

## Third Generation Organic Light Emitting Diodes -Design for Molecular and Device Architectures-

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### Abstract

Although typical organic molecules are simply composed of carbon (C), hydrogen (H), nitrogen (N) and oxygen (O) atoms, their unique bonding manners based on  $sp^3$ ,  $sp^2$  and  $sp$  hybrid orbitals enables very sophisticated molecular architectures, leading to unique functions. By using unlimited freedom of molecular structures, we designed new light emitting molecules, the hyper fluorescence-highly efficient delayed fluorescence. With the proper molecular design, the energy levels of the excited states, i.e., singlet ( $S_1$ ) and triplet ( $T_1$ ) excited states, are minimized, promoting efficient up-conversion from  $T_1$  to  $S_1$  states, resulted in an ultimate EL efficiency.

### 1. Introduction

The recombination of holes and electrons can produce light, which is referred as an electroluminescence (EL). The first EL in organic materials was discovered by M. Pope et al. in 1963 using an anthracene single crystal equipped with high field carrier injection electrodes. Carriers of both signs were injected into organic layers and the subsequent carrier transport and recombination produced EL that is originating from singlet exciton fluorescence. The carrier recombination can produce both singlet and triplet excitons in the ratio of 1:3. A 3:1 ratio of triplet to singlet excitons is expected from spin statistics, and the relationship was demonstrated for many cases. The produced singlet excitons decay promptly, yielding prompt EL (fluorescence) while the two triplet excitons can fuse to form singlet excitons through the triplet-triplet annihilations, yielding delayed EL. On the other hand, while the direct radiative decay of triplet excitons results in phosphorescence, phosphorescence emission in conventional organic aromatic compounds usually occurs only at very low temperature and virtually it is useless in most cases. In 1999, Forrest and Thompsons' group firstly demonstrated efficient electrophosphorescence using iridium complexes that promote efficient radiative decay rate of  $\sim 10^6/s$  by taking the advantage of heavy metal effect, spin-orbital coupling. In fact, nearly 100% internal EL efficiency was demonstrated, consolidating the OLED technology useful for display and lighting applications.

### 2. TADF

In this report, we demonstrate a novel pathway to open an ultimate EL efficiency by using simple aromatic compounds displaying efficient thermally activated delayed fluorescence (TADF) having high photoluminescence (PL) efficiency. Fig. 1 shows the energy diagram of a conventional organic molecule, depicting singlet ( $S_1$ ) and triplet ( $T_1$ ) excitons with a ground state ( $S_0$ ) and our strategy for harvesting triplet excitons. While we suppose that the  $S_1$  level should be higher than the  $T_1$  level due to the presence of exchange energy, a proper design of organic molecules enables the formation of a rather small energy gap between them ( $\Delta E_{ST}$ ). A molecule displaying efficient TADF requires a small  $\Delta E_{ST}$  between its singlet ( $S_1$ ) and triplet ( $T_1$ ) excited states, resulting in the enhanced  $T_1 \rightarrow S_1$  reverse intersystem crossing (ISC). Such an excited state is attributable to the intramolecular charge transfer (CT) of the spatially separated donor and acceptor system. Further, to enhance the quantum efficiency of a TADF material, geometrical change between its ground ( $S_0$ ) and  $S_1$  states should be restrained.

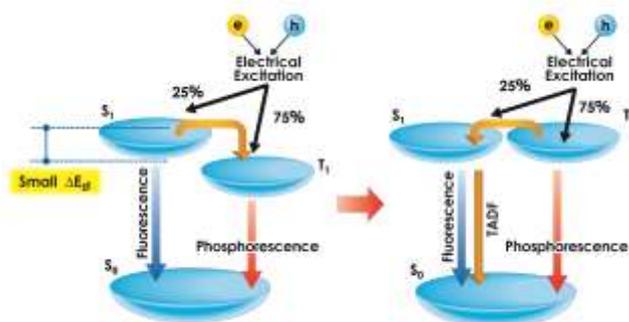


Fig. 1 Energy diagram of typical organic molecule and concept of TADF.

### 3. Conclusion

In this work, we designed a novel series of highly efficient TADF emitters having donor and electron acceptor units. The localization of HOMO and LUMO around the donor and the acceptor moieties, respectively, leads to a small  $\Delta E_{ST}$ . Moreover, the systematic combination of donor and acceptor units results in high quantum efficiency and various emission colors. We introduce our recent molecular design and high performance EL based on TADF<sup>1-8</sup>.

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