Supporting Information for: Heterofission mechanism for pure organic room temperature phosphorescence

Qi Sun[1], Jiajun Ren[3], Qian Peng[4] and Zhigang Shuai[1,2*]

[1*]MOE Key Laboratory of Organic Optoelectronics and Molecular Engineering, Department of Chemistry, Tsinghua University, Beijing, 100084, P. R. China..
[2]School of Science and Engineering, The Chinese University of Hong Kong, Shenzhen, Guangdong, 518172, P. R. China..
[3]MOE Key Laboratory of Theoretical and Computational Photochemistry, College of Chemistry, Beijing Normal University, Beijing, 100875, P. R. China..
[4]School of Chemical Sciences, University of Chinese Academy of Sciences, Beijing 100049, P. R. China..

*Corresponding author(s). E-mail(s): shuaizhigang@cuhk.edu.cn;

1 Supplementary Figures

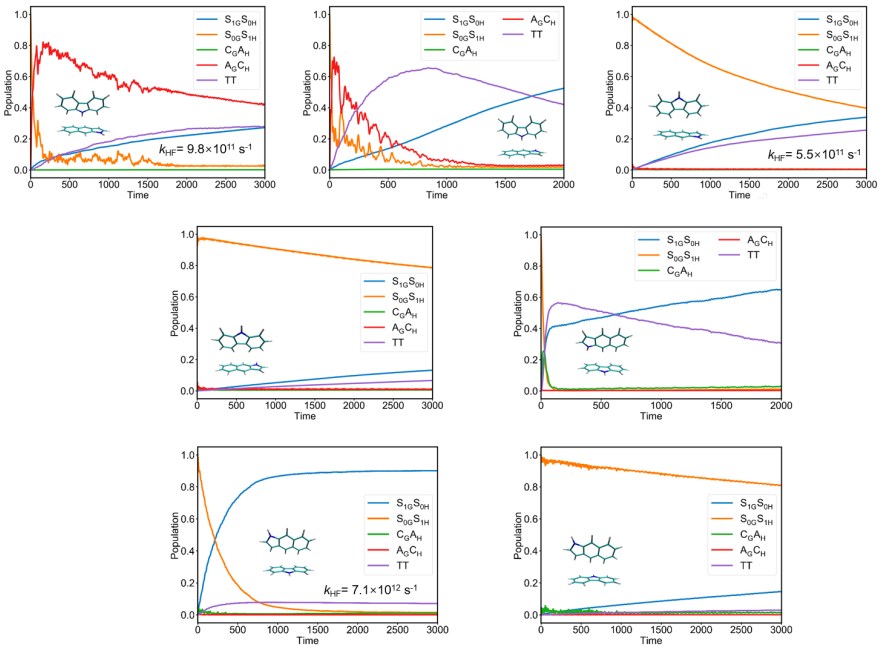


Fig. S1 Population dynamics of heterofission process in the remaining dimer (G: guest; H: host, time unit: fs).

