HL 54: Organic semiconductors

Time: Friday 9:30–12:15 Location: EW 203

HL 54.1 Fri 9:30 EW 203

Molecular origin of the anisotropic orientation of molecules in organic light emitting diodes — •Pascal Friederich[1], Vadim Rodin[2], Florian von Wrochem[2], Reinder Coehoorn[3], and Wolfgang Wenzel[1] — [1]Karlsruher Institut für Technologie, Karlsruhe, Deutschland — [2]Sony, Stuttgart, Deutschland — [3]Technische Universität Eindhoven, Eindhoven, Niederlande

Molecular orientation anisotropy of the emitter molecules used in organic light emitting diodes (OLEDs) can give rise to an enhanced light-outcoupling efficiency, when their transition dipole moments are oriented preferentially parallel to the substrate. A similar effect is observed when the anisotropic orientation of molecules with electrostatic dipole moments leads to the spontaneous buildup of an electrostatic potential perpendicular to the substrate. This so-called giant surface potential (GSP) effect can as well be exploited in organic electronics applications. Here, the orientation anisotropy of widely used organic semiconductors is investigated using a simulation approach which mimics the physical vapor deposition process of amorphous thin films [1]. Our simulations reveal for all studied systems significant orientation anisotropy which is in agreement with experimental results for the emitter orientation as well as the GSP effect. We find that the electrostatic interaction between the dipole moments of the molecules limits the orientation strength while short range van der Waals interactions between molecules and the surface during deposition act as driving force for the anisotropic orientation. [1] P. Friederich, R. Coehoorn, W. Wenzel, Chem. Mater., 2017, 29 (21)

HL 54.2 Fri 9:45 EW 203

Investigation of charge transport in solution processed and vacuum-deposited organic semiconductors — •Deepthi K. Mangalore, Paul W. M. Blom, and Gert-Jan A.H. Wetzelaer — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Organic light emitting diodes based on pi-conjugated polymers have been instrumental in revolutionizing the area of displays and lighting in the last decade. The immense opportunity presented by this technology has driven the research to find cheaper alternatives to the traditional deposition method of thermal evaporation. At the same time, the solubility of organic semiconductors in organic solvents enables film deposition from the solutions and the charge transport in these films has not been fully investigated. This work examines the transport in solution processed organic small molecule films and presents a comparison to the charge transport in vacuum-deposited films. Temperature-dependent space-charge-limited currents in single carrier devices of two hole transporting materials α-NPD and Spiro-TAD are used to investigate the transport properties in pristine and doped devices (dopants- F4TCNQ , F6TCNNQ). After optimizing the deposition conditions, comparable hole mobilities (4*10-8 m2V-1s-1 for Spiro-TAD and 0.8*10-8 m2V-1s-1 for α-NPD) were obtained in pristine solution-processed and vacuum-deposited films. In addition, the J-V characteristics were also analyzed with the extended Gaussian disorder model.

HL 54.3 Fri 10:00 EW 203

Core-Level Excitations in Oligothiophene Crystals from *Ab-Initio* Many-Body Theory — •Konstantin Lion, Caterina Cocchi, and Claudia Draxl — Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin D-12489 Berlin

We study core-level excitations in a series of linear crystalline oligothiophenes, i.e., bithiophene, quaterthiophene, and sexithiophene. Employing the full-potential all-electron `exciting` code [1], we compute X-ray absorption spectra from first principles through the solution of the Bethe-Salpeter equation, with a fully relativistic treatment of core states [2]. We investigate transitions from the carbon K, the sulfur K, and the sulfur $L_{2,3}$ edges. Our results, in very good agreement with available experimental data [3, 4], reveal the excitonic character of the near-edge resonances and allow us to resolve the individual contributions from inequivalent atoms. Core-level excitations in these systems exhibit strong excitonic effects, with electron-hole binding energies ranging from 3 to 2 eV, going from bithiophene to sexithiophene. Only in the spectrum from the carbon K edge, the individual contributions from inequivalent atoms show distinct features. Peaks in this spectrum are attributed to transitions from two types of carbon atoms, either sharing a covalent bond to a sulfur atom or not.

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26**, 363202 (2014).
[2] C. Vorwerk *et al.*, Phys. Rev. B **26**, 155121 (2017).
[3] P. Väterlein *et al.*, Surf. Sci. **452**, 20 (2000).
[4] U. Hörmann *et al.*, J. Phys. Chem. C **118**, 26462 (2014).

