

HL 31 Organic semiconductors

Time: Wednesday 14:30–19:00

Room: POT 51

HL 31.1 Wed 14:30 POT 51

Current Limiting Mechanisms in MDMO-PPV Diodes — ●CARSTEN DEIBEL¹, VLADIMIR DYAKONOV¹, BRITTA BOHNENBUCK², ELIZABETH VON HAUFF², and JÜRGEN PARIS² — ¹Experimental Physics VI, Physical Institute, University of Würzburg, 97074 Würzburg, Germany — ²Energy and Semiconductor Research Laboratory, Department of Physics, University of Oldenburg, 26111 Oldenburg, Germany

We examined the current-voltage characteristics of poly[2-methoxy,5-(3,7-dimethyloxy)]-1,4-phenylenevinylene (MDMO-PPV) diodes in the framework of space charge limited currents (SCLC). The thickness of the MDMO-PPV layer was varied between samples, and the effect of using metal cathodes with different work functions was investigated. Since the basic SCLC model could not explain the experimental data, modifications to it were individually investigated: (1) a double Gaussian density of states to account for deep traps, (2) injection of electrons from the back contact resulting in a recombination current, and (3) the influence of the built-in potential resulting from the asymmetric work functions of the electrodes. The simple SCLC model in combination with the built-in potential and a parallel resistance was able to explain both the thickness and cathode dependence of the current-voltage characteristics.

HL 31.2 Wed 14:45 POT 51

Investigation of Frenkel and charge transfer (CT) states in PTCDA and MePTCDI crystals — ●L. GISSLÉN, M. SCHREIBER, and R. SCHOLZ — Institut für Physik, Technische Universität Chemnitz

In perylene derivatives like *N,N'*-dimethyl-perylene-3,4,9,10-dicarboximide (DiMePTCDI) and 3,4,9,10-perylene tetracarboxylic dianhydride (PTCDA), neutral molecular excitations and intermolecular charge transfer occur in the same energetic range. Their mixing via electron and hole transfer has a strong impact on the photophysical properties, including *e.g.* the absorption lineshape, the minima of the excited state potential landscape resulting in various kinds of photoluminescence (PL) [1], and the decay routes between absorption and PL.

The optical transition energies and the transfer matrix elements are determined with Hartree-Fock-based methods and with time-dependent DFT applied to molecular dimers in a geometry compatible with the crystalline phase [2]. In mixed Frenkel-CT models for the photophysical properties, the degree of mixing between Frenkel and CT states can be related to their different energetic ordering in PTCDA and DiMePTCDI. The present approach is compared to a pure Frenkel exciton model [3] and a one-dimensional model for Frenkel-CT mixing [4].

[1] A. Yu. Kobitski, R. Scholz, H.P. Wagner, and D. R. T. Zahn, *Phys. Rev. B* **68**, 155201 (2003).

[2] R. Scholz, A. Yu. Kobitski, D. R. T. Zahn, and M. Schreiber, *Phys. Rev. B* (2005) *accepted*.

[3] I. Vragović and R. Scholz, *Phys. Rev. B* **68**, 155202 (2003).

[4] M. Hoffmann and Z. G. Soos, *Phys. Rev. B* **66**, 024305 (2002).

HL 31.3 Wed 15:00 POT 51

Structural and electronic characterization of Diindenoperylene single crystals — ●ASHUTOSH KUMAR TRIPATHI and JENS PFLAUM — 3. Physikalisches Institut, University of Stuttgart, Germany

For the first time, we report on the structural and electronic characterization of DIP crystals grown by sublimation technique. X-ray diffraction measurements on uncapped as well as on Ag capped DIP crystals prove the existence of two different volume phases below and above 400 K, the high-T phase corresponding to the DIP thin film structure observed on *e.g.* oxide surfaces [1]. By temperature dependent studies the effect of the phase transition on the electronic transport properties indicates the strong correlation between the structural order and the charge carrier mobilities. Remarkably, both electron and hole transients were recorded along *c'*-direction and over the studied temperature range the electron mobility was found to be higher than that for holes by an order of magnitude. As most of the organic materials are very sensitive for oxidation in combination with trap formation, observation of electron mobility indicates this material to be a potential candidate for organic electronics. Further experiments leading to FETs based on DIP single crystals are in progress.

[1] A. C. Duerr et al., *Phys. Rev. B* **68**, 115428 (2003)

HL 31.4 Wed 15:15 POT 51

Two dimensional dispersion of electron-hole excitations in pentacene — ●ROMAN SCHUSTER and MARTIN KNUPFER — Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, D-01069 Dresden, Germany

We have investigated the dispersion of the lowest electron-hole excitation in pentacene within the a-b crystal plane using inelastic electron scattering. Surprisingly, the results indicate a significant dispersion anisotropy. The results will be discussed in consideration of different inter-molecular interactions that can cause the observed dispersions.

