

DS 16: [CPP] Organic Electronics and Photovoltaics I (Joint Session DS/CPP/HL/O)

Time: Tuesday 9:30–12:45

Location: H37

DS 16.1 Tue 9:30 H37

Side chain variations on dicyanovinyl-oligothiophenes studied by photoinduced absorption spectroscopy: consequences for small molecule organic solar cells — ●HANNAH ZIEHLKE¹, ROLAND FITZNER², CHRISTIAN KOERNER¹, EGON REINOLD², PETER BAEUERLE², KARL LEO¹, and MORITZ RIEDE¹ — ¹Institut für Angewandte Photophysik, Technische Universität Dresden — ²Institut für Organische Chemie II und Neue Materialien, Universität Ulm

Oligothiophenes capped with electron-withdrawing dicyanovinyl groups (DCVnT) are promising candidates for applications in small molecule organic solar cells. These oligothiophene derivatives can act as electron donor in blend layers with C₆₀. Single heterojunction devices reach efficiencies above 4 %. The introduction of side chains as intermolecular spacer has little effect on the energetics and mainly influences the morphology of the evaporated thin film. In addition, the distance between donor and acceptor molecules and thus the energy transfer and charge separation at the interface can be controlled. The energetic and dynamic properties of the long lived photoexcitations in pristine and blend layers can be obtained by photoinduced absorption spectroscopy (PIA). We here characterize of DCV3T with zero, two, and four alkyl chains (Methyl and Butyl) via PIA spectroscopy complemented with morphological studies. Our results indicate that the energy transfer process at the heterojunction is more efficient for smaller spatial distances between donor and acceptor molecules.

DS 16.2 Tue 9:45 H37

New multiwall molecular organic nanotubes — ●MAREN RASTEDT¹, FRAUKE KUTSCHER¹, OKKO FREY², RÜDIGER BECKHAUS², CHRISTIAN MAIBOHM³, and KATHARINA AL-SHAMERY¹ — ¹University of Oldenburg, Physical Chemistry 1, Germany — ²University of Oldenburg, Inorganic Chemistry, Germany — ³NanoSYD, Sonderborg, Denmark

Nanotubes can be described as the newest star in the evening sky of nanotechnology. Since the discovery of carbon nanotubes, this nanostructure has grasped the mind of many. This structure has many application possibilities ranging from liquid and gas storage to microelectronics and sub wavelength optical components and fibers. In our presentation we will give an introduction to multiwall nanotubes made from Tetrabenzofluorene(Tbf)-derivates. These Tbf-nanotubes have attracted interest because of their many properties, e.g. crystallization and waveguiding. Our nanotubes are prepared by the elegant and simple process of template assisted assembly. The assembly process will be presented together with specific properties of different Tbf-nanotubes. By changing growth parameters in the assembly process we have a method for probing fundamental questions and properties of our nanotubes. One future application of our nanotubes could be as an active element in a photovoltaic device.

DS 16.3 Tue 10:00 H37

Radical Molecular Wires — ●GEORG HEIMEL¹, EGBERT ZOJER², LORENZ ROMANER³, JEAN-LUC BRÉDAS⁴, and FRANCESCO STELLACCI⁵ — ¹Institut für Physik, Humboldt-Universität zu Berlin, Germany — ²Institut of Solid State Physics, Graz University of Technology, Austria — ³Chair of Atomistic Modeling and Design of Materials, University of Leoben, Austria — ⁴School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, USA — ⁵Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, USA

The technological relevance and the functionality of semiconducting materials originate in the fact that their conductivity and the band alignment at the interfaces with other materials can be controlled through doping. Here, we consider the ultimate miniaturization of functional devices by computationally investigating the doping of molecular wires suspended between two metal electrodes.¹ For representative systems we find that, upon doping, the molecular conductivity is enhanced by more than two orders of magnitude. We elucidate the microscopic origin of this dramatic effect and present an intuitive picture, which rationalizes our observations in terms of *Fermi-level pinning*. Our results shed new light on recent experimental findings and, most importantly, in-depth understanding of the doping mechanism enables the targeted development of new functional components for sensing and switching at the single-molecule scale.

[1] G. Heimel et al., *Nano Lett.* **9**, 2559 (2009).

