

# Thermally activated delayed fluorescence emitters with dual conformations for white organic light-emitting diodes: mechanism and molecular design

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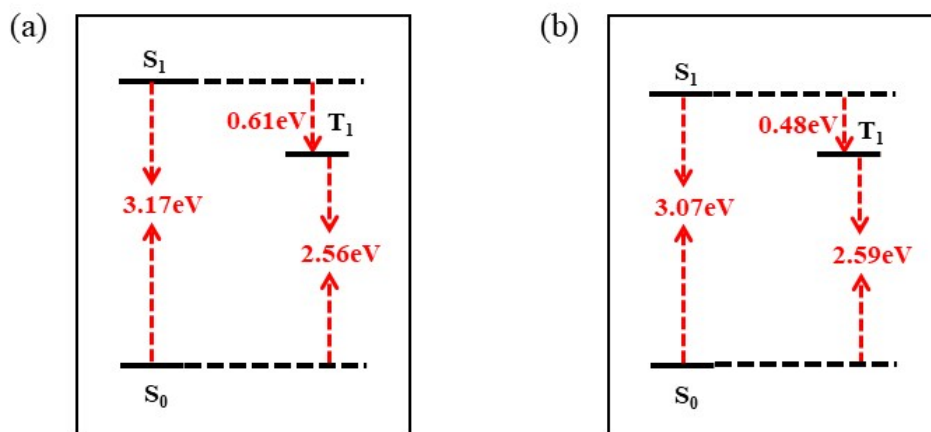


Figure S1. Energy levels for PTZ-TTR in toluene (a) and in the aggregate state (b) respectively.

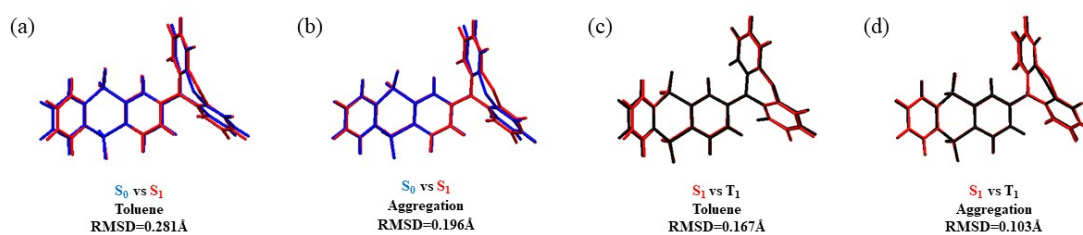


Figure S2. Geometric deviation for PTZ-TTR between  $S_0$  (blue),  $S_1$  (red) and  $T_1$  (black) in toluene (a and c) and in the aggregate state (b and d) respectively.

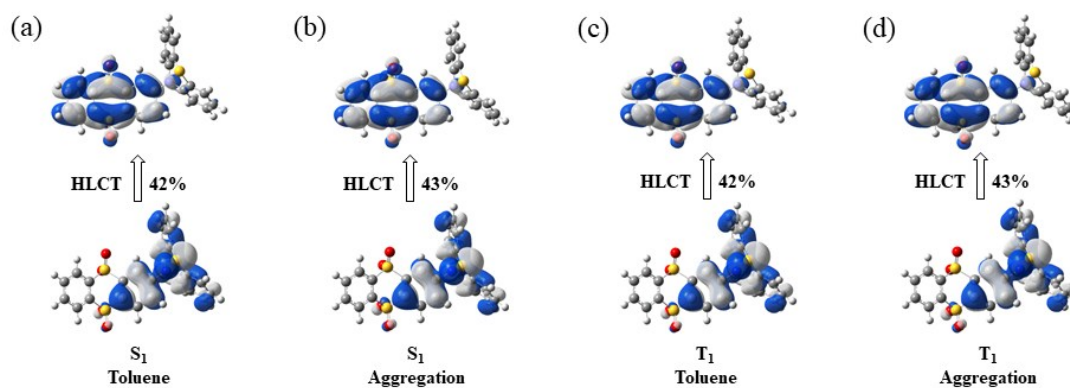


Figure S3. Transition characteristics for  $S_1$  and  $T_1$  states of PTZ-TTR in toluene (a and c) and in the aggregate state (b and d) respectively. The values to the right of the arrow are the LE proportion in excitation.

