Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

An effective method in modulating the thermally activated delayed fluorescence (TADF) emitters from green to blue emission: The role of the phenyl ring

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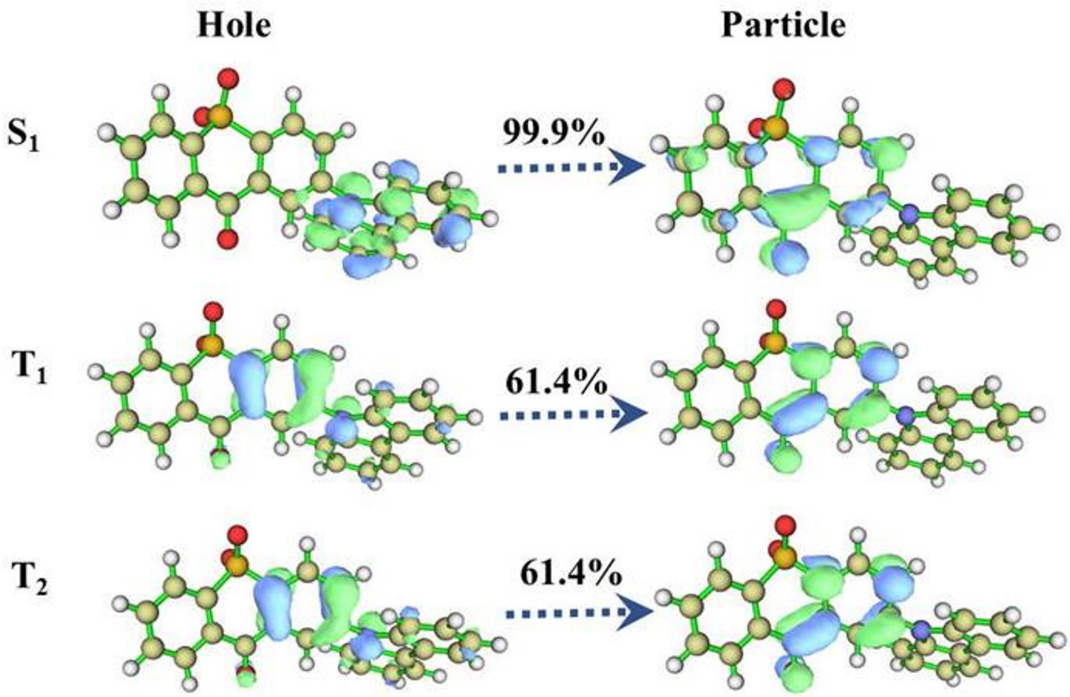

Figure S1 The natural transition orbitals (NTOs) of S_1, T_1 and higher triplet states for CzSOXO.

