CPP 22: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics I

Time: Tuesday 9:30–11:15 Location: ZEU/0260

Invited Talk CPP 22.1 Tue 9:30 ZEU/0260
From Solution to Thin Films: Structure Formation Pathways in Organic Photovoltaic Films — •Eva M. Herzig — Dynamik- und Strukturbildung - Herzig Group, University of Bayreuth, Germany

The performance of organic solar cells is governed by a delicate interplay between molecular packing, phase separation, and mesoscale connectivity in donor-acceptor blends. It is therefore highly desirable to control structure formation; however, this remains a non-trivial task. Several factors contribute simultaneously: the initial aggregation state in solution [1,2], the rapid structure formation during solution processing [2], and subsequent temperature- or solvent-annealing steps [3,4]. In this talk, I will discuss and illustrate with selected examples at which of these stages the final thin-film morphology can be controlled.

Using time-resolved and multimodal characterization methods, including grazing-incidence X-ray scattering and optical spectroscopy, we resolve the evolving structures during and after film deposition. These measurements reveal how subtle variations in processing conditions translate into distinct nanoscale morphologies.

[1] F. Eller & E. M. Herzig, J. Phys. Chem. A 2024, DOI: 10.1021/acs.jpca.4c04902

[2] F. Eller, R. Hildner, R. W. A. Havenith & E. M. Herzig, Small 2023, DOI: 10.1002/smll.202207537

[3] F. Eller, C. R. McNeill & E. M. Herzig, Adv. Energy Mater. 2024, DOI: 10.1002/aenm.202304455

[4] M. Kuhn, X. Huang, M. Gebert, L. Thomsen, C. R. McNeill & E. M. Herzig, Adv. Funct. Mater. 2025, DOI: 10.1002/adfm.202509532

CPP 22.2 Tue 10:00 ZEU/0260
DBTTF:HATCN Cocrystals – experimental details on influence of crystal solvents on crystal structure and on charge transfer — •Andreas Opitz[1], Ana M. Valencia[2], Lisa Schraut-May[3], Marie Siegert[3], Sebastian Hammer[3], Beatrice Cula[4], Alexandra Friedrich[5], Holger Helten[5], Jens Pflaum[3], and Caterina Cochi[6] — [1]Institut für Physik, Humboldt-Universität zu Berlin — [2]Institute of Physics, Carl-von-Ossietzky Universität Oldenburg — [3]Experimental Physics VI, Julius-Maximilians-Universität Würzburg — [4]Department of Chemistry, Humboldt-Universität zu Berlin — [5]Institute of Inorganic Chemistry & Institute for Sustainable Chemistry and Catalysis with Boron, Julius-Maximilians-Universität Würzburg — [6]Institute of Condensed Matter Theory and Optics, Friedrich-Schiller-Universität Jena

Donor-acceptor (D:A) cocrystals offer a promising platform for next-generation optoelectronic applications, but the impact of residual solvent molecules on their properties remains an open question. We investigate six novel D:A cocrystals of dibenzotetrathiafulvalene (DBTTF) and 1,4,5,8,9,11-hexaazatriphenylenehexacarbonitrile (HATCN), prepared via solvent evaporation, yielding 1:1 molar D:A ratios with solvent molecules in the structure, and horizontal vapor deposition, resulting in solvent-free 3:2 cocrystals. Optical properties of these materials are largely unaffected by solvent inclusion. The vibrational energy of the cyano mode depends on the dipole moment of the incorporated solvent molecules, but the degree of charge transfer is consistent across all analyzed cocrystals.

CPP 22.3 Tue 10:15 ZEU/0260
Reassessing Mobility Imbalance in Organic Photodetectors for High-Speed Applications — •Felix Hergenhan, Tianyi Zhang, Karl Leo, and Johannes Benduhn — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, Technische Universität Dresden

Organic photodetectors (OPDs) are emerging candidates for diverse optoelectronic applications, yet their use in high-speed technologies such as optical communication remains largely believed to be restricted by low effective charge carrier mobilities. To address this challenge, we investigated how the transient behavior of OPDs depends on the mobilities of the respective charge carriers. This relationship is examined through drift-diffusion simulations and experiments across various material systems, under varied bias and illumination conditions. We show, contrary to common assumptions, that obtaining only one fast charge carrier mobility is sufficient to achieve high response speed. Likewise, in systems with pronounced mobility imbalance, the slower carriers do not necessarily govern the maximum operation speed of the device. Leveraging these insights, we demonstrate an OPD tailored for optical communication that achieves data transmission rates up to 170 Mbps, representing one of the highest reported transmission rates for organic-based optical communication systems. These findings establish a refined design framework for ultrafast OPDs, providing guidance on material selection, device design, and operation regimes.

