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

Electronic Supplementary Information

The study of intramolecular decay and intermolecular energy transfer for phosphorescent organic light-emitting devices

Wanlin Cai, Kai Ren, Ancong Zhao, Xiulan Wu, Rongxing He, Ming Li and Wei Shen *
Key Laboratory of Luminescence and Real-Time Analytical Chemistry (Southwest University), Ministry of Education, School of Chemistry and Chemical Engineering, Southwest University, Chongqing 400715, China

*Corresponding author. E-mail: shenw@swu.edu.cn

MD simulation details

The initial substrates were constructed by randomly placing 300 TAPC molecules. After energy minimization, the system were heated from 0 to 500 K in 5 ns, followed by a 10 ns equilibration at 500 K. The subsequently simulations of these systems were rapid cooling from 500 to 300 K in 200 ps. The finally systems were kept a 10 ns equilibration at 300 K. Then, one PtON7 and 73 26mCPy (approximately 2 wt % of emitter) molecules were deposited within a 2 nm height from the top to the frozen substrate; for another system, one PtOO7 and 64 26mCPy molecules were deposited. After deposition of all molecules, the system was equilibrated at 298 K for 15 ns. Here, the velocity rescaling thermostat and the Berendsen barostat were conducted to control temperature and pressure, respectively. The long range electrostatic interactions performed by the particle-mesh Ewald (PME) method and vdW interactions were computed at a cutoff distance of 1.4 nm.

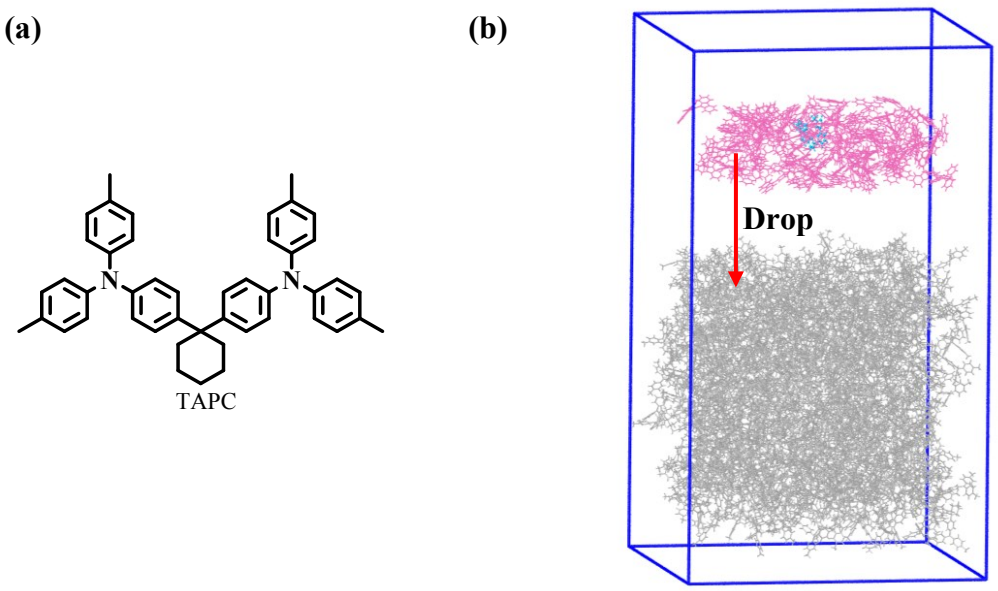

Figure S1. (a) Chemical structures of hole-transporting material TAPC. (b) Schematic diagram of vacuum deposition.

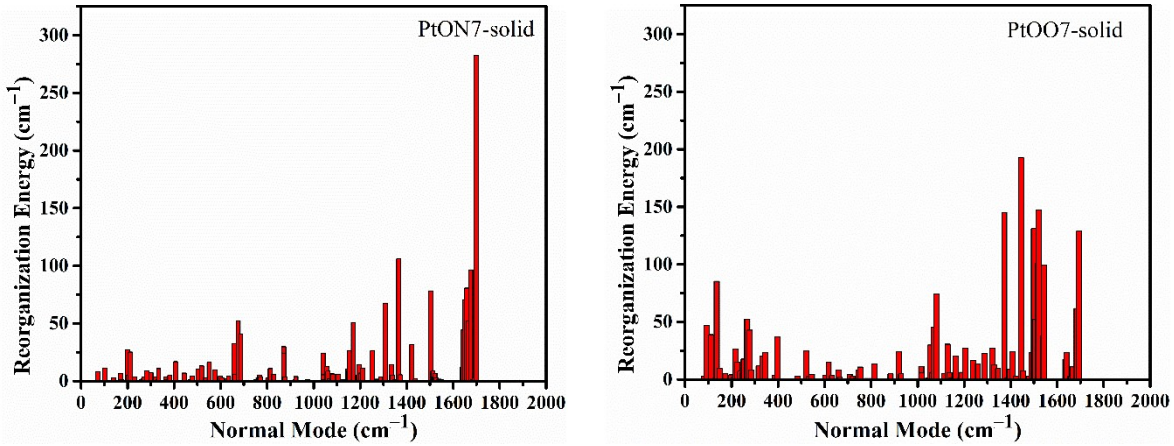

Figure S2. The contribution of different normal modes to reorganization energy.

