HL 41: Organic Semiconductors 2

Time: Friday 9:30–10:45 Location: H34

HL 41.1 Fri 9:30 H34

Understanding structure-to-property relationships for phonons and thermal transport in hydrogen-bonded organic semiconductors. — •Lukas Legenstein, Lukas Reicht, Tomas Kamencek, Sandro Wieser, and Egbert Zojer — Institute of Solid State Physics, Graz University of Technology, Graz, Austria

Research on organic semiconductors (OSC) has primarily focused on their (opto-)electronic properties. The understanding of phonons in these materials is, however, still rather poorly developed, despite their crucial role for charge and heat transport processes. Of central importance in this context are lattice phonons dominated by translations and rotations of entire molecules, which are coupled through non-covalent interactions. To elucidate how non-covalent bonding types such as H-bonding and π-π interactions affect phonons in otherwise vdW-stacked OSCs, we simulate the phonon bands of crystalline quinacridone (QA), as a prototypical H-bonded OSC. Notably, QA forms polymorphs with fundamentally different crystal structures, which strongly impact the observed phonons. The obtained phonon bands show complex dispersions with avoided crossings and mode hybridisations due to a mixing of inter- and intra-molecular vibrations. The phonons are simulated combing the phonopy package with density-functional theory employing the FHI-aims and VASP codes. The calculated phonon band structures are also used for benchmarking on-the-fly trained machine learning force fields calculated with VASP, which are then employed for modelling thermal transport within the Green-Kubo formalism.

HL 41.2 Fri 9:45 H34

Regiochemistry of Donor-Dendrons Controls the Performance of TADF Dendrimer based OLEDs — •Rishabh Saxena[1], Dianming Sun[2], Stavros Athanasopoulos[1], Eli Zysman-Colman[2], and Anna Köhler[1] — [1]University of Bayreuth, Germany — [2]University of St. Andrews, UK

The potential of dendrimers exhibiting thermally activated delayed fluorescence (TADF) as emitters in solution-processed organic light-emitting diodes (OLEDs) has to date not yet been realized. This in part is due to a poor understanding of the structure-property relationships in dendrimers where reports of detailed photophysical characterization and mechanism studies are lacking. In this study, we investigated dendrimers with multiple dendritic electron-donating moieties connected to a central electron-accepting core via a para- or a meta-phenylene bridge. Characterization of host-free OLEDs revealed the superiority of meta-dendrimers as compared to the already reported para-analogue. Photophysical investigations in the films showed that, although all the dendrimers possess similar singlet-triplet energy gap, normally implying similar reverse intersystem crossing (RISC) rate, better TADF properties are obtained for meta-dendrimers when compared to para-dendrimers. In this regard, what this study reveals is that the reorganization energy can play an important role in enhancing RISC rate and that this can be modulated as a function of the regiochemistry of donor dendron about the acceptor. This is a heretofore unexploited strategy and can be used as a general chemical design principle, especially in the case of bulky dendrimers.

HL 41.3 Fri 10:00 H34

Optical Vortices in Hemispherical Organic Microcavities — •Johannes Düreth[1], Simon Betzold[1], Marco Dusel[1], Monika Emmerling[1], Jürgen Ohmer[2], Utz Fischer[2], Christian Schneider[3], Sven Höfling[1], and Sebastian Klembt[1] — [1]Technische Physik, RCCM and Würzburg-Dresden Cluster of Excellence ct.qmat, University of Würzburg, Germany — [2]Department of Biochemistry, University of Würzburg, Germany — [3]Institute of Physics, University of Oldenburg, Germany

Light can carry two different kinds of angular momentum: spin angular momentum (SAM), which is associated with polarization, and orbital angular momentum (OAM), which occurs in light with spiral phase fronts. In recent years, it has been shown that rotational symmetry of a microcavity systems leads to an effective spin-orbit coupling of the SAM and the OAM of photons, resulting in new polariton eigenstates.

Here, we study helical Laguerre-Gaussian modes $LG_{0\pm1}^{\sigma_\pm}$ formed in such systems. For a total angular momentum of $J = 0$, both eigenstates are radially and azimuthally polarized, respectively. Due to the spatial dependence of the linear polarization, we measure spin vortices for these modes. In contrast, the energetically degenerate modes with $J = 2$ exhibit opposite circular polarization and carry an optical OAM with opposite chirality. Accordingly, phase vortices with opposite sign were measured by polarization-dependent interference measurements.

Moreover, we show that the preservation of pump polarization allows selection of the optical OAM of ±1.

HL 41.4 Fri 10:15 H34

Experimental and theoretical studies of the occupied density of states distribution of charge carriers at low temperatures in disordered organic semiconductors — •Andrei Stankevych, Rishabh Saxena, Heinz Bässler, Andrey Kadashchuk, and Anna Köhler — Soft Matter Optoelectronics and Bavarian Polymer Institute (BPS), Universitätsstrasse 30, 95448 Bayreuth, Germany

The thermally-stimulated luminescence (TSL) technique has been applied to determine the width of density of state (DOS) distribution σ_{DOS} in pristine amorphous films of 18 common OLED materials. The high-temperature wing of the TSL curve in amorphous materials is an exact replica of the deeper portion of the DOS distribution and yields the effective DOS width. In addition, we measured the width of the TSL curves σ_{TSL} and found that it scales linearly with σ_{DOS} parameter, suggesting an existence of a universal ratio σ_{TSL} / $\sigma_{DOS} \approx 2/3$ observed for a large set of organic materials. The low-temperature energy relaxation of photogenerated carriers within a Gaussian DOS implies a significant narrowing of the ODOS distribution. In order to gain a deeper insight into this effect, we performed extensive Monte-Carlo simulations of charge-carrier energetic relaxation process and found that such "spectral narrowing" effect is a genuine property of the hopping carrier relaxation at low temperature within a Gaussian DOS. Moreover, we found that spatial energy correlation effects, which are indeed present in organic media, must be considered for the quantitative description of experimental observations.

HL 41.5 Fri 10:30 H34

Exploring the interplay of oriented molecules and device performance by post-annealing studies of organic light-emitting diodes — •Dinara Samigullina, Christian Hänisch, Karl Sebastian Schellhammer, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, Technische Universität Dresden, Germany

Organic light-emitting diodes (OLEDs) have been widely investigated in the last decades exploring strategies to enhance their performance. Nevertheless, a thorough understanding of the microscopic processes during the thin-film formation and morphology evolution is quite challenging and under debate in many facets. In this work, we present a comprehensive study of the influence of post-annealing on the optoelectronic performance of OLEDs. In addition to standard characterisation techniques such as spectroscopy and electrical measurements, we use impedance spectroscopy in order to probe the change in polarisation of organic thin films depending on the annealing temperature. We show, how the orientation of permanent dipole moments (PDMs) in thin films can be manipulated by post-annealing and connect this to improved electrical performance. Moreover, angle-resolved emission spectra reveal the influence of heating on the orientation of the transition dipole moment (TDM) of emitting molecules. In such manner, the correlation between annealing temperature and orientation of PDMs and TDMs is studied while taking into consideration the optoelectronic properties of OLEDs.