

Supporting information

Transition density matrix (TDM) refers to the transition density matrix in basis function representation. The TDM between ground state and an excited state can be calculated as

$$P_{\mu\nu}^{tran} = \sum_a^{vir} W_i^a C_{\mu i} C_{\nu a}$$

where $C_{\mu i}$ denotes the expansion coefficient of basis function μ in MO i . The TDM in real space representation, can be constructed easily via TDM in basis function representation:

$$T(r;r') = \sum_{\mu} \sum_{\nu} P_{\mu\nu}^{tran} \chi_{\mu}(r) \chi_{\nu}(r')$$

where χ stands for basis function. The off-diagonal elements of TDM essentially represent the coupling between various basis functions during electron excitation.

Table S1. The long-range separation parameter of the LC-PBE0 functional.

Molecule	ω	α	β
Y6	0.01	0.10	0.90
PM6	0.01	0.19	0.81
Y6:PM6 complex	0.01	0.10	0.90