate the Si towards oxidation and exhibit a much better stability than H-terminated Si surfaces in ambient air.

SYSA 5.69 Tue 14:30 Poster A

Monolayer to multilayer transition of hexa-peri-hexabenzocoronene on Ag(111) — •Hendrik Glowatzki[1], Gianina N. Gavrila[2], Stefan Seifert[2], Robert L. Johnson[3], Hans Joachim Räder[4], Klaus Müllen[4], Dietrich R.T. Zahn[2], Jürgen P. Rabe[1], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Institut f. Physik, Newtonstr. 15, D-12489 Berlin — [2]Technische Universität Chemnitz, Institut f. Physik, Reichenhainer Str. 70, D-09126 Chemnitz — [3]Universität Hamburg, Institut f. Experimentalphysik, D-22761 Hamburg — [4]Max Planck Institut für Polymerforschung, D-55021 Mainz

The properties of hexa-peri-hexabenzocoronene (HBC) deposited on Ag(111) in the mono- and multilayer regimes were investigated by several complementary techniques. The molecular orientation was determined by near-edge x-ray absorption fine structure spectroscopy (NEXAFS), scanning tunneling and scanning force microscopy (STM, SFM), and the electronic structure by ultraviolet photoelectron spectroscopy (UPS). We found that the molecular orientation changed as a function of coverage; at monolayer coverage the HBC molecules were aligned parallel to the substrate whereas in the multilayer the molecules were tilted by 43°. This structural transition was accompanied by a rigid shift of the molecular energy levels by 0.3 eV towards higher binding energy between mono- and multilayer coverage. In addition, the highest molecular levels in the multilayer were broadened by 0.35 eV, suggesting the formation of extended intermolecular energy bands.

SYSA 5.70 Tue 14:30 Poster A

Cu-Adatom-Mediated Bonding in close-packed Benzoate/Cu(110) Systems — •Maria Christina Lennartz, Nicolae Atodiresei, Silvia Karthäuser, and Stefan Blügel — Institute for Solid State Research, Research Centre Juelich, Juelich, Germany

Copper is an established metal in electronics industry and the special linkage between carboxylates and Cu(110) surfaces justifies that this system is regarded as an alternative to the well-known and intensively studied thiol/gold system. Therefore our aim is to investigate the structure and the electronic transport through the carboxylate/Cu(110) interface, experimentally and theoretically, and to use these data to build up molecular devices. Especially the electronic transport properties depend crucially on the molecular orientation and the crystalline structure. Therefore a major point of our interest is to control the lateral order of the molecular arrangements while determining the corresponding molecular transport properties. We will present a microscopic evidence for a new Cu-adatom stabilized high density phase of benzoate molecules on Cu(110) surfaces. Using UHV-STM investigations and density-functional theory calculations two different chemical species building the new structure, benzoate molecules and benzoate copper-adatoms molecules, could be identified. The energy calculations provide strong support that the benzoate copper-adatoms molecules form energetically favourable bonds with the surface, but are also more mobile on the surface.

SYSA 5.71 Tue 14:30 Poster A

Electronic coupling of organic dyes with inorganic van der Waals semiconductors — Eric Mankel, Johanna Härter, •Thomas Mayer, and Wolfram Jaegermann — FG Oberflächenforschung, FB Materialwissenschaft, Technische Universität Darmstadt

A prerequisite for tailoring organic/organic and organic/inorganic interfaces is the understanding of the electronic coupling processes. Inert van der Waals surfaces of layered chalcogenide semiconductors are free of surface states and allow to monitor free of chemical interaction charge transfer and interface dipole formation by synchrotron induced photoelectron spectroscopy. Copper phthalocyanine, CuPc and a perylene derivate, PTCDA were adsorbed in situ on UHV-cleaved n- and p-WSe2. For both molecules the HOMO position below the valence band maximum is independent of the substrate Fermi level position, SFLP, (n or p-type) and amounts to 0,64eV and 1,63eV for CuPc and PTCDA. The constancy of the HOMO position versus substrate orbitals for varied SFLP and coverages indicates the absence of an interface dipole. Both molecules induce band bending on n and on p substrates but in opposite directions in dependency of doping indicating the position of the molecule charge neutrality level between the n and p SFLP. The surface SFLP of n- and p-WSe2 for higher dye coverage do not converge to the same value. A difference of about 0,45eV is measured for both dyes indicating a shift of the dye charge neutrality level due to charge transfer.