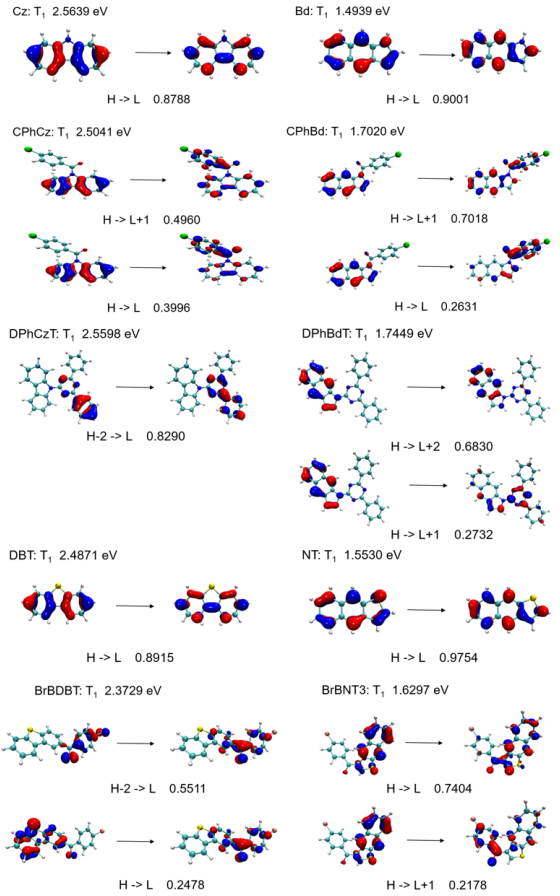


Fig. S2 Transition properties of the T_1 state in the investigate molecules

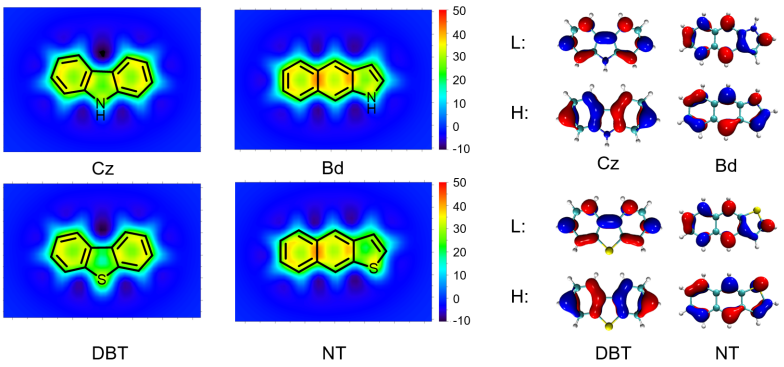


Fig. S3 The $ICSS_{zz}(1)$ values of Cz, Bd, DBT and NT and their frontier orbitals (H: HOMO; L: LUMO).

