# HL 53: Organic Semiconductors: Carrier Dynamics

Time: Friday 9:30–11:15 Location: POT/0051

**Invited Talk** HL 53.1 Fri 9:30 POT/0051

**Organic semiconductors: Opening new perspectives in sustainable electronics** — •Karl Leo — IAPP, TU Dresden

Organic semiconductors enable a variety of novel applications for flexible, lightweight, and environmentally friendly electronics. One unique advantage of these carbon-based materials is their compatibility with body tissue, thus opening perspetives for completely new medical applications on and even in the human body. Furthermore, the materials set available in this technology allows biodegradability and thus sustainable electronics without the serious environmental issue of conventional electronics. In the first part of my talk, I will show examples how organic electronic devices can be used in postsurgical monitoring, avoiding life-threatening complications. In the second part of the talk, I will address lignocellulose leaf skeleton structures (Leaftronics) as basis for a variety of novel applications, such as semitransparent electrodes.

HL 53.2 Fri 10:00 POT/0051

**Unveiling the role of disorder on carrier concentration transients in electrochemical transistors** — •Tobias Krebs and Martijn Kemerink — IMSEAM, Heidelberg University, Germany

Already the drain current transients in organic electrochemical transistors hint for not yet fully understood underlaying device physics, as they show a generally slower turn on compared to turn off, with the difference between these on- and off- switching times varying over orders of magnitude between materials and driving voltages. Tracking the charge carrier concentration during switching then completes this asymmetric picture: A sharp doping front entering the device during turn on, followed by gradual bulk de-doping during turn off. We measure these concentration transients optically, using the red-shifted absorption in the doped state of the redox active polymers we investigated. Comparison of this data with drift-diffusion simulations revealed a strong dependence of this asymmetry on the broadness of the density of states, which in our simulations both modulates the carrier density dependence of hole mobilities and influences the maximum charge carrier concentration for a set gate voltage. Our simulation framework also allowed us to study the surprisingly small effect of ionic mobilities in the semiconductor on switching times, above a device specific mobility threshold. The results can be used to guide the rational design of improved devices.

HL 53.3 Fri 10:15 POT/0051

**Simulation of Coulomb Glass Behavior in Organic Semiconductor Devices at high carrier densities** — •Magdalena Dörfler[1], Heinz Bässler[2], Anna Köhler[1,2], and Harald Oberhofer[3] — [1]Soft Matter Optoelectronics and Bayerisches Polymerinstitut (BPI), Experimental physics II, University of Bayreuth, Universitätsstr. 30, 95448 Bayreuth, Germany — [2]Bayreuth Institute of Macromolecular Research (BIMF), University of Bayreuth, Universitätsstr. 30, 95448 Bayreuth, Germany — [3]Chair for Theoretical Physics VII and Bavarian Center for Battery Technologies, University of Bayreuth, Universitätsstr. 30, 95448 Bayreuth, Germany

Recent advances in organic transistors (OFETs, EGOFETs, OECTs) enable device operation at high charge carrier densities where Coulomb interactions between carriers become significant.

Using Kinetic Monte Carlo simulations, we investigate carrier-carrier Coulomb interactions in OFET-like structures. Comparing simulations with and without these interactions reveals reduced carrier mobility and increased activation energy when interactions are included, with effects increasing for higher carrier densities.

Our results indicate a transition to correlated transport with a Coulomb gap in a dynamic density of states. The system exhibits Coulomb glass behavior, where the activation energy reflects structural reorganization of the carrier ensemble.

Notably, the Coulomb gap appears at ambient temperature and does not require variable-range hopping, unlike to the situation in electron liquids and inorganic semiconductors.

