



A new potential molecule for D/A type OLED for high luminescence: A DFT computational molecular design of study

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Abstract

A plethora of attention is being attracted on Organic Light Emitting Diodes (OLEDs) in recent years employing Thermally Activated Delayed Fluorescence (TADF) emitters which is rare metal-free, environmentally safe and highly efficient with an Internal Quantum Efficiency (IQE) of nearly 100%. We applied a theoretical design strategy for Donor–Acceptor (D/A)-type small molecules as they facilitate permit reduced exchange energy (J) hence the small energy gap (ΔE_{ST}) between singlet–triplet states, between electron-donating and accepting subunits for efficient Reverse Intersystem Crossing (RISC) which is a prerequisite for successful TADF. Our approach involves molecular design of 2,4-diphenyl-1,3,5-triazine acceptor and 9,10-dihydroacridine donor moieties connected by a 1,2-phenylene bridge which shows less ΔE_{ST} suggesting a better candidate for TADF prior to further experimental studies.

Introduction

- OLEDs based on TADF can successfully replace phosphorescent emitters which includes expensive rare metals and complex fabrication process [1].
- After electron-hole recombination, excitons are formed and transferred to lowest excited singlet and triplet states in the ratio of 1:3, respectively [2].
- With a small singlet-triplet splitting energy, (ΔE_{ST}) along with the aid of thermal activation, triplet excitons are back transferred to singlet state and thus enable delayed fluorescence for OLEDs..

