O 65: Organic Photovoltaics and Electronics

Time: Wednesday 14:45–18:30 Location: H2

Invited Talk O 65.1 Wed 14:45 H2

Ultrafast excitonic and charge transfer dynamics in nanostructured organic polymer materials — •Irene Burghardt[1], Robert Binder[1], Matthias Polkehn[1], and Hiroyuki Tamura[2] — [1]Institute for Physical and Theoretical Chemistry, Goethe University Frankfurt, Germany — [2]WPI-Advanced Institute for Material Research, Tohoku University, Japan

We present first-principles quantum dynamical studies of ultrafast photoinduced exciton migration and dissociation in functional organic materials, in view of understanding the key microscopic factors that lead to efficient charge generation in photovoltaics applications. The talk will specifically address (i) exciton dissociation and free-carrier generation in donor-acceptor materials, including models for P3HT-PCBM heterojunctions [1] as well as highly ordered thiophene-perylene diimide assemblies [2], (ii) exciton migration [3] and formation of charge-transfer excitons in oligothiophene H-aggregates, and (iii) exciton multiplication by singlet fission in acene materials [4]. Special emphasis is placed on the critical role of exciton and charge delocalization which are a sensitive function of molecular packing.

[1] H. Tamura, I. Burghardt, J. Am. Chem. Soc. 135, 16364 (2013), M. Huix-Rotllant, H. Tamura, I. Burghardt, J. Phys. Chem. Lett. 6, 1702 (2015). [2] T. Roland et al., Phys. Chem. Chem. Phys. 14, 273 (2012), J. Wenzel, A. Dreuw, I. Burghardt, Phys. Chem. Chem. Phys. 15, 11704 (2013). [3] J. Wahl, R. Binder, I. Burghardt, Comput. Theor. Chem. 1040, 167 (2014). [4] H. Tamura et al., Phys. Rev. Lett. 115, 107401 (2015).

O 65.2 Wed 15:15 H2

Non-Equilibrium Charge Carrier Dynamics in Organic Disordered Semiconductors — •Andreas Hofacker[1], Jan Oliver Oelerich[2], Alexey Nenashev[3], Florian Gebhard[2], and Sergei Baranovskii[2] — [1]Institute of Applied Photophysics, Dresden University of Technology, D-01069 Dresden — [2]Department of Physics and Materials Science Center, Philipps-University, D-35032 Marburg — [3]Institute of Semiconductor Physics, 630090 Novosibirsk, Russia

Time-dependent processes in organic semiconductors dominated by non-equilibrium physics are subject of current debate in the scientific community. The understanding of these processes promises fundamental insights into transport and recombination dynamics of charge carriers in organic semiconductor devices such as organic solar cells, and can therefore reveal possibilities for further efficiency enhancement.

Based on an analytical model developed for inorganic disordered semiconductors by Orenstein and Kastner in 1981, we formulate a description of carrier thermalization and recombination in organic disordered semiconductors. For this purpose we extend the very transparent approach of Orenstein and Kastner to enable the description of low recombination rates and applicability of the approach to arbitrary density of tail states (DOS) functions. We predict that the behavior of systems with a Gaussian DOS, which organic semiconductors are commonly believed to be, is distinctively different from systems with an exponential DOS. This fact could be used to experimentally distinguish whether a given sample possesses an exponential or a Gaussian DOS by performing a time-dependent carrier density measurement.

O 65.3 Wed 15:30 H2

Mobility-limited recombination models for organic solar cells — •Alexander Wagenpfahl and Carsten Deibel — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

Recent results of kinetic Monte Carlo simulations indicate that recombination of charge carriers in organic semiconductor blends show a strong dependence on the domain size of neat material phases [1]. Consequently, the Langevin recombination model does not generally apply and has to be modified by the geometric mean of the charge carrier mobilities. Here, we present drift–diffusion simulations to reveal the influence of such a recombination model in comparison to the Langevin theory. We discuss differences in the quality of the solar cell current–voltage characteristics and distinguish the different processes which lead to a reduction of the observed recombination rate [2].