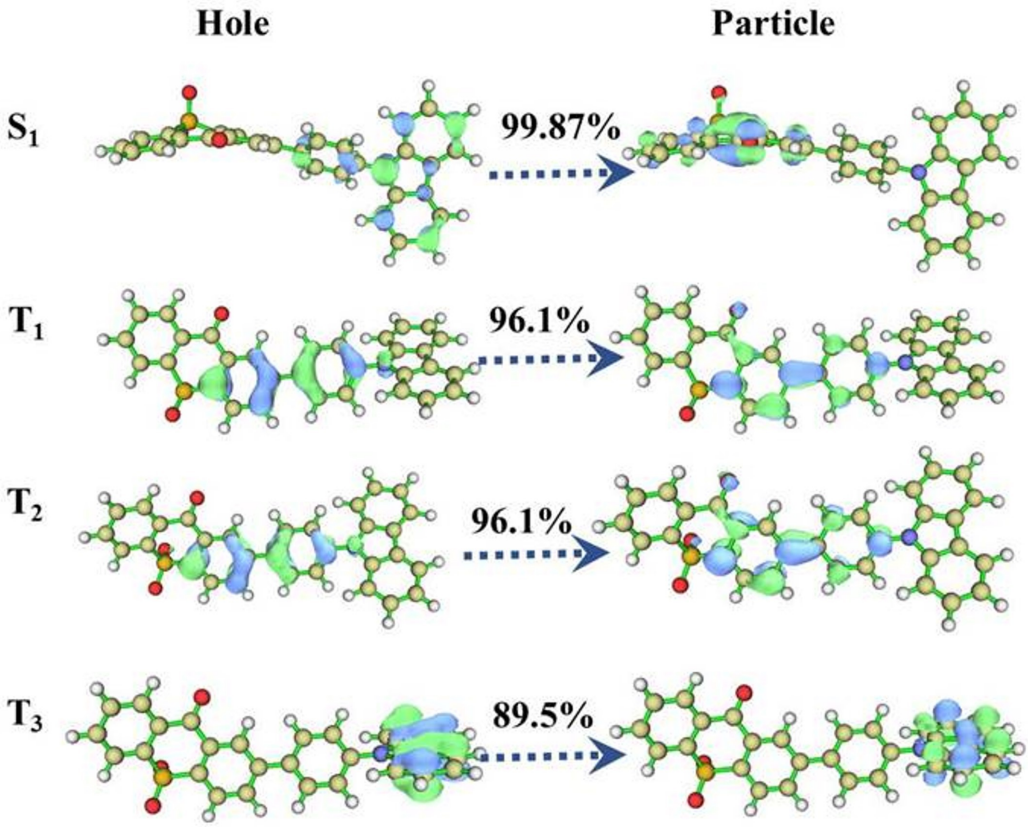

Figure S2 The natural transition orbitals (NTOs) of S_1, T_1 and higher triplet states for Cz-Ph-SOXO.

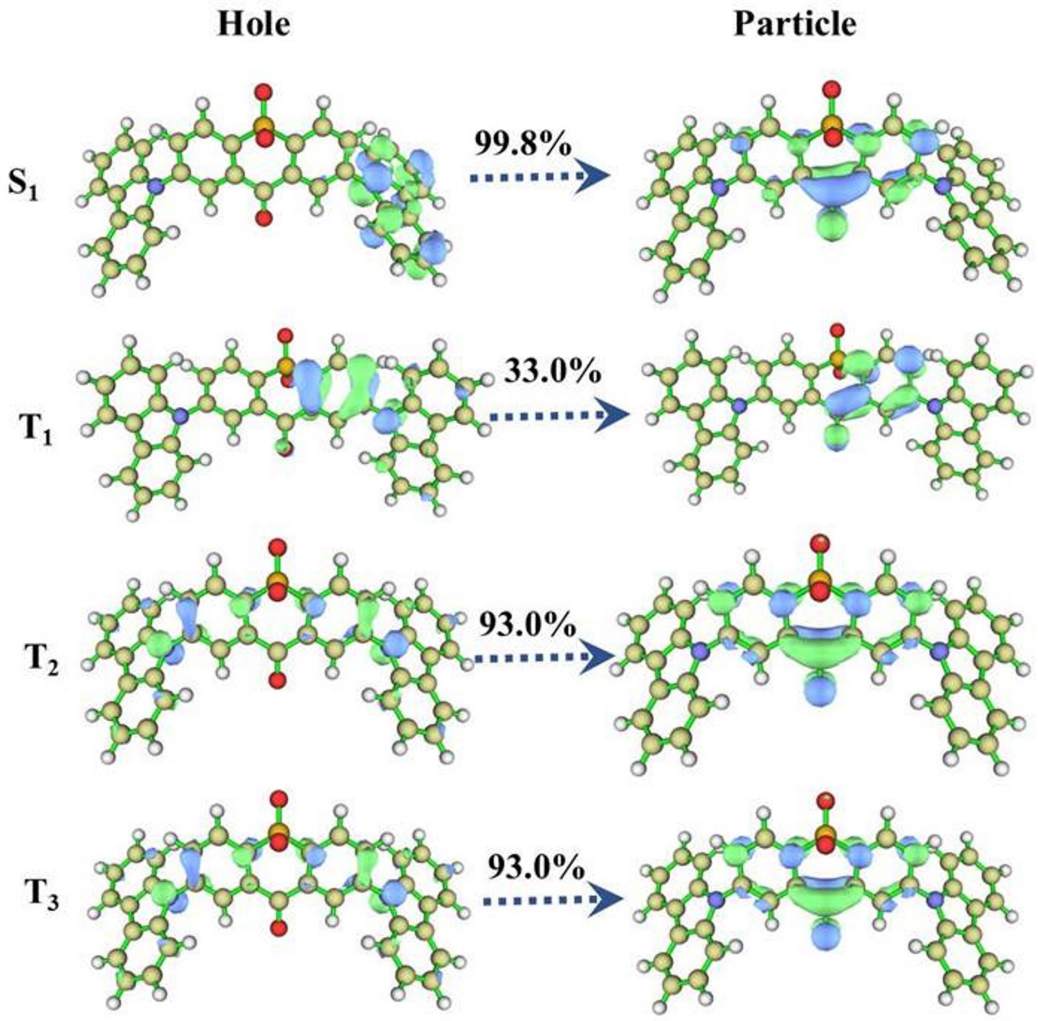

Figure S3 The natural transition orbitals (NTOs) of S_1, T_1 and higher triplet states for DCzSOXO.