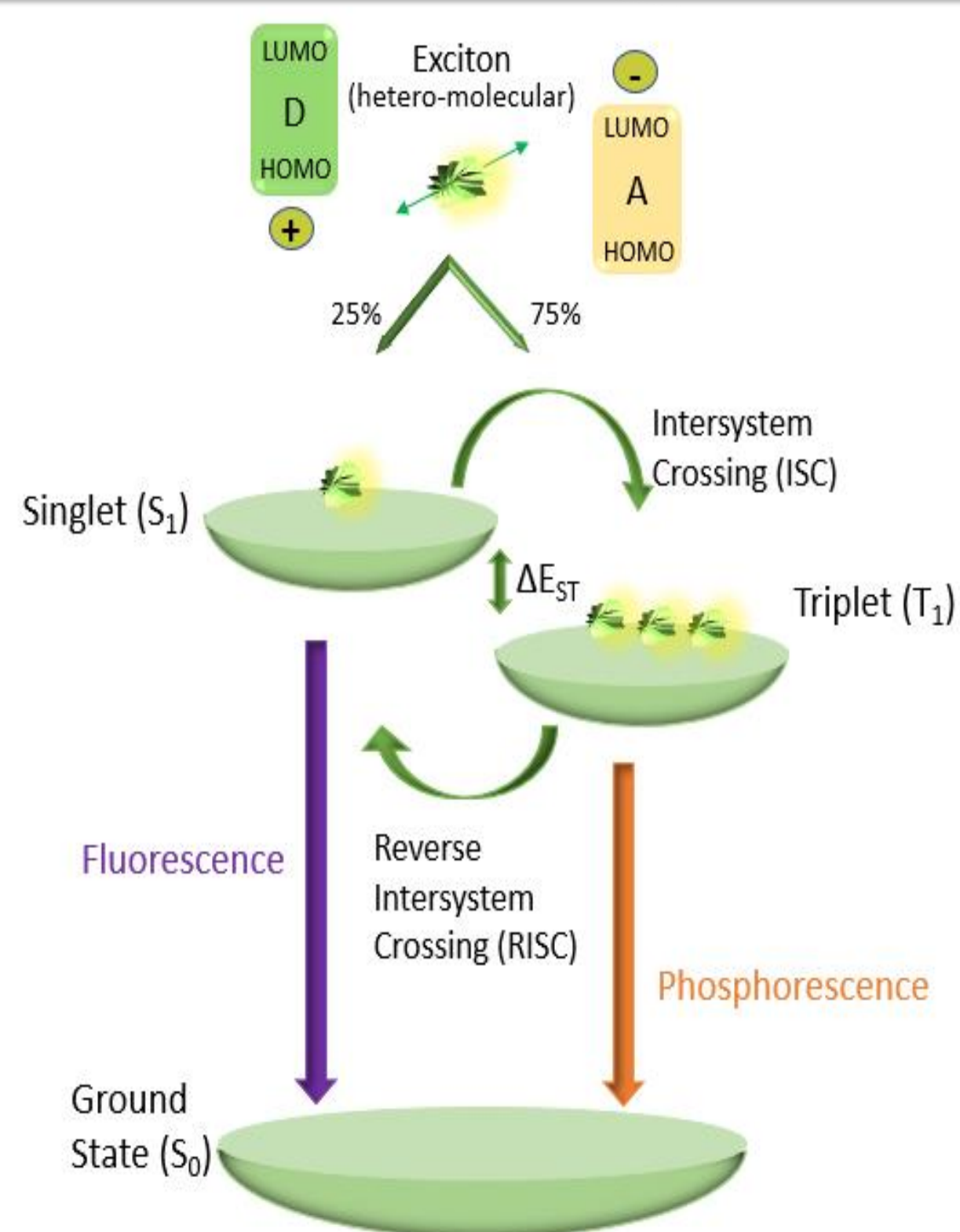


Figure 1: Illustration for thermally activated delayed fluorescence.

Methodology

- Dependence of RISC rate on temperature can be expressed in a Boltzmann distribution relation [3] : $k_{RISC} \propto \exp \frac{\Delta E_{ST}}{k_B T}$
- ΔE_{ST} is particularly important according to the above equation, which is the difference between E_S and E_T , is equal to the twice of exchange energy, J : $\Delta E_{ST} = E_S - E_T = 2J$
- Here, HOMO of donor and LUMO of acceptor of organic D-A molecular system are designed to be separated by a linker; this renders small overlap of frontier orbitals and reduced exchange energy J , resulting in a small ΔE_{ST} .
- All calculations are adopted by DFT, TD-DFT methods in Gaussian16 package for gaseous phase using APFD/LanL2MB functional.

References

- [1] Tang, X., Cui, L.S., Li, H.C. *et al. Nat. Mater.* 19, 1332–1338, 2020.
- [2] M.G. Fan, J.N. Yao, Photochemistry and Optical Function Materials, Science Press, 2009.
- [3] K. Goushi, K. Yoshida, K. Sato, and C. Adachi, *Nat. Photonics* 6, 253, 2012.