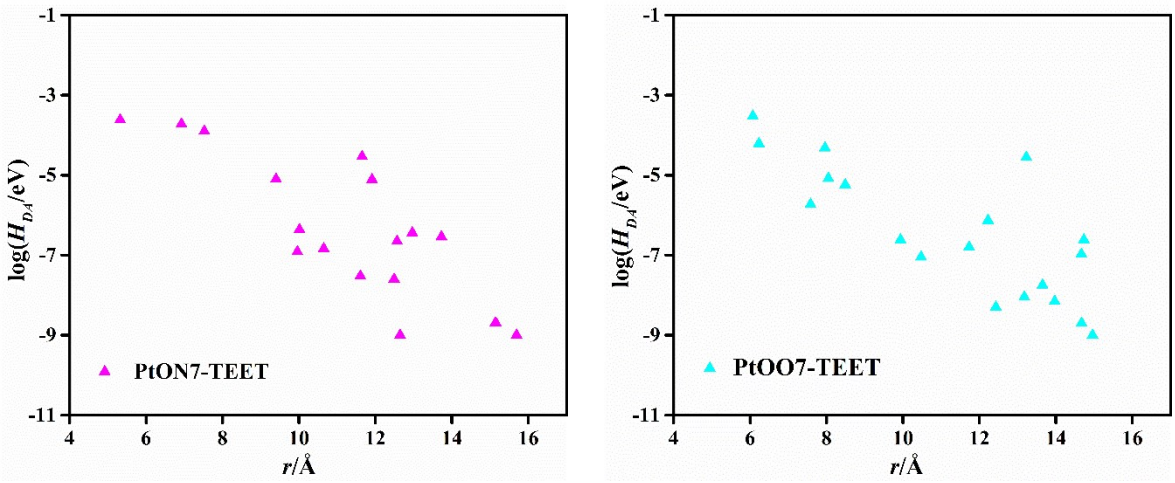

Figure S3. Calculated TEET coupling values versus centroid distances.

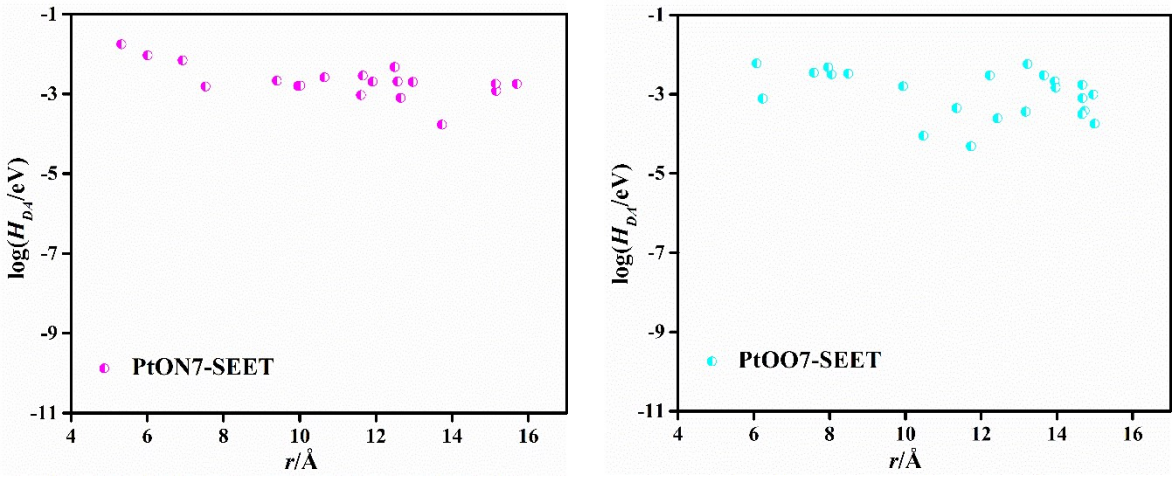

Figure S4. Calculated SEET coupling values versus centroid distances.