SYSA 5.72 Tue 14:30 Poster A

Influence of dispersion interactions on the adsorption of NTCDA on (110)-oriented noble metals — •afshin abbasi[1], Reinhard Scholz[2], and Michael Schreiber[1] — [1]Institut für Physik, Technische Universität Chemnitz — [2]Walter Schottky Institut, Technische Universität München

The chemisorption of NTCDA on noble metals is investigated with second order Møller-Plesset perturbation theory (MP2) for a single molecule adsorbed to a finite-sized Cu, Ag, or Au cluster. Contrary to Hartree-Fock and density functional theory (DFT), MP2 contains the major part of the dispersion interactions, so that the Pauli repulsion between adsorbate and substrate is largely compensated by attractive van-der-Waals forces. As a result, the adsorbate geometries are nearly flat, in sharp contrast to previous investigations with DFT [1]. The MP2 calculations provide new insight into the chemisorption of functionalized aromatic molecules on different noble metals: The binding energy and the distance between adsorbate and substrate follow opposite chemical trends.

[1] A. Alkauskas, A. Baratoff, and C. Bruder, Phys. Rev. B **73**, 165408 (2006).

SYSA 5.73 Tue 14:30 Poster A

Temperature dependence of dislocation formation in perylene films — •Phenwisa Niyamakom, Philip Schulz, Azadeh Farahzadi, Maryam Beigmohamadi, and Matthias Wuttig — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

We have recently studied the growth of highly ordered perylene thin films on top of an amorphous oxide layer at room temperature. These films show growth model, which is assisted by screw dislocation [1]. In this study, the substrate temperature is included as an important deposition parameter to investigate the temperature dependence on the evolution of dislocations in perylene films with thickness and deposition rate. The perylene films have been deposited by vacuum thermal evaporation (VTE). The film morphology and structural properties have been investigated by atomic force microscopy (AFM) and X-ray diffractometry (XRD). The surface roughness, island density and screw dislocation density have been analyzed by AFM. Our quantitative analysis also includes the determination of the lateral correlation length, extracted from AFM images. An analysis of the XRD peak profiles allowed us to determine the microstrain and vertical grain size. The comparison of the perylene thin film growth at different substrate temperatures will be presented.

[1] M. Beigmohamadi, P. Niyamakom, A. Farahzadi, S. Kremers, T. Michely and M. Wuttig, phys. stat. sol.(RRL) 2, No.1, 1-3 (2008).

SYSA 5.74 Tue 14:30 Poster A

Metal-phthalocyanine sub-monolayer films on Ag(111): An x-ray standing wave study of CuPc, TiOPc and SnPc — •Ingo Kröger[1], Christoph Stadler[1], Florian Pollinger[1], Andreas Stahl[1], Felix Erfurth[1], Benjamin Stadtmüller[1], Christian Kumpf[1], and Eberhard Umbach[1,2] — [1]Universität Würzburg, Experimentelle Physik II, 97074 Würzburg — [2]Forschungszentrum Karlsruhe GmbH, D-76021 Karlsruhe

Metal-phthalocyanine (Me-Pc) molecules adsorbed in sub-monolayer structures on Ag(111) exhibit a very interesting ordering phenomenon due to intermolecular repulsion (see contribution of C. Kumpf et al.). Key aspects for the understanding of this observation are the local bonding mechanism and the adsorption geometry of the molecules. We investigated these aspects for the planar CuPc and the non-planar TiOPc and SnPc molecules on Ag(111) using the x-ray standing wave (XSW) technique, which is a highly accurate method for getting geometric data of molecules in the monolayer regime. It yields information about (vertical) bonding distances and the deformation of the molecule upon adsorption, and therefore allows to elucidate the bonding mechanism. We present XSW data of different (disordered, commensurate, and incommensurate) phases for each of the molecules. Beside a molecule-surface interaction via the central metal atom, the data indicates chemisorption mediated by the pi-system of the molecules which decreases with increasing coverage.

SYSA 5.75 Tue 14:30 Poster A

Film formation of oligothiophenes for a molecular organic field-effect transistor — •Kinga Haubner[1], Evelin Jaehne[1], Hans-Juergen Peter Adler[1], Denny Koehler[2], Christian Loppacher[2], Lukas Eng[2], Andrei Herasimovich[3], and Susanne Scheinert[3] — [1]Institute of Macromolecular Chemistry and Textile Chemistry, Technische Universitaet Dresden, 01069 Dresden, Germany — [2]Institute of Applied Photophysics, Technische Universitaet Dresden, 01069 Dresden, Germany — [3]Solid State Electronics and Center of Micro- and Nanotechnologies, Technische Universitaet Ilmenau, 98684 Ilmenau, Germany

Novel oligomers based on β-substituted thiophene derivatives were synthesized with the aim to build-up a small molecule organic field-effect transistor (OFET). We investigated the properties of the applied films of α,ω-dicyano-β,β'-dibutylquaterthiophene (DCNDBQT) and α,ω-dicyano-β,β'-dibutylsexithiophene (DCNDBST) by different cast methods - spin-coating and vacuum sublimation - as well as thin films of two other oligothiophene derivatives, dibutylquaterthiophene (DBQT) and dibutylsexithiophene (DBST). The ultra-thin organic film formation on TiO_2 templates was effectively promoted through the specifically designed, bifunctional self-assembly molecules (SAM). Vacuum sublimated DCNDBQT, which forms a dense packed molecular layer, was used to build-up a nanoscopic OFET-structure. The resulting field mobilities of 10^{-5} cm^2 V^{-1} s^{-1} reflect a moderate current density as interpreted in the framework of the ultra-thin molecular OFET structure.