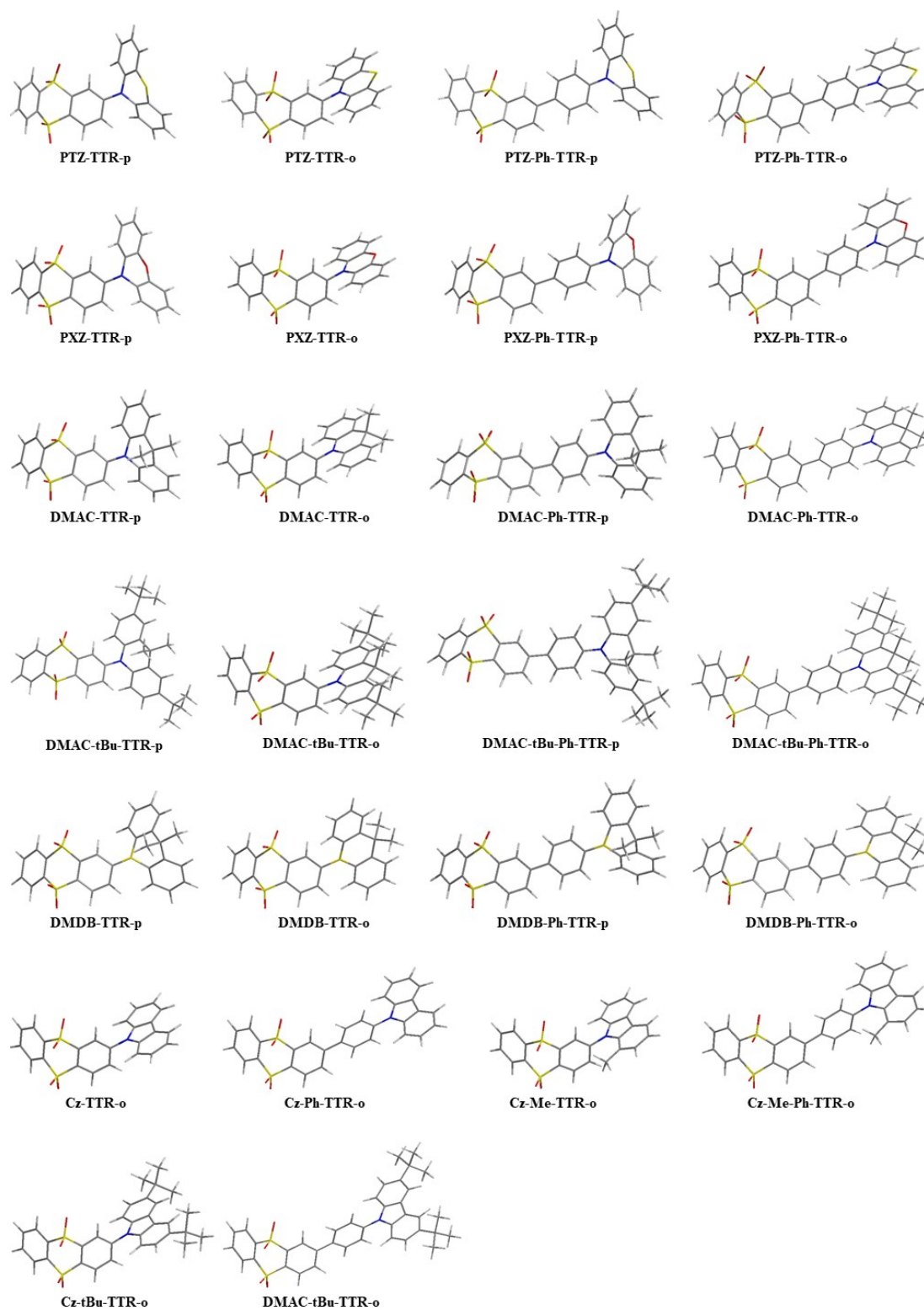


Figure S4. Chemical structures of eight different donors (PTZ, PXZ, DMAC, DMAC modified with two tert-butyl groups, DMDB, Cz, Cz modified with a methyl group, and Cz modified with two tert-butyl groups) with two conformations.