Table S1. Calculated frequency (cm^{-1}), reorganization energy (cm^{-1}) and Huang−Rhys factor of normal modes mainly involved in the vibrationally resolved spectra of PtON7.

PtON7-solid				PtON7-solution			
mode	ω	S	λ	mode	ω	S	λ
1	73.49	0.11	8.28	1	30.16	0.14	4.33
4	101.77	0.11	10.91	2	42.10	1.65	69.58
11	199.92	0.14	27.14	4	75.70	0.19	14.47
13	212.05	0.12	25.16	5	88.95	0.12	11.07
45	675.86	0.08	52.36	9	155.70	0.07	11.62
46	686.83	0.06	40.53	10	165.45	0.24	40.29
97	1308.84	0.05	67.6	13	204.28	0.43	87.28
101	1366.34	0.08	105.95	19	268.17	0.07	20.09
113	1503.01	0.05	78.15	23	329.36	0.11	36.51
126	1675.73	0.06	96.52	27	404.49	0.14	57.81
129	1699.35	0.17	282.51	30	456.60	0.25	114.09
				43	653.85	0.05	34.22
				44	657.59	0.08	52.8
				97	1303.92	0.11	147.92
				114	1494.67	0.06	91.38
				128	1681.87	0.20	334.9
				129	1694.36	0.16	267.36

Table S2. Calculated frequency (cm^{-1}), reorganization energy (cm^{-1}) and Huang−Rhys factor of normal modes mainly involved in the vibrationally resolved spectra of PtOO7.

PtOO7-solid				PtOO7-solution			
mode	ω	S	λ	mode	ω	S	λ
2	93.38	0.50	46.79	2	42.52	0.83	35.11
3	111.71	0.35	38.93	3	48.20	1.39	66.79
5	136.41	0.62	85.21	5	90.28	0.13	11.76
6	148.11	0.06	9.51	6	106.33	0.69	73.41
10	217.36	0.12	26.53	7	148.85	0.18	26.78
11	225.82	0.07	15.08	8	171.24	0.06	10.65
14	252.80	0.07	17.63	9	174.84	0.07	11.57
15	267.78	0.20	52.49	10	189.19	0.06	11.69
16	277.88	0.15	42.85	14	241.35	0.16	38.65
19	333.04	0.06	20.46	15	253.93	0.31	77.77
20	345.65	0.07	23.48	19	319.57	0.13	41.83
23	397.96	0.09	36.99	23	395.32	0.10	40.89
65	1080.84	0.07	74.21	64	1067.98	0.06	59.59
83	1372.71	0.11	144.88	65	1077.86	0.06	60.99
88	1444.99	0.13	192.54	83	1362.06	0.15	198.31
93	1500.08	0.09	131.2	88	1435.80	0.17	237.64
95	1516.99	0.07	101.07	94	1495.53	0.08	127.06
96	1521.56	0.10	147.47	95	1508.75	0.15	231.52
98	1543.92	0.06	99.41	98	1533.86	0.13	192.41
105	1694.64	0.08	128.68	104	1678.43	0.06	105.63
				106	3092.99	0.08	236.9

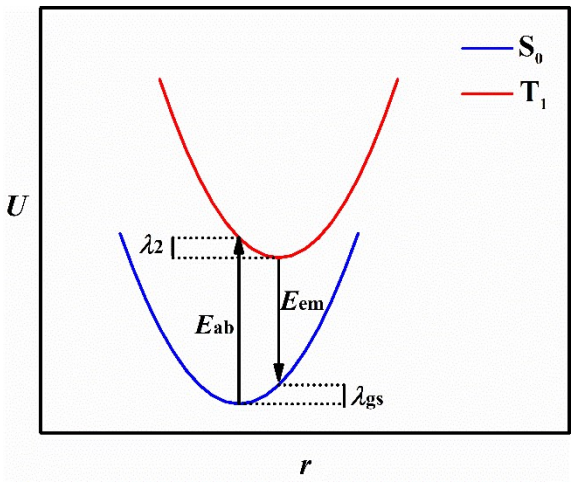

Figure S5. The adiabatic potential energy surfaces of T_1 and S_0 for emitters. Here, $\lambda_{gs/es}$ is the reorganization energy of S_0/T_1.

Table S3. Calculated reorganization energy λ_{gs} and λ_2 (see Figure S5).

	Solution		Solid	
	λ_{gs}/eV	λ_2/eV	λ_{gs}/eV	λ_2/eV
PtON7	0.283	0.209	0.211	0.178
PtOO7	0.292	0.232	0.266	0.241

[a] λ_{gs} and λ_2 were calculated by the four-point technique.