Symposium Organic Photovoltaics: From Single Molecules to Devices (SYOP)

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

Silke Rathgeber
Johannes Gutenberg-Universität Mainz
Staudingerweg 7
55099 Mainz
rath@mpip-mainz.mpg.de

Karl Leo
Technische Universität Dresden
George-Bähr-Straße 1
01069 Dresden
karl.leo@iapp.de

Thomas Thurn-Albrecht
Martin Luther-Universität Halle-Wittenberg
Hoher Weg 8
06099 Halle (Saale)
thomas.thurn-albrecht@physik.uni-halle.de

Overview of Invited Talks and Sessions

(lecture rooms BAR SCHÖ and ZEU 222)
Poster area P1A: all posters should be in place at 14:30; kernel time of the poster session is 16:30-19:00

Invited Talks

SYOP 2.1	Thu	9:30–10:00	BAR SCHÖ	**Material Design for Organic and Hybrid Solar Cells – structural to functional control on all length scales –** — •Mukundan Thelakkat, Michael Sommer, Ruth Lohwasser, Sebastien Maria
SYOP 2.2	Thu	10:00–10:30	BAR SCHÖ	**Triplet exciton formation in organic photovoltaics** — Xudong Yang, Sebastian Westenhoff, Ian Howard, Thomas Ford, Richard Friend, Justin Hodgkiss, •Neil Greenham
SYOP 2.3	Thu	10:30–11:00	BAR SCHÖ	**Charge Carrier Dissociation and Recombination in Polymer Solar Cells** — •Vladimir Dyakonov, Carsten Deibel
SYOP 2.4	Thu	11:00–11:30	BAR SCHÖ	**Modeling exciton diffusion and dissociation at organic-organic interfaces** — •David Beljonne
SYOP 2.5	Thu	11:30–12:00	BAR SCHÖ	**Correlation of Interfacial Composition and Bulk Morphology to Device Performance in Organic Bulk Heterojunction Solar Cells** — David Germack, •Joseph Kline, Daniel Fischer, Lee Richter, Calvin Chan, David Gundlach, Michael Toney, Dean DeLongchamp
SYOP 2.6	Thu	12:00–12:30	BAR SCHÖ	**Developments on the acceptor side in plastic PV** — •Jan C. Hummelen

Sessions

SYOP 1.1–1.12	Wed	14:00–17:00	ZEU 222	**Organic Photovoltaics I**
SYOP 2.1–2.6	Thu	9:30–12:30	BAR SCHÖ	**Organic Photovoltaics: from Single Molecules to Devices**
SYOP 3.1–3.8	Thu	14:00–16:00	ZEU 222	**Organic Photovoltaics II**
SYOP 4.1–4.79	Thu	16:30–19:00	P1A	**Organic Photovoltaics: from Single Molecules to Devices**
SYOP 5.1–5.11	Fri	10:30–13:15	ZEU 222	**Organic Photovoltaics III**

SYOP 1: Organic Photovoltaics I

Time: Wednesday 14:00–17:00 Location: ZEU 222

SYOP 1.1 Wed 14:00 ZEU 222

Efficient Polaron Pair Dissociation in Polymer:Fullerene Blends — •Carsten Deibel[1], Thomas Strobel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Institute of Physics, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg

Organic bulk heterojunction solar cells already achieve energy conversion efficiencies of up to 6%. To a significant part, this is due to the very efficient separation of the bound electron–hole pairs, also called polaron pairs. This event is the intermediate but crucial step between exciton dissociation and charge transport to the electrodes. Using a simple model of Coulomb attraction of the bound charge carrier pair, the electric field needed to overcome the mutual attraction with a probability of 90% is larger than 10^8V/m. In contrast, in good organic solar cells, almost all polaron pairs are separated at fields smaller by a factor of around 50. We attempt an explanation of this significant discrepancy by performing Monte Carlo simulations of hopping transport in a bulk heterojunction blend system. We discuss the influence of phase separation and recombination rate on the efficiency of the polaron pair dissociation.

SYOP 1.2 Wed 14:15 ZEU 222

Stability of organic electronics - P3HT as model to study general mechanistic effects. — •Holger Hintz[1], Hans-Joachim Egelhaaf[1,2,3], Christoph Brabec[3], Heiko Peisert[1], and Thomas Chassé[1] — [1]University of Tübingen, Institute for Theoretical and Physical Chemistry, Auf der Morgenstelle 8, D-72076 Tübingen — [2]Christian-Doppler Labor für oberflächenoptische Methoden, Johannes-Kepler University, Altenbergerstaße 69, A-4040 Linz — [3]Konarka Austria GmbH, Altenbergerstaße 69, A-4040 Linz

The stability of Polythiophene (P3HT) is still unsatisfactory and the degradation mechanism has not yet been fully understood. Photooxidation of thin P3HT layers was performed under ambient conditions and under varying partial pressures of oxygen, water and ozone using Xenon light. The kinetics were monitored by FTIR and UV/VIS spectroscopy and can be described by the laws of photo-oxidation of layer systems, considering the blue-shift of the absorption spectra of formed P3HT fragments. A sublinear dependence of the degradation rate on oxygen partial pressure is monitored, probably due to the formation of singlet oxygen via a long-lived triplet excited state of P3HT. This is supported by strongly reduced degradation rates upon addition of PCBM, due to the quenching of the polymer excited state. Further support comes from the comparison of the temperature dependences of photo degradation and oxygen diffusion. Photo-oxidation at different humidity levels showed enhanced degradation rates in the presence of water. As water in the absence of oxygen does not cause any degradation, this is due to either a solvent effect or a catalytic mechanism.

SYOP 1.3 Wed 14:30 ZEU 222

Molecular semiconductor blends: microstructure, charge carrier transport and application in photovoltaic cells — •Andreas Opitz[1], Julia Wagner[1], Bernhard Ecker[1], Wolfgang Brütting[1], Alexander Hinderhofer[2], and Frank Schreiber[2] — [1]Institute of Physics, University of Augsburg, Germany — [2]Institute of Applied Physics, University of Tübingen, Germany

Blends of organic donor and acceptor materials have the potential of an increase of solar cell efficiency. However, the balance between charge carrier transport in phase-separated structures and exciton dissociation at the donor-acceptor interface has to be optimized. To analyze this relation in more detail the following molecular material combinations were investigated: (i) Copper phthalocyanine (CuPc) combined with fullerene C_{60} and (ii) CuPc in combination with perfluorinated CuPc (F_{16}CuPc).

Measurements by X-ray diffraction and scanning force microscopy indicate the formation of phase-separated nanocrystals for blends of CuPc/C_{60} and the formation of mixed crystals in the CuPc/F_{16}CuPc system. The formation of mixed crystals is an interesting feature for organic blends which has not yet been explored in organic solar cells. We will discuss the implications of the different molecular arrangements on the optical and electrical properties as well as for the solar cell performance.

SYOP 1.4 Wed 14:45 ZEU 222

Interfacial adhesion in polymer blend P3HT:PCBM solar cells — •Ayse Turak[1], Jonas Hanisch[2], Esther Barrena[1,3], Erik Ahlswede[2], and Helmut Dosch[1,3] — [1]Max Planck Institute for Metals Research, Heisenbergstrasse 3, 70569, Stuttgart — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung (ZSW) Baden-Württemberg, Industriestrasse 6, 70565, Stuttgart — [3]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57/VI, 70550 Stuttgart, Germany

The nature of the contact at the electrode/organic interface has a major impact on device performance. Introduction of thin dielectric interlayers such as LiF have been successful in significantly improving device properties. However, examination of the buried interface is generally difficult as deposition of the top electrode may alter the nature of the contact. Using peel-off adhesion analysis with grazing incidence x-ray diffraction, atomic force microscopy and optical imaging, we have assessed the quality of the buried interfacial layer in P3HT:PCBM solar cells in the presence of interlayers. We see increased adhesion of the Al cathode without the interlayer, suggesting broader interfacial mixing of the Al with the polymer without LiF as a blocking interlayer. The confinement of the charge extraction to a well defined interface may be used to explain improved device performance with LiF interlayers.

SYOP 1.5 Wed 15:00 ZEU 222

Block copolymer templating: a bicontinuous double gyroid hybrid solar cell — •Edward Crossland[1], Sabine Ludwigs[1], Marc Hillmyer[2], Ulrich Wiesner[3], Henry Snaith[4], and Ullrich Steiner[5] — [1]Freiburg Institute for Advanced Studies, Germany — [2]University of Minnesota — [3]Cornell University — [4]University of Oxford — [5]University of Cambridge

The conversion of light to electrical energy in hybrid solar cells based on organic-ceramic composites demands engineering of highly distributed, yet interconnected heterojunctions on the 10nm length scale. Microphase separation of block copolymers offers an extremely versatile bottom-up approach to high aspect ratio patterning of functional materials on these macromolecular scales in thin films. We fabricated highly ordered arrays of semiconductor nanostructures using selectively degradable block copolymers as porous electrochemical templates. Cylinder-forming poly(4-fluorostyrene)-b-(D,L-lactide) films were aligned using electric fields to template freestanding vertical nanowire arrays over 1μm long and 10nm in diameter while the network phase of a bicontinuous double gyroid morphology could be replicated without external alignment. Charge transport and recombination rates as well as photovoltaic power conversion efficiencies were probed in each morphology incorporated into dye sensitized solid-state and liquid-electrolyte solar cells. These results mark the first successful application of the gyroid morphology in a functioning electronic device. This templating technique is fully extendable to a enormous range of potentially high performance heterojunction systems.

SYOP 1.6 Wed 15:15 ZEU 222

Preparation of hybrid solar cells from CdSe nanocrystals and poly(3-hexylthiophene) — •Folker Zutz, Marc-Daniel Heinemann, Irina Lokteva, Joanna Kolny-Olesiak, Ingo Riedel, Holger Borchert, and Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, Carl-von-Ossietzky Str. 9-11, 26129 Oldenburg, Germany

Colloidally prepared semiconductor nanocrystals with particle sizes of a few nanometers possess particular physical and chemical properties. One example is the size-dependent band gap which enables tuning of optical properties by controlling the particle size. One potential application is the use of nanocrystals as a component in hybrid solar cells. Similar to organic composites of polymer and fullerenes, a nanocrystal-polymer composite is a donor/acceptor system where photo-generated charge carriers can be efficiently separated because of the affinity of the nanocrystals and polymers to accept electrons and holes, respectively. In contrast to fullerenes, semiconductor nanocrystals can additionally act as absorber themselves. This offers possibilities to optimize the exploitation of the solar spectrum. In the present work, we prepared high-quality CdSe nanocrystals. Composites of the nanocrystals and polymere (P3HT) were successfully used to prepare laboratory solar cells which were characterized by I-V curves and measurements of the external quantum efficiency. Further experiments with different ratios of Cadmium to Selenium in the nanocrystals and different ratios of CdSe nanocrystals to polymere in the semiconductor blend were made. The results were compared with purely organic composites.

SYOP 1.7 Wed 15:30 ZEU 222

Hybrid Organic-Inorganic Bulk Heterojunctions with Silicon Nanocrystals for Solar Cells — •Sabrina Niesar[1], Roland Dietmüller[1], André Ebbers[2], Martin Trocha[2], Hartmut Wiggers[3], and Martin Stutzmann[1] — [1]Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching, Germany — [2]Evonik Degussa GmbH, Paul-Baumann-Str.1, 45772 Marl, Germany — [3]Institut für Verbrennung und Gasdynamik, Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

Hybrid organic-inorganic solar cells, which incorporate both, organic and inorganic semiconductors, have received a lot of attention during the last years. Such solar cells typically consist of a bulk heterostructure made of organic semiconducting polymers and semiconducting nanocrystals. These hybrid organic-inorganic solar cells can benefit from the solution processing and from the broad spectral absorption range of semiconductor nanocrystals. We have studied hybrid bulk heterojunctions between Silicon nanocrystals (Si-nc), which have been synthesized by decomposition of silane in a microwave plasma reactor, and the organic hole conductor poly(3-hexylthiophene-2,5-diyl) (P3HT). Hybrid bulk heterojunction solar cells with P3HT and Si-nc have been produced and characterized by current-voltage measurements. For these devices, we have demonstrated by spectrally resolved photocurrent measurements that both components of the solar cell, the Si-nc and the P3HT, contribute to the photocurrent. Current-voltage measurements under white light illumination with 100 mW/cm^2 show a high open circuit voltage of up to 0.7 V.

SYOP 1.8 Wed 15:45 ZEU 222

Inverted Bulk Heterojunction Solar Cells — •Sofie Khalil and Klaus Meerholz — University of Cologne, Institute for Physical Chemistry, Luxemburger Str. 116, 50969 Cologne, Germany

Solution processed polymer photovoltaics are nowadays a very promising low-cost fabrication technology for renewable energy sources. Nevertheless research made onto bulk heterojunction (BHJ) with structure: ITO/ PEDOT:PSS/ blends of regioregular poly-3-hexylthiophene (RR-P3HT) and the fullerene derivative [6,6]-phenyl C61 butyric acid methyl ester (PCBM) / Ca:Ag showed inherent lifetime limitations due the use of PEDOT:PSS and low work-function metal electrode. In this talk we will show an alternative device with a new stacking order of layers: the inverted solar cells. In these devices to avoid the air sensitive and lifetime limiting materials we use a stable transparent anode electrode with lower energy level than the stable high-work function metal top electrode. The direction of the carrier flow is therefore inverted due to the inversion of the direction of the internal field. Inverted bulk-heterojunction solar cell made RR P3HT and PCBM as the active layer in the structure: ITO / TiOx / RR-P3HT-PCBM / metal electrode were studied. The transparent TiOx acts as electron-collecting electrode and the metal electrode as hole-collecting electrode. Different parameters have been investigated: thickness and treatment of the TiOx layer, solvent, thickness of the active layer, molecular weight of the polymer, post-annealing process, work-function of the metal electrode. And then a comparison of lifetime between a regular solar cell and an inverted one will be presented.

SYOP 1.9 Wed 16:00 ZEU 222

Transparent Metal Electrodes for Organic Solar Cells — •Jan Meiss, Moritz K. Riede, and Karl Leo — Institut fuer Angewandte Photophysik, Technische Universitaet Dresden, 01062 Dresden - http://www.iapp.de

Organic solar cells (OSC) are emerging as possible inexpensive alternative to inorganic photovoltaics. Current issues of OSC are the high price of indium tin oxide (ITO), the most commonly used transparent contacting material, and the fact that glass is used as substrate in almost all cases. We are exploring alternatives to the scarce and expensive ITO and investigate alternative OSC configurations, i.e. top-illuminated and inverted solar cells.

In this contribution, top-illuminated small-molecule organic solar cells with transparent metal cathodes consisting of different combinations of Al, Ag and Au are presented. The whole device stack has been prepared by thermal evaporation under vacuum. It is shown that multi-layer metal cathodes employing surface modifying interlayers achieve by far superior performance compared to single-layer cathodes. Scanning electron and atomic force microscopy show that this can be attributed to significantly improved morphology in multi-layer devices; these conclusions are supported by the electrical properties in the current-voltage curves. By additionally enhancing light incoupling with a capping layer and utilizing microcavity effects, promising efficiencies of over 2.2% are obtained for zinc phthalocyanine / C60 bulk heterojunction solar cells containing standard materials.

SYOP 1.10 Wed 16:15 ZEU 222

Effects of geminate and bimolecular recombination on the performance of polymeric-small molecular solar cells — •Marcel Schubert[1], Chunhong Yin[1], Mauro Castellani[1], Alan Sellinger[2], and Dieter Neher[1] — [1]University of Potsdam, Institute of Physics and Astronomy, 14476 Potsdam-Golm, Germany — [2]IMRE and A*Star, 3 Research Link, 117602 Republic of Singapore

Many physical properties of organic photovoltaics are related to the nature of the geminate pair, an intermediate state that forms after dissociation of photogenerated excitons and prior to free charge carrier generation. Whereas it was found that photocurrent generation is dominated by the strong field dependent process of geminate pair dissociation, the recombination of uncorrelated free charge carriers and the formation of space charge seem to play a minor role in the prominent P3HT/PCBM combination. The situation may change, when using different D/A combinations or other soluble acceptor molecules.

We present organic solar cells comprising a novel small molecule based on 2-vinyl-4,5-dicyanoimidazole (Vinazene) as acceptor and M3EH-PPV as donor. While bilayer devices show promising results with a fill factor up to 57 %, the IU-characteristics of bulk heterojunction devices are dominated by bimolecular recombination and space charge effects even at moderate illumination intensities. Photo-CELIV measurements were performed to study the bimolecular recombination in detail. By combining photo-CELIV results with PL and IU measurements we are able to analyze the interrelation of recombination losses, free charge carrier generation and exciplex formation.

SYOP 1.11 Wed 16:30 ZEU 222

Highly doped layers as efficient electron-hole conversion contact for tandem organic solar cells — •Ronny Timmreck, Selina Olthof, Moritz Riede, and Karl Leo — Institut für angewandte Photophysik, TU Dresden, Dresden, Germany

To achieve high power conversion efficiencies with stacked organic solar cells, several requirements concerning their layer structure have to be fulfilled. A key feature is an efficient conversion contact at the interface between the single solar cells of a stacked cell: Here, an electron current has to be converted into a hole current without loss of energy. We investigate such contacts for small-molecule organic solar cells and present an approach adopted from inorganic tandem solar cells by using highly doped organic layers. We also compare metal-cluster based conversion contacts reported in literature to our new approach. For this purpose, comparable structures are characterised by UPS, by I-V-characteristics of organic p/n-heterojunctions, and by I-V-characteristics of corresponding solar cells. The experiments show that our approach is superior to the metal cluster based approach, e.g. it allows a full addition of the open circuit voltage Voc of the subcells independent from the used organic materials. It is thus possible to avoid the metal clusters which allows for a wider choice of materials and has advantages for future mass production. Using these results, a possible working mechanism of these contacts is discussed: high recombination rates at the conversion contact result in low sheet resistances and a removal of quasi-Fermi level splitting such that no reverse voltage occurs which would reduce Voc of the stacked solar cell.

