

CPP 14: Organic photovoltaics and electronics (joint session HL/CPP)

Time: Monday 15:00–17:15

Location: H31

CPP 14.1 Mon 15:00 H31

Spectroscopy of Oligoacene molecules attached to Argon clusters — ●MATTHIAS BOHLEN¹, COREY A. RICE¹, AARON LAForge^{1,2}, and FRANK STIENKEMEIER¹ — ¹Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg — ²University of Connecticut, Department of Physics, 2152 Hillside Rd, Storrs, CT, USA

Energy conversion efficiency for solar cells is generally limited by the Shockley-Queisser limit [1]. One way to circumvent this limit is through the use of organic photovoltaics (OPV), where specific charge and energy transfer processes can lead to higher conversion efficiencies. Polyaromatic hydrocarbons such as oligoacene molecules exhibit interesting quantum effects such as singlet fission, triplet-triplet annihilation, or superradiance and make promising candidates for OPV applications. Recently anthracene, tetracene and pentacene molecules adhered to the surface of neon clusters have been shown to provide interesting model systems for detailed studies of such effects [2]. We want to extend these measurements by spectroscopy of oligoacenes deposited to the surface of argon clusters.

[1] W. Shockley and H. J. Queisser, J Appl Phys 32, 510 (1961)

[2] S. Izadnia et al., J. Phys. Chem. Lett.*8,*2068 (2017)

CPP 14.2 Mon 15:15 H31

When the model description hampers the parameter extraction for organic thin-film transistors — MARKUS KRAMMER¹, JAMES BORCHERT², ANDREAS PETRITZ³, GERBURG SCHIDER³, ESTHER KARNER-PETRITZ³, BARBARA STADLOBER³, HAGEN KLAUK², and ●KARIN ZOJER¹ — ¹Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Graz, Austria — ²Max Planck Institute for Solid State Research, Stuttgart, Germany — ³Joanneum Research Materials, Weiz, Austria

When transistor parameters, like charge mobility or contact resistances, are determined from the electrical characteristics, their values are not unambiguous, but rather depend on the extraction technique and on the underlying transistor model. We propose a technique to establish whether the ambiguity arises already from the chosen transistor model. This two-step technique analyzes the electrical measurements of a series of TFTs with different channel lengths. The first step extracts the parameters for each individual transistor. The second step checks whether the channel length-dependence of the extracted parameters is consistent with the model. We demonstrate the technique for a range of organic TFTs that differ in the semiconductor, the injecting contacts, and the geometry. Independent of the transistor set, state-of-the-art transistor models fail to reproduce the correct channel length-dependence. Our technique suggests that transistor models require improvements in terms of carrier density dependence of the mobility and the consideration of uncompensated charges in the transistor channel.

CPP 14.3 Mon 15:30 H31

Vibronic coupling governs ultrafast intermolecular energy transfer in an oligomer thin film — EPHRAIM SOMMER¹, XUAN TRUNG NGUYEN¹, LYNN GROSS², THOMAS FRAUENHEIM², ELENA MENA-OSTERITZ³, PETER BÄUERLE³, ●ANTONIETTA DE SIO¹, and CHRISTOPH LIENAU¹ — ¹Institut für Physik, Universität Oldenburg — ²BCCMS, Universität Bremen — ³Institut für organische Chemie II und neue Materialien, Universität Ulm

Organic photovoltaic(OPV) materials are complex molecular systems with many vibrational degrees of freedom. In such large molecules, vibronic coupling may result in conical intersections(CIs) of potential energy surfaces. Close to CIs, large vibronic couplings induce efficient ultrafast transition between electronic states. Hence CIs may profoundly influence the dynamics and yield of energy and charge transfer processes. So far, however, the importance of CIs for OPV materials has not yet been discussed. Here we use ultrafast two-dimensional electronic spectroscopy to study the light-induced dynamics in an oligomer thin film for OPV. Upon impulsive excitation, we detect a grid-like peak pattern suggesting coherent wavepacket motion in the excited state. After <50fs, the pattern transforms into a broad, featureless single peak. We observe an increase of oscillation period with an abrupt vanishing of the optically excited wavepacket, followed by the emergence of a new wavepacket with different oscillation. These results,

together with ab-initio molecular dynamics calculations, show that intermolecular energy transfer in stacked dimers of this oligomer involves passage of the optically excited wavepacket through a CI within <50fs.

CPP 14.4 Mon 15:45 H31

Influence of thermal transport parameters on operation temperature of OLEDs — ●GEORGII KRİKUN and KARIN ZOJER — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Graz, Austria

Utilizing organic light emitting diodes (OLEDs) for lighting requires a homogeneous operation across large surface areas. This poses the challenge to suppress local variations in temperature and current density. While OLED research mostly focuses on electric and optical properties, thermal properties are highly relevant, as charge transport in organics is thermally activated. Due to the peculiar coupling between thermal and charge transport, related properties cannot be decoupled from each other.

We investigate how thermal conductivity and heat transfer between OLED surface and environment impact current voltage relations and device temperature for a given ambient temperature. By using self-consistent drift-diffusion based simulations, that simultaneously account for thermal and charge transport and their coupling, we establish how excess heating can be effectively counteracted. Despite a strong coupling between charge and heat transport, heat transport is essentially governed by layers that not participate in charge transport. Hence, electrical and thermal properties can be tuned with separate layers.