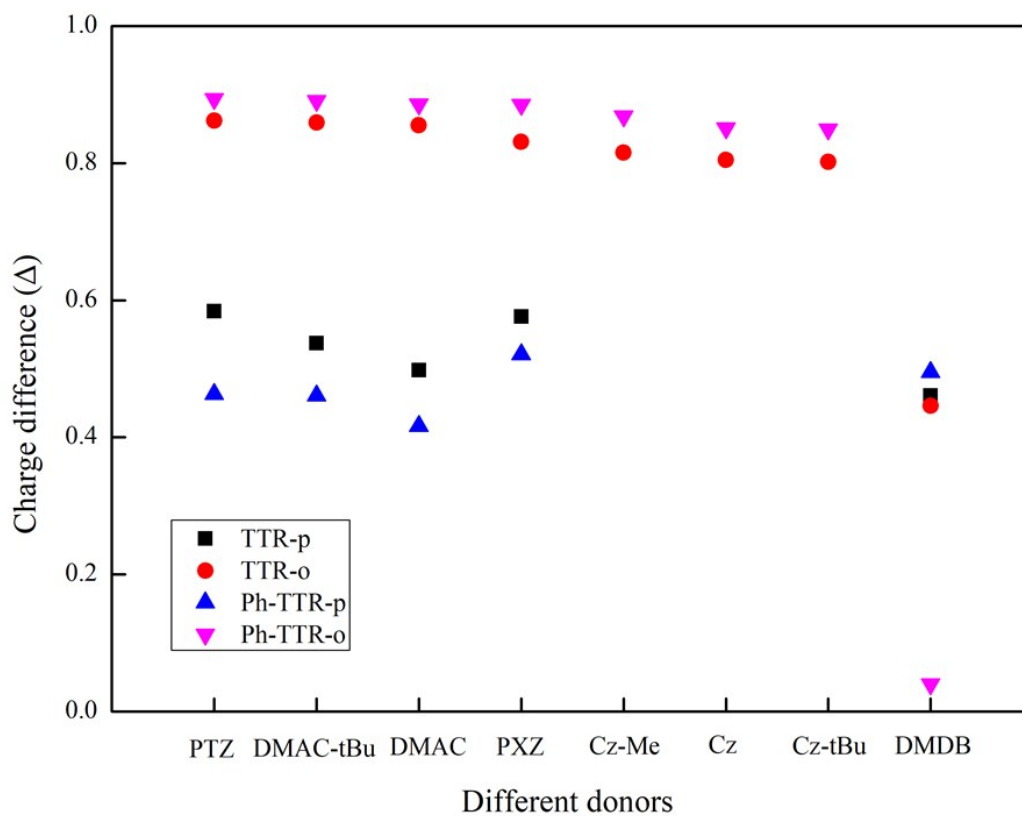


Figure S5. Calculate the charge difference between the  $S_0$  and  $S_1$  states of the electron-donating group of each system.