SYOP 1.12 Wed 16:45 ZEU 222

Light- and touch-point localization using flexible large area organic photodiodes — •Petr Bartu[1], Robert Koeppe[1,2,3], Siegfried Bauer[1], and Niyazi Serdar Sariciftci[2] — [1]Department of Soft Matter Physics (SoMaP), JKU Linz, Altenbergerstr. 69, A-4040 Linz, Austria — [2]Linz Institute for Organic Solar Cells (LIOS), JKU Linz, Altenbergerstr. 69, A-4040 Linz, Austria — [3]isiQiri interface technologies GmbH i.G., c/o tech2b, Hafenstr. 47-51, A-4020 Linz, Austria

A large area photodiode using a heterojunction of zinc-phthalocyanine and fullerene C60 as active layer sandwiched between resistive electrodes of Poly(ethylenedioxythiophenes) Polystyrenesulfonate (PEDOT:PSS) and semitransparent aluminum can be used as a two dimensional position sensitive device for detecting light spots. The current generated in the photodiode drops over resistive electrodes to the edges of the device and depends on the distance between the excitation and the point where the resistive electrode is connected with the outer circuit. For precise tuning of the device, a variation of the electrode sheet resistance as well as a change in modulation of the frequency can be used. Additionally, localized out-coupling of light from a waveguide of silicone rubber by pressure allows the construction of a pressure sensitive optical touchpad.

SYOP 2: Organic Photovoltaics: from Single Molecules to Devices

Time: Thursday 9:30–12:30 Location: BAR SCHÖ

Invited Talk SYOP 2.1 Thu 9:30 BAR SCHÖ
Material Design for Organic and Hybrid Solar Cells – structural to functional control on all length scales – — •Mukundan Thelakkat, Michael Sommer, Ruth Lohwasser, and Sebastien Maria — Applied Functional Polymers, Department of Macromolecular Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany

One of the challenging aspects in designing and developing novel functional materials is to incorporate the desired optical and /or electrical properties maintaining their film-forming and thermal characteristics which make them suitable for thin film device applications. An important criterion for photovoltaic applications is that these materials should have well-defined nanostructured morphology in thin films in order to be capable of fulfilling the complex functions of charge transfer and transport simultaneously. This morphological control on a nanoscopic level controls the interface between the functional domains as well as the long term stability of such devices. We have demonstrated the chain of control on all length scales using the self-assembly principle of a fully functionalised block polymer for photovoltaic applications.

This contribution covers the design, synthesis and properties of some novel low molecular weight semiconductors as well as poly(3-hexylthiophene) -block- Poly(perylenebisimide acrylate. Block copolymers those allow the incorporation of semiconductor quantum dots or nanocrystals to get hybrid systems with morphology control will also be discussed. The characterization of these materials in thin films and their application in devices will be presented.

Invited Talk SYOP 2.2 Thu 10:00 BAR SCHÖ
Triplet exciton formation in organic photovoltaics — Xudong Yang, Sebastian Westenhoff, Ian Howard, Thomas Ford, Richard Friend, Justin Hodgkiss, and •Neil Greenham — Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom

We have recently found that the formation of triplet excitons can be an important loss mechanism in organic photovoltaics, particularly in donor-acceptor blends designed to have high open-circuit voltages. This can occur when the intrachain triplet state lies lower in energy than the charge-transfer state formed at the heterojunction. We find that in a blend based on the polyfluorene derivatives F8BT and PFB, triplet excitons are formed after photoexcitation with much higher efficiency than in the component polymers. We use transient absorption spectroscopy to study the dynamics of charges and triplet excitons on timescales from picoseconds to microseconds. This allows us to determine a characteristic time of $\sim$ 40 ns for intersystem crossing in the charge-separated state, and to estimate that as many as 75% of photoexcitations lead to the formation of triplet states. To avoid losses to triplet excitons in photovoltaic devices, it is necessary to separate charge pairs before intersystem crossing can occur. We also present photophysical measurements of saturation and relaxation of the triplet excited state absorption used to quantify triplet populations.

Invited Talk SYOP 2.3 Thu 10:30 BAR SCHÖ
Charge Carrier Dissociation and Recombination in Polymer Solar Cells — •Vladimir Dyakonov[1,2] and Carsten Deibel[1] — [1]Julius-Maximilians University Würzburg, Institute of Physics, Experimental Physics VI, 97074 Würzburg, Germany — [2]Bavarian Center for Applied Energy Research e.V. (ZAE Bayern), 97074 Würzburg, Germany

We determined the dominant polaron recombination loss mechanisms in pristine and annealed polythiophene:fullerene blend solar cells by applying the photo-induced charge extraction by linearly increasing voltage (photo-CELIV). In pristine samples, we find a strongly temperature dependent bimolecular polaron recombination rate, which is strongly reduced as compared to the Langevin theory. For the annealed sample, we observe a polaron decay rate which follows a third order of carrier concentration almost temperature independently. We will discuss the impact of a reduced bimolecular recombination rate on the main characteristics of the polymer solar cells.

Invited Talk SYOP 2.4 Thu 11:00 BAR SCHÖ
Modeling exciton diffusion and dissociation at organic-organic interfaces — •David Beljonne — Chemistry of Novel Materials, University of Mons-Hainaut, Place du Parc 20, B 7000 Mons, Belgium

Increasing the performances of organic photovoltaic (OPV) cells requires the simultaneous optimization of various processes involved in their working principle. We will first briefly overview these processes, comment on the theoretical limits for quantum efficiencies and identify possible directions for improvement. Among other factors, the excitation diffusion length and the fraction of excitons undergoing charge generation at the interface are key to the overall OPV quantum yield. We will assess both thermodynamic and kinetic aspects of these phenomena in the case of oligoacenes:C60 bilayer devices. In particular, on the basis of quantum-chemical calculations and phenomenological models, we will discuss the reasons for the unexpected quasi-quantitative external quantum yield for charge generation that has been measured for such devices.

Invited Talk SYOP 2.5 Thu 11:30 BAR SCHÖ
Correlation of Interfacial Composition and Bulk Morphology to Device Performance in Organic Bulk Heterojunction Solar Cells — David Germack[1], •Joseph Kline[1], Daniel Fischer[1], Lee Richter[1], Calvin Chan[1], David Gundlach[1], Michael Toney[2], and Dean DeLongchamp[1] — [1]National Institute of Standards and Technology, Gaithersburg, USA — [2]Stanford Synchrtron Radiation Lightsource, Menlo Park, USA

Organic and hybrid inorganic/organic photovoltaic cells promise to drop solar energy costs low enough to compete with conventional technologies such as coal. Direct measurements of the morphology of bulk heterojunction blends are critical to future efficiency improvements. We have developed strategies to measure the orientation, distribution and dimension of morphological features in materials for organic thin film transistors and photovoltaic devices that have led to rational guidelines for the design of new polymeric materials and processing techniques. By using Near Edge X-Ray Absorption Fine Structure (NEXAFS) and ultra-violet variable angle spectroscopic ellipsometry (UV-VASE) in combination with grazing incidence X-ray diffraction (GIXD) and atomic force microscopy (AFM) we have developed models of interfacial composition and morphology and the vertical composition of a P3HT:PCBM blend. We will describe our ongoing efforts to correlate the electrical performance of P3HT/PCBM blend devices to measurements of interfacial composition and morphology and bulk morphology.

Invited Talk SYOP 2.6 Thu 12:00 BAR SCHÖ
Developments on the acceptor side in plastic PV — •Jan C. Hummelen — Molecular Electronics, Zernike Institute for Advanced Materials & Stratingh Institute for Chemistry, University of Groningen, Nijenborgh 4, 9747AG Groningen, The Netherlands

The intensity of R&D on solar cells based on the bulk heterojunction principle is rapidly increasing during the last 5 years. Much progress has been reported lately on especially bulk heterojunction cells based on the combination of conjugated polymers and fullerene derivatives. One of the present issues in materials design of donor-acceptor combinations is that of the relative energies of the frontier orbitals. Recently, there is increasing discussion concerning the optimum offset between the two LUMO energies, and, related to that, whether molecular (donor-acceptor) based PV would have lower theoretical maximum efficiency then standard inorganic PV. We will address these issues and give an overview of some recent developments. Since most of the energy tuning has been performed on the acceptor components, we will report on the developments with respect to the palette of available acceptor LUMO energies, as well as some latest device results, obtained with new acceptor materials

SYOP 3: Organic Photovoltaics II

Time: Thursday 14:00–16:00 Location: ZEU 222

SYOP 3.1 Thu 14:00 ZEU 222

Interplay between morphology and energy levels in conjugated polymers: A theoretical view — •Georg Heimel[1], Ingo Salzmann[1], Steffen Duhm[2], Jürgen P. Rabe[1], and Norbert Koch[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489, Berlin, Germany — [2]Graduate School of Advanced Integration Science, Chiba University, Japan

Conjugated polymers are important constituents of organic electronic devices and it is both the bulk properties and the interfaces, which decisively determine device performance. For example, the preparation conditions are know to crucially impact the thin-film morphology of the prototypical π-conjugated polymer region-regular poly(3-hexylthiophene) and, consequently, also the device characteristics of, e.g., organic solar cells based on this material (rr-P3HT). We present first-principles calculations on highly ordered monolayers of rr-P3HT and a fluorinated derivative with the backbone orientations varying continuosly from face-on to edge-on. Supported by electrostatic modeling, we find that the backbone orientation importantly influences the energy-level positions in these films due to intra-molecular surface dipoles; we find variations of up to 1.5 eV. As a consequence, also the energy-level alignment at ubiquitous inorganic/organic and organic/organic interfaces can be expected to depend critically on thin-film morphology. Our results provide further insight into the structure-property relationship in an important class of materials and imply novel strategies for molecular, polymer, and device design.

SYOP 3.2 Thu 14:15 ZEU 222

Investigation of the preparation process of dye sensitized photovoltaic cells by AFM, Kelvin Probe Force Microscopy and X-ray diffraction — •Harald Graaf[1], Carsten Mädler[1], Mirko Kehr[1], and Torsten Oekermann[2] — [1]Institute of Physics, University of Technology Chemnitz, 09107 Chemnitz, Germany — [2]Institute of Physical Chemistry and Electrochemistry, Leibniz University Hannover, 30167 Hannover, Germany

Dye-sensitized photovoltaic cells with zinc oxide (ZnO) as the inorganic semiconductor and organic dye molecules as the sensitizer are well known devices with high efficiency. Such cells are prepared by electrochemical deposition of an aqueous zinc salt solution including dye molecules. After deposition the dye is desorbed to obtain a porous ZnO network followed by re-adsorption of the dye as a sensitizer. Up to now studies concerning the influence of different processing steps on the structure of the ZnO are sparse. We discuss the growth mechanism during film deposition and the crystal structure changes of the ZnO accompanying the desorption process, which is performed in an alkaline aqueous solution. X-ray investigation shows the influence of the dye on the structure of the formed ZnO/dye hybrid film. AFM topography and Kelvin Probe Force Microscopy investigations suggest the following deposition process: at first dye molecules are adsorbed on the electrode followed by ZnO formation within the pores of the organic network. This ZnO, which shows high crystallinity, seems to be oriented with the zinc face up.

SYOP 3.3 Thu 14:30 ZEU 222

Nanoscale Near-field Spectroscopic Investigation of the Interplay between Local Film Morphology and the P3HT/PCBM Organic Solar Cell Efficiency — •Dai Zhang[1], Xiao Wang[1], Kai Braun[1], Hans-Joachim Egelhaaf[2], and Alfred J. Meixner[1] — [1]Institute of Physical and Theoretical Chemistry, University of Tuebingen, Germany — [2]Christian-Doppler-Lab for Surface Optical Methods, Johannes-Kepler-University and Konarka GmbH, Linz, Austria

The interplay between the local film morphology and the organic solar cell efficiency is systematically investigated by apertureless near-field scanning optical microscopy (SNOM). A home-built parabolic mirror assisted SNOM is used to collect both the topography and optical (Raman and photoluminescence (PL)) information from the Poly (3-hexylthiophene) (P3HT) and [6,6]-phenyl C61 butyric acid methyl ester (PCBM) blend film. Molecular domains composed of either PCBM or P3HT at nanometer scale are successfully determined by their corresponding Raman fingerprint information and PL information. The regioregularity of P3HT polymer influenced by the clustering of PCBM during thermal annealing is compared considering the FWHM broadening of the C=C vibration Raman peak. The influences of the local film morphology and the local distribution of P3HT/PCBM on the solar cell efficiency are discussed based on the different PL quenching levels induced by the exciton dissociation and electron transfer at P3HT/PCBM interfaces.

SYOP 3.4 Thu 14:45 ZEU 222

Ultrahigh time resolution nonlinear spectroscopy of polymer/fullerene blends — •Sarah Maria Falke[1], Daniele Brida[2], Giulio Cerullo[2], and Christoph Lienau[1] — [1]Insitut für Physik, Carl von Ossietzky Universität Oldenburg, 26129 Oldenburg, Germany — [2]Dipartimento di Fisica, Politecnico di Milano, 20133 Milano, Italy

Blends of polymers and fullerene derivatives are important prototype structures for efficient photoinduced charge generation and transport in organic photovoltaic devices. It is well established that photoexcitation of polymer/fullerene blends can result in an efficient ultrafast charge transfer from the excited polymer to the electron accepting fullerene moiety. It is generally believed that this charge transfer occurs within 50-100 fs [1]. Here we study ultrafast nonlinear spectra of pristine polymers (poly(3-hexylthiophene-2,5-diyl, P3HT) and polymer/fullerene ([6,6]-phenyl-C_{61} butyric acid methyl ester, PCBM) blends with a high time resolution of only 5 fs using a novel two-color pump-probe setup with broadband detection range. By comparing transient spectra of polymers and the polymer blend we observe an extremely rapid buildup of a band between 450 nm and 525 nm in the blend, occuring on a sub-10-fs time scale. Since the band is generally assigned to the stimulated emission from the indirectly excited fullerene moiety, our results indicate excitation transfer from the photoexcited polymer to the fullerene moiety on a sub-10-fs time scale, much faster than previously thought. The implications of these results for the microscopic charge generation processes in polymer/fullerene blends are discussed. [1] C.J. Brabec, Chem. Phys. Lett. **340**, 232 (2001).

SYOP 3.5 Thu 15:00 ZEU 222

A synthetic way towards rational design of discotic liquid crystals with high charge carrier mobilities — •Denis Andrienko[1], Xinliang Feng[1], Valentina Marcon[1], Wojciech Pisula[1], James Kirpkpatrick[2], Ferdinand Grozema[3], Kurt Kremer[1], and Klaus Muellen[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Imperial College London, UK — [3]Delft University of Technology, The Netherlands

Conjugated materials offer the revolutionary prospect of producing semiconductor devices at low cost. The best to date discotics are built around the coronene unit and possess six fold symmetry. In the discotic phase six fold symmetric molecules stack with an average azimuthal twist of 30 deg, whereas the angle which would lead to the greatest electronic coupling and hence highest charge mobility is 60 deg. Here, a molecule with three fold symmetry and alternating hydrophilic/hydrophobic side chains is synthesized and X-ray scattering is used to prove the formation of the desired helical microstructure. Pulse radiolysis time resolved microwave conductivity measurements show that the material has indeed a very high mobility in the plastic crystalline phase, in the range of $0.1 - 0.2\,\mathrm{cm}^2/\mathrm{Vs}$. The physical structure of the assemblies of molecules are simulated using molecular dynamics. This, together with quantum chemical techniques, allows the computation of charge mobilities without fitting parameters. The calculations prove that mobility is still limited by structural defects and that a defect free assembly would lead to mobilities in excess of $10\,\mathrm{cm}^2/\mathrm{Vs}$.

SYOP 3.6 Thu 15:15 ZEU 222

Absorption enhancement in excitonic solar cells by a photonic crystal top layer — •Stefan Guldin[1], Nicolas Tetreault[1,3],

Mathias Kolle[1], Sven Hüttner[1], Mark Welland[2], Peter Müller-Buschbaum[4], Richard Friend[1], and Ullrich Steiner[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]Nanoscience Center, University of Cambridge, UK — [3]LPI, Ecole Polytechnique Federale de Lausanne, CH — [4]Physik-Department, E13, TU München

Photonic crystal structures have been identified by theorists as a candidate to enhance the still relatively low response of excitonic photovoltaic cells in the near infrared. We present a new material route that enables the fabrication of a double layer dye-sensitised solar cell, including a mesoporous TiO_2 underlayer with high surface area and an optically active TiO_2 photonic crystal layer. A diblock copolymer acts as a structural directing agent for the mesoporous TiO_2, arranging the sol-gel-derived material into a highly ordered nanostructure. The hybrid underlayer is not porous in its unannealed state and thus allows the self-assembly and infiltration of a photonic crystal template. This approach represents, to our knowledge, the first successful method that couples a photonic crystal top layer into a functioning dye-sensitised solar cell with front illumination, opening up a vast parameter space for effective light management. In this first attempt an increase in normalised photon to electron conversion of 20.4% was observed in the range from 520 nm to 725 nm (at the tail of the dye absorption spectrum).

SYOP 3.7 Thu 15:30 ZEU 222

Investigation of ageing processes in bulk-heterojunction P3HT:PCBM organic solar cells by means of impedance spectroscopy — •Uli Würfel[1,3], Bas v. d. Wiel[2], Birger Zimmermann[1,3], and Michael Niggemann[3] — [1]Freiburg Materials Research Centre, Freiburg, Germany — [2]Universiteit Utrecht, Netherlands — [3]Fraunhofer Institute for Solar Energy Systems, Freiburg, Germany

The improvement of the long term stability is one important task in the development of organic photovoltaic (OPV) devices. Although promising device stabilities in the order of years can be expected the degradation mechanisms are not understood completely. They have to be identified to define conditions for accelerated degradation experiments to predict the lifetime of a device. Oxygen and water are well known as most harmful chemical species for OPV devices. We will present results of accelerated ageing experiments done on bulk-heterojunction P3HT:PCBM solar cells. The cells were placed in a gas tight flow cell and exposed either to ambient air, pure dry oxygen or nitrogen saturated with water vapour. They were repeatedly measured by recording dark and illuminated current-voltage characteristics and a series of impedance spectra for different applied bias voltages. By means of the impedance spectra it is possible to distinguish between different degradation phenomena - like e.g. doping and interface degradation - and gain a deeper understanding of the underlying processes. Finally, simulations were carried out to model the change in the physical properties of the organic semiconductor and its impact on the device performance.