SYSA 5.76 Tue 14:30 Poster A

Dipole orientation of the P[VDF-TrFE] co-polymer films: A NEXAFS study — •Dipankar Mandal, Klaus Müller, and Dieter Schmeisser — Brandenburgische Technische Universität Cottbus, Angewandte Physik - Sensorik, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany

Ferroelectric properties of copolymers of vinylidene fluoride with trifluoroethylene (P[VDF-TrFE]) has become great deal of interest due to potential use in non volatile memory technology. Permanent dipoles (formed between the alternating hydrogen and fluorine atom within the copolymer) ordering of orientation are crucial for device efficiency. Here we focus on thickness dependence dipole orientation in these copolymer films. In our systematic studies, we found there is prominent dipole re-orientation effect also for the intrinsic films (˜10 nm thickness) before applying the electric field. It is observed after the application of the field, the dipoles re-oriented in opposite direction. Therefore, we conclude that the lowest thickness of the film should have well grown crystalline lamellae structure. As a result, c-axis of crystallites acts as well define manner in plane of the surface and for that reason the b-axis is more free. Because the b-axis is parallel to the polarization direction, it is easy to get a preferred orientation of the dipoles. For thicker films (here up to 100 nm), the average orientation effect is hindered, so a very low re-orientation effect has been observed. For this investigation, we used Near Edge X-ray Absorption Spectroscopy, at the U 49/2-PGM beam line of BESSY-II, Berlin. This work is supported by DFG within SPP1157 (SCHM 745/11-2).

SYSA 5.77 Tue 14:30 Poster A

High Resolution Photoelectron Spectroscopy at the SnPc/Ag(111) interface — C. Scheuermann, M. Haeming, I. Kröger, C. Stadler, C. Kumpf, •A. Schöll, F. Reinert, and E. Umbach — Universität Würzburg, Experimentelle Physik II, 97074 Würzburg

Phthalocyanines are interesting for applications in organic devices due to the potential of tailoring their properties by introducing different metal ligands into the heterocycle. Some derivates offer the potential of tuning the work function of metal contacts due to an intrinsic dipole moment. We present a high resolution photoelectron spectroscopy study on SnPc submonolayers on Ag(111). Based on a structural analysis, which shows the existence of different adsorption phases with different orientation of the molecular dipoles depending on temperature and coverage, the PES data indicate a significant effect on the surface work function. The valence and core spectra allow identifying a covalent interaction at the interface with the appearance of a new state at EF. Moreover, the data provide evidence for a systematic weakening of the interfacial interaction with increasing coverage. This is accompanied by a constriction of the substrate-adsorbate charge transfer, which becomes evident from an analysis of the core level line shapes. As a consequence, a comprehensive description of the electronic structure in the contact regime, of the resulting interface dipole, and of work function effects needs to account not only for structural properties such as the intrinsic molecular geometry, but also for intermolecular- and interfacial interactions which may involve significant charge transfer.

SYSA 5.78 Tue 14:30 Poster A

Metal work function tuning with new molecular acceptors — •Benjamin Bröker[1], Ralf-Peter Blum[1], Antje Vollmer[2], Oliver Hofmann[3], Steffen Duhm[1], Hendrik Glowatzki[1], Ralph Rieger[4], Hans Joachim Räder[4], Klaus Müllen[4], Jürgen P. Rabe[1], and Norbert Koch[1] — [1]Institut für Physik, Humboldt-Universtität zu Berlin, D-12389 Berlin, Germany — [2]Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung mbH, D-12489 Berlin, Germany — [3]Institut für Festkörperphysik, Technische Universität Graz, A-8010 Graz, Austria — [4]Max Planck Institut für Polymerforschung, D-55128 Mainz, Germany

The interfaces between metal electrodes and electroactive organic materials are important for the performance of organic electronic devices. One way of optimizing the anode/organic interface is the insertion of a (sub-)monolayer of molecular acceptors. Here we present an UPS study of new electron acceptor molecules deposited on Au(111), Cu(111) and Ag(111). This study intends to improve the understanding of how the interactions of specific electron withdrawing groups with metal surfaces are correlated with observed modifications of interfacial electron density distribution, work function change ($\Delta\Phi$), and the energy level alignment. We find that $\Delta\Phi$, which is the difference between the work function (Φ) of the clean metal surface and Φ after formation of a molecular monolayer, is a monotonic function of initial Φ of the metal. Two different slopes were observed for acceptors with cyano and those with keto or nitro groups. This work is financially supported by the European Community project "IControl" (EC-STREP-033197).