Result and Discussion

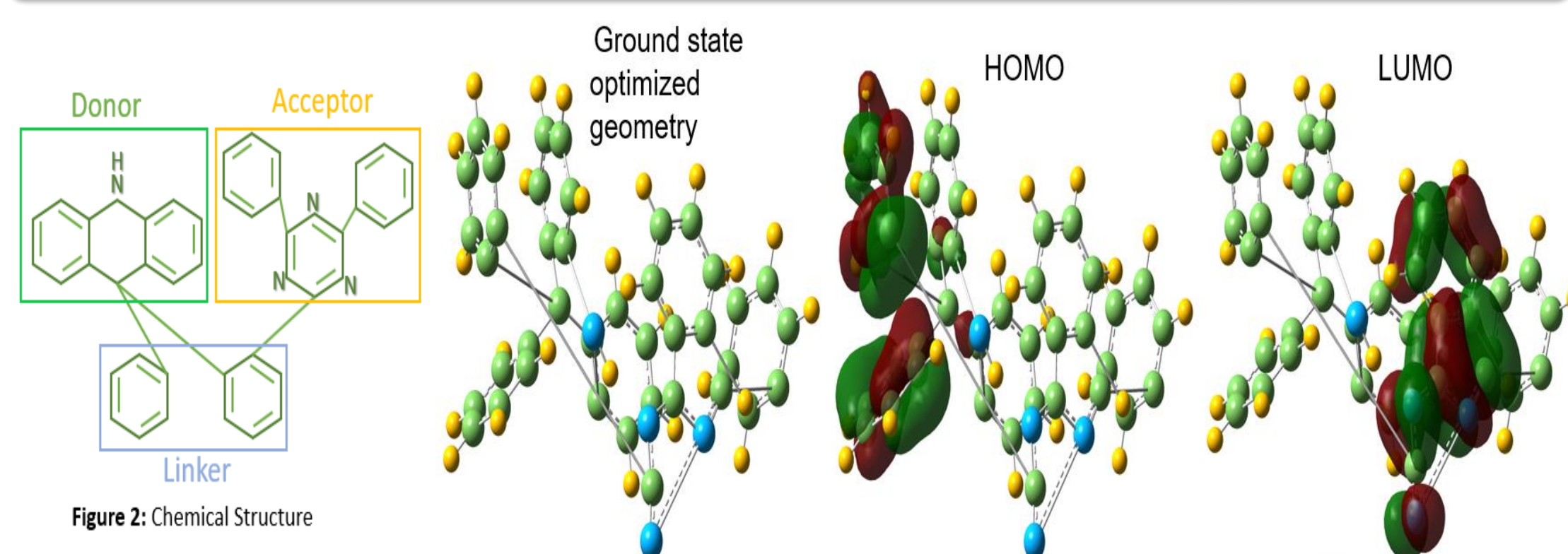


Figure 2: Chemical Structure

Figure 3: Optimized structure, HOMO and LUMO. c: C, H: H, N: N

- Calculated HOMO and LUMO are allocated on donor and acceptor units, respectively and their overlap is negligible. Dipole moment of S_1 is 7.33 Debye.
- We observe two triplet bands corresponding to $S_0 \rightarrow T_1$ transition. Higher lying triplet band may involve RISC from triplet to singlet.

