CPP 37: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics III

Time: Wednesday 15:00–16:45 Location: ZEU/LICH

Invited Talk CPP 37.1 Wed 15:00 ZEU/LICH

Predicting molecular ordering in deposited molecular films — •Denis Adrienko — Max Planck Institute for Polymer Research, Mainz, Germany

Thin films of molecular materials are commonly employed in organic light-emitting diodes, field-effect transistors, and solar cells. The morphology of these organic films is shown to depend heavily on the processing used during manufacturing, such as vapor co-deposition. However, the prediction of processing-dependent morphologies has until now posed a significant challenge, particularly in cases where self-assembly and ordering are involved. In this work, a method is developed based on coarse-graining that is capable of predicting molecular ordering in vapor-deposited films of organic materials. The method is tested on an extensive database of novel and known organic semiconductors. A good agreement between the anisotropy of the refractive indices of the simulated and experimental vapor-deposited films suggests that the method is quantitative and can predict the molecular orientations in organic films at an atomistic resolution [1]. The methodology can be readily utilized for screening materials for organic light-emitting diodes.

[1] C. Scherer, N. Kinaret, K.-H. Lin, M. N. Qaisrani, F. Post, F. May, D. Andrienko, Adv. Energy Mater., 14, 2403124, 2024

CPP 37.2 Wed 15:30 ZEU/LICH

A Universal Soft Upper Limit to the Seebeck Coefficient in Organic Thermoelectrics — •Dorothea Scheunemann[1], Zelong Li[2], Dennis Derewjanko[1], Yuqian Liu[2], Martijn Kemerink[1], and Guangzheng Zuo[2] — [1]Heidelberg University, Germany — [2]Fudan University, Shanghai, P.R. China

Organic thermoelectrics have the potential to convert waste heat into electricity by utilizing lightweight and flexible polymers. Despite over a decade of intensive research, significant progress remains limited. A key factor is the trade-off between conductivity (σ) and Seebeck coefficient (S), which dictates the extent to which the power factor ($PF = \sigma S^2$) can be optimized. Here, we combine an experimental data set for different polymers at variable doping levels to show that the S vs. σ curve is universal up to the maximum PF, followed by a material-dependent roll-off, when S and σ are normalized to their values at maximum PF. Furthermore, it is demonstrated that there is a soft upper limit for S ($\sim$200μV/K), at which the optimal power factor is achieved. Combining tight-binding and kinetic Monte-Carlo modeling, we quantitatively explain this behavior in terms of quasi-free charges moving in a renormalized density of states of Gaussian shape, where the renormalization accounts for the screened interaction with the ionized dopants. These findings suggest that the trade-off only exists at the single-material level, which subsequently gives rise to practical design rules.

CPP 37.3 Wed 15:45 ZEU/LICH

Nanoscale Dry-Processed Phosphorescent Films for Programmable Photonic Applications — •Yana Bui Thi, Sebastian Schellhammer, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, Technische Universität Dresden

Room-temperature phosphorescence (RTP) of organic materials provides a versatile basis for applications in environmental detection, security features, and optical data storage. Many of these concepts, including programmable luminescent tags (PLTs) [1], rely on precise control of triplet states, which poses certain challenges in terms of stability and processing. While polymer matrices are commonly used to suppress non-radiative decay, their processing limitations have restricted the miniaturization and control of devices. Here, we introduce ultrathin RTP tags that are produced entirely solvent-free and use organic materials as active layer. These nm-sized stacks exhibit higher efficiency and can be more than twenty times thinner than polymer-based structures. We characterize the resulting activation dynamics, stability, and reusability and discuss how the processing enables improved uniformity and the possible integration with structuring techniques. These results demonstrate a path toward compact, low-energy, and precisely controllable luminescent tags for future photonic technologies.

[1] Gmelch et.al. High-Speed and Continuous-Wave Programmable Luminescent Tags Based on Exclusive Room Temperature Phosphorescence (RTP). Adv Sci. 2021 (23):e2102104.