SYSA 5.79 Tue 14:30 Poster A

Exploring the binding of the strong organic acceptor F4TCNQ to coinage metals — •Gerold Rangger[1], Lorenz Romaner[1], Georg Heimel[2], Steffen Duhm[3], Ralf-Peter Blum[3], Benjamin Bröker[3], Norbert Koch[3], Alexander Gerlach[4], Frank Schreiber[4], and Egbert Zojer[1] — [1]Institut für Festkörperphysik, Technische Universität Graz, 8010 Graz, Austria. — [2]Department of Material Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02143, USA — [3]Institut für Physik, Humboldt-Universität zu Berlin, 12389 Berlin, Germany — [4]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany

Organic/metal interface properties are of high interest for the application of molecular (sub)monolayers to modify surface properties. They are applied for, e.g., molecular electronics, chemical sensing, or the tuning of injection barriers in organic electronic devices.

We present a joint theoretical and experimental study of F4TCNQ adsorbed on Cu(111). The electronic and structural properties were determined by ultraviolet photoelectron spectroscopy (UPS) and X-ray standing wave (XSW) measurements. To better understand the complex process of binding, we modelled the system using density-functional theory. We find forward-donation from the lone pairs of the molecule into metallic states and back-donation from the metal into the LUMO of the molecule. The data on Cu(111) are compared to F4TCNQ on Au(111) and Ag(111) as well as to investigations of pyrenetetraone on various coinage metals.

SYSA 5.80 Tue 14:30 Poster A

Self-assembly and tunneling transport characteristics of phenylthio-substituted coronenes on graphite — •Peter Kowalzik[1], Silvia Karthäuser[1], Jean-Manuel Raimundo[2], Marc Gingras[2], and Rainer Waser[1] — [1]Institute of Solid State Research and CNI, Research Center Juelich GmbH, 52425 Juelich, Germany — [2]Département de Chimie, GCOM2, Université de La Méditerranée Aix-Marseille II, Case 901, 13288 Marseille Cedex 09, France

The use of conjugated (macro)molecules as components in molecular electronic devices is favoured because of the possibility to tune their electron transport properties through modifications of the size of the aromatic system and appropriate functionalisations in the periphery. Here we study the self-assembly and tunneling transport properties of dodecakis(phenylthio)coronene (DPTC) on graphite. DPTC shows an effective delocalisation of negative charges throughout the molecular system despite its overall nonplanarity. Layers of DPTC were deposited on the graphite surface from solution and characterised via UHV-STM/STS resulting in large highly ordered two dimensional supramolecular structures with several phases. Monolayers of DPTC adsorb with the coronene disc of the molecules lying flat on the graphite surface and arrange in stuctures with hexagonal symmetry. In addition clusters of several DPTC molecules of definite size are observed which again assemble into hexagonaly ordered films on the substrate. STS measurements reveal orbital mediated tunneling processes which were analysed by current-voltage curves.

SYSA 5.81 Tue 14:30 Poster A

Ordering and morphology of CoPc (FePc) thin films grown on Au(001)-5x20 — •Olga V. Molodtsova[1], Victor Yu. Aristov[1,2], and Martin Knupfer[1] — [1]IFW Dresden, Dresden, Germany — [2]ISSP RAS, Chernogolovka, Russia

The molecular orientation and ordering in the organic semiconductor cobalt- and iron-phtalocyanine (CoPc and FePc) thin films in situ grown on a Au(001)-5x20 surface has been studied by a combination of Low Energy Electron Diffraction (LEED) and near-edge x-ray absorption spectroscopy. The results indicate that the molecular planes of CoPc and FePc (up to 60 Å) deposited at substrate temperatures ranging from room temperature (RT) to 300°C are mainly laying parallel to the substrate surface. The LEED patterns from the thin films show that the overlayers are highly ordered with a square unit cell of approximately 14 Å x14 Å aligned along the <110> axes of the Au(001) surface. The additional high resolution photoelectron spectroscopy data prove that CoPc and FePc overlayers on (001) single crystal gold substrates remain stoichiometric and molecular.

Acknowledgements: This work was supported by the DFG (no. 436RUS17/52/06), SFB 463 and RFBR (Grant No 05-02-17390).