HL 31.5 Wed 15:30 POT 51

Novel fullerene-derivatives for plastic solar cells — ●TOBIAS ERB¹, ULADZIMIR ZHOKHAVETS¹, HARALD HOPPE¹, PAUL DENNER¹, GERHARD GOBSCH¹, STEFFI SENSFUSS², LARS BLANKENBURG², and ELISABETH KLEMM³ — ¹Institute of Physics, Ilmenau Technical University, 98693 Ilmenau, Germany — ²TITK Institut Rudolstadt, Physical Material Research and Functional Polymer Systems, 07407 Rudolstadt, Germany — ³Institut für Organische Chemie und Makromolekulare Chemie, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany

We have investigated several fullerene-derivatives in pristine films or in bulk heterojunctions with polymers. Their structural properties were studied by X-ray diffraction in grazing incidence geometry. The lattice symmetry and the size of the fullerene and polymer nanodomains were determined. Furthermore, the optical properties were studied with spectral ellipsometry. The influence of various annealing steps on the film properties were investigated, too. The X-ray findings show particularly, under which conditions fullerene-derivatives crystallize. Solar cells have been optimised using the results from X-ray and were characterized under AM 1.5 standard solar irradiation simulation.

HL 31.6 Wed 15:45 POT 51

Time resolved luminescence quenching experiments with dicyanovinylene-terthiophene — ●ANDRÉ HOLZHEY, KARL LEO, and MICHAEL HOFFMANN — Institut für Angewandte Photophysik, TU Dresden

Dicyanovinylene-terthiophene (DCV3T) as a new promising material for solar cell applications [1] shows intensive luminescence and exciton diffusion but also photo-degradation. CW and time-resolved photoluminescence and luminescence quenching of DCV3T shows exciton diffusion properties of DCV3T and permits a detailed view on the exciton diffusion mechanism. Using a spectrofluorometer and a streak camera setup, the surface luminescence quenching in double layers is investigated for various layer thicknesses and temperatures. By investigation of various degradation processes, the influence of degradation on the experiment could be minimized. The results indicate that luminescence quenching affects at least two different exciton levels in DCV3T.

[1] C. Uhrich, R. Schüppel, A. Petrich, K. Leo and M. Pfeiffer, E. Brier, P. Kilickiran, P. Bäuerle, to be submitted.

HL 31.7 Wed 16:00 POT 51

The Transport Gap of Organic Semiconductors Studied Using the Combination of Direct and Inverse Photoemission — ●GIANINA N. GAVRILA, MIHAELA GORGOI, and DIETRICH R.T. ZAHN — Chemnitz University of Technology, Semiconductor Physics, D-09107, Chemnitz, Germany

Direct valence band photoemission spectroscopy in combination with inverse photoemission spectroscopy is applied to study the densities of occupied and unoccupied electronic states of organic semiconductor materials *e.g.* perylene derivatives and phthalocyanines. The energy separation derived from the difference between Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) in an organic solid is called HOMO-LUMO gap or transport gap. The charge injection processes require promotion of an electron or a hole from the electrodes into one of the charge transport (HOMO or LUMO) states of the organic film therefore their determination is vitally important. It is proposed that the transport gap of organic materials can be obtained from the edge-to-edge distance between the HOMO and LUMO features. The resulting values of the transport gaps are in good agreement with results of electrical measurements and another method of deriving the transport gap employing measurements of the interface dipole at inor-

ganic/organic interfaces.

HL 31.8 Wed 16:15 POT 51

Anodized gate dielectrics: Preparation, characterization and organic-based transistor application — ●J. PFLAUM¹, S. GOETTLING², J. BRILL², N. FRUEHAUF², and E. MARGALLO-BALBÁS³ — ¹3rd Inst. of Physics, Stuttgart University, 70550 Stuttgart — ²Chair of Display Technol., Stuttgart University, 70550 Stuttgart — ³Electr. Instr. Lab., TU-Delft, 2628 CD Delft, The Netherlands

