

CPP 32: Poster: Organic Semiconductors

Time: Wednesday 16:30–18:30

Location: Poster C

CPP 32.1 Wed 16:30 Poster C

Organic Magneto-optoelectronics: Magnetoresistive Organic Field-Effect Transistors — •THOMAS REICHERT, CAROLIN ISENBERG, TOBAT SARAGI, and JOSEF SALBECK — Macromolecular Chemistry and Molecular Materials (mmCmm), Department of Mathematics and Science and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Strasse 40, 34132, Kassel, Germany.

In organic semiconductors the spin-correlation between quasiparticles can be influenced by low magnetic fields, which leads to large (up to 20% at 10mT) magnetoresistance at room temperature. This organic magnetoresistance (OMAR) is not only highly interesting for addressing fundamental questions about spin-transport and spin-manipulation in organic materials, but also for the realization of lightweight, flexible, multifunctional magneto-optoelectronic applications. We were able to develop different types of magnetoresistive organic field-effect transistors (OFETs) and present an overview about the corresponding magnetic-field dependent effects (Photoinduced magnetoresistance; Magnetoresistance based on donor/acceptor blends; Photoinduced sign change of magnetoresistance) as well as the underlying fundamental physical processes. These results do not only pave the way for the application of organic semiconductors in future multifunctional magneto-optoelectronic devices but also help to identify the details of spin-dependent processes in organic semiconductors.

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Self-aggregation of fullerene derivatives in water: a molecular dynamics simulation study — •SRINIVASA RAO VARANASI¹, OLGA GUSKOVA¹, ANDREAS JONN¹, PETER FRIEDEL¹, and JENS-UWE SOMMER^{1,2} — ¹Leibniz Institute of Polymer Research, Dresden, Germany — ²TU Dresden, Dresden, Germany

Some of the amphiphilic derivatives of fullerene are known to self-assemble in solution at the nanoscale into various shapes (spherical, rod-like and vesicle depending on the length of the side chain, functionality of the substituent, concentration and temperature). This self-aggregation behaviour seems to determine their photophysical as well as photochemical activities. The understanding of self-aggregation behaviour in water is not only useful in photovoltaic applications but also in biomedical applications (for example, effects on lipid membranes). We present here a molecular dynamics simulation study on amphiphilic fullerene derivatives in water. We used PCFF force field along with Girifalco's parameters for modeling fullerene derivatives and TIP3P model for water. In this study, we analyze various structural and dynamic properties related to fullerene derivatives as well as water.

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Charge generation and loss processes in polymer-polymer solar cells — •HANNAH MANGOLD¹, IAN A. HOWARD¹, MARCEL SCHUBERT², DIETER NEHER², and FRÉDÉRIC LAQUAI¹ — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²Institute of Physics, University of Potsdam, Germany

All-polymer solar cells, where both donor and acceptor component are π -conjugated polymers, have the advantage of a broad absorption over the entire visible wavelength range. In this contribution we use broadband visible and near-infrared transient absorption spectroscopy covering the picosecond to microsecond timescale to investigate the charge generation and loss processes in various blends of the well-known donor polymer P3HT with a naphthalenediimide (NDI)-based copolymer exhibiting maximum power conversion efficiencies up to 1.4%. We demonstrate that the anticorrelation between the NDI-aggregation and solar cell performance recently reported by us [1] is caused by a variation of the fraction of contact sites between the donor and acceptor polymer that can facilitate free charge generation and that this fraction is strongly influenced by the choice of solvents used for film preparation. [1] Schubert et al, Adv. Energy Mat. 2012, 2, 369.