DS 16.4 Tue 10:15 H37

Structure property relationship in aza-bodipy absorber materials for organic photovoltaics — ●ROLAND GRESSER, TONI MUELLER, MORITZ PHILIPP HEIN, KARL LEO, and MORITZ RIEDE — Institute of Applied Photophysics, Dresden University of Technology, Germany

In this joint experimental and theoretical study, we focus on the structure property relationship of aza-bodipy dyes as active donor materials in vacuum deposited small molecule solar cells.

The position of the materials HOMO can be intentionally varied by the choice of the functional group attached to the molecule. The absorption spectra show a red shift of the maximum with increasing donor strength of the substituents due to the increasing HOMO energy and decreasing band gap.

Based on crystal structure data, the charge carrier mobility determining parameters like reorganization energies and transfer integrals are calculated. The results show an increasing molecular orbital overlap and significant higher transfer integrals upon planarization and rigidification of the molecule. With this information, the observed charge carrier mobility differences from experiment can be explained.

In addition to the electronic properties a high thermal and photo stability is essential. From combined thermogravimetric analysis and mass spectroscopy we could determine the degradation process of the material and were able to increase the thermal stability by substitution of the involved species.

DS 16.5 Tue 10:30 H37

Dicyanovinyl sexithiophenes: self-organization and photovoltaic properties — ●MARIETA LEVICHKOVA¹, DAVID WYNANDS¹, ALEXANDR LEVIN¹, KARL LEO¹, KARSTEN WALZER², DIRK HILDEBRANDT², PETER BÄUERLE³, ROSINA RENTENBERGER⁴, and MORITZ RIEDE¹ — ¹Institut für Angewandte Photophysik, TU Dresden, Germany — ²Heliatek GmbH, Dresden, Germany — ³Institut für Organische Chemie II und Neue Materialien, Universität Ulm, Germany — ⁴Institut für Physik, TU Ilmenau, Germany

Recently, vacuum deposited films consisting of conjugated dicyanovinyl-capped (DCV) oligothiophenes have shown significant potential as photoactive layers in small molecule solar cells [1]. Here, we study the structural and optical properties of films of two DCV-derivatives both comprising six thiophene rings (DCV6Ts) but having different side groups. For both derivatives, neat DCV6T and mixed DCV6T:C60 films are compared using UV-VIS absorption and photoluminescence spectroscopy, X-ray diffraction (XRD), and Atomic Force Microscopy. It is shown that the modification of the molecular structure results in a structured and red shifted absorption band, which indicates better molecular arrangement in the solid state. The improved self-organization at room temperature deposition is confirmed by XRD. Furthermore, the nanomorphology of the mixed DCV6T:C60 films is optimized using substrate heating. Bulk heterojunction solar cells with power conversion efficiencies exceeding 4% are presented.

[1] K. Schulze et al., *Adv. Mater.* **2006**, *18*, 2872-2875

15 min. break

DS 16.6 Tue 11:00 H37

Hexaazatriphenylene and hexaazatrinaphthylene derivatives as electron transport materials in organic solar cells — ●CHRISTIANE FALKENBERG¹, MARTIN BAUMGARTEN², RALPH RIEGER², SELINA OLTHOFF¹, KARL LEO¹, MORITZ RIEDE¹, and KLAUS MÜLLEN² — ¹Institut für Angewandte Photophysik, TU Dresden, 01069 Dresden — ²MPI für Polymerforschung, 55128 Mainz

There is increasing interest in molecularly doped organic materials for the fabrication of efficient organic electronic devices. In small molecule organic solar cells, the so-called p-i-n concept is advantageous for the independent optimization of electrical and optical properties. Here, the absorbing donor-acceptor heterojunction is sandwiched between a p-doped hole transport layer and an n-doped electron transport layer. The design of suitable functional molecules for the transport layers is currently an important issue, however, the choice of available wide-

gap materials for the n-side of organic solar cells is very limited. Here, we investigate hexaazatriphenylene and hexaazatrinaphthylene derivatives as substitutes for the common electron transport materials C₆₀ or BPhen and BCP. Having bandgaps of > 2.7eV the new materials are transparent which, in combination with a suitable position of the energy levels, enables exciton blocking. Furthermore molecular doping with either acridine orange base (AOB) or NDN1 (Novaled AG) leads to an increase of the conductivity by several orders of magnitude, reaching values beyond 1·10⁻⁶ S/cm. Altogether the beneficial optical and electrical properties allow the fabrication of organic solar cells with increased efficiency compared to the standard devices.