SYOP 3.8 Thu 15:45 ZEU 222

Influence of polymer solar cell geometry on device parameters — Burhan Muhsin[1], Joachim Renz[1], Karl-Heinz Drüe[2], Gerhard Gobsch[1], and •Harald Hoppe[1] — [1]Institute of Physics, Ilmenau Technical University, Weimarer Str. 32, 98693 Ilmenau, Germany — [2]Electronic Technology, Ilmenau Technical University, Gustav-Kirchhoff-Str. 7, 98693 Ilmenau, Germany

In order to study the influence of the device shape on the solar cell device parameters, we systematically varied its geometry. By determining all sheet and contact resistances in the device, we were able to correlate the series resistance with the geometry of the device using a simple model for its calculation. As a result, rules for optimal design of solar modules were derived. However, further refinement of the calculation is required in order to minimize the deviation between calculus and experiment.

SYOP 4: Organic Photovoltaics: from Single Molecules to Devices

Time: Thursday 16:30–19:00 Location: P1A

SYOP 4.1 Thu 16:30 P1A

"Equipment for flexible solar cells and parameters for coating and printing processes" — •Thomas Kolbusch — Solarcoating Machinery GmbH

The lecture titled gives an overview on flexible PV markets and possible products which could be made of flexible PV. The author compares different flexible technologies presenting advantages and still existing challenges. He also gives an outlook on the development of different technologies during the next years.

Furthermore a summary of different approaches in simultaneous engineering for scaling-up processes in renewable technologies is given. The author compares pros and cons of the batch approach in comparison to the roll-to-roll approach combined with an insight on different machine building concepts and news in that field, e.g. the Click&Coat* concept for highest flexibility in the field of pilot lines. Then he gives an outlook on possible production methods to bond flexible solar cells to flexible substrates and how to draw up consumer products. Another topic are parameters for coating and printing processes in the field of flexible electronics.

At the end the author summarizes the results of the above mentioned points.

SYOP 4.2 Thu 16:30 P1A

Temperature dependence of organic solar cell parameters — •Matthias Richter, Klaus Müller, Shine Philip, Ioanna Paloumpa, Karsten Henkel, and Dieter Schmeisser — Brandenburgische Technische Universität Cottbus, Angewandte Physik - Sensorik, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany

The influence of an annealing step on the parameters of bulk heterojunction organic solar cells is investigated. In order to fabricate the solar cells we use glass coated with ITO (Indiumtinoxide) as a substrate on which the active layer consisting of P3HT and PCBM is spincoated. Al-electrodes are evaporated on top of the active layer. We use PEDOT:PSS as buffer layer. Each sample is annealed at different temperatures for a short time. Between every temperature step the I-V characteristic of the cell is measured. The following parameters are derived afterwards: FF, Isc (density), Voc. Also the efficiency is estimated. The results show a maximum cell efficiency for drying at 100°C for 20sec. A further important step for preparation is the drying procedure of the PEDOT:PSS layer. Here an improvement of about 50% in cell efficiency is measured after drying at 50°C for 5 days under inert gas atmosphere.

SYOP 4.3 Thu 16:30 P1A

Investigation of light induced charge carrier generation in polymer/nanoparticle blends — •Florian Witt, Marc Daniel Heinemann, Folker Zutz, Xiaoping Jin, Karsten von Maydell, Joanna Kolny-Olesiak, Holger Borchert, and Jürgen Parisi — Institute of Physics, Energy and Semiconductor Research Laboratory, University of Oldenburg, 26111 Oldenburg

Organic photovoltaics are a promising approach for a cheap and easy-to-produce alternative for inorganic semiconductor solar cells. In such cells the photoactive layer consists of a polymer donor and a fullerene acceptor. Their disadvantage lies in a low power conversion efficiency wich has to increase significantly for industrial purposes. For such a performance improvement, new approaches were suggested, e.g. the exchange of the acceptor material with semiconducting inorganic nanoparticles (NP). A detailed knowledge of the internal electronical processes like exciton separation and charge carrier transport in such hybrid systems is needed to find ways for further cell optimization. An important technique to investigate the charge separation process between the acceptor and donor materials is Light induced Electron Spin Resonance (LESR). Photoinduced excitons are separated at the interface of NP and polymer. These free polarons have a net spin which can be detected by ESR.

We present LESR measurements on polymer:CdSe and polymer:CdTe blends. Time resolved experiments show an increased amount of trap states in comparison to polymer:PCBM blends.

SYOP 4.4 Thu 16:30 P1A

Structure control of conjugated block copolymers via adding a homopolymer — •Matthias A. Ruderer[1], Robert Cubitt[2], and

Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department LS E13, James-Franck-Str. 1, 85747 Garching (Germany) — [2]Institute Laue Langevin, 6 Jules Horowitz, 38042 Grenoble (France)

Conjugated polymers have shown to be interesting candidates for organic photovoltaics due to their high absorption coefficient and easy processibility. Nevertheless there are stringent constraints in the morphology of the active layer due to the short exciton diffusion length (on the order of 10 nm). While polymer blends tend to form structure sizes in the range of hundred nanometers, one promising approach are conjugated block copolymers which generate nanostructures in the desired range due to micro-phase separation.[1] Instead of changing the composition of the block copolymer via synthesis, an alternative approach is offered by blending the conducting block copolymer with a homopolymer which is equal to one of the blocks to adapt the morphology and match the desired spatial dimensions. A diblock copolymer with a rigid conjugated block and a conventional coiled block is focused. We investigate the structural changes due to blending this block copolymer with the coiled block homopolymer of smaller degree of polymerization using the non destructive methods grazing incidence small angle neutron scattering (GISANS) and neutron reflectivity.[2] The investigations are completed with AFM and UV/Vis measurements.

[1] S. Günes et al., Chem. Rev. 107, 1324 (2007); [2] P. Müller-Buschbaum et al., Langmuir 22, 9295 (2006)

SYOP 4.5 Thu 16:30 P1A

Silicon organic dye composites for photovoltaic applications — •Andreas Decker[1], Ulrich Weiler[2], Maxime Monnoyer[3], Thomas Mayer[1], and Wolfram Jaegermann[1] — [1]Darmstadt University of Technology, Institute of Materials Science, Surface Science Division — [2]now Calyxo GmbH, Thalheim — [3]now Arcelor, Lüttich

We have introduced the concept of bulk sensitization of the indirect semiconductor Si with direct absorbing organic dye molecules in order to enhance light absorption and decrease absorber film thickness in thin film μc-Si solar cells. With Raman spectroscopy it was shown that the pigments like ZnPc are not damaged by the hot wire activated μc-Si CVD from hydrogen diluted silane. Photoemission measurements prove the band line up of F_4ZnPc and F_8ZnPc to provide a driving force for the hole as well as electron transfer from the dye to the Si valence and conduction band respectively.

In a first attempt towards an electronic device films of bulk sensitized Si have been deposited on p+ doped μc-Si substrates and Au back contacts have been sputter deposited. In the composites optical transmission shows absorptivity of the pigments. Due to pinholes that were detected by AFM, results of I-V curves measured in the dark and under illumination are not yet representative of the film characteristics.

SYOP 4.6 Thu 16:30 P1A

Influence of image force effects on the recombination in organic bulk heterojunction solar cells — •Jędrzej Szmytkowski — Institut für Angewandte Physik, Universität Karlsruhe (TH), Karlsruhe, Germany

It has been recently reported that an experimental bimolecular recombination coefficient in PCBM:P3HT blend solar cells is about four orders of magnitude lower than the Langevin recombination coefficient. This effect is not sufficiently explained. We present a theoretical model based on the electrical polarization effects, which is able to explain the observed discrepancies between experiment and theory. The interface recombination of one sign charge carriers located in a material with lower permittivity competes with the bimolecular recombination of electrons and holes, leading to the reduction of bimolecular recombination. We have derived an analytical formula which describes the interface recombination coefficient.

SYOP 4.7 Thu 16:30 P1A

Preparation and Characterisation of Mixed Films of a Subphthalocyanine and a Perfluorinated Phthalocyanine — •Dominik Klaus, Christopher Keil, Robin Knecht, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, 35392, Gießen, Germany. E-mail: schlettwein@uni-giessen.de; Fax: +49 641 9933409; Tel: +49 641 9933400

Mixed films consisting of two different organic semiconductors were studied that were prepared by physical vapour deposition on electrode structures on glass. A planar perfluorinated phthalocyanine ($F_{16}PcCu$) absorbing in the red was used as an electron acceptor and a cone-shaped subphthalocyanine ($SubPcBCl$) absorbing in the green as electron donor. Electrical conduction measurements revealed the development of the conductivity in different phases of the experiment. Further, the change of the photocurrent in dependence on different wavelengths of illumination was measured. The observed photocurrents showed light-induced charge transfer and even the direction of the photocurrent changed in different parts of the solar spectrum. A photovoltaic effect even across the electrode gap was indicated and the applicability of such films in organic bulk heterojunction solar cells is discussed.

SYOP 4.8 Thu 16:30 P1A

Mixed films of phthalocyanines and perylene imids as bulk heterojunction materials — •André Dragässer[1], Robin Knecht[1], Christopher Keil[1], Günter Schnurpfeil[2], and Derck Schlettwein[1] — [1]Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392, Gießen. eMail: schlettwein@uni-giessen.de — [2]Institut für Organische und Makromolekulare Chemie, Universität Bremen, D-28334 Bremen.

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 phthalocyanines as electron donors absorbing in the red part of the spectrum and perylene imids as electron acceptors absorbing in the green part of the spectrum providing almost perfect coverage of the visible range. Mixed films were successfully created by simultaneous physical vapour deposition of the molecules to create an evaporated organic bulk heterojunction. The films were studied for their potential as materials in organic photovoltaic devices. Using transmission spectroscopy, structure analysis and photoconductivity measurements electronic and optical properties were investigated and compared with the properties of the pure films and solution spectra. The observed spectral dependence of the photoconductivity indicates a potential use of such materials in organic photovoltaic cells. First attempts to create a sandwich structure with indium tin oxide, the mixed organic layer and a metal contact will be discussed.

SYOP 4.9 Thu 16:30 P1A

Dye-sensitized solar cells based on nanostructured zinc oxide — •Jonas Conradt[1], Jędrzej Szmytkowski[1,2], Florian Maier-Flaig[1], Janos Sartor[1], Johannes Fallert[1], Manuel Reinhard[4], Alexander Colsmann[4], Uli Lemmer[2,4], Teodor Silviu Balaban[2,3], and Heinz Kalt[1,2] — [1]Karlsruhe Institute of Technology (KIT), Universität Karlsruhe (TH), Institute of Applied Physics, Karlsruhe, Germany — [2]Center for Functional Nanostructures (CFN), Karlsruhe, Germany — [3]Karlsruhe Institute of Technology (KIT), Forschungszentrum Karlsruhe, Institute for Nanotechnology, Karlsruhe, Germany — [4]Karlsruhe Institute of Technology (KIT), Universität Karlsruhe (TH), Lichttechnisches Institut, Karlsruhe, Germany

Hybrid solar cells represent a promising (cost-efficient) alternative to pure inorganic solar cells. We present dye-sensitized solar cells (DSSC) which are based on a zinc oxide (ZnO) electrode covered with a ruthenium dye. Our work focuses on the morphology of the ZnO electrode and its impact on the photovoltaic performance of the solar cell. Nanocrystalline ZnO powder layers and arrays of nanorods are incorporated into the DSSCs. The ZnO nanorods are grown by vapor transport deposition. The morphology and doping concentration of the rods can be controlled by the choice of substrate material, growth condition and catalytic metal layers. The nanorod arrays are expected to fasten the electron transport towards the anode and thereby improve the solar cell efficiency. In addition, novel self-assembling (porphyrin) dyes are tested as sensitizer within a DSSC.

SYOP 4.10 Thu 16:30 P1A

Photoinduced absorption studies on dicyanovinyl-oligothiophene thin films for application in small molecule organic solar cells — •Hannah Ziehlke[1], Rico Schüppel[1], Moritz Riede[1], Egon Reinold[2], Peter Bäuerle[2], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden — [2]Insitut für Organische Chemie II und neue Materialien, Universität Ulm

Oligothiophenes capped with electron-withdrawing dicyanovinyl groups are promising candidates for applications in small molecule organic solar cells with reached efficiencies of 3.4 % [1]. In blend layers with fullerene C_{60} as acceptor material, the dicyanovinyl-oligothiophenes (DCVnT) act as donor material. The variation of the HOMO energies along the series $n = 3...6$ have significant influence on the charge separation process at the donor acceptor interface.

The energetic and dynamic properties of the long lived photoexciations present at this interface can be obtained by photoinduced absorption (PIA) spectroscopy . We here present the characterisation of DCVnT with varying chain length via PIA spectroscopy. By analyzing recombination dynamics of the triplet excitons and cation states with respect to the existing models of mono- and bimolecular recombination processes, lifetimes and generation efficiencies can be compared. Likewise the temperature dependence of the lifetimes of triplet excitons and cations is evaluated.

[1] K. Schulze, M. Riede, E. Brier, E. Reinold, P. Bäuerle, and Karl Leo, J. Appl. Phys. **104**, 074511 (2008)

SYOP 4.11 Thu 16:30 P1A

Theoretical study of morphology and charge transport in amorphous Alq3 — •Alexander Lukyanov[1], Christian Lennartz[2], and Denis Andrienko[1] — [1]Max Planck Institute for Polymer Research, Mainz — [2]Department of Scientific Computing, BASF, Ludwigshafen

A force-field for tris(8-hydroxyquinoline) aluminium (Alq3) - a compound widely used in organic light emitting diodes [1] - is developed and verified by comparing classical and first principles (DFT, B3LYP functional) molecular dynamics simulations. This force-field is then used to simulate large scale morphologies of amorphous Alq3. Given the realistic morphology, charge transport in thin films of amorphous Alq3 is analyzed withing the framework of high temperature non-adiabatic Marcus' theory [2].

1. J.J. Kwiatkowski, J. Nelson, H. Li, J.-L. Bredas, W. Wenzel, and C. Lennartz, Phys. Chem. Chem. Phys. 14, 1852 (2008)
2. J. Kirkpatrick, V. Marcon, J. Nelson, K. Kremer and D. Andrienko, Phys. Rev. Lett. 98, 227402 (2007)

SYOP 4.12 Thu 16:30 P1A

Charge transport in carbazole-based crystals — •Thorsten Vehoff[1], James Kirkpatrick[2], Alessandro Troisi[3], and Denis Andrienko[1] — [1]Max Planck Institut für Polymerforschung, Mainz — [2]Imperial College London, London, UK — [3]Department of Chemistry and Center of Scientific Computing, University of Warwick, UK

We compare two descriptions of charge transport in organic semiconducting crystals. The first approach is based on a semi-classical Hamiltonian with the non-local electron-phonon coupling. The second is the variable range hopping model based on the Marcus' charge transfer theory. Molecular dynamics (MD) simulations of the crystalline phase of 6,12-dimethoxy-5,11-dihydroindolo[3,2-b]carbazole are performed. The transfer integrals for nearest neighbor pairs are calculated with the molecular orbital overlap method. Charge dynamics is simulated using kinetic Monte Carlo technique with rates calculated from Marcus' theory [1]. Based on the same MD trajectory, the mobility is calculated by monitoring the spread of a wave function over a few neighboring molecules using numerical integration of the small polaron model Hamiltonian [2]. Both results are compared to time of flight measurements.

1. J. Kirkpatrick, V. Marcon, J. Nelson, K. Kremer and D. Andrienko, Phys. Rev. Lett. 98, 227402 (2007)
2. A. Troisi, Adv. Mater. 19, 2000-2004, (2007)

SYOP 4.13 Thu 16:30 P1A

Investigation of the Nanomorphology and Device Performance of Organic Solar Cells based on Polymer:Fullerene Bulk Heterojunctions — •Thomas Madena, Uli Wischnath, Achim Kittel, Jürgen Parisi, and Ingo Riedel — Energy- and Semiconductor Research Laboratory, Department of Physics, University of Oldenburg, Carl-von-Ossietzky-Strasse 9-11, D-26111 Oldenburg

The coherences between structural layout of P3HT:PCBM bulk heterojunction (BHJ) solar cells and the electrical properties are not fully understood so far. The morphology of such BHJ-thin films determines the efficiency balance between separation of electron hole pairs at the phase boundary of PCBM and P3HT and the charge transport along continuous paths in the pure materials. The optimization of both fundamental mechanisms is a challenge and plays a crucial role for the efficiency of the photovoltaic device. In this presentation we investigate the interplay of nanomorphology and device properties of P3HT: PCBM solar cells. AFM measurements were carried out to profile the nanomorphology of differently composed polymer: fullerene composite films. In these films we observed substantial growth of micronsized crystallites in the PCBM moiety upon thermal annealing which severely limits the device performance. Based on these studies we discuss the influence of the nanomorphology of different thin film formulations on the electrical characteristics of P3HT: PCBM solar cells.

SYOP 4.14 Thu 16:30 P1A

Surface effects on organic solar cell characteristics — •Alexander Wagenpfahl, Carsten Deibel, and Vladimir Dyakonov — Experimental Physics VI, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg

For an economic competition with other energy sources, the power conversion efficiency of polymer:fullerene solar cells has to be increased. Limiting factors on this efficiency are diverse and range from influence of the charge carrier mobility, gaussian disorder of energies to recombination effects of charges and excited states. Surface effects, however, have been mostly neglected so far. Using a numerical device simulation, we examine the influence of the surface recombination on the solar cell characteristics. Under consideration of different models, such as the well known injection model of Scott and Malliaras (Chem. Phys. Lett. 299 (1999) 115), we discuss the relevance of surface recombination for bulk heterojunction photovoltaic devices.

SYOP 4.15 Thu 16:30 P1A

Integrated approaches in templated functional oxide materials — Maria Lechmann[1], Mine Memesa[1], Philipp Lellig[1,2], Jan Perlich[3], Peter Müller-Buschbaum[3], and •Jochen Stefan Gutmann[1,2] — [1]Max-Planck Istitute for Polymerresearch, Ackermannweg 10, 55128 Mainz (Germany) — [2]Inst. f. Physik. Chem., Johannes Gutenberg Universität, Welderweg 11, 55099 Mainz (Germany) — [3]TU München, Physik Department LS E13, James-Franck Str. 1, 85748 Garching (Germany)

Templating of functional oxide materials via block copolymers is a technique that currently progresses towards a mature state. While it is therefore readily possible to obtain nanomaterials from functional oxides with are well defined in terms of their structure, morphology and function, it is furthermore possible to integrate a second function into the (hybrid) material. With this approach even mutually orthogonal functions can be integrated into the same material. We have used this integrated templating approach to obtain integrated barrier materials for photo electronic devices as well as functional oxide materials for hybrid solar cells. Doing so, we covered the whole materials science development cycle from chemical synthesis via structural characterization to application. We'll demonstrate why each of these steps is synergistic and how a rational materials design can evolve from basic research.