[1] Phys. Rev. Lett. 114, 136602 (2015)
[2] Phys. Rev. B 80, 075203 (2009)

O 65.4 Wed 15:45 H2

Energy-Gap Law of Non-Radiative Voltage Losses in Organic Solar Cells — •Johannes Benduhn[1], Kristofer Tvingstedt[2], Fortunato Piersimoni[3], Olaf Zeika[1], Donato Spoltore[1], Dieter Neher[3], and Koen Vandewal[1] — [1]IAPP, TU Dresden, Germany — [2]EP VI, Julius-Maximillian University of Würzburg, Germany — [3]IPA, University of Potsdam, Germany

The open-circuit voltage of organic solar cells is low as compared to their optical gap, indicating large energy losses per absorbed photon. These losses arise from the necessity of an electron transfer from an electron donor to an electron acceptor to dissociate the excitons, and furthermore from the recombination of the resulting free charge carriers. It has been shown that the energy loss in the electron transfer event can be below 0.1 eV, while radiative recombination losses are in principle unavoidable.

In this work, we investigate the remaining voltage losses due to non-radiative decay of charge carriers. We find that the non-radiative voltage losses increase when the energy difference between charge transfer (CT) state and ground state decreases. This behaviour is consistent with the "energy gap law for non-radiative transitions", which implies that internal conversion from CT state to ground state is facilitated by molecular vibrations. With this work, we identify a possibly intrinsic loss mechanism, which until now has not been thoroughly considered for organic photovoltaics, and which is different in its very nature as compared to the commonly considered inorganic photovoltaic loss mechanisms of defect, surface, and Auger recombination.

O 65.5 Wed 16:00 H2

Development of a photocapacitor based on printed solar cells and supercapacitors — •Katrin Anneser[1], Lukas Hörlin[2], Stephan Braxmeier[1], Andreas Baumann[1], Gudrun Reichenauer[1], and Vladimir Dyakonov[1,2] — [1]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg — [2]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

The main drawbacks of renewable energy sources such as wind and solar energy are unpredictable power fluctuations presenting a major challenge to stability and efficiency of the grid. With increasing fraction of these intermittent energy sources it is necessary to smooth the power before feeding it into the grid without just cutting off the fluctuations. We are following the few previous research activities aiming at combining a fast energy storage device, a supercapacitor, and a solar cell. Rather than developing a modular system our objective is an integrated layered system provided by printing the components from solution processed precursors. Those combined cells will provide a more constant power output compared to stand-alone photovoltaic systems and thus allow feeding into storage units with far slower kinetics (e.g. batteries) or the grid. We present the concept and the related boundary conditions and problems to be solved. Furthermore, we show experimental data from solar cells measured at a high frequency (every second) and derive the basic requirements in terms of power and energy density required for the storage unit per m^2 of the integrated system from these data.

O 65.6 Wed 16:15 H2

Passivation and modification of silicon nanowires towards hybrid solar cells — •Jessica Hänisch[1], Carola Klimm[1], Marc A. Gluba[1], Karsten Hinrichs[2], Iver Lauermann[3], Wolfram Calvet[3], Norbert H. Nickel[1], and Jörg Rappich[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium-Photovoltaik, Berlin, Germany — [2]ISAS e.V. - Leibniz-Institut für Analytische Wissenschaften, Berlin, Germany — [3]BESSY, Berlin, Germany

Hybrid solar cells combine inorganic and organic materials to benefit from both areas, particularly in terms of production costs and material consumption. The inorganic-organic interface needs to be well passivated, especially if nanowires with a high surface area are implemented to enhance light absorption. The silicon nanowires were prepared by metal assisted chemical etching (MACE). The etching procedure leads to surface damaging and thereby generates surface defects. These defects reside in the band gap and act as recombination centers. As a consequence, the amount of collected charge carriers is reduced and

therefore, the power conversion efficiency decreases. We applied electropolishing procedures to the silicon surface to minimize the amount of surface defects. Changes in the density of surface defects were directly monitored by in-situ photoluminescence measurements. To preserve the improved surface passivation obtained after the electropolishing process we used (electro-)chemical grafting of small molecules and investigated the surfaces by infrared spectroscopy, x-ray photoelectron spectroscopy and photoluminescence measurements.