SYSA 5.82 Tue 14:30 Poster A

Molecular Wires and Assemblies on Ionic Surfaces — •Lars Zimmerli, Thilo Glatzel, Bartosz Such, Pascal Steiner, and Ernst Meyer — Department of Physics, Klingelbergstr. 82, 4056 Basel, Switzerland

The adsorption of functional organic molecules on insulating surfaces offers fascinating perspectives for novel nanometer sized electronic and optoelectronic devices. However, the growth of ordered molecules is often hampered by the strength of the intermolecular interaction compared to molecule-surface interaction [1].

In this contribution we report on the self assembly of cyanoporphyrin based molecules deposited on in-situ cleaved and annealed ionic (KBr and NaCl) surfaces. The molecular arrangements on the terraces and steps are analyzed in detail using an ultrahigh vacuum nc-AFM operated at room temperature. Ordered molecular assemblies grown out of a bunch of disordered molecules at step edges are typically found. Single molecular wire-like structures were resolved within the assemblies. The arrangement as well as the orientation of the ordered molecules with respect to the atomic lattice of the substrate has been determined from measurements showing atomic and molecular resolution simultaneously. Along straight monatomic steps single molecular wires of several hundred nanometers length were found.

[1] L Zimmerli et al., J. Phys.: Conf. Ser. 61 (2007) 1357.

SYSA 5.83 Tue 14:30 Poster A

The unoccupied electronic structure of potassium doped cobalt- and iron phthalocyanines studied by near edge absorption fine structure — •Victor Yu. Aristov[1,2], Olga V. Molodtsova[1], Victor N. Sivkov[3], Sergei V. Nekipelov[3], Victor M. Zhilin[2], and Martin Knupfer[1] — [1]IFW Dresden, Dresden, Germany — [2]ISSP RAS, Chernogolovka, Russia — [3]Syktyvkar State University, Syktyvkar, Russia

Magnetic transition metal phthalocyanines, which are organometallic complexes, have already obtained substantial attention of researchers due to many different potential applications. In particular, CoPc is often utilizing in the fields of gas and radiation sensors, optoelectronics and in medical applications. Nowadays CoPc is considered as a material for development of low dimensional molecular magnets. Such important potential applications give a strong motivation to characterize and study the electronic structure, molecular orientation and ordering in the organic semiconductor transition magnetic metal phthalocyanines thin films which is relevant to the organic film performance. The ability to incorporate electron acceptors and donors into molecular crystals enables the control of their electronic properties by introducing charge carriers. In this presentation we report the evolution of unoccupied electronic levels and electronic properties of the organic semiconductor cobalt- and iron phthalocyanines with potassium doping, which has been studied by near-edge x-ray absorption.

Acknowledgements. This work was supported by the DFG (no. 436RUS17/52/06), SFB 463 and RFBR (Grant No 05-02-17390).

SYSA 5.84 Tue 14:30 Poster A

Time-resolved investigations on reversible single-crystal-to-single-crystal photodimerisation — •Jörg Hallmann, Jav Davaasambuu, and Simone Techert — MPI for biophysical Chemistry, Am Fassber 11, 37070 Göttingen

Compounds like cinnamic acid and their derivates are known for their ability to dimerise upon light irradiation. In the following the work will concentrate on time-resolved structural studies of α-styrylpyrylium (TFMS) salts. These systems preserve periodicity upon photodimerisation and transform thermally back to the initial phase and structure. Therefore these systems are attractive candidates for optical switcher and information storage materials using light, respectively. In the following kinetic studies are presented for crystals with an edge length in the millimeter range as well as studies on single crystal films with a thickness of a few hundred nanometers. The studies concern time-resolved diffraction studies and spectroscopy of fluorescence, absorption in the VIS and IR range, and single-photo-counting. The thin crystalline films of some hundred nanometer size were used for ultrafast time-resolved optical pump - x-ray probe experiments revealing that the photo-switchable process occurs in the (sub) picosecond time regime beyond the resolution of the apparatus used. Investigations on macroscopic crystals allowed determining the time-resolved light-induced changes of the molecular structures down to electron densities.

SYSA 5.85 Tue 14:30 Poster A

Long term aging behavior of ZnPc:C60 Organic Solar Cells under controlled conditions — •Rudolf Lessmann[1], Ziruo Hong[2], Moritz K. Riede[1], and Karl Leo[1] — [1]IAPP - Institut Für Angewandte Photophysik, Technische Uniservität Dresden, Germany — [2]Department of Materials Science & Engineering, University of California, Los Angeles, USA