DS 16.7 Tue 11:15 H37

Structure - property relationship of thiophene based materials bearing different accepting groups — ●MARION WRACKMEYER, MARKUS HUMMERT, HORST HARTMANN, KARL LEO, and MORITZ RIEDE — Institut für Angewandte Photophysik, Technische Universität Dresden, Germany

Organic solar cells require new materials for improved efficiencies. The relationship of molecular structure and properties is very important to optimise the devices. An interesting class of materials are thiophene block co-oligomers. The materials obtain electron donating (D) and accepting (A) groups and have the general structure A-D-A or D-A-D. In particular, the investigation of electron accepting groups is very important, because they have a high influence on the electronic structure of an organic molecule and are therefore an influential impact in the performance of a small molecule p-i-n solar cell. We present investigations on thiophene based materials bearing different accepting groups. The accepting groups are eg dicyanovinyl, dioxaborine, and benzthiadiazole. The materials were synthesised by Stille-coupling. Basic precondition for all materials is the thermal stability for deposition by vacuum-techniques. Subsequent investigations focus on absorption (solution and thin films), electrochemical behaviour (cyclic voltammetry to investigate the frontier molecular orbital energy levels), DFT-calculations (to show the location of HOMO and LUMO), mobility, morphology, dopability, and the properties of a solar cell.

DS 16.8 Tue 11:30 H37

Charge transport in self-assembled semiconducting organic layers: role of dynamic and static disorder — ●THORSTEN VEHOFF¹, YEON SOOK CHUNG², KAREN JOHNSTON¹, ALESSANDRO TROISI³, DO YEUNG YOON², and DENIS ANDRIENKO¹ — ¹Max Planck Institut fuer Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany — ²Department of Chemistry, Seoul National University, Seoul 151-747, Republic of Korea — ³Department of Chemistry and Centre of Scientific Computing, University of Warwick, Coventry, CV4 7AL, United Kingdom

Partial disorder is an inherent property of self-assembled organic semiconductors that complicates their rational design, since electronic structure, self-assembling properties and stability all have to be accounted for simultaneously. Therefore, the understanding of charge transport mechanisms in these systems is still in its infancy. A theoretical study of charge transport in organic semiconductors was performed on self-assembled layers of [1]Benzothieno[3,2-b]benzothiophene functionalized with alkyl side chains. Analysis showed that semiclassical dynamics misses static (on timescales of charge transport) disorder while the solution of the master equation combined with the high-temperature limit Marcus theory for charge transfer rates does not take into account molecular dynamic modes relaxing on a timescale of charge hopping. A comparison between predictions based on a perfectly ordered and a realistic crystal structure reveals the strong influence of static and dynamic disorder. The advantage of two-dimensional charge transporting materials over one-dimensional ones is clearly shown.

DS 16.9 Tue 11:45 H37

Charge Transport in rr-P3HT:PCBM Blends - The Impact of Ultrahigh Regioregularity on Hole Transport and Device Performance — ●RALF MAUER and FRÉDÉRIC LAQUAI — Max-Planck-Institut für Polymerforschung, Mainz, Deutschland

Blends of poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl C₆₁ butyric acid methyl ester (PCBM) have emerged as a prototypical material system for bulk heterojunction solar cells with reasonable efficiencies during the past five years. Despite tremendous engineering efforts to push devices to 5% power conversion efficiency (PCE), the correlation between charge carrier mobility and device performance is still up for debate. Theoretical models range from "the higher - the better" over

optimum finite mobilities to no effect of mobility on PCE at all.

We investigate charge transport in pristine P3HT films and in blends with PCBM by the time of flight (TOF) technique and analyse the results in the framework of the Gaussian disorder model. In order to understand the effect of charge transport on solar cell efficiency, we examine P3HT with three different regioregularities, i.e. regiorandom P3HT, rr-P3HT with high (rr=94%) and with ultrahigh (rr>98%) regioregularity. While the regioregularity is known to have a strong influence on the charge carrier mobility, its effect on other transport parameters, especially on the energetic disorder of hole transport in P3HT, is reported by us for the first time.

Finally, we correlate the TOF results and spectroscopic measurements with device performance to determine the influence of charge transport on the power conversion efficiency.