30 min. Coffee Break

O 65.7 Wed 17:00 H2

Vertical Organic Field-Effect Transistors - Functional Principles and Applications — •Alrun Aline Günther[1], Michael Sawatzki[1], Christoph Hossbach[2], Petr Formánek[3], Daniel Kasemann[1,4], Johannes Widmer[1], Johann W. Bartha[2], and Karl Leo[1,5] — [1]Institut für Angewandte Photophysik, TU Dresden, Germany — [2]Institut für Halbleiter- und Mikrosystemtechnik, TU Dresden, Germany — [3]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [4]currently: CreaPhys GmbH, Dresden, Germany — [5]Fellow of the Canadian Institute for Advanced Research, Toronto (ON), Canada

Vertical organic field-effect transistors (VOFETs) are a means to overcome the limitations of conventional organic field-effect transistors (OFETs). At present however, they often suffer from two major drawbacks: performance limitation by contact effects and limitation to certain materials and processing techniques, making a controlled shift of parameters such as the transistor threshold voltage difficult. Here, we present p- and n-type VOFETs operating in the accumulation and inversion regimes. By introducing contact doping, we are able to increase the transconductance and On/Off ratio of VOFETs by an order of magnitude. We further show that the realisation of inversion VOFETs is possible and can shift the threshold voltage in a controlled manner, while reducing the Off state current of VOFETs through reduction of the source-drain leakage current.

O 65.8 Wed 17:15 H2

Vertical Organic Light Emitting Transistors for Investigation of Charge Transport in VOFETs — •Franz Michael Sawatzki[1], Alrun Günther[1], Duyhai Doan[2], Christoph Hossbach[3], Petr Formánek[4], Daniel Kaseman[1,5], Johannes Widmer[1], Thomas Kopprucki[2], and Karl Leo[1,6] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, Germany — [2]Weierstraß-Institut für Angewandte Analysis und Stochastik, Leibniz-Institut im Forschungsverbund Berlin e. V., Germany — [3]Institut für Halbleiter- und Mikrosystemtechnik, Technische Universität Dresden, Germany — [4]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [5]currently: CreaPhys GmbH, 01257 Dresden, Germany — [6]Fellow of the Canadian Institute for Advanced Research (CIFAR), Toronto, Ontario M5G 1Z8, Canada

The vertical organic field effect transistor (VOFET) offers many technological advantages due to its very short geometric channel length. However, in contrast to the standard lateral organic field effect transistor (OFET), the basic physics and working principles are not yet well known. Here, we compare results regarding the charge transport obtained from simulations with measured charge carrier density distributions. The latter ones are obtained from the light emission of vertical organic light emitting transistors (VOLETs). These devices are a combination of an organic light emitting diode (OLED) and a VOFET, which allow to locally resolve the current path. We show the dependence of the channel size and geometry on the gate-source voltage, the drain-source voltage, and the source geometry.

O 65.9 Wed 17:30 H2

Ultra-High Current Densities in Organic Transistors — •Markus P. Klinger, Axel Fischer, Felix Kaschura, Daniel Kasemann, Johannes Widmer, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr Str. 1, 01069 Dresden

Organic transistors are considered for flat panel or flexible displays, radio identification systems, and sensor arrays. Much effort has been spent to optimize the charge carrier mobility and to reduce the channel length of organic field-effect transistors (OFETs). Likewise, new device concepts have been introduced based on charge transport perpendicular to the substrate utilized in so-called vertical organic transistors. One representative is the high-performing organic permeable-base transistor (OPBT) [1,2]. Here, we show that this device is determined by space-charge limited current (SCLC) in the on-state. Thus, OPBTs can drive as much current as possible for a certain thickness of semiconducting material. Using C_{60} with a low charge carrier mobility of about $0.025\,\mathrm{cm^2\,V^{-1}s^{-1}}$ in the vertical direction, current densities of more than $600\,\mathrm{A\,cm^{-1}}$ are reached at voltages below 6 V. This performance can be achieved as the total thickness of the device is in the range of 100 nm. With that, OPBTs can easily outperform OFETs in terms of current per footprint area.