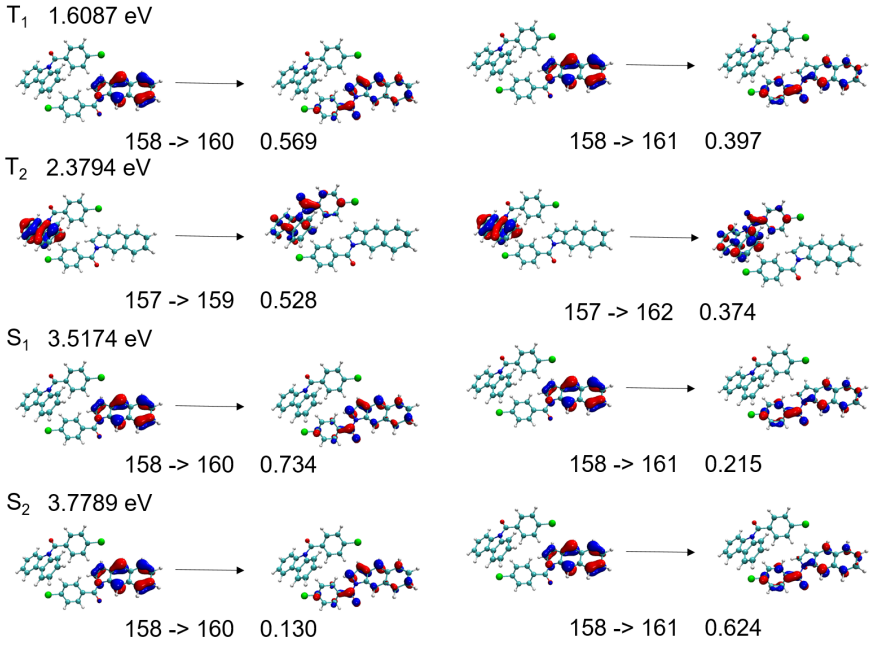


Fig. S4 Transition properties of the hetero-dimer CPhCz/CPhBd at T_1 geometry

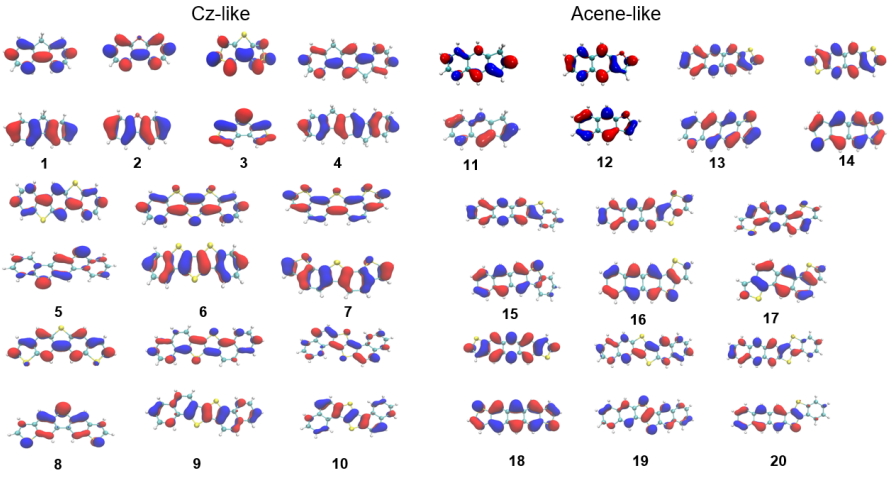
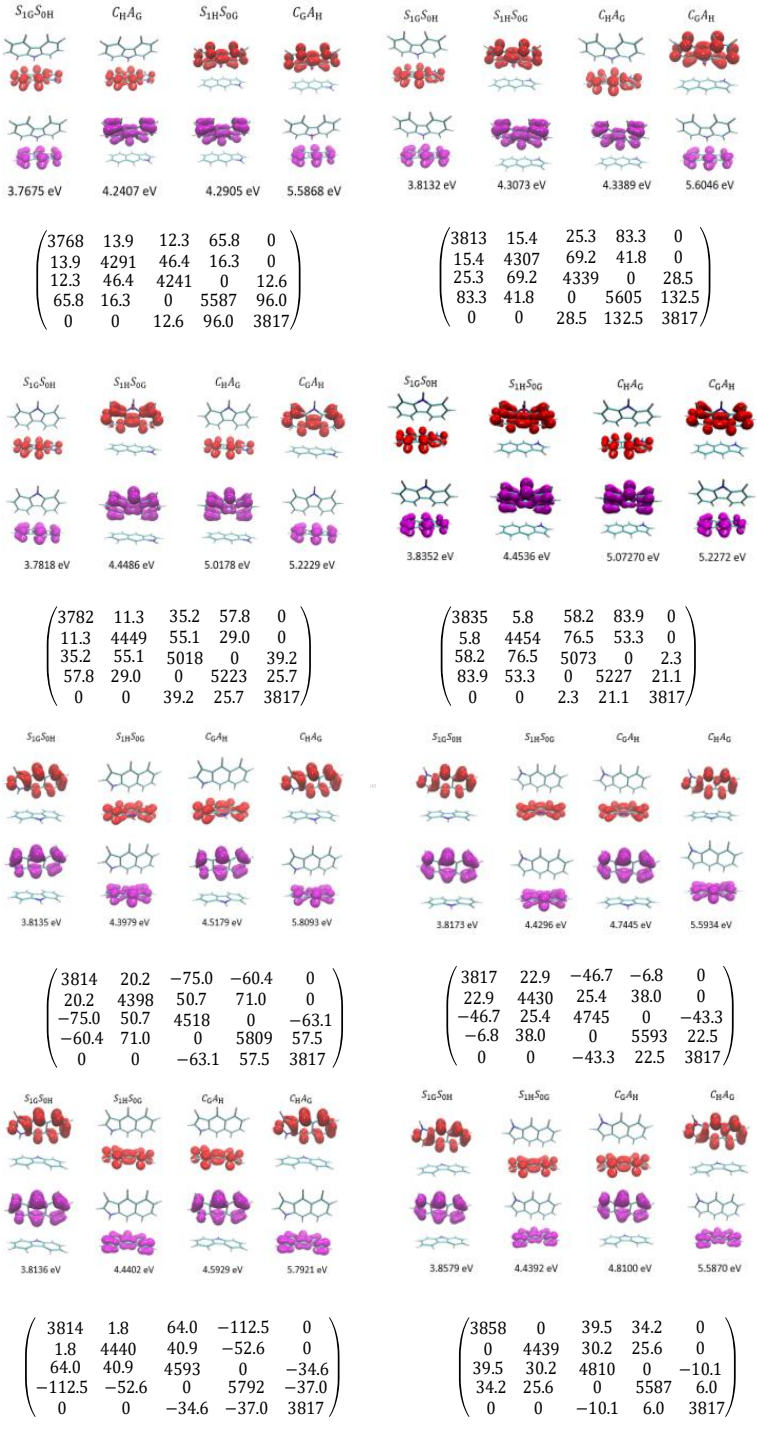