SYOP 4.16 Thu 16:30 P1A

X-ray Diffraction Studies of Different Polythiophene based Polymers Thin Films — •Shabi Thankaraj Salammal[1], Souren Grigorian[1], Ullrich Pietsch[1], Niel Koennen[2], and Ullrich Scherf[2] — [1]Solid State Physics, University of Siegen, Siegen, Germany — [2]Macromolecular Chemistry, University of Wuppertal, Wuppertal, Germany

Poly(thiophenes) and its derivatives have received special considerations for organic device applications. One open question to solve in what extend the crystalline structure is responsible for the conductive properties of the polymers. Our aims are to understand the crystallinity and interface induced ordering of such thiophene based family by exploiting surface sensitive X-ray diffraction technique and its correlatation to charge carrier mobility. Our primarily results have shown the variation of in inter-planar distances of these different polythiophene based derivatives, for P3PT = 1.52 nm, P3HT = 1.65 nm, P3HepT = 1.79 nm and P3OT = 1.99 nm. We have found that P3HT is indeed the derivate with highest crystallinity compared to the other three thiophene derivatives. It is the only one showing the second and third order Bragg peak in addition to the first order. Our current studies indicate that by keeping the substrate and solution at low temperature while growing, one can increase the crystallinity of the thiophene derivatives.

SYOP 4.17 Thu 16:30 P1A

Hybrid Organic-Inorganic Heterojunctions made of Doped

Crystalline Silicon and a Hole Conducting Polymer — •Helmut Nesswetter, Sabrina Niesar, Roland Dietmüller, and Martin Stutzmann — Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching, Germany

There is an increasing research activity in hybrid heterojunctions made of organic semiconductors and inorganic semiconductors, due to their possible applications for photovoltaic and optoelectronic devices. However, a fundamental understanding of such material systems is still lacking. As a model system, we have studied hybrid heterojunctions made of crystalline silicon (Si) and the organic hole conductor poly(3-hexylthiophene-2,5-diyl) (P3HT) to gain insight into the electronic processes at the heterojunction. The heterojunctions were fabricated by spin coating a P3HT layer from solution on n-type or p-type Si wafers with an ohmic metal back contact. Afterwards, a semitransparent aluminium or a transparent indium tin oxide (ITO) front contact was applied on top of the P3HT layer. These devices were characterized via current-voltage and spectrally resolved photocurrent measurements. Depending on the use of n-type or p-type Si and on the use of Al or ITO as a front contact, we have observed different current-voltage characteristics for the P3HT/Si heterojunctions. This can be explained by the interplay of the Si/P3HT heterojunction, which is influenced by the doping level of the Si substrate and the P3HT/Metal contact, which can form a Schottky diode.

SYOP 4.18 Thu 16:30 P1A

Investigation of the effects of doping concentration in a p-doped organic semiconductor — •Selina Olthof, Björn Lüssem, and Karl Leo — Institut für Angewandte Photophysik, TU Dresden, George-Bähr-Straße 1, 01069 Dresden

Thin films of organic materials are widely investigated for the use in electronic and optoelectronic devices for instance solar cells and light emitting diodes. Like in the field of inorganic semiconductors, the technique of doping can greatly increase the performance of such devices.

However, so far little is understood of the underlying mechanisms of doping organic layers with molecules and whether they are comparable to the doping in inorganic semiconductors. Using UV- photoelectron spectroscopy (UPS) and X-ray photoelectron spectroscopy (XPS), we study the properties of a p-doped organic thin film using as a model system MeO-TPD doped by the strong electron acceptor F4-TCNQ.

We investigate how the doped layer aligns with different contact materials by performing interface resolved measurements. By varying the doping concentration, changes in the position of the Fermi energy in the band gap and the influence of the free carrier concentration on the width of the depletion layer can be studied.

As expected from inorganic semiconductors, we find that for higher doping ratio the Fermi level moves closer to the HOMO and furthermore this distance is independent on the contact material used.

SYOP 4.19 Thu 16:30 P1A

Efficiency increase of two-step-sensitized inorganic / organic hybrid absorber materials — •Eric Mankel, Thomas Mayer, and Wolfram Jaegermann — Technische Universität Darmstadt, Materials Science Institute, Surface Science Division, Petersenstraße 23, 64287 Darmstadt

Photovoltaic third generation concepts promise a significant increase of energy conversion efficiency. Two-step sensitization of inorganic wide band gap matrices by incorporated organic donor-acceptor molecules (e.g. dyads) has been suggested as possible means of creating third generation absorbers. Based on the model of Shockley and Queisser we calculate the rise of the ultimate efficiency and the detailed balance limit of a sensitized p-n-junction by adding a sensitization current provided by the organic molecules to the photocurrent provided by the matrix material. The model includes the dependence of a number of parameters namely the band gap of the matrix material, the energetic position of the organic frontier orbitals relative to the matrix band edges, the lifetime of the first excited molecular state and the Gaussian width of the absorption curve of the dye. For a width of 0.25eV an overall maximum efficiency of 45% has been calculated. To reach this limit under AM1.5 conditions the lifetime of the excited state must be longer than 10ms. Finally the calculations have been applied on ZnSe / CuPc / PTCDA composites using the band alignment as experimentally determined by XPS/UPS measurements.

SYOP 4.20 Thu 16:30 P1A

Electronic properties of doped CuPc layers — •Johanna Härter, Eric Mankel, Corinna Hein, Thomas Mayer, and Wolfram Jaegermann — Technische Universität Darmstadt, Materials Science Institute, Surface Science Division, Petersenstraße 23, 64287 Darmstadt

Doping of molecular organic materials is important for the functionality of organic electronic devices as e.g solar cells. We investigated the doping behaviour of the acceptor molecules Cl_2-DCNQI and F_{16}CuPc incorporated into a CuPc matrix. In-situ XPS/UPS measurements were performed on coevaporated films. Doping by Cl_2-DCNQI was not successful. The molecule lost its chlorine atoms during thermal evaporation. For pristine F_{16}CuPc layers we observe a strong broadening of the photoemission features with increasing deposition rate indicating different domains probably of different molecular structure of differing electric interface potential. F_{16}CuPc incorporated into CuPc shows sharp photoemission features. With increasing F_{16}CuPc content Fermi level shifts are observed in both phases. In CuPc the maximum shift is about 0.45eV towards the HOMO level indicating p-doping. Simultaneously the Fermi level in F_{16}CuPc shifts 0.15eV towards the LUMO level. The opposite Fermi energy shifts can be explained by charge transfer between separate CuPc and F_{16}CuPc phases. The HOMO offset is 1.23eV. Compared to the electron affinity rule this offset differs by approximately 100meV indicating an interfacial dipole between CuPc and F_{16}CuPc in the same order of magnitude.

SYOP 4.21 Thu 16:30 P1A

Temperature induced structural changes of P3HT thin films — •Souren Grigorian[1], Siddharth Joshi[1], Patrick Pingel[2], Tobias Panzner[1], Ullrich Pietsch[1], Achmad Zen[3], Dieter Neher[2], Michael Forster[4], and Ullrich Scherf[4] — [1]Solid State Physics, Universität Siegen — [2]Institute of Physics and Astronomy, University of Potsdam — [3]Inst. of Mat. Res.&Eng., Research Link, Singapore — [4]Macromolecular Chemistry, University of Wuppertal

Current study is focus on the temperature dependent crystalline structure of spin coated thin films of high molecular weight regioregular poly(3-hexylthiophene) (P3HT) (Mn ˜ 30000) and its correlation with charge carrier mobility [1]. Crystalline structure reveal temperature-dependent anisotropy: interlayer lattice spacing (100) along the film normal continuously increases up to a temperature of about 180 ° C and in opposite the in-pane p-p distance becomes smaller compared to the values measured at room temperature. These structural changes are reversible and can be repeated several times. Regarding the electrical properties we find a rather constant mobility up to a temperature of ca. 100-120 °C, followed by a continuous decrease. Upon cooling back to room temperature, the electrical properties almost recover. The drop of the charge carrier mobility at higher temperatures is explained by the creation of numerous small crystallites at the film-substrate interface reducing the number of long polymer chains bridging crystalline domains.

1.S. Joshi, S. Grigorian, P. Pingel, T. Panzner, U. Pietsch, A. Zen, D. Neher, M. Forster, U. Scherf, Macromolecules, 2008, (submitted)

SYOP 4.22 Thu 16:30 P1A

Charge transport in conjugated polymers: a multiscale picture — •Victor Rühle[1], James Kirkpatrick[2], Kurt Kremer[1], and Denis Andrienko[1] — [1]Max Planck Institute for Polymer Research, Mainz — [2]Imperial College London

A framework to study charge transport in conjugated polymers using realistic morphologies is developed. First, the atomistic force field is refined using first-principles calculations. Systematic coarse graining is then performed to extend simulation times and system sizes accessible to molecular dynamics simulations. Material morphologies are generated using the coarse grained and atomistic models. Finally, the charge mobility is obtained using temperature activated hopping picture for charge transport [1]. The framework is tested on neutral and oxidized polypyrrole with different structural ordering [2].

[1] J. Kirkpatrick, V. Marcon, J. Nelson, K. Kremer, D. Andrienko, Phys. Rev. Lett. 98, 227402 (2007)

[2] V. Ruehle, J. Kirkpatrick, K. Kremer, D. Andrienko, Phys. Stat. Solidi B, 245, 844 (2008)

SYOP 4.23 Thu 16:30 P1A

Organic Photovoltaic Cells Employing Diindeno-Perylene Thin Films — •Martin Meseth[1], Tobias Roller[2], and Jens Pflaum[1,3] — [1]Julius-Maximilians-University of Würzburg, Experimental Physics VI, D-97074 Würzburg — [2]Universität Stuttgart, 3. Phys. Inst., D-70569 Stuttgart — [3]Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg

A crucial factor for the efficiency in organic photovoltaic (OPV) cells made of small molecules is the exciton diffusion length of the absorbing material. Diindenoperylene (DIP) has shown to have an exciton diffusion length in the order of 100nm which can be attributed to its high crystallinity [Kurrle et al., APL 92(2008), 133306]. However, its use in OPV cells is limited by the weak absorption due to the disadvantageous orientation of the optical transition dipole.

In our study we examined OPV cells using DIP as donor material in combination with various acceptor molecules such as C_{60}. By this combinative approach, the degree of crystallinity in DIP could be varied and the impact of the corresponding cell efficiencies will be discussed.

The properties of the respective organic-metal contacts will also be adressed.

SYOP 4.24 Thu 16:30 P1A

Charge transfer of organic complexes — •S. Shahabedin Naghavi, Gerhard H. Fecher, and Claudia Felser — Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz

In the present work the binding energy of some polyaromatics which can be used as a donor or acceptor in charge transfer systems are calculated. Among many calculated molecules, hexamethoxycoronen as a donor and coronene-hexaone as a strong acceptor are investigated. Calculations were done with respect to finale state. All calculations were performed using Gaussian 03. The energies and geometries of different molecules were calculated and optimized with Lee, Yang and Parr correlation functional, denoted B3LYP, which the most successful one based on the hybrid functional method. In coronene-hexaone bond length of different C–C bonds increase with respect to hexamethoxycoronen.Because of presence of carbonyl groups in coronene-hexaone, the aromatic ring feels a higher deficiency of electrons than hexamethoxycoronen; therefore, C–C bond lengths are increased in the acceptor.

Financial support of SFB (Project B10 in TRR49) is gratefully acknowledged.

SYOP 4.25 Thu 16:30 P1A

Energy levels and work function of ultra-thin polythiophene films on conductive polymer electrodes — •Johannes Frisch[1], Norbert Koch[1], Jürgen P. Rabe[1], and Antje Vollmer[2] — [1]Humboldt-Universität zu Berlin, Institut f. Physik, 12489 Berlin — [2]BESSY GmbH, 12489 Berlin

Because poly(ethylenedioxythiophene):poly(styrenesulfonate) (PEDT:PSS) as transparent anode and poly(3-hexylthiophene) (P3HT) as prototypical donor polymer are prototypical materials in modern organic photovoltaic cells (OPVCs), knowledge about the energy levels at interfaces between PEDT:PSS and P3HT is essential to identify the influence of these on the efficiency of OPVCs. In the present work, the morphology, work function, and energy level alignment of ultra-thin films of P3HT on PEDT:PSS was investigated using X-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS). Ultra-thin films (down to sub-monolayer range) were produced by spin coating P3HT films from chloroform solution on PEDT:PSS and a subsequent washing process. The deposition of such ultra-thin P3HT film on PEDT:PSS lowered the sample work function (Φ) by 0.4 eV due to doping of P3HT film with positive charges from the PEDT:PSS layer. The valence band edge (VBE) was found only 0.1 eV below the Fermi-level. For thicker P3HT films (ca. 10nm), Φ further decreases by 0.2 eV and the VBE was observed 0.2 eV below the Fermi-level. These observations are discussed within existing concepts of local work function fluctuations and energy level bending at the P3HT/PEDT:PSS interface.

SYOP 4.26 Thu 16:30 P1A

Transport and noise in organic field effect devices — •Klaus Morawetz[1,2], Sibylle Gemming[1], Regina Luschtinetz[4], Tim Kunze[1], Pavel Lipavsky[3], Lukas Eng[5], and Gotthard Seifert[4] — [1]Forschungszentrum Dresden-Rossendorf, PF 51 01 19, 01314 Dresden, Germany — [2]International Center for Condensed Matter Physics, 70904-910, Brasília-DF, Brazil — [3]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic — [4]Institute of Physical Chemistry and Electrochemistry, TU Dresden, 01062 Dresden, Germany — [5]Institute of Applied Photophysics, TU Dresden, 01062 Dresden, Germany

The transport and fluctuation properties of organic molecules ordered parallel between two Au contact leads are investigated by the method of surface Green function. From first-principles simulation the relevant hopping parameters are extracted and used to calculate nonlinear transport coefficients with respect to an external bias voltage. A staggering of conductance is found in dependence on the number of molecules squeezed in-between the contacts. The thermal properties show an anomalous behavior whenever the voltage reaches the values of the molecular energy levels active for transport. The thermoelectric figure of merit shows a resonance allowing to reach values even larger than one.

SYOP 4.27 Thu 16:30 P1A

Modelling the transport through organic layers on a ferroelectric substrate — •Tim Kunze[1], Sibylle Gemming[1], Regina Luschtinetz[2], Volker Pankoke[1], Klaus Morawetz[1,3,4], Michael Schreiber[5], Lukas Eng[6], and Gotthard Seifert[2] — [1]Forschungszentrum Dresden-Rossendorf, P.O. Box 51 01 19, D-01314 Dresden, Germany — [2]Physical Chemistry and Electrochemistry, TU Dresden, D-01062 Dresden, Germany — [3]International Center for Condensed Matter Physics, 70904-910, Brasilia-DF, Brazil — [4]Max-Planck-Institute for the Physics of Complex Systems, D-01187 Dresden, Germany — [5]Institute of Physics, TU Chemnitz, D-09107 Chemnitz, Germany — [6]Institute of Applied Photophysics, TU Dresden, D-01062 Dresden, Germany

Organic semiconductors, which might be suitable for logical as well as optical applications, have attracted a lot of scientific effort in recent years. This includes the understanding of the underlying transport mechanisms, the improvement of the transport characteristics and possible fields of application. The electronic transport through stacks of functionalized quaterthiophene molecules as part of a novel organic device is presented and investigated by means of a phenomenological approach called multilayer organic light-emitting diode (MOLED) [1]. Numerical results including the tuning of carrier injection and optical activity will be discussed.

[1] Houili et al., Comp. Phys. Comm. 156, 103-122 (2003)

SYOP 4.28 Thu 16:30 P1A

Organic p-n heterostructures and superlattices — •Stefan Kowarik[1], Alexander Hinderhofer[2], Alexander Gerlach[2], Oriol Osso[3], Cheng Wang[4], Alexander Hexemer[4], and Frank Schreiber[2] — [1]Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720, USA — [2]Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen, Germany — [3]MATGAS 2000 A.I.E., Esfera UAB, 08193 Bellaterra, Barcelona, Spain — [4]Advanced Light Source, 1 Cyclotron Road, Berkeley, CA 94720, USA

For many applications of organic semiconductors two components such as e.g. n and p-type layers are required, and the morphology of such heterostructures is crucial for their performance. Pentacene (PEN) is one of the most promising p-type molecular semiconductors and recently perfluoro-pentacene (PFP) has been identified as a good electron conducting material for complementary circuits with PEN. We use soft and hard x-ray reflectivity measurements, scanning transmission x-ray microscopy (STXM) and atomic force microscopy for structural investigations of PFP-PEN heterostructures. The chemical contrast between PEN and PFP in STXM allows us to determine the lateral length scales of p and n domains in a bilayer. For a superlattice of alternating PFP and PEN layers grown by organic molecular beam deposition, X-ray reflectivity measurents demonstrate good structural order. We find a superlattice reflection that varies strongly when tuning the X-ray energy around the fluorine edge, demonstrating that there are indeed alternating PFP and PEN layers.

SYOP 4.29 Thu 16:30 P1A

Nanotomography of organic heterojunction solar cells — •Mario Zerson[1], Andreas Sperlich[2], Carsten Deibel[2], Vladimir Dyakonov[2], and Robert Magerle[1] — [1]Chemische Physik, TU Chemnitz, D-09107 Chemnitz — [2]Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg

The morphology of organic heterojunction solar cells based on blends of P3HT and PCBM is an important factor determining the power conversion efficiency. For a good charge carrier generation the interface between the two components should be as large as possible. Furthermore, bicontinuous networks of both components are required for an efficient charge carrier extraction. We investigate the three-dimensional structure of blends of P3HT and PCBM with Nanotomography based on scanning force microscopy (SPM). The specimen is ablated layer by layer using plasma etching and imaged with tapping mode SPM after each etching step. From the resulting series of images the three-dimensional structure is reconstructed. We will present first volume images of P3HT:PCBM blends and discuss the structure of the interface between donor and acceptor components in view of the charge generation efficiency.