HL 53.4 Fri 10:30 POT/0051

**Dual Ferroelectric and Semiconducting behaviour in supramolecular organics** — •Tara Vollus[1], Sophia Klubertz[1], Shyamkumar Vadakket Haridas[2], Oleksandr Shysho[2], Max von Delius[2], and Martijn Kemerink[1] — [1]IMSEAM, Heidelberg University, Germany — [2]Institute of Organic Chemistry, Ulm University, Germany

The combination of interacting conductive and ferroelectric properties, resulting in a multifunctional material, has the potential to simplify the structure of memory devices. It has been demonstrated that the organic ferroelectric material C6H6F5O-C3-amide (M3) exhibits both these properties, showing ferroelectricity and an unexpected DC conductivity.[1][2] It has been shown that the latter is related to the presence of interfacial dipoles that allow efficient charge injection from (oxidation and/or reduction by) metal contacts and is enhanced by a supramolecular arrangement formed at higher temperatures and under an applied electric field. Here, we demonstrate the effects of alignment and, especially, the presence of both n- and p-type doping-like processes, suggesting that M3 is a wide-bandgap organic semiconductor that reversibly can be reduced and oxidized. Kelvin probe force microscopy measurements revealed filament-like potential structures that may act as pathways for bipolar charge transport, and suggest the formation of dynamic pn-junctions.[3]

[1] Mager et al., arXiv:2507.11309 [cond-mat.mtrl-sci] [2] Mager et al., arXiv:2506.02673 [cond-mat.mtrl-sci] [3] Matyba et al., DOI:10.1038/nmat2478

HL 53.5 Fri 10:45 POT/0051

**Backbone Alignment and Morphology Formation in PBTTT Thin Films: Insights from In-Situ GIWAXS** — •Robin M. Teichgreber[1], Christopher R. McNeill[2], and Eva M. Herzig[1] — [1]Dynamics and Structure Formation - Herzig Group, University of Bayreuth, Universitätsstraße 30, 95447 Bayreuth, Germany — [2]Material Science and Engineering, Monash University, 20 Research Way, Clayton

The performance of organic electronic devices strongly depends on the morphology of the organic semiconductor thin film [1]. Enhancing the understanding on fundamental structure-function relationships is therefore crucial to improve the performance of such devices in the future. Highly aligned films can furthermore be used to study fundamental charge separation processes. Controlling the alignment of polymer backbones is a challenge in the first place, demanding further research on the processes of structure formation resulting in aligned films. Using PBTTT as a model system, the influence of different coating parameters on the kinetics of film formation during the deposition thin films via blade-coating is investigated by employing time-resolved in-situ GIWAXS measurements. Furthermore, the formation of high degrees of alignment during the post-deposition annealing process was studied with temperature-resolved GIWAXS. [1] Herrmann, N.J., von Coelln, N., Teichgreber, R.M., Höfener, S., Huck, C., Ghalami, F. et al. (2023) J. Mater. Chem. C, 11, 10185-10197.

HL 53.6 Fri 11:00 POT/0051

**Multiscale Modelling of the Density of States in PEDOT:Tosylate Films** — •Melissa Kim Meinel and Igor Zozoulenko — Laboratory of Organic Electronics, Linköping University, Norrköping, Sweden

A key descriptor of the electronic structure is the density of states (DOS), which directly affects properties such as charge mobility, intrinsic capacitance, and optical absorption. Structural disorder and the local electrostatic environment strongly influence the DOS but are rarely captured in full detail in computational studies that often rely on small model systems or simplified methods. We present a multiscale modelling approach for computing the DOS of realistic PEDOT:Tosylate films. Molecular dynamics simulations generate film structures that capture the complex packing and disorder of PEDOT chains and counterions. These configurations are analysed within a quantum mechanical/molecular mechanical (QM/MM) framework, where molecular mechanics accounts for large-scale heterogeneity while quantum calculations resolve local electronic states under explicit electrostatic embedding of the environment. Steric effects are treated at the MM level, while the QM region can be limited to a single chain. Accurate results require optimally tuned range-separated hybrid functionals, geometry optimisation of the QM chain, and iterative adaptation of charge distributions to capture realistic environmental effects. This framework enables quantitatively realistic, morphology-sensitive predictions of the electronic structure and has been applied to systems at different oxidation levels.