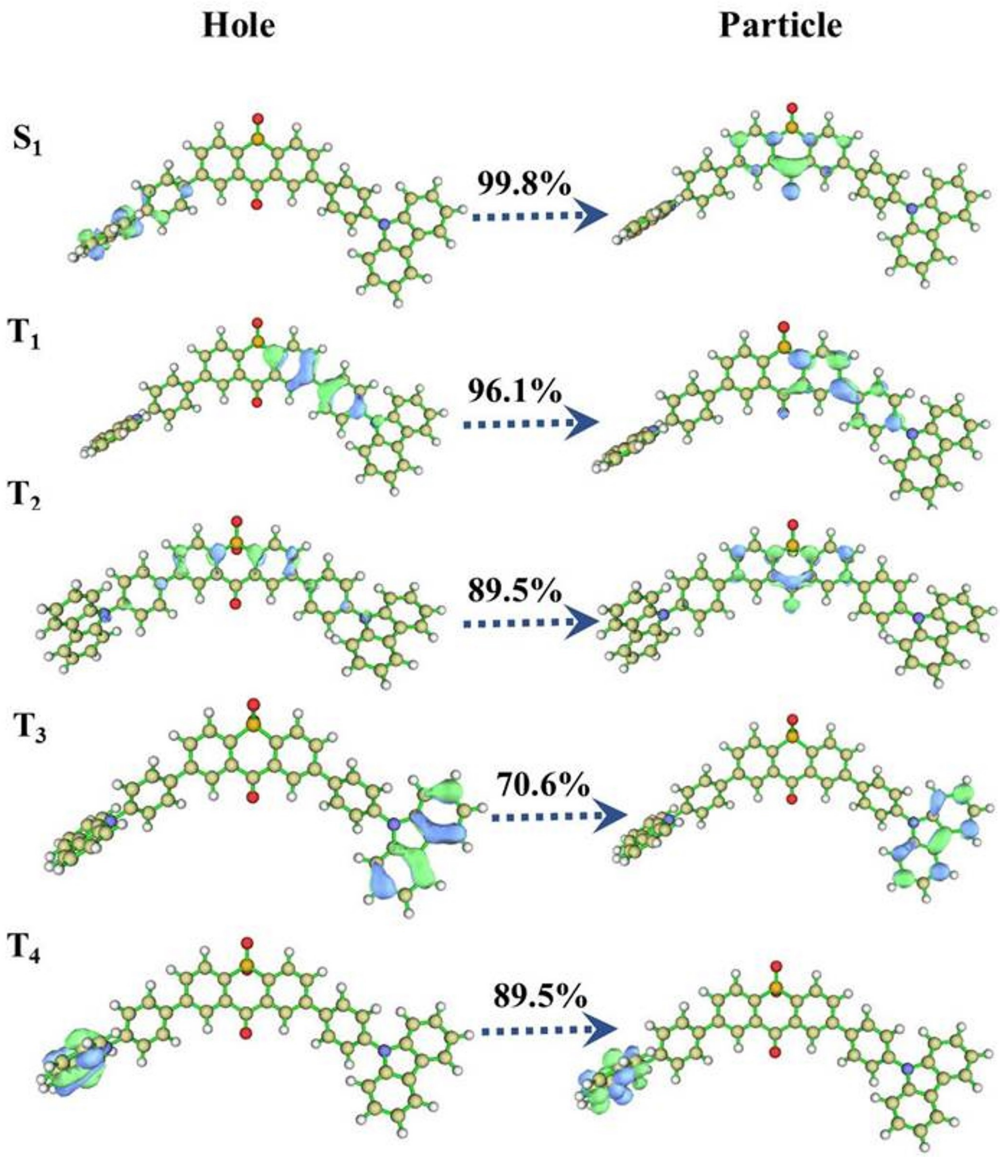

Figure S4 The natural transition orbitals (NTOs) of S_1, T_1 and higher triplet states for DCz-DPh-SOXO.

Table S1 The SOC values between T_1 and S_0 states and the calculated phosphorescence rates (k_p) from T_1 to S_0 state for investigated molecules.

Molecules	$\langle T_1\|H_{SO}\|S_0\rangle$ (cm^{-1})	kp (s^{-1})
CzSOXO	3.34	1.38
DCzSOXO	3.66	2.83
Cz-Ph-SOXO	2.63	0.11
DCz-DPh-SOXO	2.69	0.11