Cu or Zn Phtalocyanines (CuPc and ZnPc) and C60 are frequently used for organic solar cells, since their energy levels form a donor-acceptor hetero junction and they have high absorption coefficients and a complementary absorption in the sun spectrum. Its known from literature that strong degradation is induced by oxygen diffusion in C60 wich acts as an exciton quencher, drastically reduces the mobility, and eventually decomposes C60. Here, we analyze the long term aging behavior of solar cells based on flat and bulk ZnPc/C60 heterojunctions under controlled conditions. The starting structure is ITO(120 nm)/ZnPc(15 nm)/C60(40 nm)/buffer(4 nm)/Al(100 nm). Devices encapsulated with glass and UV epoxy were aged under controlled temperature and illumination at 475 nm (intensities $> 10\ mW/cm^2$), corresponding to the maximum photo-response of C60 in the visible spectra for this device structure. We experimentally address new ways to stabilize the C60 - oxygen interaction in the device. The overall degradation is quite fast, the fitted time to half of initial value (t_H) of I_{SC} is on the order of 1000 h. After that time $I(-1V)$ is still around 95% of its initial value, indicating that the degradation is mainly driven by changes of the transport properties.

SYSA 5.86 Tue 14:30 Poster A

Phenyl-thiophene co-oligomer growth on dielectrics — •Frank Balzer[1], Manuela Schiek[1], Arne Lützen[2], and Horst-Günter Rubahn[1] — [1]Mads Clausen Institute, NanoSYD, University of Southern Denmark, Sønderborg, Dänemark — [2]Kekulé-Institute of Organic Chemistry and Biochemistry, Universität Bonn, Deutschland

Light emitting thiophene/phenylene co-oligomers have attracted quite some interest in the past due to their fortunate optical and transport properties. Here the growth of 2,5-bis(4-biphenylyl)thiophene on alkali halide (001) surfaces as well as on muscovite mica (100) is investigated by atomic force microscopy (AFM), by low energy electron diffraction (LEED), and by fluorescence microscopy. Profound differences in the growth morphology are observed. On, e.g., KCl both needle-like crystallites with several ten nanometers width and height, but several micrometers length from lying molecules are formed. These needles cover the substrate surface together with platelets from upright molecules. Needles aggregate into box-like structures with several micrometers side length. On muscovite only uniaxially aligned needles are observed by AFM and by fluorescence microscopy. However, LEED demonstrates the formation of an epitaxial wetting layer from lying molecules. In all cases needles emit polarized light after UV excitation. Formation mechanisms of such different types of self-assembled structures are discussed and compared to thin films from *para*-phenylenes and from α-thiophenes.

SYSA 5.87 Tue 14:30 Poster A

Reversible Temperature Induced Switching of Grafted Poly-N-isopropylacrylamide Brushes — •Petra Uhlmann, Eva Herold, Sina Burkert, Martin Müller, and Manfred Stamm — Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, D-01069 Dresden

Polymer brushes, as linear polymer chains tethered by one end to a solid surface with sufficient grafting density, represent a special case of grafted polymer thin films and a versatile tool to control and switch the properties of polymer interfaces. Poly-N-isopropylacrylamide (PNiPAAM) which is known to undergo conformational changes due to temperature alterations (stretched below and coiled above the lower critical solution temperature (LCST) of 32°C) represents a very interesting mean to reversibly switch the physico-chemical properties of polymer interfaces when immobilized in a brush-like conformation at solid interfaces. The switching process and mechanism of collaborative acting PNiPAAM brushes was investigated using ellipsometry, dynamic contact angles and attenuated total reflectance infrared spectroscopy (ATR). The phase transition mechanism of the PNiPAAM brushes observed near the LCST was found to be independent of the molecular weight of the polymer. Using ATR-FTIR the formation of internal hydrogen bonds due to switching, by ellipsometry the deswelling of the brush in aqueous environment above the LCST and by wetting measurements changing hydrophilicity in dependence of temperature could be followed. The influence of molecular weight and grafting density on switching process and mechanism will be discussed.

SYSA 5.88 Tue 14:30 Poster A

The Potential of the Horizontal ToF-Neutron Reflectometer REFSANS at FRM-II Munich Highlighted by Recent Experimental Results — •Reinhard Kampmann[1], Haese-Seiller Martin[1], Moulin Jean Francois[1], Nickel Bert[2], Müller-Buschbaum Peter[3], Papadakis Christine[3], Sackmann Erich[2], Rädler Joachim[2], and Schreyer Andreas[1] — [1]GKSS-Forschungszentrum Geesthacht GmbH, D-21502 Geesthacht, Germany — [2]Lehrstuhl für Experimentelle Physik/Biophysik, Sektion Physik, Ludwig-Maximilians-Universität, D-80539 München, Germany — [3]Physik-Department E13, TU-München, D-85748 Garching, Germany

The horizontal neutron reflectometer REFSANS allows to perform comprehensive analyses of vertical and lateral surface and interface structures by means of specular and off-specular neutron reflectivity as well as small-angle neutron scattering at grazing incidence (GISANS). All measurements can be performed on the air-water interface (horizontally aligned sample). The performance of this novel instrument is highlighted by means of recent measurements of weak off-specular scattering, GI-SANS and extremely low specular reflectivity including the case of a strong incoherent substrate scattering. This work has been supported by the German Federal Ministry of Education, Research and Technology (BMBF) under contracts 03-KA5FRM-1 and 03-KAE8X-3.