SYOP 4.30 Thu 16:30 P1A

Interfacial structure modifying interlayers: Time dependent changes in the structure of inorganic/organic interfaces — •Felix Maye[1,2], Ayse Turak[1], Jonathan Heidkamp[1,2], and Helmut Dosch[1,2] — [1]Max-Planck-Institut für Metallforschung, Stuttgart — [2]Institut für Theoretische und Angewandte Physik, Universität Stuttgart

Organic molecules are in focus because they are a serious low-cost alternative to many products in the inorganic based semiconductor industry with the advantage of flexibility and ease of production. We are studying the structure of a thin film of Diindenoperylene, an organic semiconducting molecule, and Lithium Fluoride, an inorganic crystalline molecule, using SPM and X-Ray techniques. The inorganic film is assumed to improve the charge transport of light-induced excitons created in the active organic layer. Since the system will act as a basic model for organic solar cells, we are interested in the structural changes and stability of the system with time.

SYOP 4.31 Thu 16:30 P1A

Electronic properties of potassium doped CoPc and FePc — •Olga Molodtsova[1], Martin Knupfer[1], Alexander Chaika[2], Denis Vyalikh[3], Alexei Preobrajenski[4], and Victor Aristov[1,2] — [1]IFW Dresden, D-01069 Dresden, Germany — [2]ISSP RAS, Chernogolovka, 142432 Russia — [3]IFP, TU Dresden, D-010169 Dresden, Germany — [4]MAX-Lab, 22100 Lund, Sweden

Magnetic transition metal (MTM) phthalocyanines are interesting due to their many different potential applications. In particular, FePc and CoPc are often utilized in optoelectronics and medical applications. Nowadays such phthalocyanines are considered as materials for development of low dimensional molecular magnets and quantum computers. To make further progress in development of this and other similar kinds of devices both the understanding and the tailoring of the physical, chemical and transport properties of the organic semiconductor components are required. The later is based on information about their electronic structure. Moreover the ability to incorporate electron acceptors and donors into molecular crystals enables the control of their electronic properties by introducing charge carriers. This special aptitude represents a promising route for technology as well as for the investigation of the fundamental properties of molecular crystals. In this work we have studied the electronic properties of potassium-doped organic semiconductor MTM phthalocyanines thin films CoPc and FePc using photoelectron spectroscopy. Acknowledgements: This work was supported by the DFG (no.436RUS17/52/06), SFB 463 and RFBR (Grant N°08-02-01170).

SYOP 4.32 Thu 16:30 P1A

The properties of metastable PcVO modifications in evaporated thin-films — •Indro Biswas, Heiko Peisert, and Thomas Chassé — Institut f. Phys. u. Theor. Chemie, Universität Tübingen

Vanadyle phthalocyanine (PcVO) and perfluorinated vanadyle phthalocyanine (F_{16}PcVO) are small molecule organic semiconductors with a nonplanar distortion and a permanent dipole. The nonfluorinated material can be evaporated in two different thin-film modifications, (one of which is metastable and is transformed into its stable form by heating up to 200°C.) [1] In this work we present radiative (photoemission spectroscopy) and non-radiative (Kelvin probe measurements) investigations of evaporated thin-films. Depending on the method two different types of interface formation are observed. It can be shown, that the metastable form is converted under the influence of irradiation, i.e. the UV light provides the energy for the phase transition.

The Kelvin probe method gives the possibility to examine samples with a minimum amount of perturbation, where common spectroscopic techniques may change a sample due to the applied radiation.

[1] C. H. Griffiths, M. S Walker, P. Goldstein, Mol, Cryst. Liq. Cryst. 33 (1976) 149.

SYOP 4.33 Thu 16:30 P1A

Bipolar Charge Transport in Poly(3-hexylthiophene)/ Methanofullerene Blends: A Ratio Dependent Study — •Andreas Baumann[1], Jens Lorrmann[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Julius-Maximilians-University of Würzburg, Institute of Physics, Experimental Physics VI, D-97074 Würzburg — [2]Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg

One of the most promising candidates for bulk heterojunction (BHJ) solar cells nowadays is the material combination of poly(3-hexylthiophene) (P3HT):[6,6]-phenyl-C_{61} butyric acid methyl ester (PCBM). One of the prerequisites for a well-performing BHJ solar cell is that the respective mobilities for transporting electrons on the fullerene and holes on the polymer are rather balanced, in order to avoid a space charge building up. We investigated the charge carrier mobility in P3HT:PCBM blend devices by applying the time resolved photoconductivity experiment as a function of the donor:acceptor ratio. We observed bipolar transport in all studied samples ranging from pure polymer to polymer:fullerene with 90% PCBM content. Furthermore, two transit times in the hole and electron current transients were found [1]. We discuss their origin in terms of electron (hole) transport on P3HT (PCBM), respectively and simulate the hopping transport by using Monte Carlo simulation.

[1] Baumann et al., accepted for publication in Appl. Phys. Lett.

SYOP 4.34 Thu 16:30 P1A

Transient photovoltage and photocurrent of polymer:fullerene solar cells — •Alexander Förtig[1], Daniel Rauh[1], Carsten Deibel[2], and Vladimir Dyakonov[1,2] — [1]Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg — [2]Julius-Maximilians-University of Würzburg, Institute of Physics, Experimental Physics VI, D-97074 Würzburg

Improvements in the performance of organic solar cells based on polymer:fullerene blends are strongly dependent on understanding dominant loss processes within these devices, such as bimolecular recombination. Especially measurements under working conditions of the solar cell are attracting legitimate interest. Therefore, we used transient photovoltage and transient photocurrent measurements in order to determine the charge carrier lifetime and density of poly(3-hexylthiophene):[6,6]-phenyl-C_{61} butyric acid methyl ester solar cells. Transients were performed over a wide range of light intensities. The experimental results are discussed with respect to recent findings concerning the order of the charge carrier decay rate in organic solar cells.

SYOP 4.35 Thu 16:30 P1A

Investigation of charge carrier transport and recombination in polymer:fullerene solar cells using transient current injection and extraction techniques — •Cristina Urs[1], Andreas Baumann[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Julius-Maximilians-University of Würzburg, Institute of Physics, Experimental Physics VI, D-97074 Würzburg — [2]Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg

The charge carrier transport and recombination processes are important factors for the efficiency of organic bulk heterojunction solar cells. We study these mechanisms in poly(3-hexylthiophene) (P3HT): [6,6]-phenyl-C_{61} butyric acid methyl ester (PCBM) photovoltaic devices, using the experimental techniques double injection current and plasma extraction. Both, the charge carrier mobility as well as the recombination rate can be determined simultaneously. We find that the major loss mechanism is due to nongeminate charge recombination, with at least second order decay rates. Our findings will be discussed in view of recent publications concerning bimolecular and trimolecular recombination.

SYOP 4.36 Thu 16:30 P1A

Photocurrent in organic solar cells obtained by pulsed IV-measurements — •Moritz Limpinsel[1], Daniel Rauh[2], Markus Mingebach[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Julius-Maximilians-University of Würzburg, Institute of Physics, Experimental Physics VI, D-97074 Würzburg — [2]Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg

The photocurrent in organic solar cells gives insight into fundamental device physics, as it allows determination of the field dependence of the photogeneration of charges. Its dependence on factors like absorber thickness and light intensity were observed and analysed. The magnitude of the photocurrent was obtained by IV-measurements under illumination by pulsed LEDs, which eliminate the overestimation of the device performance due to temperature effects made by sequential IV-measurements under constant illumination. We investigated bulk heterojunction solar cells with P3HT:PCBM blends as absorber layers, prepared by spin-coating. The built-in potential and the saturation photocurrent will be discussed in view of the internal field necessary to dissociate polaron-pairs.

SYOP 4.37 Thu 16:30 P1A

Investigation of novel organic n-type semiconductors in photovoltaic bulk heterojunction — •Moritz Liedtke[1,2], Andreas Sperlich[1], Carsten Deibel[1], Vladimir Dyakonov[1,2], Patrick Witte[3], and Alexander Hirsch[3] — [1]Julius-Maximilians-University of Würzburg, Institute of Physics, Experimental Physics VI, D-97074 Würzburg — [2]Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg — [3]Friedrich-Alexander-University Erlangen-Nürnberg, Department of Chemistry and Pharmacy & Interdisciplinary Center for Molecular Materials, D-91054 Erlangen

Two novel organic n-type semiconductors are investigated due to their function as electron acceptor for applications in organic electronic devices to widen the knowledge of how molecule structure influences the excitation processes in organic electronics. Bispyrenylfullerene and Octadecyl-Capronacidesterfullerene are C60 derivates with sidechains more featured compared to the commonly used [6,6] phenyl-C61-butyric acid methyl ester (PCBM). In bulk heterojunction devices regioregular poly(3-hexylthiophene) (P3HT) was used as donor. The materials, pristine and in blend, were studied in view of light absorption, their quenching abilities of the P3HT photoluminescence as well as excited states. Furthermore, the spinstate of the excited states was determined by light-induced electron spin resonance. Combining these complimentary experimental techniques, we obtained information on the generation of excited states, their nature, and the efficiency of the subsequent charge carrier separation.

SYOP 4.38 Thu 16:30 P1A

Investigation of s–shaped current–voltage characteristics of organic bulk heterojunction solar cells — •Daniel Rauh[1], Stefan Geissendörfer[1], Carsten Deibel[2], and Vladimir Dyakonov[1,2] — [1]Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg — [2]Julius-Maximilians-University of Würzburg, Institute of Physics, Experimental Physics VI, D-97074 Würzburg

In order to achieve a high performance in organic solar cells, reaching a reproducibly high fill factor – the solar cell parameter which depends on internal device structure and electrodes mostly sensitive – is crucial. Depending on the preparation conditions, sometimes the problem of s–shaped current–voltage (IV) curves arises, causing a low fill factor and therefore a low power conversion efficiency. In order to investigate this double diode behaviour, we prepared poly(3-hexyl thiophene):methanofullerene bulk heterojunction solar cells with a blend ratio of 1:1, varying the processing conditions. We discovered two different types of s–shapes, one with an increasing slope after the inflexion point and the other with a decreasing slope. We discuss space charged limited currents, trap states and internal energy barriers as as potential origin of the double diode behaviour.

SYOP 4.39 Thu 16:30 P1A

Influence of morphology modification on device performance of conjugated polymer solar cells — •Philipp Oberhumer[1], Justin Hodgkiss[1], Guoli Tu[2], Wilhelm Huck[2], and Richard Friend[1] — [1]Cavendish Laboratory, Cambridge, UK — [2]Melville Laboratory for Polymer Synthesis, Cambridge, UK

The device efficiency of bulk heterojunction solar cells greatly depends on the morphology of the conjugated polymer blend system. The addition of a third conjugated material to a binary blend of polyfluorene copolymers shows significant morphological changes on the mesoscale and its further effect on the nanoscale, exciplex formation, charge generation and device performance is studied by atomic force microscopy, photoluminescence, femtosecond transient absorption and device efficiency measurements.

SYOP 4.40 Thu 16:30 P1A

Infrared Ellipsometry for determination of molecular orientation in DCV6T films — •K. Hinrichs[1], M. Levichkova[2], M. Riede[2], M. Pfeiffer[3], E. Brier[4], E. Reinold[4], P. Baeuerle[4], and K. Leo[2] — [1]ISAS - Institute for Analytical Sciences, Department Berlin, 12489 Berlin, Germany — [2]Institut für Angewandte Photophysik, TU Dresden, 01062 Dresden, Germany — [3]Heliatek GmbH, 01187 Dresden, Germany — [4]Institut für Organische Chemie II und Neue Materialien, Universität Ulm, 89081 Ulm, Germany

For improving the electronic properties of organic solar cell devices the molecular structure of the organic compounds is of high interest. Films of DCV6T-Eth4(2,2,5,5): α,ω-Bis-(Dicyanovinylen)-Sexithiophene with different thicknesses were prepared by Physical Vapor Deposition (PVD) on silicon substrates. Infrared spectroscopic ellipsometry (IRSE) was used for characterisation. From evaluation of the ellipsometric data in an optical layer model, the film thickness and the anisotropic optical constants of the DCV6T films were determined. It was found that the optical constants strongly depend on the film thickness. Different average molecular orientations were determined for thin and thick (d=4-17.5 nm) films. The deposition at higher substrate temperatures (80 °C) resulted in a higher average molecular tilt angle.

SYOP 4.41 Thu 16:30 P1A

Donor-Acceptor Block Copolymers for their Application in Organic Photovoltaics. — •Sven Hüttner[1,2], Michael Sommer[2], Ullrich Steiner[1], and Mukundan Thelakkat[2] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]Angewandte Funktionspolymere, Universität Bayreuth, Germany

Organic photovoltaic cells rely on two different materials, a donor (p-type) and an acceptor (n-type) material. In conventional approaches, both materials are blended together to form the active layer. We use a block copolymer instead, where a donor and an acceptor polymer are covalently linked. Block copolymers are well known to phase separate in highly ordered nanostructures on lengthscales of the exciton diffusion length. The acceptor block consists of perylene bisimide moieties and shows excellent electronic properties. Different donor blocks have been synthesized - one of the block copolymers features poly(3-hexylthiophene) (P3HT). We demonstrate photovoltaic devices based on these polymers with high external quantum efficiencies up to 30%.

The investigation of the morphology is accompanied by transient absorption spectroscopy resolving the exciton formation, separation and recombination processes on a time scale from ps to ms. Furthermore organic thin film transistors are used to characterize the transport properties in these materials displaying unique properties: Initially all materials exhibit p-type character after processing. However, depending on the post treatment and on the molecular weight ratios of blocks, we can switch the polarity of the transistor or achieve ambipolar transport.

SYOP 4.42 Thu 16:30 P1A

Negative Capacitance for various electrode materials in organic solar cells — •Roland Rösch[1], Almantas Pivrikas[2], Niyazi Serdar Sariciftci[2], and Harald Hoppe[1] — [1]Institute of Physics, TU Ilmenau, 98693 Ilmenau, Germany — [2]LIOS, Johannes Kepler University Linz, 4040 Linz, Austria

Electrical behaviour of bulk heterojunction polymer solar cells is strongly influenced by their contacts. Charge carrier injection/extraction at contact-active layer interface depends on type of contact. In the literature different models - Schottky-contact, thermionic injection and injection via hopping processes - for the cathode contact are discussed. We use different contact materials and investigate the resulting capacitance via impedance spectroscopy, a non-invasive technique for electrical analysis. We observe a dependence of Negative Capacitance on contact type.

SYOP 4.43 Thu 16:30 P1A

Morphology Optimization of Diblock Copolymer Based Polymer Solar Cells — •Chetan Raj Singh, Martin Kunz, and Harald Hoppe — Institute of Physics, TU Ilmenau, 98693 Ilmenau, Germany

Diblock copolymers have emerged during the last few years as single active layer material in polymer solar cells with extraordinary high morphological stability. The immiscibility of two covalently bonded donor and acceptor blocks drives the nanoscale phase separation between them and leads to self organized nanometer-scale morphology. The desired perpendicular orientation of donor and acceptor phases on the substrate is aimed by various treatments including thermal annealing and solvent vapor annealing. We analyzed the success of the post-production treatments via optical absorption, photoluminescence spectroscopy, atomic force microscopy and light-induced electron spin resonance.

SYOP 4.44 Thu 16:30 P1A

Exciton dynamics in a hybrid TiO2-polymer bilayer structure — •Beate Reinhold, Sylvia Paul, and Dieter Neher — Universität Potsdam, Institut für Physik und Astronomie, Physik weicher Materie

Exciton diffusion plays an important role for the performance of polymeric optoelectronic devices like organic light emitting diodes and polymer based solar cells. Therefore, understanding the exciton transport processes is a key parameter to improve device performance and to develop new interface architectures. Here, we present our results of spectroscopic investigations on bilayer structures consisting of a soluble PPV derivative as the electron donor and an acceptor layer formed from nanocrystalline TiO2. From these experiments, the exciton diffusion length and the probability for exciton dissociation at the heterojunction are determined. The results are discussed with regard to the morphology of the bilayer structure and the energetic conditions at the heterojunction.

SYOP 4.45 Thu 16:30 P1A

Probing ultrafast charge transfer dynamics in a P3HT:PCBM blend via photoluminescence quenching — •Theo Hoyer[1], Stefan Trotzky[2], Wilfried Tuszynski[1], Christoph Lienau[1], and Jürgen Parisi[1] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz, Germany

So far the ultrafast charge transfer dynamics in polymer/fullerene blends for solar cell device applications have mostly been studied by nonlinear photoinduced absorption techniques. Time-resolved photoluminescence (PL) methods have the potential to yield additional information about the charge separation dynamics as they give direct access to the exciton relaxation dynamics and provide higher sensitivity.

Here, we present an experimental study of the donor-acceptor charge transfer in a polymer/fullerene blend by means of a femtosecond PL up-conversion technique. The exciton dynamics of pristine P3HT and a P3HT:PCBM blend with a weight ratio of 1:1 were measured by recording PL decay traces at $\lambda = 650\,\mathrm{nm}$ after two-photon excitation at excitation densities of up to $6\cdot10^{18}\,\mathrm{cm}^{-3}$. Both samples show clearly nonexponential decay traces compatible with diffusion-limited exciton-exciton annihilation and charge transfer in the polymer blend. A fast PL decay in this blend on a time scale of about 150 fs indicates that about 50% of the photogenerated excitons undergo a prompt charge transfer process.

SYOP 4.46 Thu 16:30 P1A

Model studies on the injection of charge carriers into organic semiconductors: The case of pentacene single crystals grown on self-assembled monolayers (SAMs) — Zhihong Wang[1], Asif Bashir[1], Daniel Käfer[1], Alexander Birkner[1], Gregor Witte[2], and •Christof Wöll[1] — [1]Physik. Chemie, Ruhr-Universität Bochum — [2]AG Molek. Festkörperphysik, Philipps-Universität Marburg

SEM and STM micrographs reveal that the deposition of the organic semiconductor (OSC) pentacene on Au-supported SAMs with different termination yields similar morphologies, namely multilayer islands containing upright-oriented molecules. Charge transport across the SAM / within the OSC was studied using the STM-tip as a second electrode. For films on alkanethiol SAMs the I-V characteristics show not only a pronounced asymmetry, but also a strong dependence on temperature and film thickness [1]. An explanation was provided by numerical simulations which found a dominance of p(n)-transport at neg. (pos.) bias. A different behaviour is found for films on a mercaptoundecanol SAM. Here, stable images could only be obtained for neg. substrate bias; for pos. bias the tip was found to penetrate the OSC-island resulting in a complete removal during scanning. We explain this unexpected behaviour by electron trapping at OH-groups (SAM) and by quenching of n-transport in the OSC. This is in accord with the observation that in pentacene devices n-type transport is only found in absence of OH groups [2]. Possible microscopic mechanisms for the trapping of charges at the OH-groups will be discussed.