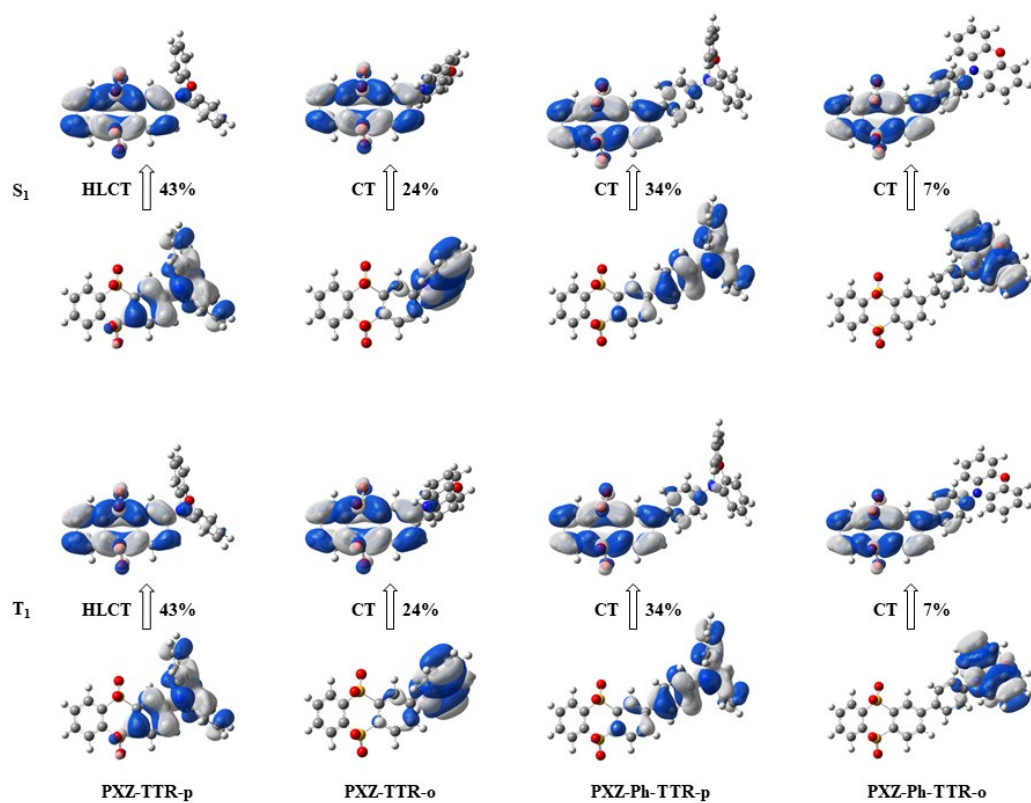


Figure S6. NTOs of PXZ-TTR and PXZ-Ph-TTR for  $S_1$  (up) and  $T_1$  (below) states in toluene.

