CPP 40: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics IV

Time: Wednesday 17:00–18:30 Location: ZEU/LICH

CPP 40.1 Wed 17:00 ZEU/LICH

Morphological Disorder Boosts Charge Separation in Single-Component OPDs — •Michel Panhans[1], Jakob Wolansky[2,3], Karl Leo[2], Johannes Benduhn[2,3], and Frank Ortmann[1] — [1]TUM School of Natural Sciences and Atomistic Modeling Center, Munich Data Science Institute, Technische Universität München, 85748 Garching b. München, Germany — [2]Dresden Integrated Center for Applied Physics and Photonic Materials, Technische Universität Dresden, 01069 Dresden, Germany — [3]DZA, Görlitz, Germany

Single-component organic photodetectors (OPDs) provide a simplified alternative to donor-acceptor heterojunctions, yet their operation mechanisms remain theoretically underexplored. We investigate the molecular origin of charge generation in vapor-deposited DCV2-5T by modeling the excitonic density of states with an effective exciton Hamiltonian that incorporates electronic coupling, Coulomb interaction, and structural disorder. Disorder is introduced through lateral shifts between π-stacked molecules, which notably modulates electronic and excitonic couplings. Simulations show that intermediate disorder reproduces the experimental external quantum efficiency, while strong disorder enhances hybridization between excitonic states. This hybridization enables exciton delocalization via a superexchange-like mechanism, increasing the probability of charge separation. Counterintuitively, disordered domains exhibit stronger coupling than crystalline ones, suggesting that reduced structural order can facilitate charge generation. These insights highlight morphology-dependent excitonic interactions as a design principle for self-driven OPDs.

CPP 40.2 Wed 17:15 ZEU/LICH

Limiting factors to free charge generation in low-bandgap organic blends for photovoltaic applications and beyond — •Manasi Pranav[1], Atul Shukla[1,2], and Dieter Neher[1] — [1]University of Potsdam, Potsdam, Germany — [2]University of Queensland, Brisbane, Australia

Despite possessing similar theoretical limits, state-of-the-art organic solar cells outshine low-bandgap organic blends (absorption edge beyond 1000 nm) in their exciton harvesting efficiency. An understanding of these free charge generation mechanisms is needed to tap into the potential of such low-bandgap non-fullerene acceptors (NFAs) for photovoltaic and photodetector applications. To this end, we probe the pathways of exciton dissociation and charge-transfer state separation in multiple D:NFA systems with varying absorption edges, and varying extents of energy-transfer or charge-transfer prior to free charge generation. This is done by combining transient and steady-state optoelectronic techniques, to resolve the losses incurred between photon absorption and carrier extraction. For some of these systems, namely in blends using Y6 derivatives with extended pi-conjugation, we find that the kinetic competition between geminate charge-transfer state decay and its separation is a major limiting role in the overall photon harvesting capability of the devices. As part of ongoing work, these investigations aim to reveal the underlying geminate loss pathways, which limit overall internal quantum efficiency of the blends and, in turn, limit the figures of merit of the resulting devices.

CPP 40.3 Wed 17:30 ZEU/LICH

Consistency of Electron-Vibrational Coupling Across Methods? A Comparative Study — •Maximilian F. X. Dorfner, Konrand Merkel, and Frank Ortmann — Department of Chemistry, TUM School of Natural Sciences, and Atomistic Modeling Center, Munich Data Science Institute, Technical University of Munich, München, Germany

Characterizing electron-vibrational interaction in materials is a non-trivial theoretical task, owing to the differing definitions of coupling constants and the variety of available methods for computing these. This diversity naturally raises questions about the consistency and reliability of the methods used and their interrelation.

To address this issue, this contribution presents a systematic comparison of electron-vibrational coupling calculations. We summarize our findings on the relationship between density functional theory approaches and quasi-particle methods [1], study the influence of different exchange and correlation functionals, and investigate the impact of various ab initio methodologies [2] on the resulting electron-vibrational coupling constants.

Our findings provide guidelines and data for validating methodologies and estimating theoretical errors in coupling constant calculations.