The application of organic-based thin film transistor (TFTs) requires the controlled preparation of thin high-k gate dielectrics in combination with low-cost, large-area processes. As a possible approach, we investigated the growth and morphology of the anodized gate dielectrics Al₂O₃ and Ta₂O₅. The anodization was carried out for glass and plastic substrates using various electrolytes. For the analysis of thickness, interface roughness and chemical composition, small-angle X-ray diffraction was exploited and modelled by the Parratt-formalism. The resulting data indicate the formation of oxide layers with defined stoichiometry and sharp interfaces. An influence of the respective electrolyte on the structural properties and on the breakthrough field strength could be clearly deduced. The obtained breakthrough fields up to 5MV/cm indicate the suitability of anodized gate-dielectrics in organic-electronic devices. First application of anodized dielectrics in pentacene TFTs on glass and plastic substrates will be demonstrated. As a key result, pentacene TFTs on Al₂O₃ on glass and on plastic substrates provide reliable transistor characteristics with hole mobilities of 0.1cm²/Vs and on/off-ratios of 10⁷-10⁸. Financial support by DFG (Project Pf 385/2), EU (FlexiDis) and Landesstiftung Baden-Württemberg is acknowledged.

— 15 min. break —

HL 31.9 Wed 16:45 POT 51

Efficient photosensitization of C₆₀ microcrystals with II-VI and III-V semiconductor nanocrystals — ●A. BIEBERSDORF¹, R. DIETMÜLLER¹, A. S. SUSH¹, A. L. ROGACH¹, S. K. POZNYAK², D. V. TALAPIN³, H. WELLER³, T. A. KLAR¹, and J. FELDMANN¹ — ¹Photonics and Optoelectronics Group, Physics Department and CeNS, Ludwig-Maximilians-Universität, München — ²Physico-Chemical Research Institute, Belarusian State University, 220050 Minsk, Belarus — ³Institute of Physical Chemistry, University of Hamburg

Photoconductors are essential and common components of optoelectronic devices such as photodetectors or photocopying machines. The sensitivity and spectral range of photoconductors can be drastically improved by sensitizers, which absorb light and provide additional charge carriers to the photoconducting material.

In the present report we demonstrate that semiconductor nanocrystals (NCs) such as CdSe, CdTe and InP can efficiently photosensitize needle-like C₆₀ microcrystals. A significant increase in photocurrent (by 3 orders of magnitude) is observed for C₆₀ microcrystals covered with NCs, in comparison with C₆₀ microcrystals without NCs. The photocurrent spectrum of C₆₀ / NCs composites is close to the NC absorption spectrum and can be tuned precisely by the NC size. Maximum external quantum efficiency was estimated by calculating the number of photoelectrons per incident photon and is about 10% for the CdSe / C₆₀ composites and about 3% for InP / C₆₀ composites.

We explain the increased photoconductivity in the following way: The photoexcited electrons in the NCs are transferred to the C₆₀ microcrystals causing photoconductivity, while the holes remain trapped in the NCs.

HL 31.10 Wed 17:00 POT 51

Charge modulation spectroscopy and electrical transport in single crystalline OFETs — ●MATTHIAS FISCHER¹, BRUNO GOMPF¹, ASHUTOSH TRIPATHI², JENS PFLAUM², and MARTIN DRESSEL¹ — ¹Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart. — ²Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart.

Transport in organic thin films is limited by grain boundaries, traps and imperfections of the film morphology. To get access to the intrinsic properties of organic semiconductors, for example the maximum possible mobility, investigations on single crystals are essential. We have fabricated organic field effect transistors (OFETs) on sublimation grown high quality single crystals of rubrene, tetracene and anthracene. As gate insulator we use PPX. To avoid photoreaction at the surface all inves-

tigations were carried out under yellow light. In the case of rubrene these crystals show hole mobilities well above 1 cm²/Vs in surface space charge limited current and in FET measurements, respectively. Charge-modulation spectroscopy in the far- and mid infrared of the accumulation layer in the conductive channel gives additional information of the high frequency conduction and the physics of the charge transport in these presumably small bandwidth materials. *Supported by the DFG through Go 642/6-1,2 and PF385/2.*

HL 31.11 Wed 17:15 POT 51

Comparison of two-dimensional device simulations with potentiometry measurements on pentacene OFETs — ●R. SCHOLZ¹, F. MÜLLER^{1,2}, A.-D. MÜLLER^{1,2}, M. HIETSCHOLD¹, I. THURZO¹, D. R. T. ZAHN¹, C. PANNEMANN³, and U. HILLERINGMANN³ — ¹Institut für Physik, TU Chemnitz — ²Anfatec Instruments AG, Oelsnitz — ³Elektrotechnik und Informationstechnik, Universität Paderborn

Potentiometry with a Kelvin probe atomic force microscope is used to investigate the contact resistances of pentacene OFETs. The potentiometry measurements are performed *ex situ* under atmospheric conditions after storing the samples in air for several weeks. At room temperature, the device performance is limited by the resistance at the Au/pentacene injection contact, so that the mobility in the channel region as deduced from potentiometry is about one order of magnitude higher than the value obtained from the output characteristics [1].