[1] M. P. Klinger et al., Adv. Mater. (2015), 27(47);
[2] A. Fischer et al., Appl. Phys. Lett. (2012), 101, 213303

O 65.10 Wed 17:45 H2

Controlling the electronic properties in liquid crystal conjugated small molecules for application in electronics — •Nadine Tchamba Yimga[1], Holger Borchert[1], Peer Kirsch[3], Jürgen Parisi[1], and Elizabeth von Hauff[2] — [1]Department of Physics, University of Oldenburg, Germany — [2]Department of Physics and Astronomy, VU University Amsterdam, The Netherlands — [3]Merck KGaA, Liquid Crystals R&D Chemistry, Germany

Organic semiconductors offer numerous advantages for electronics. However, carrier mobilities in organic semiconductors are generally orders of magnitude lower than in inorganic semiconductors. This is a major bottle neck for device efficiency. The electrical properties are additionally dependent on thin film morphology which is challenging to control in solution deposited films. We studied structure-function relationships in a novel liquid crystal molecule. The molecular films demonstrate phase changes from crystalline to nematic to isotropic phases at temperatures of 140 C, 165 C and 250 C, respectively. We demonstrate the influence of temperature on the structure of solution processed films with cross polarized microscope (CPM) and X-ray diffraction (XRD). Current-voltage measurements and impedance spectroscopy were performed on films annealed to temperatures above the crystalline - nematic phase change and subsequently cooled. The mobility increases from 10^{-4} cm^2 V^{-1} s^{-1} to 10^{-3} cm^2 V^{-1} s^{-1}. We demonstrate that controlled structural manipulation of the film can be used to reduce electronic disorder. These results show the potential of liquid crystal conjugated materials in electronic applications.

O 65.11 Wed 18:00 H2

Photodetectors Based on an Anilino Squaraine for Efficient Detection of Light in the 700 nm Region — •Andre Pries[1], Matthias Schulz[2], Arne Lützen[2], Jürgen Parisi[1], and Manuela Schiek[1] — [1]Institute of Physics, Energy and Semiconductor Research Laboratory, Oldenburg, Carl von Ossietzky University, Germany — [2]Kekulé Institute of Organic Chemistry and Biochemistry, Bonn, Rheinische Friedrich-Wilhelms-University, Germany

In this work the squaraine derivative 2,4-bis[4-(N,N-diisobutylamino)-2,6-dihydroxyphenyl] squaraine (SQIB) is analyzed in a conventional bulk-heterojunction photodiode architecture, Glass/ITO/MoO_3/SQIB:PCBM/LiF/Al. This architecture shows a power conversion efficiency of ≈2.5 % and a peak external quantum efficiency (EQE) of ≈50 % at 700 nm, making the device highly sensitive in the red wavelength region. In order to even further increase the EQE a negative bias voltage is used. Next the time-dependent response of the device is measured, to find, e.g. the rise- and fall time. Finally, the bandwidth of the device is determined and the cut-off frequency.

[1] G. Chen et. Al, Optical and electrical properties of a squaraine dye in photovoltaic cells, Applied Physics Letters, Vol. 101, No.8 2012, 083904

[2] M.Binda et. Al, Fast and air stable near-infrared organic detector based on squaraine dyes, Organic Electronics, 2009, Vol. 10, Issue 7, p. 1314-1319

O 65.12 Wed 18:15 H2

First results of an implementation of GW of reduced complexity for organic semiconductors — •Saber Gueddida and Dietrich Foerster — LOMA, Université de Bordeaux, France

We have implemented a GW algorithm of reduced complexity (N^3 rather than N^4) for crystals containing N»1 atoms in their unit cell. The main ideas of the algorithm and first results of its implementation will be given. Our code aims at contributing to optimizing organic solar cells by predicting the bands and gaps of their constituents.