CPP 37.4 Wed 16:00 ZEU/LICH

Probing the percolating charge transport network in organic semiconductors by noise spectroscopy — •Sebastian Klein, Priya Viji, Constantin Tormann, Clemens Göhler, and Martijn Kemerink — IMSEAM, Heidelberg University, Germany

In disordered organic semiconductors (OSCs), a suppression of shot noise is expected due to the internal charge carrier transport mechanisms, which is relevant for, e.g., their application in photodetectors. The charge transport in OSCs, which occurs by hopping between localized sites, can be described by percolation theory, from which it follows that so-called hard hops form the bottleneck that charge carriers have to overcome to progress through the device. The tunneling through one singular hard hop is a random uncorrelated poissonian process which leads to OSCs displaying shot noise. Since multiple hard hops sit in series in the charge transport path in macroscopic OSCs, it is expected that shot noise in OSC is suppressed, inversely proportional to the number of hard hops, which in turn depends on disorder, temperature and thickness of the OSC. This suppression is quantified by the Fano factor, which we directly measure by current cross-correlation noise spectroscopy. Temperature- and current-bias-dependent Fano factor measurement results are compared with kinetic Monte Carlo simulations. From the measurements and simulations, it can consistently be concluded that Fano factor measurements give direct and otherwise inaccessible insight into the internal structure as well as the disorder and correlation length of OSC.

CPP 37.5 Wed 16:15 ZEU/LICH

Charge transfer dynamics in PBDB-T blends studied by time-resolved optical spectroscopy — Beatriz Molinaro Guerra[1], Federico Cilento[2], Maria Luiza Miranda Rocco[1], and •Wibke Bronsch[2] — [1]Institute of Chemistry, Federal University of Rio de Janeiro, 21941-909, Rio de Janeiro-RJ, Brazil — [2]Elettra-Sincrotrone Trieste S.C.p.A., 34149 Basovizza, Trieste, Italy

Charge transport processes in conjugated polymers are an important key for the production of more efficient organic optoelectronic devices, such as organic solar cells. Specially, the study of electron charge transfer dynamics in excited states may help us to understand charge transport properties in these materials. We studied the ultrafast response of different blends of PBDB-T polymers with small molecules after NIR excitation. Time-resolved optical spectroscopy measurements with broad-band probe pulses performed in the T-ReX facility at Elettra reveal clear changes in the ultrafast response when comparing the results for the pure molecule films and the blends, suggesting that charges are transferred between the two components of the blend on the femto- to picosecond timescale. After exciting the HOMO-LUMO transition of the ITIC molecule, the exciton population decay time drastically reduces due to the presence of the PBDB-T polymer, while the decay constant at photon energies in the range corresponding to the PBDB-T HOMO-1-LUMO transition increases. This behavior indicates hole injections in PBDB-T after primary excitation of ITIC, as it was also discussed for PBBF:ITIC blends [1]. [1] Liu et al. Advanced Science 6, 1802103 (2019).

CPP 37.6 Wed 16:30 ZEU/LICH

Analysis of Charge Carrier Dynamics in Organic Solar Cells via Optical Impedance Spectroscopy — •Elias Wassmer, Jan Phillip Ott, Brian Hinz, Clemens Göhler, and Martijn Kemerink — IMSEAM, Heidelberg University, Germany

Understanding the complex dynamics of charge carriers in organic solar cells (OSCs) is essential to identify the mechanisms that lead to voltage, current and fill factor losses. In this work, we investigate these dynamics by combining conventional electrical impedance spectroscopy (EIS) with the newly implemented optical impedance spectroscopy (OIS). In OIS, in addition to a constant background illumination, a small alternating light signal is applied to investigate the photogenerated charge carriers under quasi-steady-state conditions. The results of both EIS and OIS of PM6:Y6 OSCs across a range of operating conditions are used to compare the two methods and allow us to track changes during device degradation. To interpret the measured impedance spectra, two established models are applied: an equivalent-

circuit model, which maps the behaviour of the OSC onto a network of resistances and capacitances, and a rate-equation model that describes carrier generation, recombination and extraction through differential equations. Comparing these modelling approaches allows us to evaluate how well the charge-carrier dynamics are captured by each model and how this relates to the physical processes inside the OSCs. Our results show that the equivalent-circuit model is insufficient for describing OIS, indicating that a more physically motivated rate-equation model is needed to reproduce photogenerated carrier dynamics.