From two-dimensional device simulations in the accumulation regime, we can deduce the hole mobility close to the interface between the active channel and the SiO₂ gate insulator. In the pinchoff regime, the charge carriers are pushed away from the gate towards the interface pentacene/air. The comparison between the device simulation and the potentiometry traces reveals a larger mobility in this region of the pentacene film. This finding indicates trap states at the pentacene/SiO₂ interface, probably related to adsorbed water molecules.

[1] R. Scholz, A.-D. Müller, F. Müller, I. Thurzo, B. A. Paez, L. Mancera, D. R. T. Zahn, C. Pannemann, and U. Hilleringmann, Proc. of SPIE 5940 (2005), 59400I.

HL 31.12 Wed 17:30 POT 51

Relation between chain length, disorder and conductivity in Polypyrrole films — ●THOMAS HEINZEL¹, CESAR BOF BUFON¹, PAMELA ESPINDOLA², and JÜRGEN HEINZE² — ¹Heinrich-Heine-Universität Düsseldorf — ²Albert-Ludwigs-Universität Freiburg

The effects of polymerization temperature, electrosynthesis current density and voltammetric cycling on the transport properties of polypyrrole (PPy) films are investigated. PPy films are prepared by galvanostatic electropolymerization at a variety of experimental conditions. The films are investigated by UV-VIS spectroscopy, cyclic voltammetry and temperature-dependent transport measurements. It is observed that as the current density is reduced or the growth temperature is increased, the formation of short oligomers (PPy II) is favored, at the expense of the formation of long polymer chains (PPy I). Surprisingly, we observe a higher conductivity in films with a higher fraction of PPy II. In samples containing predominantly PPy II, quasi-metallic behavior is found. Furthermore, PPy II can be transferred in PPy I by voltammetric cycling, which goes along with a decrease of the conductivity and a localization of the states at the Fermi level. We interpret these results in terms of a disorder-dominated conductivity.

HL 31.13 Wed 17:45 POT 51

Influence of the active layer morphology on the device performance of polymer-fullerene bulk heterojunction solar cells — ●INGO RIEDEL¹, CARSTEN DEIBEL², and VLADIMIR DYAKONOV^{1,2} — ¹Bavarian Centre for Applied Energy Research (ZAE-Bayern e.V.), Div. Functional Materials for Energy Technology, Am Hubland, D-97074 Würzburg — ²Experimental Physics VI, Institute of Physics, University of Würzburg, Am Hubland, D-97074 Würzburg, Germany

Recent achievements in organic photovoltaics demonstrate the high potential of using polymer-fullerene blends, such as P3HT:PCBM, as photoactive films for PV applications. Blending of the two materials introduces new effects, which have direct impact on the performance of the solar cell: Thermal annealing of P3HT:PCBM devices results in drastic efficiency improvement. The relevant effect is a thermally induced ordering of the P3HT phase, accompanied with molecular diffusion of PCBM out of the polymer matrix to form isolated semicrystalline domains. Their size and concentration is correlated with the amount of PCBM available. We show that the nanoscaled morphology additionally

influences the open circuit voltage V_{OC} . This is shown by comparing devices based on two fullerene derivatives with identical redox potentials, each blended with the same donor polymer. Films of both composites exhibit different morphologies, which are represented by different values of V_{OC} . Analysis of the dark diode characteristics yields different ideality factors, which reflect the dominant internal recombination mechanism, e.g., electron back transfer from the fullerene moiety into the polymer phase.

HL 31.14 Wed 18:00 POT 51

Modified quinolates for pH-probes and high performance light emitting devices — ●STEPHAN RENTENBERGER¹, STEFAN KAPPAUN², ALEXANDER POGANTSCH¹, FRANZ STELZER², EGBERT ZÖJER¹, and CHRISTIAN SLUGOVIC² — ¹Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — ²Institute for Chemistry and Technology of Organic Materials, Graz University of Technology, Stremayrgasse 16, 8010 Graz, Austria

Aluminum quinolates (AlQ3) were first reported by Tang and VanSlyke in 1987 to possess electroluminescent properties and are currently widely used as light emitting electron transport materials for organic light emitting devices (OLEDs). As recent studies revealed, boron compounds are in general more stable than the corresponding aluminum compounds. While ligand precursors of those complexes exhibit characteristic features that can be used for pH-sensing purposes, the corresponding boron complexes display impressive properties as emitting layers in OLEDs. In our presentation we demonstrate both, the influence of protonation on the emission characteristics of the ligand precursors, and the application of the corresponding boron complexes in highly stable OLEDs. Additionally color-tuning by controlling the extension of the pi-conjugated system is achieved.

