Structure-property relationship of thermally activated delayed fluorescence (TADF) materials: Carbazole based organic emitters.

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Thermally activated delayed fluorescence (TADF) phenomenon has attracted a great deal of attention; triplet excitons can be harnessed via TADF in organic light emitting diodes (OLEDs), which leads to a low device fabrication cost. For an effective TADF phenomenon, the facile intersystem crossing (ISC) from the triplet to the singlet excited states is imperative; to this end, the singlet and triplet energy gap, ΔE_{ST}, should be considerably suppressed. It has been long believed that ΔE_{ST} is equivalent to $2K$, twice the exchange energy, and hence reduced via a spatial separation of the HOMO and LUMO. However, the singlet and triplet states are often of different nature, and the triplet states tend to favor the local excitation (LE) character, related to a large K value.[1]

In this presentation, based on the results of carbazole-based emitters, we will present how multiple carbazole units have influences on the nature of the triplet excited states, and thus the ΔE_{ST} values.[1] we will also discuss how such multiple molecular units can give rise to the quasi-degeneracy of the excited states and enhance the ISC rate.[2] Consequently, we propose a design rule for efficient TADF emitters.

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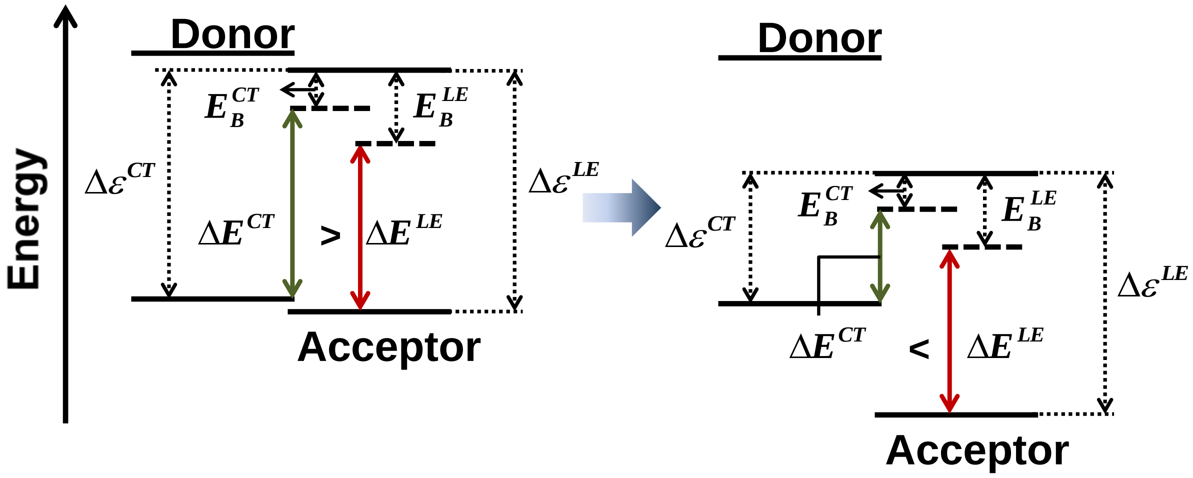

Figure 1: Schematic illustration of the evolution of the excited-state nature as a function of the HOMO and/or LUMO energy offsets between the donor and acceptor units.

References

1. K. Lee and D. Kim, *J. Phys. Chem. C* **120** (2016), 28330.
2. C. H. Ahn and D. Kim, *ChemPhotoChem in press*.