HL 54.4 Fri 10:15 EW 203

Design of high mobility molecular organic semiconductors — Pascal Friederich[1], Franz Symalla[1], Velimir Meded[1], Vadim Rodin[2], Christian Sprau[1], Florian von Wrochem[2], Alexander Colsmann[1], Mario Ruben[1], and •Wolfgang Wenzel[1] — [1]Karlsruher Insitut für Technologie , Karlsruhe, Germany — [2]Sony Europe Ltd, Stuttgart, Germany

Small-molecule organic semiconductors are used in a wide spectrum of applications, ranging from organic light emitting diodes to organic photovoltaics. A number of factors determine mobility, such as molecular packing, electronic structure, dipole moment and polarizability. Presently, quantitative ab-initio models to assess the influence of these molecule-dependent properties, including the influence of dopants, are lacking. Here, we present a multi-scale model, which provides an accurate prediction of experimental data over ten orders of magnitude in mobility and demonstrate the de novo designg of a novel organic semicodunctor with improved mobility. The availability of first-principles based models to compute key performance characteristics of organic semiconductors may enable in-silico screening of numerous chemical compounds for the development of highly efficient opto-electronic devices.

HL 54.5 Fri 10:30 EW 203

High current density vertical electrolyte gated organic transistors — •Jakob Lenz[1] and Ralf Thomas Weitz[1,2] — [1]Physics of Nanosystems, Physics Department, Ludwig Maximilians Universität München — [2]NanoSystems Initiative Munich (NIM), Center for NanoScience (CeNS), Solar Technologies go Hybrid(SolTech)

In some areas of renewable energy high currents must be handled. For example, in the case of charging an electrical vehicle, currents of multiple Ampere need to be switched. Using conventional transistors for such a switching purpose is not an option since here typical current levels are in the muA to mA range. However, when utilizing a comparably novel concept, the so called vertical organic transistors (VOFETs), allows to reach current densities in the 1 A/cm^2 regime [1] where typically small molecules as semiconductor and conventional gating is utilized. Here, we show that using organic semiconducting polymers in combination with an ionic liquid even higher current densities up to 100 A/cm^2 can be realized.

[1] A. Fischer et al. Appl. Phys. Lett. 2012, 101, 213303

15 min. break.

HL 54.6 Fri 11:00 EW 203

Doping-induced Optimization of Organic Field Effect Transistors — •Marc-Michael Barf[1,2], Christian Willig[1,2,3], Robert Lovrincic[1,2], and Wolfgang Kowalsky[1,2,3] — [1]IHF, TU Braunschweig — [2]InnovationLab, Heidelberg — [3]KIP, Heidelberg University

Doping of organic semiconductors has become a common method to improve the efficiency of devices like organic light emitting diodes, organic solar cells and more recently also organic field effect transistors (OFETs). By increasing conductivity or creating space charge regions charge transport within such can be enhanced. Here, metal oxides are used to optimize charge carrier injection in p-type OFETs. Through the implementation of molybdenum oxide layers, it was possible to fabricate OFETs consisting of the polymer Poly[[(2,4-dimethylphenyl)imino]-1,4-phenylene(6,12-dihydro-6,6,12,12-tetraoctylindeno[1,2-b]fluorene-2,8-diyl)-1,4-phenylene] (PIF8-TAA) which are, to the best of our knowledge, the first of their kind that can be operated with silver contacts. This paves the way towards all-solution-processed devices. n-type OFETs were optimized using small molecules as dopants. The performance of OFETs consisting of the polymer Poly([N,N*-bis(2-octyldodecyl)-1,4,5,8-naphthalenedicarboximide-2,6-diyl]-alt-5,5*-(2,2*-bithiophene)) (N2200) could be improved significantly through a contact treatment with derivatives of 1,3-Dimethyl-2-phenyl-2,3-dihydro-1H-benzoimidazole (DMBI).

HL 54.7 Fri 11:15 EW 203

Three-dimensional photonic confinement in imprinted liquid crystalline pillar microcavities — •Marco Dusel[1], Simon Betzold[1], Sebastian Brodbeck[1], Stefanie Herbst[2], Frank Würthner[2], Daniel Friedrich[3], Bert Hecht[3], Christof P. Dietrich[1], and Sven Höfling[1,4] — [1]Technische Physik, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institut für Organische Chemie and Center for Nanosystems Chemistry, Universität Würzburg — [3]Nano-Optics and Biophotonics Group, Universität Würzburg — [4]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, UK

Organic semiconductors are used as an active material in laser cavities for more than 50 years where they have shown great versatility and flexibility and furthermore enable measurements to be conducted at room temperature. The most common organic cavity design is given by sandwiching an organic material between two highly reflective mirrors. However, those planar microcavities suffer from photonic losses within the layer plane.

Alternatively, we demonstrate three-dimensional photonic confinement in a planar organic microcavity by using thermal imprint technology to structure pillars in an organic liquid crystal (LC) on top of a mirror. After structuring, we evaporate Au on top to form the cavity. The so-fabricated pillar microcavities achieve three-dimensional photonic confinement. Our developed process brings the investigation of optical phenomena in much more complicated photonic potentials such as coupled pillars, chains or lattices, into reach.