CPP 32.4 Wed 16:30 Poster C

Linear X-ray dichroism of perylene diimide derivatives and its correlation with their transport properties — •NINA ZEILMANN¹, SUSANNE BACKES², BENEDIKT RÖSNER¹, ANDREAS SPÄTH¹, KATRIN LUDWIG¹, ANDREAS HIRSCH², and RAINER H. FINK¹

— ¹FAU Erlangen-Nürnberg, Physical Chemistry II and ICMM, Erlangen, Germany — ²FAU Erlangen-Nürnberg, Organic Chemistry II and ZMP, Erlangen, Germany

The development of organic semiconductors for organic electronic applications has undergone notable progress during the last years. While hole transporting p-type semiconductors have already shown performances comparable to their inorganic analogues, competitive electron transporting n-type materials still pose a challenge. Among these materials, perylene diimide derivatives are very promising and interesting candidates. Since the transport properties are often strongly correlated with the microstructure of the organic films, microscopic probes that provide high chemical specificity and sensitivity to molecular orientation at high spatial resolution are required. Scanning transmission X-ray microspectroscopy (STXM) ideally combines these requirements. Within this contribution we present a microspectroscopic analysis of thin films of various perylene diimide derivatives prepared on Si₃N₄ membranes. Polarization dependent light microscopy gives clear evidence on the growth of large domains with preferential molecular orientations. Using STXM, film and orientational homogeneities can directly be correlated with the electronic transport properties. The project is funded by the BMBF, contract 05K10WEA.

CPP 32.5 Wed 16:30 Poster C

Structural Aging and Degradation of Polymer Solar Cells — •CHRISTOPH SCHAFFER¹, JAN PERLICH², STEPHAN V. ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹Technische Universität München, Physik-Department - Lehrstuhl Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching — ²HASYLAB at DESY, Notkestr. 85, 22607 Hamburg

One of the major challenges in OPV is to elongate their lifetimes. Several mechanisms of organic solar cell degradation have been proposed in literature within the last years. Most of the mechanisms are related to chemical alteration of the applied materials, such as photo-bleaching and oxidation of the active organic layer and the metal contacts or the diffusion of oxygen or water into the organic layer. However, insufficient research has been done on determining transitions of the nanomorphology of the active layer of bulk heterojunction (BHJ) polymer solar cells as an effect of aging. These transitions are expected to strongly affect the properties of solar cells since the active layer morphology plays a crucial role in the energy conversion process. In our investigations, we study the influence of illumination on the morphology of the active layers of PCPDTBT:PC71BM solar cells. Therefore, advanced scattering techniques such as grazing incidence small angle x-ray Scattering (GISAXS) are performed both in-situ on operating PCPDTBT:PC71BM solar cells and ex-situ on pre-aged polymer-blend films. The findings are supplemented with UV/Vis and characteristic IV curve measurements.

CPP 32.6 Wed 16:30 Poster C

The influence of processing additives on the morphology of bulk heterojunction films — •WEIJIA WANG¹, MARTINE PHILIPP¹, DAVID MAGERL¹, JEAN-FRANCOIS MOULIN², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany — ²HZ Geesthacht at FRM II, Lichtenbergstr.1, 85748 Garching, Germany

In the last decades, photoactive polymers and its applications in organic photovoltaic have attracted tremendous attention. Compared with standard inorganic solar cells, there are plenty of advantages for these materials, such as light weight, easy processibility and low cost. Currently the main drawback is still the low efficiency. It is already observed that the morphology of the heterojunction film plays an important role in organic solar cells. In this work, in order to modify the morphology, different amount of additives are applied in blend system rrP3HT:C61-PCBM. The internal structure is investigated with grazing incidence small angle neutron scattering (GISANS) in time-of-flight (TOF) mode. Additionally, the surface morphology is probed with optical microscopy and atomic force microscopy. The effect on molecular level is investigated by absorption.

