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A7

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D3

D4

Thermally activated delayed fluorescence (TADF) plays a key role in the design of high efficiency organic lightemitting diodes[1]. The mechanism of the process consists in both, direct fluorescence (25%) and delayed fluorescence produced after thermal transformation of triplet to singlet excited states (75%), known as reverse intersystem crossing (rISC). Increasing the triplet-singlet states energy degeneracy, facilitating the rISC, the efficiency of the system increases[2]. In this regard, we aim to use mechanochemistry (that is the application of an



external force) as a versatile tool to modulate the properties and enhance the efficiency of TADF systems.

Reference system:



- The initial singlet-triplet gap is 0.23 eV (5.07 kcal/mol), demonstrating the inefficiency of the system.
- The analysis of the spin density in T_1 let us conclude that it is a local excited (LE) state as this density is mainly located in the donor moiety.
- In contrast, by analyzing the natural transition orbitals describing the S1 state, we can conclude that it is a charge transfer (CT) state.

With the aim of improving the rISC of the PTZ-DBTO2 reference system increasing the CT character and shifting to the blue its emission color, we have proposed concrete substitution patterns, attending to the substitution position and electronic nature of the substituent.

APPLICATIONS

EDG



Phenothiazine modifications:



Substituent effect:

The substituent effect can be divided into two contributions, on the one hand the effect caused by the change of geometry in the original PES and on the other hand the change of the relative stability between the surfaces:







$$\Delta E_{T_1-S_1}^M = E_{T_1-S_1}(q_0) - E_{T_1-S_1}(q_0^R) \quad \Delta E_{T_1-S_1}^D = E_{T_1^R-S_1^R}(q_0^R) - E_{T_1-S_1}(q_0^R)$$

 $\Delta E_{T_1-S_1}^{Total} = \Delta E_{T_1-S_1}^M + \Delta E_{T_1-S_1}^D$

Bibliography

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