

Shining Light on Triplet States:

When The Triplet Excitons Shape Recombination, Voc and Efficiency Limits

Safa Shoaee*

University of Potsdam and Paul Drude Institute for Solid State Electronics

shoaee@pdi-berlin.de

Organic solar cells have recently exceeded 20% power-conversion efficiency, prompting a key question: how much further can we push performance? Despite rapid advances, progress is limited by photophysical loss channels that are not yet described within a unified framework. At the heart of the problem lies the intricate excited-state dynamics at the donor–acceptor interface, where excitons, charge-transfer states and fully separated charges are in constant interconversion, governed by the materials' energetic landscape. A central challenge is to understand and mitigate loss pathways involving singlet and triplet charge-transfer states and local triplet excitons, which ultimately constrain the open-circuit voltage. This talk will outline recent insights into these processes and discuss how mastering them could unlock the next efficiency gains in organic photovoltaics.

In this talk, we share our experimental data and kinetic model that, for the first time, explicitly incorporates the formation and re-splitting of local triplet excitons. Fully parameterised by the interfacial energy offset, this unified framework reproduces key photovoltaic observables – such as the charge-generation efficiency, photoluminescence, electroluminescence and the Langevin reduction factor. Our results show that the triplet-state dynamics may govern device performance. In systems with short triplet lifetimes, triplet decay emerges as the dominant recombination pathway, reconciling long-standing experimental findings, including those in benchmark systems like PM6:Y6. In systems with long triplet lifetimes, triplets can be recycled to mitigate this loss channel. The model further offers a mechanistic explanation for the empirically observed link between energy offset, radiative singlet-exciton decay and reduced-Langevin recombination as well as a correlation, and accurately predicts the device efficiency across different material systems.

By connecting excited-state kinetics with macroscopic device metrics, our work provides a unified mechanistic picture of the photophysics in organic semiconductors.