HL 54.8 Fri 11:30 EW 203

Tuneable Light-Matter Hybridization in Open Organic Microcavities — •Simon Betzold[1], Marco Dusel[1], Stefanie Herbst[2], Jürgen Ohmer[3], Utz Fischer[3], Aurelien A. P. Trichet[4], Jason M. Smith[4], Frank Würthner[2], Sven Höfling[1,5], and Christof P. Dietrich[1] — [1]Technische Physik, University of Würzburg, Germany — [2]Institut für Organische Chemie and Center for Nanosystems Chemistry, University of Würzburg, Germany — [3]Institut für Biochemie, University of Würzburg, Germany — [4]Department of Materials, University of Oxford, United Kingdom — [5]SUPA, School of Physics and Astronomy, University of St Andrews, United Kingdom

Strong interaction between excitons and photons, e.g. in a semiconductor microcavity, lead to the formation of hybrid light-matter quasiparticles called exciton-polaritons. Frenkel excitons, characteristic of organic semiconductors, possess large binding energies, making polariton experiments at ambient conditions possible. Organic materials further exhibit large oscillator strenghts and thus strongly interact with a cavity field. Open cavities are tunable systems rendering non-invasive investigation possible and allow independent control of the excitonic and the photonic part (e.g. mode detuning). Here, we demonstrate the versatility of open cavities and examine the strong exciton-photon coupling between different organic systems (J-aggregates, proteins) and the dielectric cavity for 2D (planar) and 0D (hemispherical) cavities. We further analyzed the transversal mode patterns of the emission of hemispherical cavities.

HL 54.9 Fri 11:45 EW 203

Fano resonance in hybrid nanostructures - result of exciton-surface plasmon polaritons coupling — •Xuan Trung Nguyen[1], Antonietta De Sio[1], James Lim[2], Alexandra Markovic[3], Julia Witt[3], Moritz Gittinger[1], Martin Silies[1], Gunther Wittstock[3], Susana Huelga[2], Martin Plenio[2], and Christoph Lienau[1] — [1]Institut für Physik, Universität Oldenburg, Germany — [2]Institut für Theoretische Physik and IQST, Universität Ulm, Germany — [3]Institut für Chemie, Universität Oldenburg, Germany

The coupling between excitons and surface plasmon polaritons in organic-metal hybrid nanostructures has been subject of many studies. Using broadband spectral interferometry, we observe that the linear optical spectrum of a J-aggregate cyanine dye transforms from a symmetric Lorentzian into an asymmetric Fano line shape in the presence of an ultrathin gold layer. Reconstruction of both amplitude and phase of the linear optical response function in the time domain allows us to determine the Fano asymmetry parameter q as a phase shift with respect to the Lorentzian response function. We show that, in the frequency domain, q results in a rotation of the optical response in the complex plane . We explain the formation of the Fano resonance as the result of coupling between the J-aggregate excitons and surface plasmon supported by the dielectric-metal interface and quantitatively extract the coupling strength. This introduces a new and straightforward technique for probing the interaction between plasmons and quantum emitters, also at the single nanoparticle level.

HL 54.10 Fri 12:00 EW 203

Ultrafast dynamics through a conical intersection in a donor-acceptor oligomer thin film — Ephraim Sommer[1], •Antonietta De Sio[1], Johannes Krantz[2], Elena Mena-Osteritz[2], Peter Bäuerle[2], and Christoph Lienau[1] — [1]Institut für Physik, Universität Oldenburg, Germany — [2]Institut für organische Chemie II und neue Materialien, Universität Ulm, Germany

Conical intersections (CoIns) arising from strong multimode vibronic coupling are a universal feature of molecular systems. They are predicted to play a key role for the ultrafast dynamics of ubiquitous processes such as charge transfer in donor-acceptor (D-A) systems. However, clear experimental signatures of nonadiabatic dynamics at CoIns are challenging to obtain. Here we use ultrafast two-dimensional electronic spectroscopy to track the initial dynamics in an A-D-A oligomer thin film used in efficient organic photovoltaics (OPV). Upon impulsive excitation, we observe a clear grid-like peak pattern suggesting coherent wavepacket motion in the excited state. After only 40 fs, this peak structure transforms into a broad, nearly featureless peak. The data show an increase of oscillation period and concurrent, abrupt amplitude drop of the optically excited wavepacket within 40 fs, followed by the appearance of a new wavepacket with different oscillation. These results cannot be described in a single mode vibronic coupling scenario, as recently reported for some polymers [1,2]. They instead show that the initial intramolecular charge separation in this OPV material is governed by strong multimode vibronic coupling via a CoIn. [1] Nature Commun. 7,13742(2016), [2] PCCP 19,18813(2017)