SYSA 5.89 Tue 14:30 Poster A

Crystallisation of acetaminophen in nanoporous glasses — •Gopalakrishnan T. Rengarajan, Dirk Enke, and Mario Beiner — Naturwissenschaftliche Fakultät II, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle/Saale, Germany

Pharmaceuticals are polymorphic materials existing in different crystalline forms like many other small molecules. Selection of a particular crystalline form and stabilization of amorphous pharmaceuticals are important issues for specific drug applications. DSC and X-ray scattering methods are used to study the crystallization behavior of acetaminophen used as model drug in nanoporous glasses with well defined pore diameters in the range 4-100nm. We will show that nanoconfinement is a strategy to produce the metastable form III of acetaminophen, which is usually inaccessible in bulk samples. Thermodynamic quantities like melting temperature and heat of melting of form III are reported for the first time [1]. We will also show that nanoconfinement can be used to increase the life time of the amorphous phase, which has better solubility and bioavailability compared to crystalline states. Thermodynamic, nucleation and kinetic effects contributing to changes in the crystallization behaviour in nanoscopic host systems will be discussed.

[1] M. Beiner, G.T. Rengarajan, S. Pankaj, D. Enke, M. Steinhart, Nano Letters 7 (2007) 1381-1385.

SYSA 5.90 Tue 14:30 Poster A

Long-ranged steric forces between poly(styrene sulfonate) covered surfaces — •Stephan Block and Christiane A. Helm — Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17487 Greifswald, Germany

We investigate distance dependent surface forces with Colloid Probe Technique (CPT) between poly (styrene sulfonate) (PSS) coated surfaces in salt solutions between 1 mM and 1 M, after the PSS was adsorbed from 1 M NaCl solution onto Si surfaces positively charged by silanization. A non-flat conformation is observed [1]. The theory of Alexander and de Gennes for interacting surfaces covered with neutral anchored polymers describes the long-ranged steric interaction between the PSS layers. A lack of electrostatic interaction and the scaling of the layer thickness similar to polyelectrolyte brushes suggest that the polyelectrolytes are neutralized by counterions incorporated into the layer. Investigation of asymmetric surfaces (one PSS covered surface against a silica colloidal probe or a silicon tip) supports this picture, since decay length and amplitude of the force are halved compared to the forces between two identical surfaces. After drying (0% r.h.) and reimmersion into solution the surface forces between the PSS layers are almost unchanged, suggesting strong local bonds between few monomers and the substrate. Furthermore, on increase of the PSS molecular weight (78kDa, 350kDa and 1.3MDa) the PSS layer thickness as well as the distance between adsorption points increases.

[1] S.Block and C.A.Helm, PRE 76 (2007) 030801(R).

SYSA 5.91 Tue 14:30 Poster A

Lamellar phase of polyectrolyte chains adsorbed onto oppositely charged lipid monolayers — •Jens-Uwe Günther, Heiko Ahrens, Olaf Soltwedel, and Christiane A. Helm — Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17487 Greifswald, Germany

At the air-water interface, the polyanion PSS (Poly styrene sulfonate) is adsorbed onto positively charged TAP or DODAB monolayers (1,2-Dipalmitoyl-3-Trimethylammonium-Propane, dioctadecyammonium bromide), respectively. By compressing the lipid monolayer, the surface charge is varied. In-plane order is investigated with grazing incidence X-ray diffraction, the lipid phases with fluorescence microscopy. When the alkyl chains of DODAB and TAB are ordered, an additional superstructure peak of the aligned PSS chains is observed provided the PSS concentration is 1 mM or less. For DODAB in the fluid phase, PSS in a lamellar phase with a much wider spacing is found. On decrease of the PSS concentration, the spacing of the chains is larger, since the monolayer charge is no longer compensated. The influence of the kind of counterion as well as the polymer length is less pronounced. If the PSS concentration or the ion concentration is larger than 1 mM no chain ordering is observed, suggesting that both large intra- and interchain electrostatic interactions are necessary to obtain a lamellar polyelectrolyte phase.