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Systematic investigation on ternary bulk heterojunction so-

lar cells based on PTB7:PC70BM — ●CHRISTIAN JENDRZEJEW-SKI, SHUAI GUO, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany

Organic solar cells hold great promise for future applications in photovoltaics as they have several advantages, like the potentially lower production costs, much lower weight and flexibility in comparison to inorganic solar cells. In the present investigation the new, high efficient chlorobenzene based PTB7:PC71BM bulk heterojunction system are prepared and investigated with the addition of different third components. These kind of ternary systems have shown a promising result, which combines the advantages of the host material as well as the third component, and therefore improves the final power conversion efficiency. The inner structure of the ternary blend films is probed via X-ray reflectivity (XRR) and grazing incidence small angle X-ray scattering (GISAXS). The surface morphology is investigated with atomic force microscopy (AFM) and scanning electron microscopy (SEM). Via integrating XRR, GISAXS, AFM and SEM data, the inner 3D structure of the ternary films is obtained. As a consequence, the correlation between the nano-morphology of the films and the efficiency of the polymer-based solar cells is addressable.

CPP 32.8 Wed 16:30 Poster C

Molecular orientation and growth mode of organic molecular beam deposited ultrathin HBC films on SiO₂ — ●PAUL BEYER^{1,2}, TOBIAS BREUER³, SALIOU NDIAYE³, GREGOR WITTE³, and STEFAN KOWARIK² — ¹Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — ²Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — ³Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany

Hexa-peri-hexabenzocoronene (HBC) is a polycyclic aromatic hydrocarbon that is investigated in supramolecular electronics due to its high electron mobility of up to $1\text{cm}^2/\text{Vs}$. We examine the real-time growth kinetics of organic molecular beam deposited ultrathin HBC films on silicon dioxide using x-ray diffraction and x-ray spectroscopy.

With grazing incidence x-ray diffraction (GIXD) we observe a larger crystallinity at higher substrate temperatures of 150°C but rough films. We observe smooth films as indicated by growth oscillations of specular x-ray reflectivity (XRR) during growth of HBC at lower temperatures of 25°C . The growth oscillations show changes in the molecular arrangement during the first monolayers. To test whether the molecular orientation changes we use near edge x-ray absorption fine structure (NEXAFS) spectroscopy at the BESSY II synchrotron. NEXAFS is used to determine the orientation of the π^* orbitals and therefore the orientation of the HBC molecules in (sub)mono- and multilayer films. We find that the molecules on average are tilted by an angle of 74° relative to the surface plane.

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Vibronic spectra of excitons in 2-D polyacene lattices — ●CHRISTOPH WARNS¹, THOMAS HARTMANN¹, IVAN LALOV^{2,1}, and PE-TER REINEKER¹ — ¹Institute for Theoretical Physics, Ulm University, 89069 Ulm, Germany — ²Faculty of Physics, Sofia University, Sofia 1164, Bulgaria

Vibronic spectra of excitons in various 2-dimensional lattices, which model the (ab)-plane of polyacene crystals, have been investigated. We have considered interacting FEs and molecular vibrations, taking into account linear and quadratic coupling. The linear optical susceptibility of the 2-D crystal was calculated using the Green's function method and the vibronic approach. Various 2-D crystal lattices were assumed: actual anthracene, tetracene and pentacene crystal lattices, a hypothetical graphene-like lattice, all with two molecules per unit cell, and a simple hexagonal lattice with only one molecule per unit cell. In the computation of the vibronic spectra we used the measured excitonic and vibrational parameters of polyacene crystals (based on data by Petelenz et al.).

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Aggregate Structures and Electron Transport Anisotropy in High Mobility n-type Low Bandgap Copolymer — ●ROBERT STEYRLLEUTHNER¹, RICCARDO DI PIETRO¹, SCOTT HIMMELBERGER², BRIAN COLLINS³, FRANK POLZER⁴, HOLM KIRMSE⁴, MARCEL SCHUBERT¹, ZHIHUA CHEN⁵, HARALD ADE³, ALBERTO SALLEO², ANTONIO FACCHETTI⁵, and DIETER NEHER¹ — ¹University of Potsdam, Institute of Physics — ²Stanford University, Materials Science and Engineering — ³North Carolina State University, Department of Physics, — ⁴Humboldt University Berlin, Institute of Physics — ⁵Polyera Cor-