[1] Ruppel et al., J.Appl.Phys. 102, 033708 (2007), [2] Chua et al., Nature 434, 194 (2005)

SYOP 4.47 Thu 16:30 P1A

Limitating factors in Phenyl-substituted rylenes as electron acceptors associated with P3HT donor in bulk heterojunction solar cells. — •Julien Gorenflot[1], Maria Hammer[1], Andreas Sperlich[1], Andreas Baumann[1], Aleksey Vasilev[3], Martin Baumgarten[3], Chen Li[3], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Julius-Maximilians-University of Würzburg, Institute of Physics, Experimental Physics VI, D-97074 Würzburg — [2]Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg — [3]Max-Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz

In the quest for new efficient electron acceptor/donor couples for bulk heterojunction organic solar cells, we report the study of an important family of electron acceptors: rylenes were investigated as associated with P3HT. Photophysical studies including photoluminescence, steady-state photo-induced absorption ans electron spin resonance confirmed the good charge generation properties of TDI:P3HT blends. Nevertheless no correlation could be established between generated charges and devices performances. Further studies of this mismatch were carried out by investigating the charge transport properties of the materials using Charge Extraction by Linearly Increasing Voltage as well as Field Effect Transistor measurements. The acceptors and donor were varied in order to maximize the charge separation driving force. Those experiments enabled to emphasize two key limiting factors for bulk heterojunction solar cells: charge transport ability of each material and morphological compatibility of the blended components.

SYOP 4.48 Thu 16:30 P1A

Photophysical properties of novel small acceptor molecules and their application in hybrid small-molecular/polymeric organic solar cells — Sahika Inal[1], •Mauro Castellani[1], Alan Sellinger[2], and Dieter Neher[1] — [1]Universität Potsdam, Institut für Physik und Astronomie, 14476 Potsdam-Golm — [2]Institute of Materials Research & Engineering, Singapore 117602

Recent experimental investigations revealed that the photovoltaic properties of our devices are related to the balance between recombination and field-induced dissociation of interfacial excited states such as exciplexes or geminate polaron pairs. This balance was shown to be affected by the nanomorphology at the heterojunction [J. Phys. Chem. C 2008, 112, 14607]. We have analyzed the photophysical properties of a new materials couple comprising an electron-donating PPV copolymer and a vinazene-based small molecule acceptor [Chem. Mater. 2007, 19, 1892]. Steady state and time-resolved photoluminescence (PL) spectroscopy in solution and in the solid state showed the formation of excimers within the acceptor. The associated long-range diffusion promise efficient energy harvesting at the heterojunction. On the other hand, blends of the PPV-derivative and the small molecule revealed strong exciplex formation. Therefore, bilayered hybrid small-molecular/polymeric solar cells have been fabricated by consequently spin-coating the macromolecular donor and the small molecule acceptor from two different solvents. The bilayer architecture limits recombination processes enabling high FFs of around 44% and a technologically important open circuit voltage of 1Volt.

SYOP 4.49 Thu 16:30 P1A

Electronic characterization of photoactive conjugated polymers — •Stefan M. Prams, Matthias A. Ruderer, and Peter Müller-Buschbaum — TU München, Physik-Department LS E13, James-Franck-Str. 1, 85747 Garching (Germany)

It is well known that in organic photovoltaics the molecular conformations as well as the polymer phase morphology in the active layer define the performance of a device. Typically the systems are optimized via pre- and postproduction treatments like the choice of the solvent or annealing steps. Furthermore ageing and degradation influence the performance during operation. In this work we characterized the electronic behavior of a system of selected photoactive conjugated polymers depending on pre- and postproduction treatments and ageing with a solar simulator. The investigations are completed with UV/Vis, FT-IR and thickness measurements.

SYOP 4.50 Thu 16:30 P1A

Unsymmetrically substituted n-type perylene bisimides with liquid crystalline properties — André Wicklein and •Mukundan Thelakkat — Universität Bayreuth, Applied Functional Polymers, Universitätsstrasse 30, 95440 Bayreuth (Germany)

Perylene bisimides (PBIs) represent an important class of organic n-type semiconductors exhibiting a relatively high electron affinity among large-band-gap materials. Herein synthesis and characterization of several unsymmetrical N-substituted PBI dyes is presented and the thermotropic behavior, which is strongly affected by the respective N-substituents was investigated. Two different series of highly soluble and fluorescent derivatives have been synthesized: (1) PBIs bearing swallow-tailed alkyl chains, different in size or (2) one swallow-tailed alkyl chain and one branched oligoethylenglycolether. Synthesis of these PBIs is generally feasible by two distinct divergent synthesis approaches. Thermotropic behavior was studied by DSC, POM and XRD measurements. Inherent π-π interactions between cofacially orientated perylene molecules and the elliptic shape of the molecule favor the ordering in columns and self-organized architectures. Among them hexagonal columnar Colh mesophases, large spherulitic crystals or formation of stable amorphous phases upon rapid cooling from the isotropic phase can be observed. Due to high solubility in organic solvents, film preparation by solution processing is readily feasible. The interesting optical and thermal properties of these compounds allow these organic n-type semiconductors as potential materials for application in organic electronic devices, such as photovoltaics or OFETS.

SYOP 4.51 Thu 16:30 P1A

Novel Concepts in Solid-State Dye-Sensitized Solar Cells — •Katja Willinger[1], Johannes Brendel[1], Yan Lu[2], and Mukundan Thelakkat[1] — [1]Makromolekulare Chemie I, Angewandte Funktionspolymere, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Physikalische Chemie I, Universität Bayreuth, 95440 Bayreuth, Germany

We combine two major concepts to improve the performance of solid-state dye-sensitized solar cells (SDSC). In concept I, we synthesize novel heteroleptic Ru(II)bis(bipyridyl)(NCS)2 dyes carrying donor-antenna groups. These dyes typically comprise of an efficient anchoring group to guarantee a proper connection between the dye and the mesoporous TiO2 surface, two NCS-groups to cause a bathochromic shift of the absorption spectra and novel donor-antenna groups. These groups effect very high extinction coefficients and as a consequence of this a distinctive light harvesting behaviour. To prove the performance of this new dyes they were applied in SDSCs consisting of FTO coated glass, mesoporous TiO2 and for regeneration of the dyes Spiro-OMeTAD as hole transport layer. In concept II, we developed novel porous TiO2 network using polymer electrolyte brushes as templates to control the morphology of the network and thus to provide best conditions for a sufficient pore filling and an effective electron transport. The facile tuning of the brush length as well as core size of the template and defined amounts of TiO2 hydrolysed within the brushes finally provide exact control on the resulting morphology of the porous network.

SYOP 4.52 Thu 16:30 P1A

Theoretical investigation of the competition between electron-hole generation and recombination effects in organic and hybrid organic-inorganic solar cells — •Benjamin A. Stickler[1,2], Manfred Gruber[1,2], Ferdinand Schürrer[1], Gregor Trimmel[2], and Karin Zojer[1] — [1]Department of Theoretical and Computational Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — [2]Christian Doppler Pilotlabor for Nanocomposite Solar Cells, Institute for Chemistry and Technology of Materials, Graz University of Technology

Electron-hole generation and recombination in bulk heterojunctions profoundly influence the performance of the solar cell, independent whether organic-organic or inorganic-organic heterojunctions are considered. In this work, a drift diffusion based transport model implemented in one as well as two dimensions was used to simulate these processes and to compute the corresponding I-V curves of the device. Furthermore, intensity-dependent exciton generation (via Lambert-Beer's law), exciton diffusion, and field- dependent dissociation into electrons and holes are considered.The influence of field-dependent carrier mobilities, recombination and generation models is discussed in terms of exciton, charge carrier, and electric field distribution.

SYOP 4.53 Thu 16:30 P1A

Investigation of heterojunction morphology in organic solar cells by 2D drift-diffusion simulations — •Manfred Gruber[1,2], Bejamin A. Stickler[1,2], Ferdinand Schürrer[1], Gregor Trimmel[2] und Karin Zojer[1] — [1]Department of Theoretical and Computational Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — [2]Christian Doppler Piotlabor für Nanokompositsolarzellen - Institut für Chemische Technologie von Materialien, Graz University of Technology, Stremayrgasse 16, 8010 Graz, Austria

The interface morphology of bulk heterojunctions in organic solar cells plays a crucial role in determining the fill factor and, thus, the quantum efficiency. To gain a better understanding of the influence of the interface morphology on the performance of solar cells, we calculated their I-V curves by means of a two-dimensional drift-diffusion model. The corresponding system of equations containing the Poisson equation and the continuity equations for electrons and holes is solved self-consistently on a two-dimensional rectangular mesh. The mesh cell extensions reflect the aspect ratio of the modelled device cross-section. By means of an idealized comb-shaped heterojunction, i.e., interdigited donor and acceptor phases, we discuss the influence of the digit aspect ratios, the recombination rates, and mobilities in the light of the local charge carrier and electric field distributions

SYOP 4.54 Thu 16:30 P1A

Reliable Electron-Only Devices and Electron Transport in n-type Polymers — •Robert Steyrleuthner, Sebastian Bange, and Dieter Neher — Universität Potsdam, Institut für Physik und Astronomie, Karl-Liebknecht-Strasse 24-25, D-14476 Potsdam

Charge transport properties of conjugated polymers have received increasing attention during the last years as a possibly limiting factor for solar cell performance. While hole transport properties have been extensively studied using single-carrier current-voltage measurements, only few reports can be found where this was applied to electron transport. Here, we summarize the experimental difficulties associated with electron-only single-carrier devices. The role of leakage currents and nonlinear differential resistance is discussed and the physical origin of these effects analyzed. We present a preparation technique for the metal electrodes which significantly improves the reliablity of electron-only devices. Using this method, electron transport was studied for two representative n-type polymers over a wide range of layer thickness and temperature. The results are explained in terms of established trapping models with exponential trap distribution.

SYOP 4.55 Thu 16:30 P1A

Study of the Performance of Hybrid Solar Cells Incorporating Dense TiO2 Layers — •Sylvia Paul and Dieter Neher — University of Potsdam, Institute of Physics, Karl-Liebknecht- Street 25, 14476 Potsdam, Germany

Hybrid solar cells combine an organic with a suitable inorganic semiconductor (TMO*s). Hereby, the morphology and surface characteristics of the TiO2-films are of great importance, as they affect the exciton diffusion length and carrier transport properties of the TMO in the inorganic/polymeric hybrid-cell. It is expected that the way of layer preparation has a large impact on these properties. We have systematically investigated different techniques for the preparation of the TiO2 layers with regard to the performance of hybrid photovoltaic cells using a soluble derivative of PPV as the hole acceptor. The following processes were applied: TiO2 layers compounded via sputtering, dip-coating of preformed crystalline nanoparticles, dip-coating of preformed TiO2 by sol-gel process and the combination of all methods. Structural characteristics were investigated by atomic force microscopy (AFM), transmissions electron microscope (TEM), scanning electron microscope (SEM), infrared and Raman spectroscopy while the optical properties were studied with ellipsometry. In particular we show that dense and defect-free layers could be prepared from preformed crystalline TiO2 nanoparticles and that these layers, in combination with a sol-gel buffer substrate layer, gave the best performance in our hybrid photovoltaic devices: an open circuit voltage Voc of approximately 0.9 V and a fill factor of more than 40%.

SYOP 4.56 Thu 16:30 P1A

CT-State Dissociation and Charge Recombination in OPVs — •Roger Häusermann[1], Nils Reinke[1], Evelyne Huber[1], Thomas Flatz[2], Michael Moos[2], and Beat Ruhstaller[1] — [1]ZHAW, Inst. of Computational Physics, Winterthur, Switzerland — [2]Fluxim AG

The dissociation of the charge-transfer-state (CT) into free charge carriers is a very important process in the modeling of OPVs. A theoretical description of this mechanism has been developed by Onsager and Braun. The implications of this theory in real OPVs is not completely clear. Recently there was the proposition to reduce the whole device physics to the mechanisms at the donor-acceptor interface. This has been verified for a wide range of OPV materials, but it also raises questions about the universality of this simplification.

In this study we developed a comprehensive device simulator. Our simulations have shown that a good agreement with measured J-V curves can be found by omitting any dissociation mechanism but at the same time increasing the influence of the Langevin recombination. This shows that distinct features of J-V curves are multi-causal and therefore a simplification by leaving out some of the mechanisms leads to an overestimation of the influence of other processes.

We present the influence of the input parameters (CT-state dissociation, recombination and mobility) on the J-V curves and discuss in detail where and if each parameter can be seen separately in the shape of the J-V curve. The contributions of the different loss mechanisms, namely decay of excitons and CT-states as well as charge recombination will be addressed as function of material properties.

SYOP 4.57 Thu 16:30 P1A

The effect of polymer-fullerene interaction on film morphology and performance of polyfluorene-based solar cells — •Ana Sofia Anselmo[1], Ellen Moons[1], Krister Svensson[1], Mats Andersson[2], Andrzej Budkowski[3], and Andrzej Bernasik[4] — [1]Karlstad University, Karlstad, Sweden — [2]Chalmers University of Technology, Göteborg, Sweden — [3]Jagiellonian University, Kraków, Poland — [4]AGH - University of Science and Technology, Kraków, Poland

In our research project, we focus on morphological issues in thin-films spin-coated from blends of low-bandgap polyfluorenes and a fullerene derivative (PCBM). Characterization of the thin-film topography is performed through AFM, and the in-depth organization of the blend components through dynamic SIMS. Solar cell devices are fabricated to correlate device performance and film morphology.

Previous studies have shown multilayer-structured films of polyfluorene:fullerene blends to form spontaneously under specific conditions, which improved solar cell performance [1]. The mechanisms leading to these results can be rationalized with thermodynamic and kinetic models of nucleation and phase separation [2]. Recently an increased tendency for self-stratification was found in a series of films prepared from PCBM blended with polyfluorene copolymers that had been especially synthesized with a varying fraction of a phenolic monomer for enhanced polymer-fullerene interaction.

[1] Björström, C.M. et al J. Phys.:Condens. Matter 2005, 17, L529-L534; [2] Nilsson, S. et al Macromol. 2007, 40, 8291-8301.

SYOP 4.58 Thu 16:30 P1A

2d-gisaxs investigation of the crystal structure in thin polymer films — •Yun Gu[1], Ullrich Pietsch[1], Ingolf Hennig[2], and Walter Cox[2] — [1]FKP Universität Siegen — [2]BASF-Ludwigshafen

Structure and crystallinity of thin polymer film made from PDI8CN2 on silicon substrates were investigated by Grazing Incidence Small Angle X-ray Scattering using synchrotron radiation. The samples were prepared by spin-coating at different temperatures onto native SiO2 or substrates treated with OTS. The measurements were performed at DELTA in Dortmund. From the two dimensional GISAXS pictures, a large number of distinct Bragg spots appeared above a low diffuse background which refer to a high degree of crystallinity. The position of Bragg peaks was transformed in a set of d-values and used for the determination of the triclinic space group and respective lattice parameters. Based on this structure model all Bragg peaks could be indexed which allows for the determination of crystal orientations. Our data give evidence that all crystals coincides with one axis [100] parallel to surface normal; the other two axes show random orientation within the surface plane. Based on Scherrer equation the out-of plane crystallite size is same as the layer thickness and the average in-plane size is about 30nm. Comparing the different samples, we found that both crystal structure and orientation do not depend on film thickness.

SYOP 4.59 Thu 16:30 P1A

Spatially resolved luminescence measurements on polymer photovoltaic cells — •Marco Seeland[1,2], Florian Kühnlenz[1], Harald Hoppe[1], Gerhard Gobsch[1], Martin Kasemann[2], and Wilhelm Warta[2] — [1]Institute of Physics, Technical University Ilmenau, 98673 Ilmenau, Germany — [2]Fraunhofer Institute for Solar Energy Systems (ISE), 79110 Freiburg, Germany

We applied spatially resolved luminescence measurements for studying degradation of P3HT:PCBM bulk heterojunction polymer solar cells. This technique is useful to clarify the influence of impurities that are imposed on the solar cell during its production. Upon application of a forward bias to the photovoltaic devices the generated electroluminescence is detected in a CCD-Camera. The obtained images allow us to get a direct view on the advancing degradation patterns and also to study the influence of varying processing parameters.

SYOP 4.60 Thu 16:30 P1A

Electrical modeling of organic solar cells — •Wolfgang Tress, Moritz Riede, and Karl Leo — TU Dresden Institut für Angewandte Photophysik, George-Bähr-Straße 1, 01069 Dresden

We report on realistic modeling of small molecule solar cells based on ZnPc/C_{60}. For this purpose, samples with systematically varied parameters like layer thicknesses are prepared in a pin structure, i.e. active layer(s) sandwiched in between doped transport layers.

For a comprehensive description of the whole solar cell stack, a drift-diffusion model has been developed to simulate the current-voltage characteristics of organic solar cells. As input an exciton profile is used, obtained from optical modeling via a thin-film-optics algorithm. In the electrical simulation, Poisson, transport, and continuity equations for electrons and holes are solved numerically under boundary conditions describing the contacts. The iterative algorithm itself is based on [1]. The multi-layer structures are treated using different recombination and mobility models, modified Onsager theory for charge carrier dissociation, and tunneling assisted barrier crossing. Additionally exciton processes like diffusion and quenching are implemented.

The experimental data is compared to simulation results, where parameter variations allow to estimate the influence of distinct effects. Different recombination and mobility models are evaluated and the limitations of the models shown. Finally, values for exciton diffusion lengths and other electrical properties of the used materials can be extracted.

[1] J. Staudigel et al, J. Appl. Phys. 86, 3895 (1999)

SYOP 4.61 Thu 16:30 P1A

Investigating aza-bodipy for organic electronics: A chemist's view. — •Roland Gresser, Toni Müller, Horst Hartmann, and Karl Leo — Institut für Angewandte Photophysik, TU Dresden

Current research on organic photovoltaics aims for broader photoactive spectral ranges of the organic solar cells, and the synthesis and investigation of new, appropriate low band gap absorbers are essential.

The focus of this study is on the material class of 4,4-difluoro-4-bora-3a,4a,8-triazaindacene (aza-bodipy) as active donor material in vacuum deposited small molecule solar cells. Due to the straightforward synthesis, an aza-bodipy series with different substituents is prepared and investigated.