SYSA 6: Organic Interfaces (further abstracts see DS 19.2-11)

Time: Wednesday 14:30–17:30 Location: H 2013

Invited Talk SYSA 6.1 Wed 14:30 H 2013

Organometallic Nanojunctions Probed by Different Chemistries: Thermo-, Photo, and Mechanochemistry — •I. Stich[1,2], M. Konopka[1], R. Turansky[1], J. Reichert[3], N. L. Doltsinis[4], H. Fuchs[3], and D. Marx[4] — [1]Slovak Tech. Univ. (FEI STU), Slovakia — [2]Inst. of Phys., Slovak Acad. of Sci., Slovakia — [3]Uni. Muenster, Germany — [4]Ruhr-Uni. Bochum, Germany

Different methods of activation of chemical reactions are compared for organometallic nanojuctions. The study is based on density functional theory simulations. First we provide a comparison of thermal activation with mechanical activation, or mechanochemistry. Study of thiolate/copper junctions and interfaces provides evidence for vastly different reaction pathways and products. The differences are understood in terms of mechanical manipulation of coordination numbers and system fluctuations in the process of mechanical activation. Next we compare photo- and mechanochemistry. Azobenzene is an optically switchable molecule. Laser light is normally used to achieve molecular switching between the cis and trans isomers. We study azobenzene optomechanical switch which combines photo excitation with external pulling force to manipulate optical switching properties of the azobenzene molecule anchored to gold tips by thiolate bonds. We focus on the separation between ground (S0) and first excited (S1) singlet states. We observe a pronounced dependence of the S0-S1 separation on the applied strain. Furthermore we find that ground-state mechanochemistry alone can be used to achieve switching. For instance, mechanochemistry with modest applied forces leads to cis -> trans reisomerization.

Joined session with DS: Further abstracts are listed under DS 19.2-11

SYSA 7: Organic Polymer-Metal Interfaces (further abstracts see DS 20.2-6)

Time: Wednesday 17:45–19:30 Location: H 2013

Invited Talk SYSA 7.1 Wed 17:45 H 2013

Designing the nanostructure of the organic polymer - metal interface — •Stephan V. Roth — HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany

Thin film organic-metallic nanocomposites play an important role in biosensoring [1], solar cell applications [2] or organic electronics [3]. Depending on the desired application, one must tailor the interface metal - organic layer, e.g. selective contacting [4] or exploiting the plasmon resonances of the nanostructured metal layer [2,5,6]. Therefore, understanding the growth kinetics of the nanoparticle layer during deposition is of utmost importance to be able to design the nanocomposites' properties [6].

We exploited different deposition methods ranging from vacuum deposition [5,7] to solution casting [8] to install different metal layer morphologies. In combination with grazing incidence small-angle x-ray scattering we were able to observe the metal nanolayer growth kinetics on different organic and inorganic layers in real-time and present first results.

[1] B. Dubertret et al., Nat. Biotechnol. 19, 365 (2001)
[2] M. Westphalen et al., Sol. Energy Mater. Sol. Cells 61, 97 (2000)
[3] S. Gamerith et al., Adv. Funct. Mater. 17, 3111 (2007)
[4] T. L. Morkved et al., Appl. Phys. Lett. 64, 422 (1994)
[5] S.V. Roth et al., Appl. Phys. Lett. 88, 021910 (2006)
[6] A. Biswas et al., Vac. Techn. & Coat. 7, 54 (2006)
[7] S.V. Roth et al., Appl. Phys. Lett 82, 1935 (2003)
[8] S.V. Roth et al., Appl. Phys. Lett 91, 091915 (2007)

Joined session with DS: Further abstracts are listed under DS 20.2-6

SYSA 8: Nanostructured Block Copolymer Films (further abstracts see DS 35.2-5)

Time: Thursday 17:00–18:30 Location: H 2032

Invited Talk SYSA 8.1 Thu 17:00 H 2032

Nanostructure and transport in regioregular polythiophenes and their block copolymers — Rui Zhang[1], Bo Li[1], Jessica R. Cooper[1], Mihaela Iovu[1], Genevevie Sauve[1], David N. Lambeth[1], Detlef-M. Smilgies[2], Richard D. McCullough[1], and •Tomasz Kowalewski[1] — [1]Department of Chemistry, Carnegie Mellon University , 4400 Fifth Avenue, Pittsburgh, PA 15213 — [2]Cornell University, Ithaca, NY, USA

This presentation will describe the results of combined atomic force microscopy (AFM) and grazing incidence small and wide angle x-ray scattering (GISAXS/GIWAXS) studies of narrow polydispersity regioregular poly(alkyltiophenes) (PATs) and their block copolymers. Well-defined PATs were shown to have a high tendency to form nanofibrillar structures with the nanofibril widths closely related to the contour lengths of polymer molecules. Moreover, carrier mobilities in field effect transistors fabricated from PATs exhibiting nanofibrillar morphologies exhibited exponential dependence on nanofibril width. The significance of this relationship as well as the morphology of block copolymers of PATs with immiscible segments and its impact on transport properties will be also discussed.

Joined session with DS: Further abstracts are listed un-

der DS 35.2-5