[1] M.F.X. Dorfner and F. Ortmann, J. Chem. Theory Comput. 2025, 21, 5, 2371-2385; [2] K. Merkel, M.F.X. Dorfner and F. Ortmann, J. Phys. Mater. 8 045014

CPP 40.4 Wed 17:45 ZEU/LICH

Enhanced Photo-multiplication Effect through Synergistic Hole Blocking and Traps Engineering in OPDs — •Awais Sarwar[1], Louis Conrad Winkler[1,2], Karl Leo[1], and Johannes Benduhn[1,2] — [1]IAPP, TU Dresden, Germany — [2]DZA, Görlitz, Germany

Photomultiplication-type organic photodetectors (PM-OPDs) are highly effective for detecting weak light. However, they often face a significant trade-off: high gain usually results in excessive noise and slow response times. To overcome these limitations, we introduce a vacuum-deposited broadband photodetector architecture that utilizes the synergistic integration of hole-blocking layers and precise traps engineering. By strategically controlling the charge injection barriers and trap distribution, this design effectively separates the gain mechanism from the noise floor. The resulting device achieves a peak external quantum efficiency (EQE) exceeding 1100 per cent, while maintaining a specific detectivity of 4.4*10e12 Jones at a bias of -2 V. Unlike slow trap-dominated systems, our optimised architecture keeps a cut-off above 25 kHz. Vacuum-deposited PM-OPDs offer high sensitivity and fast response, ideal for real-time sensing.

CPP 40.5 Wed 18:00 ZEU/LICH

Wavelength-dependent charge carrier extraction of organic solar cells under operational conditions — •Lara Bartnick, Martijn Kemerink, and Clemens Göhler — IMSEAM, Heidelberg University, Germany

Organic solar cells (OSCs) have recently achieved power-conversion efficiencies of about 20%, making them increasingly promising for renewable energy applications despite still falling behind silicon photovoltaics. To understand the mechanisms that limit their performance, highly sensitive external quantum efficiency (EQE) measurements are essential, as they show how efficiently photons of different energies generate extractable charge carriers across the UV- to near-infrared spectrum.

We have measured the EQE of current standard PM6:Y6 OSCs under different initial conditions including bias voltage in both reverse and forward direction, bias illumination, and temperature, to investigate how open-circuit voltage- and fill-factor losses can be attributed to wavelength-dependent charge carrier generation efficiencies. These measurements reveal that the spectral shape of the EQE is highly sensitive to biasing conditions. By relating the voltage dependent EQE to collection fields, we have been able to identify charge carrier extraction losses under typical working conditions, which are dependent on the incident photon energy. These findings, as well as wavelength- and voltage-dependent exciton generation and recombination rates, contribute to understanding the loss mechanisms and charge extraction behaviour of OSCs.

CPP 40.6 Wed 18:15 ZEU/LICH

Current Generation in Photomultiplication-type Organic Photodetectors — •Louis Conrad Winkler[1,2], Jonas Kublitski[1,3], Awais Sarwar[1], Hrisheekesh Thachoth Chandran[1], Wolfgang Tress[4], Urs Aeberhard[5], Karl Leo[1], and Johannes Benduhn[1,2] — [1]IAPP, TU Dresden, Germany — [2]DZA, Görlitz, Germany — [3]Departamento de Fisica, UTFPR, Curitiba, Brazil — [4]ZHAW, Winterthur, Switzerland — [5]FLUXiM, Winterthur, Switzerland

Organic photodetectors (OPDs) utilizing intrinsic gain promise enhanced performance in regard to faint light detection. While this gain mechanism boosts the external quantum efficiency (EQE), the associated noise often negates the net improvement of the specific detectivity D*. Nonetheless, the simplified readout circuitry and associated cost savings hold high potential for the market. Crucially, the origin of this photomultiplication (PM) effect is currently attributed to tunnel injection of charge carriers, driven by internal band bending due to trapped charge carriers. Here, we challenge this prevailing tunnel injection model based on comprehensive experimental evidence. We propose an alternative mechanism that offers a unified explanation for the gain observed across diode-like OPD architectures and validate it by drift-diffusion simulations. This model successfully provides general predictive capabilities regarding the magnitude and dependencies of the photocurrent gain. We rigorously tested this proposed mechanism across 29 diverse material systems, including both vacuum-processed and solution-processed devices.