CPP 22.4 Tue 10:30 ZEU/0260
Rational Design of Donor-Acceptor Oligomers for Enhanced Charge Separation — •Jannik Theile[1], Michele Guerrini[2], Surender Kumar[2], and Caterina Cocchi[2] — [1]Physics Department and Center for Nanoscale Dynamics, Carl von Ossietzky Universität Oldenburg, Germany — [2]Physics Department for Solid-State Physics and Optics, Friedrich-Schiller Universität Jena, Germany

Intramolecular charge transfer (ICT) in donor-acceptor (D-A) oligomers is central to organic optoelectronics, yet symmetric D-A-D and A-D-A systems often suffer from delocalized frontier molecular orbitals (FMOs) that hinder efficient photoinduced charge separation. To address this, we present a first-principles study based on (time-dependent) density functional theory of 22 dithieno[3,2-b:2',3'-d]pyrrole oligomers, exploring the interplay between structural asymmetry and site-selective fluorination. Donor fluorination widens the electronic gap, while acceptor fluorination enhances charge imbalance and promotes confinement and spatial segregation of FMOs onto distinct molecular segments. The resulting optical properties reveal asymmetric, acceptor-fluorinated systems as optimal for ICT due to strong charge-transfer excitations with large oscillator strengths in the visible region. This work establishes rational design rules for conjugated D-A oligomers, showing that combining asymmetry with targeted halogenation is key to achieving robust, directional ICT and enabling high-performance organic semiconductors.

CPP 22.5 Tue 10:45 ZEU/0260
Substituted Benzo[*b*]fluorenes as Emitters for OLED With Tunable Electroluminescence in the Full Visible Range — •Pascal Schweitzer[1], Christopher M. Leonhardt[2], Cazibe Arslan[1], Hermann A. Wegner[2], and Derck Schlettwein[1] — [1]Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen — [2]Justus-Liebig-Universität Gießen, Institut für Organische Chemie, Heinrich-Buff-Ring 17, D-35392 Gießen

Organic light emitting diodes (OLED), despite widespread application in displays, still exhibit major challenges. The search for stable and efficient emitting molecules continues, especially in the blue range. Substituted benzo[*b*]fluorenes (BF) show high stability of photoluminescence in solution over months. By exchanging the substitutional pattern, we show that this group of molecules allows for preparation of OLED with tunable emission bands in the full range of the visible spectrum. Thin films of BF can be prepared by solution-based methods or physical vapor deposition, allowing for easy integration into different layer stacks. Photoluminescence spectroscopy of showcase BFs revealed a multi-band emission that is found in line with electroluminescence spectra of the corresponding devices. Contact formation at relevant device interfaces was studied by in-situ Kelvin-probe force microscopy and gave insight into details of film growth and alignment of transport levels. Based on these findings we demonstrate working OLED devices with intense blue or red emission, respectively.

CPP 22.6 Tue 11:00 ZEU/0260
Electrically switchable chiroptical responses in organic ferroelectric thin films — •Lorenz Friedrich Meier[1], Sophia Klubertz[1], Victor Rodriguez[2], Miguel García-Iglesias[2], David González-Rodríguez[3], and Martijn Kemerink[1] — [1]Heidelberg University, Germany — [2]Universidad de Cantabria, Spain — [3]Universidad Autónoma de Madrid, Spain

Organic ferroelectrics potentially allow to introduce switchable polarization into an easily processable material, enabling their integration into next-generation electronic devices. We investigate a liquid-crystalline organic ferroelectric that additionally can exhibit electrically controlled chiroptical responses, relevant for optical data storage, photonic components, and chiroptical sensing. We investigate thin films of trialkylbenzene-1,3,5-tricarboxamide (BTA). These molecules self-assemble into supramolecular columns by forming a triple helix of dipoles connected via hydrogen bonds. By incorporating chirally-biased sidechains, the handedness of the supramolecular helix can be defined. We experimentally show ferroelectric behavior in both in-plane and out-of-plane geometries by double wave and CV measurements. We demonstrate how the unpractically high coercive fields for pure chiral BTA can be reduced by mixing with achiral BTA. Previous simulations show that the energetically preferred mechanism of polarization reversal of a supramolecular column will simultaneously change its chirality. Thus, an electrically switchable chirality is possible. We present an experimental investigation of this mechanism, discussing the challenges including the need for dipole pre-alignment.