HL 31.15 Wed 18:15 POT 51

Paracrystalline structure of P3HT thin films: X-ray studies — ●ROSINA A. STANEVA^{1,2}, THOMAS HABER¹, ATTILA J. MOZER³, NIYAZI S. SARICIFTCI³, and ROLAND RESEL¹ — ¹Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria — ²Institute of Physics, Technical University of Ilmenau, Unterpörlitzer Str. 38, D-98693 Ilmenau, Germany — ³Linz Institute for Organic Solar Cells (LIOS), Physical Chemistry, Johannes Kepler University Linz, Altenbergerstr. 69, A-4040 Linz, Austria

The paracrystalline structure of poly(3-hexylthiophene) (P3HT) thin films was studied by integral breadth evaluation of X-ray diffraction patterns. The 30-40 μm thin films were cast on low reflectance Si substrate by doctor blade technique. The wide angle X-ray diffraction (WAXD) measurements were done on as-prepared films and after annealing at elevated temperatures. The crystallite size and the lattice distortions were obtained taking in account the first, the second and the third order of the (100) reflection. Two approaches were compared: the paracrystalline model of Hosemann and the method of Williamson and Hall for size and strain analysis. It was found that the method of Hosemann fits better to the most of the scattering curves. The crystallite size of as prepared films was found to be 7-9 nm. It increases to 9-12 nm for the annealed films. The lattice distortions were obtained to be 3-4%. The both parameters do not show any clear dependence on the molecular weight Mw in the range of 20000-58000.

HL 31.16 Wed 18:30 POT 51

In situ stability studies of long-life organic field-effect transistors — ●M. MICHELFEIT, M. LEUFGEN, G. SCHMIDT, J. GEURTS, and L. W. MOLENKAMP — Physikalisches Institut der Universität Würzburg, Experimentelle Physik III

In spite of numerous investigations, degradation of organic field effect transistors (OFETs) due to contamination, ageing and voltage stressing remains a hot issue. We report on stability studies, performed in situ in UHV in order to avoid extrinsic contamination effects. For this purpose we fabricated high-performance OFETs with UHV deposited dihexylquaterthiophene (DH4T) as active material. Using UHV-processed Au/Ti electrodes, mobility values of 0,12 cm^2/Vs are achieved and the in-situ performance data show negligible ageing effects on a time scale of at least several weeks. Thus they allow age independent measurements of the effect of applied voltage stress (both at gate/source and drain/source) on the OFET performance. We discover the carrier mobility to be independent of the voltages and the time of their application. In contrast, the threshold voltage exhibits a strong dependence on these parameters, although its shift turns out to be almost reversible. We explain this

behaviour by the existence of traps at the organic/insulator interface.

HL 31.17 Wed 18:45 POT 51

High-mobility organic thin-film transistors with low operation voltage — ●GÜNTHER LEISING, BARBARA STADLOBER, URSULA HAAS, ANJA HAASE, VALENTIN SATZINGER, JOSEF KRISCHE, HANNES MARESCH, MARTIN ZIRKL, HEINZ PICHLER, and GEORG JAKOPIC — Institut für Nanostrukturierte Materialien und Photonik, Joanneum Research GmbH, Franz-Pichler Strasse 30, A-8160 Weiz

Highly integrated consumer products are the main drivers for down-scaling electronic devices. We work on the miniaturization of organic thin film transistors (TFT) for its application in plastic electronics. We have produced a series of bottom-gate organic (pentacene) TFTs with channel lengths (L) in the range 0.3 - 2.4 μm by means of nanoimprinting techniques, to investigate the effects of the channel length on the device characteristics (short channel effects). Organic sub- μm TFTs showed similar characteristics as comparable long-channel devices (carrier mobilities in the range of 0.1 cm^2/Vs). Drain current saturation is observed for devices with L as small as 0.3 μm . The morphology of the pentacene domains is determined by the channel size and is studied by AFM. In the sub- μm regime we observe only a few pentacene crystallites filling the channel region. To achieve TFTs with a driving voltage below 5 Volts, we utilized a double-layer dielectric technique using a combination of inorganic and organic dielectric thin layers. Due to low leakage currents and the excellent growth of the pentacene thin films on the organic dielectric we could achieve carrier mobilities of up to 1 cm^2/Vs in our miniaturized organic TFTs.