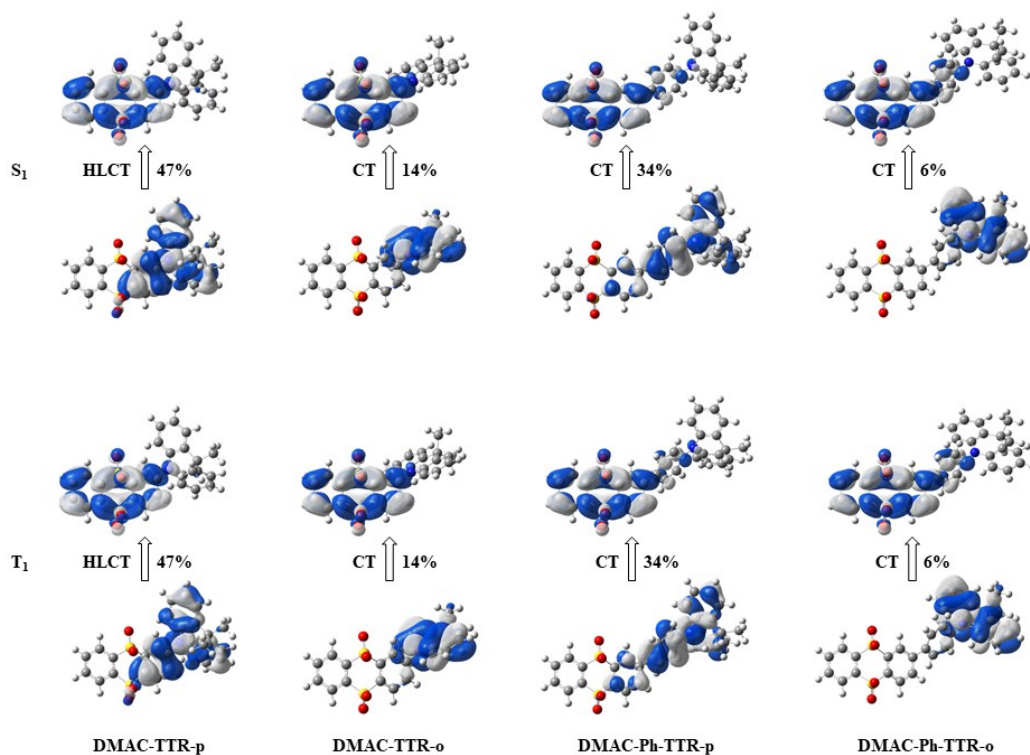


Figure S7. NTOs of DMAC-TTR and DMAC-Ph-TTR for S<sub>1</sub> (up) and T<sub>1</sub> (below) states in toluene.

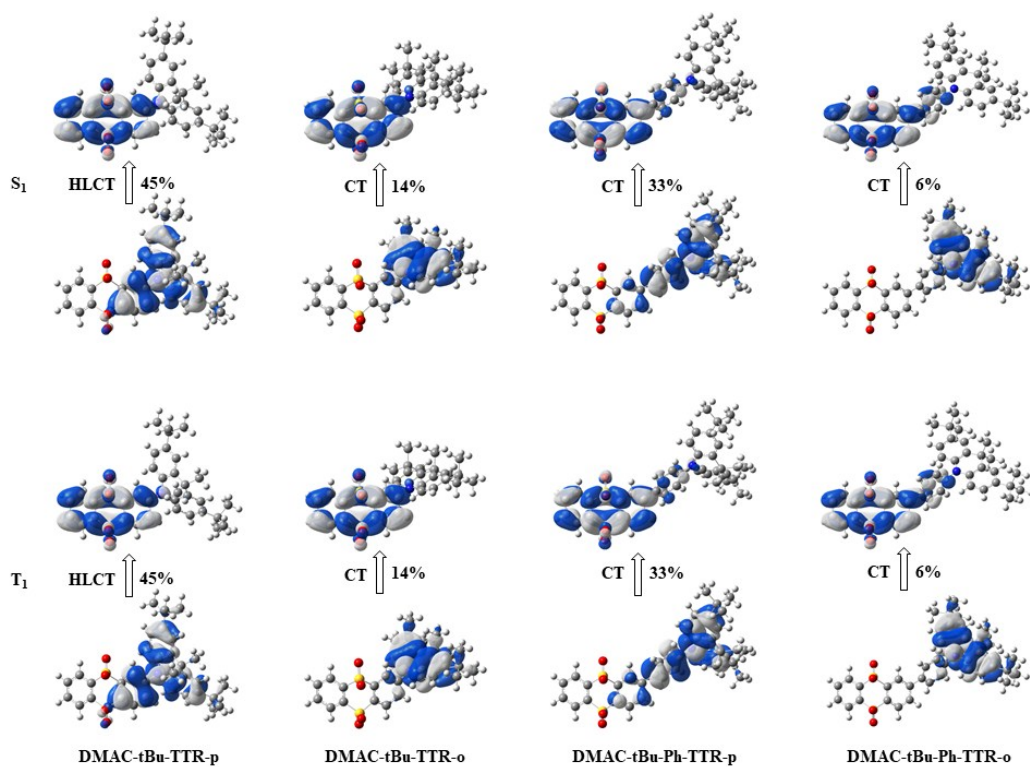


Figure S8. NTOs of DMAC-tBu-TTR and DMAC-tBu-Ph-TTR for S<sub>1</sub> (up) and T<sub>1</sub> (below) states in toluene.