

Thermally activated delayed fluorescence (TADF) molecular and macromolecular materials based on through-space donor-acceptor interactions

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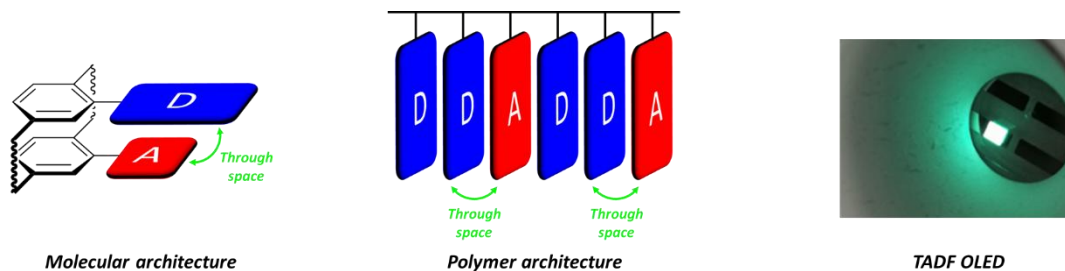
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TADF materials have been intensively studied this last decade because they can show 100% of internal quantum efficiency (IQE) in OLED configuration due to an effective up-conversion from the triplet excited state to the singlet excited state by reverse-intersystem crossing (RISC) using thermal energy.^[1] In general, the key method is to decrease the overlap occurring between the highest occupied and the lowest unoccupied molecular orbitals (HOMO and LUMO), which are generally distributed onto the electron-donating (D) and electron-accepting (A) units, respectively. Thus, the common strategy when designing TADF emitters consists in separating such D and A groups by a central core. Some overlap between the HOMO and LUMO is then maintained by a weak electronic communication occurring through an intensely twisted conjugated linker.^[1]

Recently, a novel molecular design, based on through-space interactions, was successfully utilized to prepare efficient TADF emitters. This alternative approach allows to physically separate D and A moieties and leads to a small HOMO and LUMO overlap.^[2] In such design, intramolecular through-space D-A interactions occur and the D and A electronic clouds mainly communicate via spatial charge transfer interactions. This strategy leads to very small ΔE_{ST} and enhanced radiative decay rates.

In this context, we propose to explore new (macro)molecular designs for the preparation of through-space TADF emitters (see Figure). Regarding the molecular approach, we propose to use paracyclophane building-blocks as versatile 3D platforms to promote through-space interactions between D and A units and TADF emission properties.^[3] Regarding the polymer approach, we propose to design side-chain copolymers incorporating different ratios of D and A side groups able to present through space interactions and self-host TADF properties.



Références

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