15 min. break

CPP 14.5 Mon 16:15 H31

Barrier Heights in Contacts to Electroluminescent Thin Films of 1-(pyridin-2-yl)-3-(quinolin-2-yl)imidazo[1,5-a]quinoline Determined by Kelvin Probe Force Microscopy

— ●CLEMENS GEIS¹, GEORG ALBRECHT¹, JULIA RUHL², JASMIN MARTHA HERR², RICHARD GÖTTLICH², and DERCK SCHLETTWEIN¹ — ¹Justus-Liebig-Universität Gießen, Institut für Angewandte Physik — ²Justus-Liebig-Universität Gießen, Institut für Organische Chemie

Thin films of 1-(pyridin-2-yl)-3-(quinolin-2-yl)imidazo[1,5-a]quinoline (*PCIC*) were prepared by physical vapor deposition and analyzed in situ by Kelvin probe force microscopy (KPFM). As contact phases, poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (*PEDOT : PSS*) and poly(9-vinylcarbazole) (*PVK*) were used as hole conductors and bathocuproine (*BCP*) as electron conductor. Charge carrier injection barriers were identified, electroluminescent layer structures were prepared and effects of contact formation on radiative recombination were studied. Aside from the expected blue emission, a significantly red-shifted emission was found and assigned to electroplex formation with *BCP*. Using *PCIC* in a host-guest system within a matrix of *PVK* led to blue emission at improved luminescence. The studied interactions of *PCIC* with typical contact materials reveal the potential and limitations of *PCIC* as an electroluminescent material.

CPP 14.6 Mon 16:30 H31

Rubrene based diodes for rectification applications —

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The development of organic electronics is usually focused on a small set of electronic components, mainly OLEDs, solar cells, and various types of OFETs. To realize circuits, additional devices are required. One such device type are high-speed diodes, in the role of rectifiers, voltage stabilizers or analog signal processing. In particular for high-frequency RFID-applications it is essential to provide fast-switching diodes. The performance of such devices is closely related to the mobility of the semiconductor materials in use. Due to the anisotropy of charge carrier transport in most high-mobility organic semiconductors,

it is necessary to find material systems that offer high vertical mobilities. We present organic diodes, optimized for transition-frequency and high driving current, utilizing highly crystalline layers of Rubrene. These diodes show record values for the transition frequency, both in open circuit and under load. The values reached are higher than for inorganic diodes based on amorphous silicon and therefore allow for a low-cost realization of medium to long range RFID-systems.

CPP 14.7 Mon 16:45 H31

Non-fullerene acceptors with tailored properties for organic solar cells — ●ANASTASIA MARKINA¹, FREDERIC LAQUAI², and DENIS ANDRIENKO^{1,2} — ¹Max Planck Institute for Polymer Research, Mainz 55128, Germany — ²King Abdullah University of Science and Technology (KAUST), KAUST Solar Center (KSC), Thuwal 23955-6900, Kingdom of Saudi Arabia

One promising method to achieve higher solar cell efficiencies is to replace fullerenes with strongly-absorbing dye molecules, namely, non-fullerene acceptors (NFAs). However, the systematic design of acceptor molecules with tailored properties has yet to be demonstrated. The main difficulty here is that, while fullerenes are electrostatically inert, new acceptor molecules typically have strong static quadrupole moments.

By exploring the long-range electrostatic interaction at the interface, we demonstrate that, for a set of recently developed NFAs, the electrostatic bias potential can be directly related to the stabilization (or destabilization) of charge-transfer (CT) states as well as changes of the photovoltaic gap.

We find that the correlation between quadrupole moments, charge separation efficiency, and CT-state energy predicted by our model, is experimentally reproduced for several different donor /acceptor combinations. This allows us to predict new NFA structures using combina-

tions of readily available molecular building blocks that can potentially reach even higher performances than those currently achieved in state-of-the-art NFA devices.

CPP 14.8 Mon 17:00 H31

The three optical signatures of p-doping in poly(3-hexylthiophene) — MALAVIKA ARVIND¹, ●CLAUDIA TAIT², JAN BEHREND², and DIETER NEHER¹ — ¹Universität Potsdam, Potsdam, Germany — ²Freie Universität Berlin, Berlin, Germany

Doping is an important process in the realization of electronic devices. Here we investigate the mechanism of p-doping of regioregular- and regiorandom- poly(3-hexylthiophene) (P3HT) using two dopants - F4TCNQ and tris(pentafluorophenyl)borane (BCF). Although both dopants exhibit Integer Charge Transfer (ICT) with rreP3HT in solution, the sub-band gap features in the UV-Vis-NIR spectra of F4TCNQ- and BCF-doped rraP3HT differ significantly.[1] The concentration and nature of paramagnetic states generated in the different systems was investigated using EPR spectroscopy. The results reveal significantly reduced spin concentrations in the doped rraP3HT solutions, in particular with F4TCNQ as dopant, supporting the existence of EPR-silent bound charge pairs. Additionally, the hole delocalization was shown to be reduced in regiorandom- compared to regioregular-P3HT. We conclude that CTC and ITC formation is not specific for thiophene-based polymers and oligomers, respectively, as suggested by earlier results. [2] Instead, the nature of the doping-induced state correlates strongly with the ability of the conjugated backbone to planarize and to delocalize the polaron along the conjugated system.

[1] Pingel P., Arvind M. et al. (2016). Adv. Electron. Mater.,2:1600204 [2] H. Méndez, I. Salzmänn, et al., Nat. Commun. 6, 8560 (2015).