All compounds indicate reversible one electron reduction and oxidation waves determined by cyclic voltammetry (CV) in solution. Corresponding absorption measurements show a clear tendency towards a red shift of the absorption maximum with increasing donor strength of the substituents. The origin of this bathochromic shift originates from the increase of the HOMO energy level which was determined by CV.

Additional quantum chemical calculations of the series with ab-initio methods show a typical donor-acceptor charge transfer behavior upon HOMO-LUMO transition. Internal reorganization energies were calculated directly from the adiabatic potential energy surfaces for hole and electron transport process respectively. The results show that aza-bodipy is a suitable material for organic electronics.

SYOP 4.62 Thu 16:30 P1A

Relationships between the charge carrier mobility and the morphology in the hybrid system composed of poly(3-hexylthiophene) and CdSe nanoparticles — •Nikolay Radychev, Folker Zutz, Irina Lokteva, Joanna Kolny-Olesiak, Holger Borchert, and Jürgen Parisi — Institute of Physics, Energy and Semiconductor Research Laboratory, University of Oldenburg, 26111 Oldenburg, Germany

It is well known that hybrid systems composed of polymers such as poly(3-hexylthiophene) and semiconductor nanoparticles like CdSe are perspective materials for solar cell applications. Light conversion efficiencies of up to ˜3 percent were reported for these systems, but low charge carrier mobility is one of the limiting processes in these structures. Therefore, research on correlations between the charge carrier mobility and the morphology of the organic-inorganic blends is one of the most important tasks which have to be addressed in order to improve the light conversion efficiency. In the present work, composites of poly(3-hexylthiophene) and CdSe nanoparticles with systematically varied parameters such as concentrations, particle size and shape were prepared. Systematic reserach with atomic force microscopy, transmission electron microscopy and absorption spectroscopy was made to study the structural properties of the systems. The charge carrier mobility was measured by MOSFET methods. Relationships between the charge carrier mobility and the morphology of the blends were analyzed.

SYOP 4.63 Thu 16:30 P1A

Degradation studies on organic pin solar cells containing ZnPc and C_{60} — •Martin Hermenau, Moritz Riede, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden, Germany

In addition to the power conversion efficiency of organic solar cells, the lifetime of these devices plays an important role for the market entry as commercial products. Therefore a detailed understanding of degradation of organic solar cells is necessary. In this work, we present ageing studies of small-molecule solar cells with a pin structure and a mixed heterojunction of Zinc-Phthalocyanine and fullerene C_{60}. These devices have an initial efficiency of 2.8% under solar irradiation.

The ageing dynamics of these solar cells are observed under different conditions, e.g. illumination and temperature, and compared to reference devices which are stored in the dark. The external quantum efficiency of these cells is measured before and after ageing studies to observe changes in different spectral ranges. The relative change of external quantum efficiency does not depend on the colour of the incident light during time of ageing, indicating the stability of the absorbing layers during the observed time span.

SYOP 4.64 Thu 16:30 P1A

Effect of π-π stacking distance in low-band-gap PPE-PPV polymers on the morphology and performance of polymer-fullerene solar cells — •Rupali Jadhav[1], Stefan Türk[3], Florian Kühnlenz[1], Daniel Egbe[2], and Harald Hoppe[1] — [1]Institute of Physics, Technical University Ilmenau, 98673 Ilmenau, Germany — [2]Institute of Organic and Macromolecular Chemistry, Friedrich-Schiller-University Jena, 07743 Jena , Germany — [3]Institute for Print and Media Technology, Chemnitz University of Technology, 09107 Chemnitz, Germany

Poly(-p-arylene-ethynylene)-alt-poly(-p-arylene-vinylene)s, (PAE-PAVs) are conjugated systems, which combine the interesting intrinsic properties of both their constituents within a single polymeric backbone and in addition show novel promising structure-specific properties. They can be effectively used as donor materials in polymer-PCBM bulk heterojunction polymer solar cells. Their photovoltaic parameters were found to be dependent on the concerting effects of backbone conjugation pattern, and the nature and size of the solubilizing alkoxy side chains. Moreover, the insertion of electron-rich thiophene leads to a reduction of the optical band gap energy. Reduction of the length of the side chains on the other hand results in a significant increase of the short circuit current, which can be explained in terms of an extended donor-acceptor interfacial area. The active layer nano-scale morphology of these polymer/fullerene blend films has been investigated using Atomic Force Microscopy and is related to the different chemical structures of the donor polymers.

SYOP 4.65 Thu 16:30 P1A

Investigations of film thickness dependence in polythiophene organic field effect measurements on device performance and charge carrier mobility using a gated four probe technique — •Ali Tunc, Fabian Johnen, Elizabeth von Hauff, and Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, Carl-von-Ossietzky Str. 9-11, 26129 Oldenburg, Germany

In this study polythiophene (P3HT) based organic field effect transistors (OFET) with different semiconductor film thickness were investigated using a gated four probe geometry. A series of P3HT OFETs with different P3HT film thicknesses (from 39 to 240nm) were fabricated by varying P3HT concentration in chloroform and varying the spin coating parameters for depositing the semiconducting layer. The OFETs were bottom contact devices with Au contacts with a thin layer of Cr for adhesion to the SiO2. The source and drain contacts as well as two thin additional electrodes protruding roughly 1/4 of the way into the channel were patterned with photolithography. The four point geometry allowed for the investigation of the effects of contact resistances on the field effect measurements. The source-drain current and the field effect mobility determined in the saturation region of the OFET current-voltage characteristics were found to increase with P3HT film thickness. The field effect mobility determined from the linear region of the IV characteristics showed less dependence on the film thickness and seemed to be influenced by inhomogeneities in the semiconducting channel at low currents.

SYOP 4.66 Thu 16:30 P1A

Microwave photoconductivity of cadmium telluride doped by gallium studied at different temperatures — Alexander Marinin, •Nikolay Radychev, Gennadii Novikov, and Mikhail Gapanovich — IPCP RAS Chernogolovka Moscow region 142432

The number of charges reaching the electrodes is a key parameter for detector quality characterestics. Solid solutions of CdTe-GaTe are considered as a perspective medium for X-ray detection. The kinetics of photogenerated charges was studied at different temperatures and for different doping concentrations. The samples were made by CdTe and GaTe vacuum sintering. The sintering temperature and duration were 1010 K and 300 h, respectively. The microwave photoconductivity (f=36 GHz) was investigated. The temporal resolution of the experimental facility was decreased to 5 ns. Investigations were made in a wide temperature range, T=140-295 K. A nitrogen laser was used for photoexcitation. Generally, the experimental curves of the photoresponse P(t) consist of fast and slow components after switching of the laser light. The temperature and the Ga content were found to influence the form, amplitude and characteristical decay time of P(t) considerably. The photoresponse decay analysis shows that a self-compensation effect is present and this effect results in a decrease of the depth of traps. The active medium parameters take a turn for the better by this effect. This work was supported by RFFI 06-03-32725, 06-08-01510

SYOP 4.67 Thu 16:30 P1A

Improved morphology of C60:ZnPc blend solar cells by using heated substrates — •Steffen Pfuetzner, Moritz Riede, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, 01069 Dresden, Germany, http://www.iapp.de

To reach higher efficiencies in organic solar cells, ideally the open circuit voltage (Voc), fill factor (FF), and the short current density (jsc) has to be further improved. It is well known from polymer based solar cells that the morphology of the photoactive layers can have a significant influence on the jsc and FF. However, only few such studies are available for small molecule based solar cells. This work investigates the effects of substrate temperature on the morphology of the photoactive layer during vacuum deposition of the organic absorber materials. AFM, SEM and TEM measurements were done to characterize the morphological changes. Complete solar cells with a 150nm thick blend layer of C60 and ZnPc were fabricated at different substrate temperatures to study the morphology. It was shown that jsc reaches a maximum at 110°C due to the balance of improved transport paths and charge carrier generation. Further optimization of the thin film optic led to a 60 nm blend solar cell which was made at 110°C. This device shows a high FF of 56% and a p.c. efficiency of 2.6%.

SYOP 4.68 Thu 16:30 P1A

Small Bandgap aza-Bodipy in Organic Solar Cells — •Toni Mueller, Roland Gresser, Moritz Riede, Horst Hartmann, and Karl Leo — Institut für Angewandte Photophysik, Technical University of Dresden, George-Bähr-Straße 1, 01069 Dresden, Germany

Extending the available part of the spectral range to the infrared plays an essential role for increasing the efficiency of organic solar cells. However, the choice of efficient organic materials absorbing above 800nm is still scarce, especially for small molecules.

In this work we have investigate a series of aza-Bodipy (4,4-Difluoro-4-bora-3a,4a,8-triazaindacene) as absorber materials in organic solar cells. UPS-data shows that the position of the materials' HOMO can be intentionally varied by the choice of the functional group attached to the aza-Bodipy, and, thus, changing the optical bandgap. Consequently, the external quantum efficiency of these solar cells is bathochromically shifted. Mobility and conduction measurements on the aza-Bodipy show good values and first heterojunction solar cells with doped transport layers (p-i-n structure) incorporating these materials, e.g. in combination with the fullerene C60, show spectral response above 800nm.

SYOP 4.69 Thu 16:30 P1A

Influence of substrate metals on the properties of electrodeposited dye- sensitized electrodes — •Kerstin Strauch, Thomas Loewenstein, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen. Phone +496419933400 FAX +496419933409 email:schlettwein@uni-giessen.de

The performance of porous sensitized semiconductor electrodes depends on both the quality of the deposited films and the electrode properties of the substrate material in contact with the active electrolyte needed for dye- sensitized solar cells. In this study we varied the substrate metal to study its electrode properties in contact with iodine- containing organic electrolytes. The electrodes were also used as substrates for the deposition of porous zinc oxide by electrochemically induced crystallization reactions. Zinc oxide serves as sensitized wide-bandgap semiconductor and properties of the obtained electrodes in dye- sensitized solar cells will be discussed.

SYOP 4.70 Thu 16:30 P1A

Room temperature sintering of organosoluble ZnO nanopar-

ticles for applications in electronic devices — •Thomas V. Richter, Felix Stelzl, Uli Würfel, Michael Niggemann, and Sabine Ludwigs — Freiburger Materialforschungszentrum Stefan-Meier-Str. 21, D-79104 Freiburg

During the last years, interest in nano-sized, inorganic semiconductors has grown due to their perspective application in electronic devices. In particular the use of inorganic semiconductor nanoparticles as acceptor phase in polymer-inorganic hybrid solar cells (h-SC) is promising. Special attention was given to nanocrystalline ZnO (n-ZnO) due to its abundance, low toxicity and easy tunability in shape and size. To obtain the full advantage of n-ZnO in h-SCs, there are two main issues to be addressed: In order to guarantee good interdispersion of the nanoparticles with the conjugated polymer in the photoactive layer, good solubility of both materials in organic solvents is necessary. Furthermore, interparticle contact has to exist after blend deposition to allow electron transport within the ZnO phase. Those requirements are often contradictory since good particle solubility requires large ligands, which in turn impede continuous percolation pathways in films. The strategy presented by us addresses both of the aforementioned problems. We synthesized n-ZnO with a weakly bound ligand that promotes solubility and allows for its post-processing removal in vacuum to establish interparticle contact. Charge carrier transport was investigated by FET measurements which indicate that ligand removal is applicable in pure n-ZnO thin films as well as in P3HT/n-ZnO blends.

SYOP 4.71 Thu 16:30 P1A

Effects of modifying active-layer/cathode interface on P3HT/PCBM based bulk-heterojunction solar cells — •Sidhant Bom and Veit Wagner — Jacobs University Bremen, School of Engineering and Science, Campus Ring 8, 28759 Bremen, Germany

The compatibility of organic photovoltaics (OPVs) with large area printing using flexible substrates offers significant cost reduction and gives the field substantial ecological and economic advantages. However, low efficiencies and inferior environmental stability has been their major setbacks. Photo-generated excitons which dissociate at donor-acceptor interface in bulk-heterojunction OPV devices are collected at the electrodes. This work focuses on interface engineering between the active layer and cathode and on environmental stability.

A series of bulk-heterojunction OPV cells were made on indium tin oxide coated glass with poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl C61 butyric acid methyl ester (PCBM) composite as the active layer using different work-function metals: Ag, Al, Au and Ca as cathodes. Furthermore, the environment was changed for different production steps between ambient air and dry nitrogen. For the devices completely processed in air, the cells with Al electrodes showed the best performance which was however much lower than completely nitrogen processed samples. The photocurrent features on the air processed sample were strongly bias dependent and indicates degradation of PCBM.

SYOP 4.72 Thu 16:30 P1A

Organic ambipolar field effect transistor as model system for light absorption in organic solar cells — •Steve Pittner and Veit Wagner — Jacobs University Bremen, Germany

Since years the interest in organic solar cells is steadily growing. The main reasons are low production costs, suitability for processing on flexible substrates and their potential to provide renewable, environmental friendly energy. Yet their efficiency is still too low and their environmental stability is not sufficient for widespread applications.

In this contribution blends of P3HT and [60]PCBM are investigated by light absorption and photocurrent spectroscopy in transistor geometry, which allow to vary charge density and carrier type systematically by varying the gate potential. In this way relevant electro-optical properties for organic blend solar cell with stacked layer geometry is investigated by using ambipolar thin film transistor (TFT) with Au contacts and a blend made of P3HT and [60]PCBM. Furthermore it is shown, that stability in air ambient can be obtained by $30\,nm$ Al_2O_3 encapsulation, which is assumed to mainly protect the air-sensitive PCBM.

The contributions of both organic semiconductors to the photocurrent spectra can be identified via their absorption spectra in the range $1.2\,eV$ to $3.7\,eV$ and is monitored for the different operation regimes. The data are interpreted in comparison with results of electrical measurements yielding the mobility for both carrier types and the trap distribution from hysteresis analysis.

SYOP 4.73 Thu 16:30 P1A

Flexible polymer solar cells: comparison between spin coating and doctor blading — •Burhan Muhsin[1], Maik Hühner[1], Karl-Heinz Drüe[2], Gerhard Gobsch[1], and Harald Hoppe[1] — [1]Institute of Physics, Ilmenau Technical University, Weimarer Str. 32, 98693 Ilmenau, Germany — [2]Electronic Technology, Ilmenau Technical University, Gustav-Kirchhoff-Str. 7, 98693 Ilmenau, Germany

The preparation of flexible polymer solar cells on plastic substrates demands the development of suitable processing conditions. Here we want to compare plastic solar cells prepared by spin coating and by doctor blading. Both, solar cells prepared by only one film formation technique, but also mixed approaches for the processing of the individual hole conducting (PEDOT:PSS) and photoactive (P3HT:PCBM) layers have been tested. After a comprehensive optimization of the blading parameters, the solar cells prepared by this technique achieve very comparable performance than those prepared by traditional spin coating. Further obstacles in the processing of flexible substrates in view of the brittle ITO-layer and thermal stability are discussed.

SYOP 4.74 Thu 16:30 P1A

Fully Coupled Opto-electronic Modelling of Organic Solar Cells — •Nils A. Reinke[1], Roger Häusermann[1], Evelyne Huber[1], Michael Moos[1], Thomas Flatz[2], and Beat Ruhstaller[1,2] — [1]ZHAW, Institute of Comp. Physics — [2]Fluxim AG (Switzerland)

Record solar power conversion efficiencies of up to 5.5 % for single junction organic solar cells (OSC) are encouraging but still inferior to values of inorganic solar cells. For further progress, a detailed analysis of the mechanisms that limit the external quantum efficiency is crucial. It is widely believed that the device physics of OSCs can be reduced to the processes, which take place at the donor/acceptor-interface. Neglecting transport, trapping and ejection of charge carriers at the electrodes raises the question of the universality of such a simplification.

In this study we present a fully coupled opto-electronic simulator, which calculates the spatial and spectral photon flux density inside the OSC, the formation of the charge transfer state and its dissociation into free charge carriers. Our simulator solves the drift- diffusion equations for the generated charge carriers as well as their ejection at the electrodes. Our results are in good agreement with both steady-state and transient OSC characteristics. We address the influence of physical quantities such as the optical properties, film-thicknesses, the recombination rate and charge carrier mobilities on performance figures. For instance the short circuit current can be enhanced by 15% to 25% when using a silver instead of an aluminium cathode. Our simulations lead to rules of thumb, which help to optimise a given OSC structure.

SYOP 4.75 Thu 16:30 P1A

Bulk-Heterojunction Solar Cells Based on Nanocrystal-Polymer Hybrid Materials — •Yunfei Zhou[1,2], Gerald Urban[2], and Michael Krueger[1,2] — [1]Freiburg Materials Research Centre (FMF), University of Freiburg, Germany — [2]Department of Microsystems Engineering (IMTEK), University of Freiburg, Germany

Organic solar cells have the promising advantages of low-cost and large-area fabrication on flexible substrates. State-of-the-art organic solar cells based on blends of conjugated polymers and fullerene derivatives achieve efficiencies up to 5-6%.

Inorganic semiconductor nanocrystals (NCs) e.g. out of CdSe, with tunable bandgaps and high intrinsic carrier mobilities, can be incorporated into conjugated polymers e.g. poly(3-hexylthiophene) (P3HT) to form bulk-heterojunction hybrid solar cells. In our group, a highly reproducible synthesis method for CdSe NCs has been developed, leading to monodisperse NCs with excellent photophysical properties. Current research is performed to control the shape and the lattice structure of the NCs within the same synthesis approach. Various solar cells based on bulk-heterojunction nanocomposite materials have been fabricated and characterized. We systematically checked how the solar cell device performance is affected by different NC ligands and by different thermal annealing treatments. Devices using spherical NCs capped with aromatic ligands and appropriate thermal annealing treatment exhibit so far power conversion efficiencies over 0.5% under standard measurement condition. Further investigations to improve the materials and device performance are currently in progress.

SYOP 4.76 Thu 16:30 P1A

Bulk-Heterojunction Organic Solar Cells Based on Merocyanine Colorants — •Nils M. Kronenberg[1], Hannah Bürckstümmer[2], Elena V. Tulyakova[2], Manuela Deppisch[2], Frank Würthner[2], Hans W. A. Lademann[1], and Klaus Meerholz[1] — [1]Department für Chemie, Universität zu Kön, Germany — [2]Institut für Organische Chemie, Universität Würzburg, Germany

To take advantage of the full potential of organic Bulk Heterojunction (BHJ) solar cells, there is a need to explore new materials. We introduced merocyanines dyes (MCs) as a new class of electron donor materials for the application in solution-processed BHJ solar cells. MCs are traditional low-molecular colorants that are widely applied in textile coloration, for printing purposes, and nonlinear optics.

