CPP 39: Focus: Triplet States in Organic Optoelectronics II

Time: Wednesday 15:00–16:30 Location: H37

Invited Talk CPP 39.1 Wed 15:00 H37

The Nature of the 'Triplet Pair State' in Singlet Exciton Fission. — •Jenny Clark[1], Andrew Musser[2], Chaw Keong Yong[2], and Daniel Polak[1] — [1]University of Sheffield, Hicks Buildling, Hounsfield Road, S3 7RH, Sheffield, United Kingdom — [2]University of Cambridge, J J Thomson Avenue, Cambridge CB3 0HE, United Kingdom

Singlet exciton fission is a process by which the bright singlet (spin-0) exciton spontaneously splits into two triplet (spin-1) excitons. The triplets are initially coupled into an overall singlet state, conserving spin. Over time the triplets lose their correlation and become 'free triplets'. The nature of the intermediate state, which may be described as a correlated (entangled) triplet pair has been the subject of debate.

In this talk, I will discuss our recent work describing the nature of the intermediate triplet-pair state and its fate: how it either (i) separates into free triplets; (ii) emits a photon; (iii) returns to the singlet manifold or (iv) in a suitable blend, undergoes double charge-transfer.

I will talk about two material classes: acenes and polyenes and highlight how their different electronic properties affect the process of singlet exciton fission and its potential to be exploited to enhance solar cell efficiency.

CPP 39.2 Wed 15:30 H37

Triplet state formation in polymer:fullerene bulk heterojunction blends — •Frédéric Laquai — Solar and Photovoltaics Engineering Research Center (SPERC), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Kingdom of Saudi Arabia — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Triplet state formation is currently being discussed as a potential loss channel in state-of-the-art bulk heterojunction organic solar cells. However, the precise mechanism of triplet state formation, the relation between the material's chemical structure, film morphology and triplet state yield, and its impact on device performance is still unknown. Here, we present recent spectroscopic results obtained by a combination of fs-ms broadband transient absorption spectroscopy and multivariate curve resolution (MCR) data analysis on two prototypic low-bandgap donor-acceptor copolymers, namely PCPDTBT and its silicon-substituted analogue PSBTBT, in blends with fullerene as acceptor indicating that not only the respective energy levels, but also the solid-state morphology and interfacial structure of the blends influence triplet state formation. These studies have very recently been extended to other common donor polymers including DPP-based materials and PBDTTT-C blends, two systems for which we observe very high triplet yields and in the latter case also recreation of charges due to fast triplet-triplet annihilation on the ns-ms timescale.

CPP 39.3 Wed 15:45 H37

Quantifying Spin-Dependent Recombination in Organic Bulk Heterojunction Solar Cells — •Stefan Väth[1], Andreas Sperlich[1], Andreas Baumann[2], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

In donor-acceptor (DA) based bulk-heterojunction (BHJ) solar cells, the splitting of singlet excitons at the DA interface is crucially important for charge generation. The reversed process, in which two initially free charge carriers meet at the DA interface and recombine is considered as the main recombination process. The intermediate charge transfer state possesses three triplet and one singlet spin configuration which makes the non-geminate recombination process spin dependent. The role of the spin, however, is under continuous discussion and still not clarified yet.

In our experiments, the influence of spin dependent recombination was investigated for organic BHJ solar cells made of the benchmark material system P3HT:PCBM at real operation conditions. For the first time, we combined electrically detected magnetic resonance (EDMR) with the quantitative technique of open circuit corrected transient charge extraction (OTRACE). Extracting photo generated charges under magnetic resonant conditions compared to non-resonant conditions yields in a spin-dependent contribution to the overall recombination of 0.01 % in this particular solar cell system.

CPP 39.4 Wed 16:00 H37

The Nature of Fluorescence Quenching in Single Conjugated Polymer Chains vs. Mesoscopic Aggregates — •Florian Steiner, Jan Vogelsang, and John M. Lupton — Department of Experimental and Applied Physics, University Regensburg, Germany

The photophysics of isolated chains and a bulk film of conjugated polymers (CP) such as poly(3-hexylthiophene) (P3HT) differ substantially. Most prominently, the fluorescence quantum yield drops by at least one order of magnitude upon the transition from dissolved chains to bulk film. The mechanisms behind these differences however are still not fully understood. Here we show that we can clarify the question of fluorescence quenching in CP by using single-particle spectroscopy techniques which can be applied to single polymer chains as well as to isolated aggregates consisting of many polymer chains. By investigating the photon statistics from one single chain at a time, we show that the fluorescence quenching mechanism in P3HT can be attributed to the efficient formation of long-lived triplet states, which are able to quench the fluorescence of the total chain by singlet-triplet annihilation [1]. By applying solvent vapor annealing we are able to grow aggregates of CP. Subsequent single-aggregate photon correlation spectroscopy identifies additional "dark" states, which are more rapidly formed compared to the triplet state. We attribute these "dark" states evolving in the mesoscopic size regime of P3HT to charge transfer states, which play the main role in the strong quenching of the fluorescence at the transition from the single molecule to the bulk film.

[1] F. Steiner et al., PRL 112, 137402 (2014)

CPP 39.5 Wed 16:15 H37

Triplet and Charge Transfer Excitons in Organic Solar Cells: Influene of Energetics and Morphology — •Andreas Sperlich[1], Stefan Väth[1], Hannes Kraus[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg

To improve organic solar cells it is necessary to develop a deeper understanding of fundamental processes, such as harvesting of singlet and charge transfer (CT) excitons, but also loss mechanisms like electron back transfer (EBT) reactions to the triplet state. These processes depend on the energy levels of constituting donor and acceptor molecules, on microscopic structure of blends but also on the relative spin orientation of charges carriers within the e-h pair. Here, we use electron paramagnetic resonance (EPR) methods to study several polymer-fullerene blend systems and found remarkable correlations between electrical performance of solar cells and formation of CT and triplet excitons. Combining results of complementary experiments, we offer a physical picture on how pushing up the LUMO level of acceptors or tailoring the blends' morphology may end up in unwanted loss mechanisms in bulk-heterojunction solar cells.