poration, Illinois

We have recently explored the photophysics of the high electron mobility ($0.85\text{cm}^2/\text{Vs}$) conjugated copolymer P(NDI2OD-T2), also known as Polyera ActivInk N2200. From these studies we could estimate, that approx 45% of the polymer chains in thin films exist in an aggregated (π -stacked) conformation mainly independent of the preparation routine [1]. However, special solvents mixtures can induce changes of the orientation and the molecular structure of the chain aggregates which we prove by GIXD and TEM measurements. We further investigate the structure property relation by correlating the morphology with the electron transport anisotropy in P(NDI2OD-T2). [1] R. Steyrlleuthner et al., J. Am. Chem. Soc., 2012, 134 (44)

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Understanding changes in optical absorption of thin organic films during growth — INES TRENKMANN¹, CHRISTOPHER KEIL², DERCK SCHLETTWEIN², and ●HARALD GRAAF¹ — ¹nanoMA (Center for nanostructured Materials and Analytics), Chemnitz University of Technology, D-09107 Chemnitz, Germany — ²Institute of Applied Physics, Justus-Liebig-University Giessen, D-35392 Giessen, Germany

The optical absorption of organic thin films changes during growth. Here mainly the lowest energy transition shows a red shift with increasing film thickness. Different explanations are given in the literature: e.g. increasing island sizes leading to larger coupled systems [1] or a change in the ratio between the numbers of molecules in the bulk compared to surface molecules [2]. We investigated three perylene derivatives showing all the expected red shift of the lowest energy transition. They are characterized by different morphologies and growth modes: One shows a layer-by-layer growth and two (an amorphous and a crystalline) show island growth. The shift for the layer-by-layer perylene can be explained by a combination of the two above mentioned explanation. The shift for the first approximately 1.5 monolayers can be understood by a two-dimensional island growth with increase of coupled chromophoric systems. Further film growth lead to an increase of the ratio between the number of molecules in the bulk with respect to the surface molecules. For the other two molecules the experimental results on the red-shift can be explained by a new theoretical model.

[1] Chau et al. J.Phys.Chem 97 (1993) 2699, [2] e.g. Heinemeyer et al. Phys.Rev.Lett. 104 (2010) 257401

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Optoelectronic Processes in Squaraine Dye-Doped OLEDs for Emission in the Near-Infrared — ●B. STENDER¹, S. F. VÖLKER², C. LAMBERT², and J. PFLAUM^{1,3} — ¹Experimental Physics VI, University of Würzburg, D-97074 Würzburg — ²Institute of Organic Chemistry and Center for Nanosystems Chemistry, University of Würzburg, D-97074 Würzburg — ³ZAE Bayern, D-97074 Würzburg

Organic light-emitting diodes (OLEDs) for emission in the near-infrared (NIR) offer the great advantage of room temperature operation due to inherently high exciton binding energies (several 100 meV) in contrast to their inorganic counterparts. Despite several approaches have been presented with reasonable efficiency, purely organic NIR-emitters are barely investigated due to degradation of the organic compound. To cope with this challenge a novel organic host-guest system consisting of the polymer SY-PPV and the squaraine dye monomer M has been investigated. Optical excitation reveals a highly efficient energy transfer from the visible range to the NIR (750 nm) with a doping concentration of less than 2.0 wt.% and an associated Förster radius of 3.8 nm. As will be demonstrated, electrically driven NIR-emission yields an efficiency of 0.65% at a current density of $2.26\text{mA}/\text{cm}^2$ with a turn-on voltage of 2.0 V at a doping concentration of only 0.05 wt.%. Comparison between steady-state photo- and electroluminescence provides access to the opto-electronic processes on molecular length scales, thereby indicating that NIR-OLED emission in this system is controlled by charge carrier dynamics rather than by exciton transfer.

