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Excited-State Non-Radiative Decay Processes in Organic Optoelectronic Materials

Xian-Kai Chen

Laboratory for Computational and Theoretical Chemistry of Advanced Materials, KAUST Solar Center
King Abdullah University of Science and Technology

Understanding excited-state non-radiative decay processes is critical for designing high-performance organic optoelectronic materials. For example, external quantum efficiencies as large as 30% have been reported recently in organic light emitting diodes (OLEDs) using intramolecular charge transfer emitters through harvesting non-emissive triplet states and converting them to singlet excited states via thermally activated reverse intersystem crossing (RISC), thus leading to delayed fluorescence. To facilitate RISC, organic emitters with nearly no gap between the first excited singlet (S_1) and triplet (T_1) states have been designed. Very recently, however, some exceptional cases have emerged where a relatively large energy gap between S_1 and T_1 states (~ 0.3 eV) also results in a high RISC rate. Here, we demonstrate that except energy gaps between S_1 and T_1 excited states, the non-adiabatic effect between low-lying excited states can play a key role in the $T_1 \rightarrow S_1$ up-conversion for TADF emitters. In addition, in organic solar cells (OSC), a major source of energy loss is attributed to non-radiative recombination from the interfacial charge transfer states to the ground state. Taking pentacene-C60 complexes as model donor-acceptor systems, we provide a comprehensive understanding of how molecular packing and charge delocalization impact these non-radiative recombination rates at donor-acceptor interfaces.

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