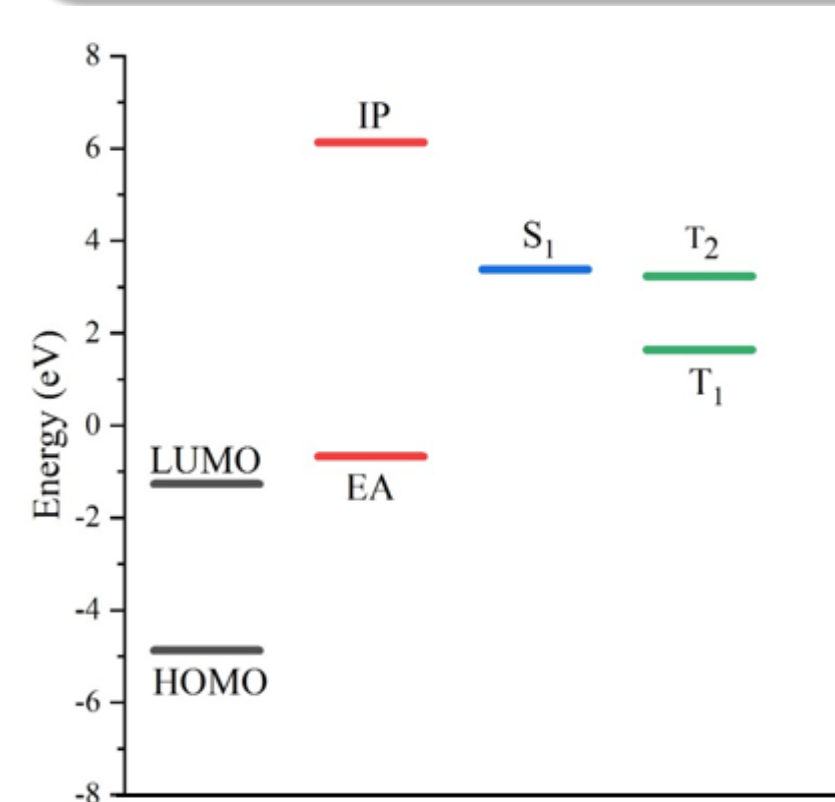


Figure 4: Energy level diagram

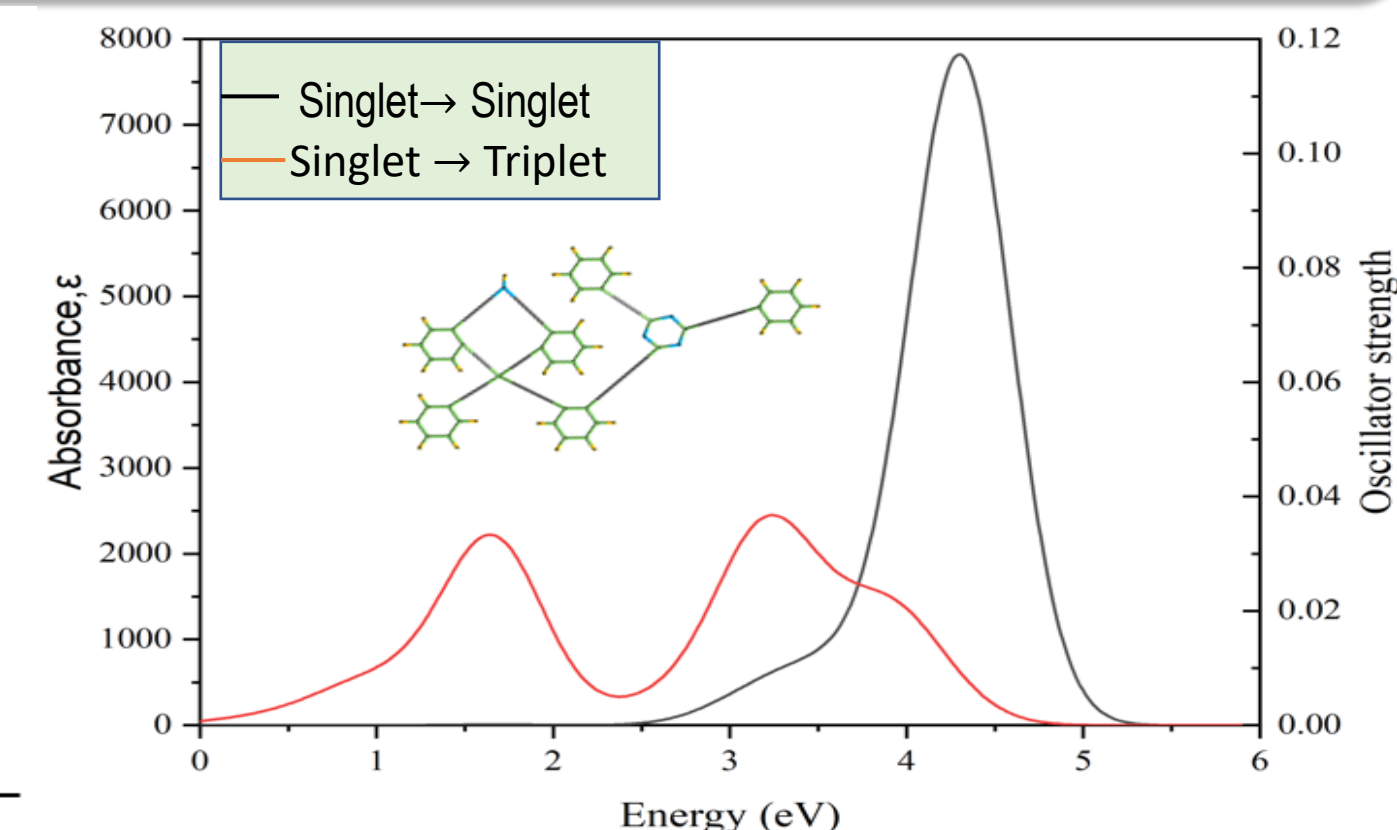


Figure 5: UV-Vis Spectra

Conclusion

The estimated ΔE_{ST} of our designed compound is 0.14 eV which is small enough to facilitate TADF process and energy gap E_g is 3.6 eV. This result suggests that, control of donor-acceptor conformation by linker can lead to effective RISC and photoluminescence yield.

Acknowledgment

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