Fig. S5 Frontier orbitals of the potential candidates (H: HOMO; L: LUMO).



$$\begin{pmatrix} 3768 & 13.9 & 12.3 & 65.8 & 0 \\ 13.9 & 4291 & 46.4 & 16.3 & 0 \\ 12.3 & 46.4 & 4241 & 0 & 12.6 \\ 65.8 & 16.3 & 0 & 5587 & 96.0 \\ 0 & 0 & 12.6 & 96.0 & 3817 \end{pmatrix} \quad \begin{pmatrix} 3813 & 15.4 & 25.3 & 83.3 & 0 \\ 15.4 & 4307 & 69.2 & 41.8 & 0 \\ 25.3 & 69.2 & 4339 & 0 & 28.5 \\ 83.3 & 41.8 & 0 & 5605 & 132.5 \\ 0 & 0 & 28.5 & 132.5 & 3817 \end{pmatrix}$$

$$\begin{pmatrix} 3782 & 11.3 & 35.2 & 57.8 & 0 \\ 11.3 & 4449 & 55.1 & 29.0 & 0 \\ 35.2 & 55.1 & 5018 & 0 & 39.2 \\ 57.8 & 29.0 & 0 & 5223 & 25.7 \\ 0 & 0 & 39.2 & 25.7 & 3817 \end{pmatrix} \quad \begin{pmatrix} 3835 & 5.8 & 58.2 & 83.9 & 0 \\ 5.8 & 4454 & 76.5 & 53.3 & 0 \\ 58.2 & 76.5 & 5073 & 0 & 2.3 \\ 83.9 & 53.3 & 0 & 5227 & 21.1 \\ 0 & 0 & 2.3 & 21.1 & 3817 \end{pmatrix}$$

$$\begin{pmatrix} 3814 & 20.2 & -75.0 & -60.4 & 0 \\ 20.2 & 4398 & 50.7 & 71.0 & 0 \\ -75.0 & 50.7 & 4518 & 0 & -63.1 \\ -60.4 & 71.0 & 0 & 5809 & 57.5 \\ 0 & 0 & -63.1 & 57.5 & 3817 \end{pmatrix} \quad \begin{pmatrix} 3817 & 22.9 & -46.7 & -6.8 & 0 \\ 22.9 & 4430 & 25.4 & 38.0 & 0 \\ -46.7 & 25.4 & 4745 & 0 & -43.3 \\ -6.8 & 38.0 & 0 & 5593 & 22.5 \\ 0 & 0 & -43.3 & 22.5 & 3817 \end{pmatrix}$$

$$\begin{pmatrix} 3814 & 1.8 & 64.0 & -112.5 & 0 \\ 1.8 & 4440 & 40.9 & -52.6 & 0 \\ 64.0 & 40.9 & 4593 & 0 & -34.6 \\ -112.5 & -52.6 & 0 & 5792 & -37.0 \\ 0 & 0 & -34.6 & -37.0 & 3817 \end{pmatrix} \quad \begin{pmatrix} 3858 & 0 & 39.5 & 34.2 & 0 \\ 0 & 4439 & 30.2 & 25.6 & 0 \\ 39.5 & 30.2 & 4810 & 0 & -10.1 \\ 34.2 & 25.6 & 0 & 5587 & 6.0 \\ 0 & 0 & -10.1 & 6.0 & 3817 \end{pmatrix}$$

Fig. S6 Attachment and detachment density plot of the results of Boys localization diabatic states and matrix elements in the unit of meV.

Molecule	$E(T_1)$	$E(S_1)$
1	2.6375	4.4643
2	2.8621	4.6389
3	2.374	4.4563
4	2.3409	3.8583
5	2.5782	3.9378
6	2.0216	3.5724
7	2.5499	3.8916
8	2.3611	3.8813
9	2.3748	3.7111
10	1.9133	3.3482
11	0.8829	3.6309
12	1.8297	3.8556
13	1.0033	2.9008
14	1.1417	3.0964
15	1.0295	2.9173
16	1.0201	2.8885
17	1.1452	3.0300
18	0.9176	2.7141
19	1.1266	2.8771
20	1.0126	2.8597

Table S1 Excited state energy of S_1 and T_1 of molecules **1-20** with TD-DFT optimized T_1 geometry calculated at the level of TDA-ωB97X-D/6-31G* (Unit: eV).