DS 16.10 Tue 12:00 H37

Charge transport in conjugated polymers with energetic disorder — ●JAMES C BLAKESLEY^{1,2}, HELEN S CLUBB¹, CHRISTOPHER GROVES¹, LOUISE M HOPKINS¹, and NEIL C GREENHAM¹ — ¹University of Cambridge, Cambridge, UK — ²Universität Potsdam, Potsdam, Germany

We investigate charge transport in sandwich-type devices with two polyfluorene-based copolymers: poly(9,9-dioctylfluorene-co-bis(N,N'-(4-butylphenyl))bis(N,N'-phenyl-1,4-phenylene)diamine) (PFB) and poly(9,9-dioctylfluorene-co-benzothiadiazole) (F8BT). A standard analysis of the data produces a poor fit to the data, with an apparent dependence of mobility on device thickness. Previously, such behaviour in electron transport has been attributed to trapping[1]. However, we find that a good fit is obtained by using a numerical simulation based on energetic disorder that takes into account the effects of electric field and carrier density on mobility (Extended Gaussian Disorder model). The amount of energetic disorder is quantified by 110+/-10meV and 100+/-10meV respectively. When the two materials are blended together, hole mobility remains constant when the fraction of PFB is 50% or greater, but drops dramatically for low concentrations of PFB. The amount of energetic disorder remains unaffected by any degree of blending, suggesting that there is no change in microscopic ordering of the polymers upon blending.

[1] R. Steyrlleuthner, S. Bange and D. Neher, J. Appl. Phys. 105, 064509 (2009)

DS 16.11 Tue 12:15 H37

Towards high charge carrier mobilities by rational design of organic semiconductors — ●DENIS ANDRIENKO¹, VALENTINA MARCON², JAMES KIRKPATRICK³, VICTOR RUEHLE¹, BJOERN BAUMEIER¹, THORSTEN VEHOFF¹, ALEXANDER LUKYANOV¹, KURT KREMER¹, JENNY NELSON³, and CHRISTIAN LENNARTZ⁴ — ¹Max Planck Institute for Polymer Research, Mainz — ²Technische Universität Darmstadt, Germany — ³Imperial College London, UK — ⁴BASF AG, Ludwigshafen

The role of material morphology on charge carrier mobility in partially disordered organic semiconductors is discussed for several classes of materials: derivatives of hexabenzocoronenes [1], perylenediimides [2], triangularly-shaped polyaromatic hydrocarbons [3], and Alq₃. Simulations are performed using a package developed by Imperial College, London and Max Planck Institute for Polymer Research, Mainz (votca.org). This package combines several techniques into one scheme: quantum chemical methods for the calculation of molecular electronic structures and reorganization energies; molecular dynamics and systematic coarse-graining approaches for simulation of self-assembly and relative positions and orientations of molecules on large scales; kinetic Monte Carlo and master equation for studies of charge transport.

[1] J. Kirkpatrick, et al, Phys. Rev. Lett., 98, 227402, 2007; [2] V. Marcon, et al, J. Am. Chem. Soc., 131, 11426, 2009; [3] X. Feng et al, Nature Materials 8, 421, 2009

DS 16.12 Tue 12:30 H37

Fully functionalized block copolymers for organic electronic applications — ●SVEN HÜTTNER^{1,2}, MICHAEL SOMMER², JUSTIN HODGKISS¹, PETER KOHN³, THOMAS THURN-ALBRECHT³, RICHARD FRIEND¹, ULLRICH STEINER¹, and MUKUNDAN THELAKKAT² — ¹Cavendish Laboratory, University of Cambridge — ²Angewandte Funktionspolymere, Makromolekulare Chemie I, Universität Bayreuth — ³Experimentelle Polymerphysik, Universität Halle-Wittenberg

Block copolymers are well known to phase separate in highly ordered nanostructures on length scales commensurate with the exciton diffusion length. We use fully functionalized block copolymers for photo-

voltaic devices, where a donor and an acceptor polymer are covalently linked. The acceptor block consists of a polyacrylate backbone with pendant perylene bisimide moieties and the donor block consists of poly(3-hexylthiophene) (P3HT). We combine temperature dependent small angle and wide-angle X-ray scattering measurements to investigate the block copolymer phase separation as well as the influence of the crystallisation kinetics of the two blocks. Intermolecular and intramolecular interactions drive the self-assembly of structures from

molecular lengthscales to larger mesostructures of some nanometers to microphase separation of some tens of nanometers. The investigation of the morphology is accompanied by steady state spectroscopy and transient absorption spectroscopy. Furthermore organic thin film transistors are used to characterize the transport properties in these novel materials which are found to exhibit unique properties such as the tunability between n-type, p-type or ambipolar transport.