Due to their structure, consisting of an electron-donating and an electron-accepting subunit, they possess high absorption coefficients which is favorable for the use in solar cells. The vast variety of the MC synthesis allows for a variation of the absorption properties in a wide range and a tuning of the solar cell absorption to the emission spectrum of the sun. Another advantage of MCs compared to some long-wavelength absorbing polymers is the relatively low HOMO-energy (down to -6.0 eV), which is beneficial for large open-circuit voltages.

We tested various different MC-dyes in the application as donor compound in BHJ solar cells in combination with the soluble C60 derivative PCBM. Power conversion efficiencies up to 2.1% under standard illumination and 2.7% at reduced intensities were achieved.

SYOP 4.77 Thu 16:30 P1A

Morphology Control of Bulk-Heterojunction Solar Cells — •Hans W. A. Lademann, Yanyan Yuan, Adam J. Moulé, and Klaus Meerholz — Department Chemie, Universität zu Köln, Germany

The most studied solar cells are based on P3HT and PCBM. Several studies concentrate on influencing and optimizing the polymer:fullerene blend morphology as well as the determination of hole mobilities and conductivities in films made with different P3HT molecular weights via OFET measurements, but the exact impact of polymer aggregation on the resulting energy levels in the thin-film blend and the performance of solar cells is still not fully understood.

In this work, we investigated the influence of the degree of polymer aggregation on the energy levels in blends of P3HT and PCBM and the resulting solar cell performance. To achieve different degrees of P3HT aggregation in the thin films (i.e. different ratios of amorphous to aggregated P3HT) several preparation methods were investigated: 1) Two primary solvents with different boiling points, namely chlorobenzene and chloroform, were used for spin coating. 2) The role of an additional secondary solvent was investigated. 3) We studied the impact of the P3HT content in the polymer:fullerene blend and 4) changed the molecular weight of P3HT. As-cast as well as annealed films were investigated. AFM and UV/VIS spectroscopy were used to analyze the polymer aggregation. Kelvin Probe measurements were carried out to investigate the energy level in the thin films. Finally we compared the results obtained by these methods to the current-voltage characteristics of the solar cells, especially the Voc.

SYOP 4.78 Thu 16:30 P1A

Novel ultra-high 3D resolution surface structuring and thin film stress investigation — •Ferdinand Messow, Daniel Todorov, Thomas Kusserow, Stefan Wittzack, Florestan Köhler, Martin Bartels, and Hartmut Hillmer — University of Kassel, Institute of Nanostructure Technologies and Analytics, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

To improve the efficiency of photovoltaic systems, functional surfaces are attractive to guide light into photo sensitive regions - capable of mass production with easy and cheap structuring. Today, NanoImprint uses 2D templates in most cases. Our novel NanoImprint templates reveal residual surface roughness and accuracies down to 0.2 nm. High-resolution 3D imprinted structures are presented.

Further efficiency increase can be achieved by anti-reflection coatings. Unfortunately most thin films provide stress and, therefore, define self-organized structures on viscoelastic organic materials due to stress release. Local stress of thin zirconium dioxide and silicon dioxide films deposited by ion beam sputter deposition was scrutinized, since these materials show no absorption in the UV-range, enlarging the range of usable light.

SYOP 4.79 Thu 16:30 P1A

STM study of organic p- and n-type Semiconductors on metal surfaces. — •Elena Mena-Osteritz and Alexey Kopyshev — Institut für Organische Chemie II und Neue Materialien

Formation of three dimensional nanostructures based on organic p- and n-type semiconductors will be presented. The electronic properties of different complexe systems have been analysed with the help of the scanning tunneling microscopy and spectroscopy.

SYOP 5: Organic Photovoltaics III

Time: Friday 10:30–13:15 Location: ZEU 222

SYOP 5.1 Fri 10:30 ZEU 222

Characterization of electroactive polymers and block copolymers with potential application in organic solar cells — •Sabine Ludwigs — Freiburg Institute for Advanced Studies & Freiburg Materials Research Center, Stefan-Meier-Str. 21, 79104 Freiburg

Organic solar cells represent a new type of solar cells based on composites of an electron-donor (p-type) and an electron-acceptor (n-type) material. The low consumption of material and the application of efficient production techniques offer great potential for cost-efficient production of these solar cells.

In my talk I will show results on the electrochemical characterization of redox polymers bearing triarylamine as pendant electroactive units and on conjugated polymers, e.g. poly(para phenylene vinylenes). We use electrochemically-gated transistors to study the electronic properties of these p-type polymers, in particular the potential of doping and the intrinsic conductivity.

Block copolymers consisting of the above-mentioned polymers and neutral, sacrificial polylactides were further polymerized and characterized. Block copolymers are particularly interesting because they typically self assemble into ordered microdomain morphologies with length scales of about 5-50 nm. Upon degradation of the sacrificial block after structure formation polymer films with nanopores can be obtained. Ultimately these nanoporous polymer films shall be employed as templates for the deposition of semiconducting inorganic materials.

SYOP 5.2 Fri 10:45 ZEU 222

Bipolar substituted spiro-bifluorenes for organic solar cells? — •Cornelia M. Brendel[1], Fernando Dias[2], Andy P. Monkman[2], and Josef Salbeck[1] — [1]Macromolecular Chemistry and Molecular Materials, University of Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany — [2]Durham Photonic Materials Institute, Department of Physics, Durham University, South Road, Durham DH1 3LN, U.K.

Substituted spiro-bifluorenes are frequently being employed in optoelectronical devices due to their tendency to build amorphous layers. Donor-acceptor compounds with a spiro-bifluorene unit as bridge have already been employed in phototransistors and have potential for application in organic solar cells.

To test their suitability for organic solar cells and clarify the role bipolar substituted spiro-bifluorenes play in phototransistors we investigated these compounds more closely by spectroscopic methods. Bipolar substituted spiro-bifluorenes show strong solvatochromism of about 100 nm when cyclohexane is exchanged by more polar solvents, e. g. methyl-THF or acetone, indicating charge-transfer emission. Charge separation by photoexcitation happens within some hundred picoseconds and has a lifetime of up to 50 ns.

We will discuss the interplay of the locally excited and the charge-transfer state on the basis of temperature dependent measurements of fluorescence and absorption as well as measurements of the fluorescence lifetime. We will also go into detail about the origin of triplett emission and its connection with the charge transfer state.

SYOP 5.3 Fri 11:00 ZEU 222

Tuning the ionization energy of organic-semiconductor films: The role of intramolecular polar bonds — •Ingo Salzmann[1], Steffen Duhm[1], Georg Heimel[1], Martin Oehzelt[2], Rolf Kniprath[1], Robert L. Johnson[3], Jürgen P. Rabe[1], and Norbert Koch[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Institut für Experimentalphysik, Johannes Kepler Universität, Linz, Austria — [3]Institut für Experimentalphysik, Universität Hamburg, Hamburg, Germany

For the prototypical conjugated organic molecules pentacene and perfluoropentacene, we demonstrate that the surface termination of ordered organic thin films with intramolecular polar bonds (e.g., -H versus -F) can be used to tune the ionization energy. The collective electrostatics of these oriented bonds also explains the pronounced orientation dependence of the ionization energy. Furthermore, mixing of differently terminated molecules on a molecular length scale allows continuously tuning the ionization energy of thin organic films between the limiting values of the two pure materials. Our study shows that surface engineering of organic semiconductors via adjusting the polarity of intramolecular bonds represents a generally viable alternative to the surface modification of substrates to control the energetics at organic/(in)organic interfaces.

SYOP 5.4 Fri 11:15 ZEU 222

Textile electrodes as substrates in the electrochemical growth of porous ZnO for application in dye-sensitized solar cells — •Thomas Loewenstein[1], Markus Mingebach[1], Melanie Rudolph[1], Kerstin Strauch[1], Yvonne Zimmermann[2], Andreas Neudeck[2], and Derck Schlettwein[1] — [1]Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, D-35392, Gießen. — [2]Textilforschungsinstitut Thüringen-Vogtland e.V., D-07973, Greiz.

The use of textile substrates for solar active electrodes is of interest in view of future applications of textile based electronics. Active structures prepared below 150 °C are needed. An approach using dye sensitized solar cells is useful for the achievable electrode distances in the micrometer range. Deposition of semiconductor films from solutions appears as an optimum technique. We will discuss the results of cathodic electrodeposition of porous ZnO films from aqueous zinc salt solutions with a structure directing agent (SDA) on metal- coated polyamide fibers leading to well- oriented single crystalline particles of ZnO with a high internal surface area. Individual fibers showed characteristics of microelectrodes and hence increased deposition rates were obtained relative to traditional planar electrodes. The modification of the diffusion layer by hydrodynamic flow or pulsed deposition had a strong effect on the morphology of the grown ZnO. Following the dissolution of the SDA in aqueous KOH, a porous ZnO structure was obtained. Sensitization studies will be presented to show the feasibility of the chosen approach. Lit.: T. Loewenstein et.al. *Phys.Chem.Chem.Phys.*, 10, 1844 (2008)

SYOP 5.5 Fri 11:30 ZEU 222

Doping of organic absorbers for application in solar cells — •Corinna Hein, Eric Mankel, Thomas Mayer, and Wolfram Jaegermann — Technische Universität Darmstadt, Materials Science Institute, Surface Science Division, 64287 Darmstadt, Germany

The band alignment of the absorbing layers of an organic bilayer heterojunction solar cell was determined by synchrotron induced photoemission (SXPS). As donor type material copper phthalocyanine (CuPc) was used, the acceptor layer consists of BPE-PTCDI (a perylene derivate). At the CuPc/BPE-PTCDI interface a band bending is induced that retains the generated charge carriers leading to recombination and a low photo current of 2.4 mA/cm2. P-doping is suggested to reverse the electric field. As dopant WO3 was used, known to be a strong electron acceptor. Doping was successfully performed by coevaporation of the CuPc matrix and the dopant showing high doping efficiency and limit. The Fermi level shifts gradually with the concentration of dopant up to 690 meV. The doping mechanism was additionally investigated by layer by layer photoemission studies. Assuming phase separation the doping limit can be explained by an interface dipole. Using the doped CuPc the field at the bilayer heterojunction was reversed to the beneficial direction.

SYOP 5.6 Fri 11:45 ZEU 222

LEEM and X-PEEM investigations of diindenoperylene on Au(100) — •Maria Benedetta Casu[1], Britt-Elfriede Schuster[1], Tevfik Onur Menteş[2], Miguel Angel Nino[2], Andrea Locatelli[2], and Thomas Chassè[1] — [1]ITPC, University of Tuebingen, Auf der Morgenstelle 8, 72076 Tübingen, Germany — [2]Sincrotrone Trieste S.C.p.A., 34012 Basovizza, Trieste, Italy

Diindenoperylene (DIP) thin films can give rise to different film phases depending essentially on the substrate, including its local morphology, and preparation conditions. By using a combination of microscopic imaging and diffraction techniques with structural and chemical sensitivity, we studied the growth of DIP on Au(100), willing to compare the results with what previously obtained on polycrystalline gold. DIP thin films were grown on Au(100) by organic molecular beam deposition at room temperature (RT) and at very low evaporation rate (˜ 0.1 Å/min). The growth and structure of DIP films of different thickness was monitored in situ and in real time by LEEM. Our investigations showed the occurrence of a Stranski-Krastanov growth mode, also establishing the influence of the local substrate morphology. Micro-LEED evidenced the different structure of the wetting layer and the islands, confirming a different molecular arrangement depending on the film thickness. Domains of different molecular orientation were identified by dark-field LEEM, following their evolution during growth. In parallel, XPEEM and micro-XPS provided information about the bond between the molecule and the substrate as well as the chemical environment.

SYOP 5.7 Fri 12:00 ZEU 222

Growth of metal thin films on conductive polymer surfaces — •Gunar Kaune[1], Matthias A. Ruderer[1], Ezzeldin Metwalli[1], Robert Meier[1], Weinan Wang[1], Sebastien Couet[2], Kai Schlage[2], Stephan V. Roth[2] und 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

Type and structure of the metal electrode deposited on top of the active layer of an organic photovoltaic cell have a strong influence on the performance of the device. Therefore it is necessary to understand the structural growth and the interaction with the photoactive polymer layer. We investigate the formation of a metal/polymer interface by deposition of gold on a poly(N-vinylcarbazole) surface [1]. The growth of the gold film is investigated in-situ with grazing incidence small angle x-ray scattering (GISAXS). In-situ GISAXS allows us to follow the spatial growth of the gold clusters from the initial stage to the formation of a continuous layer and to determine the temporal evolution of the cluster morphology. From these observations a growth model is derived, explaining the cluster growth in four steps, with a characteristic process being attributed to each step. Metal incorporation inside the semi-conducting polymer film is revealed with x-ray reflectivity measurements [1]. Finally, the results are compared with the growth of an aluminium layer on a poly(3-hexylthiophene) surface.

[1] G. Kaune et al., ACS Applied Materials and Interfaces, at press

SYOP 5.8 Fri 12:15 ZEU 222

Growth and morphology of photoactive small organic molecules on device-relevant substrates — •Jonathan Heidkamp[1], Ayse Turak[2], Felix Maye[1,2], and Helmut Dosch[1,2] — [1]Universität Stuttgart — [2]Max-Planck-Institut für Metallforschung Stuttgart

Indium-Tin-Oxide (ITO) is a commonly used electrode in organic solar cells. However, the performance of these devices depends crucially on the characteristics of the interface between the ITO and the photoactive organic layer.

To study the interface characteristics, we investigated the growth, morphology, structure and ordering of small organic molecules, diindenoperylene (DIP) and perylene tetracarboxylic di-imide (PTCDI), on SiO_2, ITO and modified ITO substrates by atomic force microscopy and x-ray measurements.

Both molecules formed well ordered multilayer structures on all investigated substrates. However, only DIP showed a substrate dependence in the growth behaviour and stability, indicating different interfacial interactions for the two molecules. These differences in growth and especially in stability for different substrates can have significant implications for the use of DIP and PTCDI in organic devices.

SYOP 5.9 Fri 12:30 ZEU 222

Excitons in Conjugated Polymers - Do we need a Paradigma Change — •Wichard J. D. Beenken — Technische Universität Ilmenau, Institut für Physik, FG Theoretische Physik I, Germany

We have previously shown that both, polymer conformation and dynamics are crucial for the exciton transport in conjugated polymers. Thereby we found that the usual Förster-type hopping transfer model – even if one applies the line-dipole approximation – fall short in two respects: (i) It is still unclear of what kind the site the excitons are transferred between is. We found that the simple model of spectroscopic units defined as segments of the polymer chains separated by structural defects breaking the π-conjugation is only justified for chemical defects like hydrogenated double bonds, or extreme gauche (90°) torsions between the monomers. Both defects are far too rare in a well prepared conjugated polymer to explain the mean spectroscopic unit length of typically 6-7 monomers. In the meanwhile, also the concept of dynamical formation of the spectroscopic units, we had previously suggested, has turned out to fail. (ii) For the ultra-fast anisotropy decay observed in films of polythiophenes, the Förster-rates are far too low. Therefore, the mechanisms resulting in initial turns of the transition-dipoles have to be different from the excitation energy transfer valid on longer time-scales. In the present talk several possible ways out of these problems will be pinpointed. It will turn out that these considerations may lead to simplified concepts for the design of polymer-based organic solar cell, with possibly higher efficiencies and longer life-times than the common polymer-fullerene blends.

SYOP 5.10 Fri 12:45 ZEU 222

The nature of charge transfer excitons in conjugated polymer-fullerene blends — •Ilka Kriegel, Enrico Da Como, Markus Hallermann, Stephan Haneder, and Jochen Feldmann — Photonics and Optoelectronics Group, Department of Physics and CeNS Ludwig-Maximilians-Universität, 80799, Munich (Germany)

Blends of conjugated polymers and fullerene derivatives are one of the most promising systems for organic photovoltaics. We have focussed our attention on the nature of the electronic interactions taking place at the heterojunction between the polymer MDMO-PPV and the fullerene PCBM. The presence of charge transfer excitons in these materials has been recently considered and it appears to have important implications for the solar cell efficiency [1]. Here we demonstrate the presence of hybrid ground- and excited-states at the MDMO-PPV:PCBM heterojunction. Evidence for such states is provided by photoluminescence (PL) spectroscopy, where a red-shifted emission is detected in the blend film, in addition to the MDMO-PPV excitonic emission. A comparison with the spectra of the pristine polymer or PCBM indicates that the new emission originates exclusively from a charge transfer exciton forming between the two materials in the blend. In contrast to exciplexes reported in polymer/polymer blends, the emission at 1.4 eV can be directly excited below the gap of the two materials, demonstrating the presence of a ground state [1].

[1] M. Hallermann, S. Haneder, E. Da Como, Applied Physics Letters 93, 053307 (2008)

SYOP 5.11 Fri 13:00 ZEU 222

Electronic properties of pristine FePc and CoPc thin films: experiment and calculations — Olga Molodtsova[1], Martin Knupfer[1], Volodymyr Maslyuk[2], Yurii Ossipyan[3], Alexander Chaika[3], Thomas Bredow[4], Ingrid Mertig[2], and •Victor Aristov[1,3] — [1]IFW Dresden, D-01069 Dresden, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Fachbereich Physik, D-06099 Halle, Germany — [3]ISSP RAS, Chernogolovka, 142432, Russia — [4]Institute for Physical and Theoretical Chemistry, Bonn University, D-53115 Bonn, Germany

Magnetic transition metal (MTM) phthalocyanines are regarded as objects for the development of low dimensional molecular magnets because they are assumed as possible candidates for potential applications in high-density information storage and quantum computers that gives a strong motivation to characterize and study the electronic structure of MTM phthalocyanine thin films. Moreover this determines also the performance of devices. In this presentation we report the results of extensive investigations of the electronic structure: core-levels and valence band of the organic semiconductors CoPc and FePc in situ grown on Au(001) surface under UHV conditions. The studies were performed by means of direct and resonant photoemission, NEXAFS and DFT calculations. The experimentally obtained electronic states appeared to be in very good agreement with DFT calculations. This work was supported by the DFG under grant no. 436RUS17/52/06 and through the DFG Priority Program 1165., by the SMWK and by RFBR (grant no. 08-02-01170).