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Modeling Mesoscale Morphology of Polymeric Semiconductors using Soft Models — ●PATRICK GEMÜNDEN^{1,2}, CARL PÖLCKING¹, KURT KREMER¹, DENIS ANDRIENKO¹, and KOSTAS DAOULAS^{1,2} — ¹Max-Planck-Institut für Polymerforschung, Mainz, Germany — ²InnovationLab GmbH, Heidelberg, Germany

Polymeric semiconductors are characterized by hierarchical structuring where the mesoscopic morphology is affected by details of molecular architecture and interactions. Here we will discuss a strategy for de-

veloping models for the description of these materials by combining systematic coarse-graining with phenomenological descriptions. As a case study we will consider a model for P3HT systems where each bead corresponds to a single hexylthiophene unit. The bonded interactions are obtained from underlying atomistic configurations using the VOTCA package. The non-bonded interactions are captured by combining soft isotropic and orientation-dependent potentials. The former controls the equation of state of the material in the amorphous state while the latter leads to liquid-crystalline mesophases with a stack-like structuring.

Using the above model, Monte Carlo simulations of systems with device-relevant dimensions (~ 50 nm) were performed. We will discuss the effect of the molecular weight on the morphology. The conformations of the polymer chains for stack-like structuring will be analyzed and related to charge transport properties.

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Morphological aspects of the exciton transport in thin films of Diindenoperylene — ●ALEXANDER STEEGER¹, ANNA KATHARINA TOPCZAK¹, and JENS PFLAUM^{1,2} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²ZAE Bayern, 97074 Würzburg

The exciton diffusion length (EDL) is a key criterion for an optimized design of organic thin film devices. As a tight correlation between morphology and charge carrier as well as exciton transport properties has been evidenced in previous studies, the extension of crystalline domains has been proposed beneficial for long range exciton transport [1]. To address this point we have varied the morphology of Diindenoperylene (DIP) thin films by means of the substrate temperature (T_S). X-ray diffraction analysis revealed an almost amorphous phase of DIP grown at $T_S = 100$ K, whereas $T_S = 300$ K and 400 K yield to long range ordered polycrystalline films of higher crystallinity with increasing T_S . Photoluminescence-quenching measurements together with an advanced modeling were performed to correlate the EDL to the DIP morphology. Long range ordered DIP layers grown at $T_S = 300$ K and

400 K show a high EDL (59 nm and 115 nm, respectively), whereas the EDL of DIP deposited at $T_S = 100$ K is significantly smaller. This result emphasizes the importance of long range structural order to achieve superior transport properties of photo-generated electron-hole pairs. Financial support by the DFG focus program SPP 1355 is gratefully acknowledged. [1] R. R. Lunt et al., *Adv. Mater* 22 (2010) 1233-1236

CPP 32.15 Wed 16:30 Poster C

Determination of molecular transition dipole orientation of organic emitters by angular-dependent photoluminescence measurements — ●CHRISTIAN MAYR, TOBIAS SCHMIDT, BERT SCHOLZ, LARS JÄGER, and WOLFGANG BRÜTTING — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Organic light-emitting diodes (OLEDs) have been investigated for more than 20 years and are standing now at the frontier to mass production. Current research focuses on the enhancement of light outcoupling efficiency which is reduced especially due to the energy dissipation to surface plasmons (SPs). Numerical simulations show that a horizontal emitter orientation with respect to the substrate can enhance the efficiency by up to 50% due to reduced coupling to SPs. An expeditious method to determine the orientation of the transition dipole moment of molecules has been developed using angular dependent photoluminescence spectroscopy. By comparing measurement with simulations, the orientation can be quantitatively determined. Although other methods to measure molecular orientation exist, the presented method not only makes it possible to study molecular orientation in neat thin films but also of small amounts of emitters doped into a matrix material without knowing any detailed information of the optical properties of the dopant. Hence, this method is particularly useful for the investigation of newly developed materials. The method is applied to Iridium-based phosphorescent emitters in order to gain a consistent efficiency analysis of OLEDs and possibilities to enhance light outcoupling.