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

Supporting information

Calculation of excited states of monolayer TPPA-COF based on First-principles

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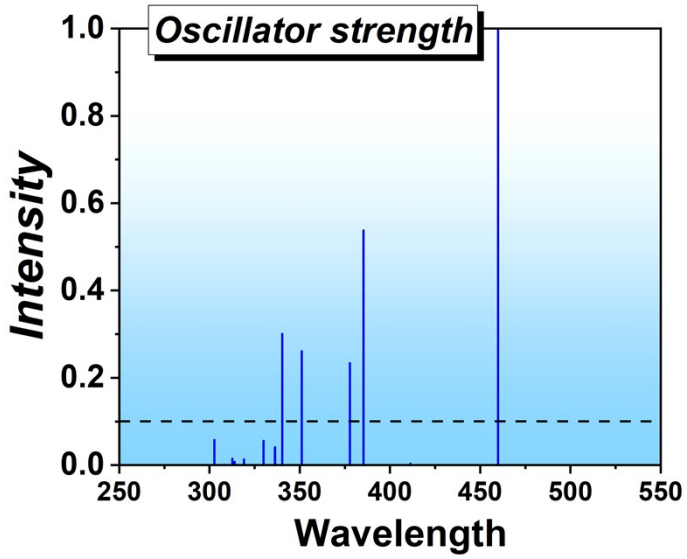
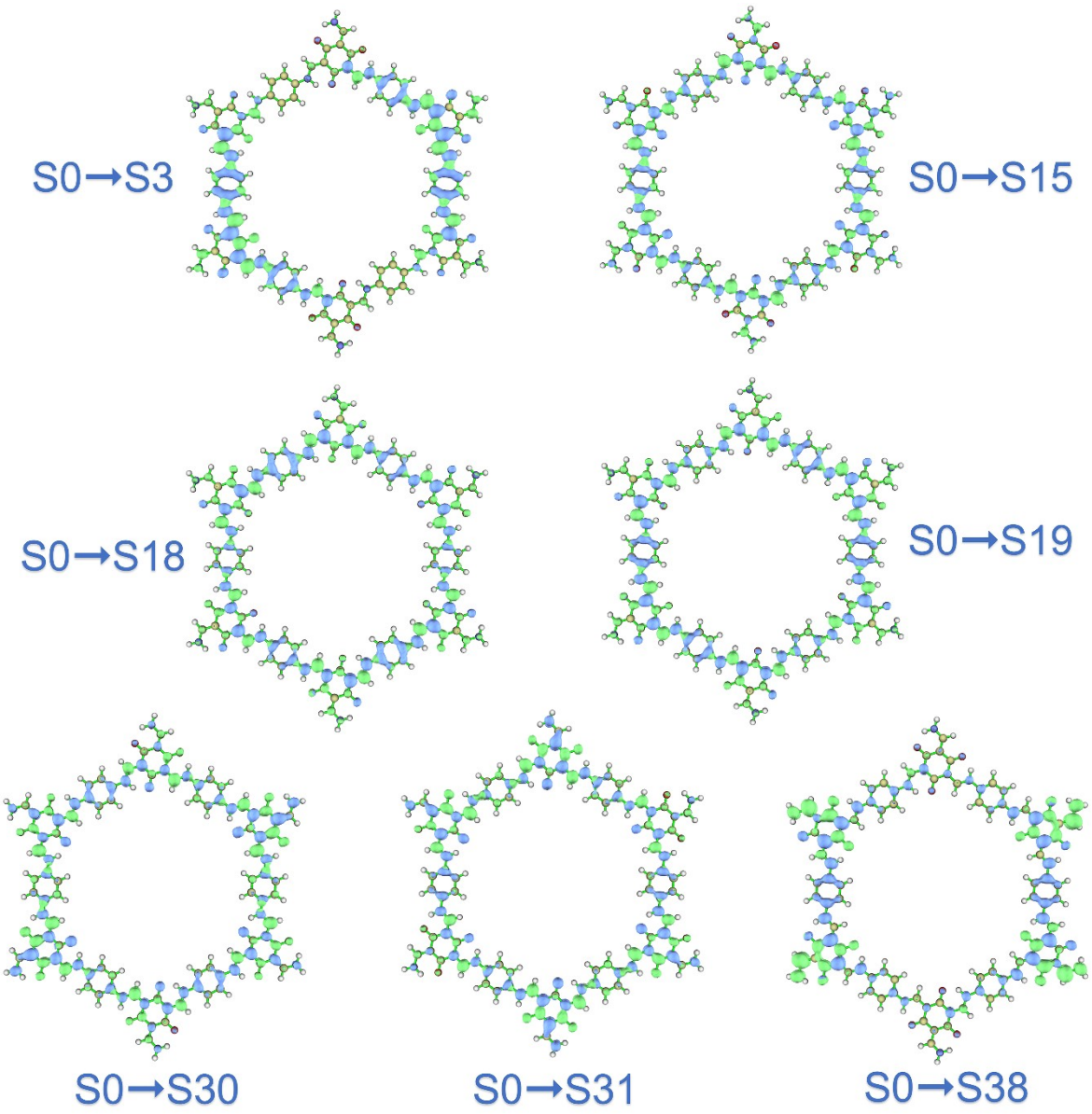
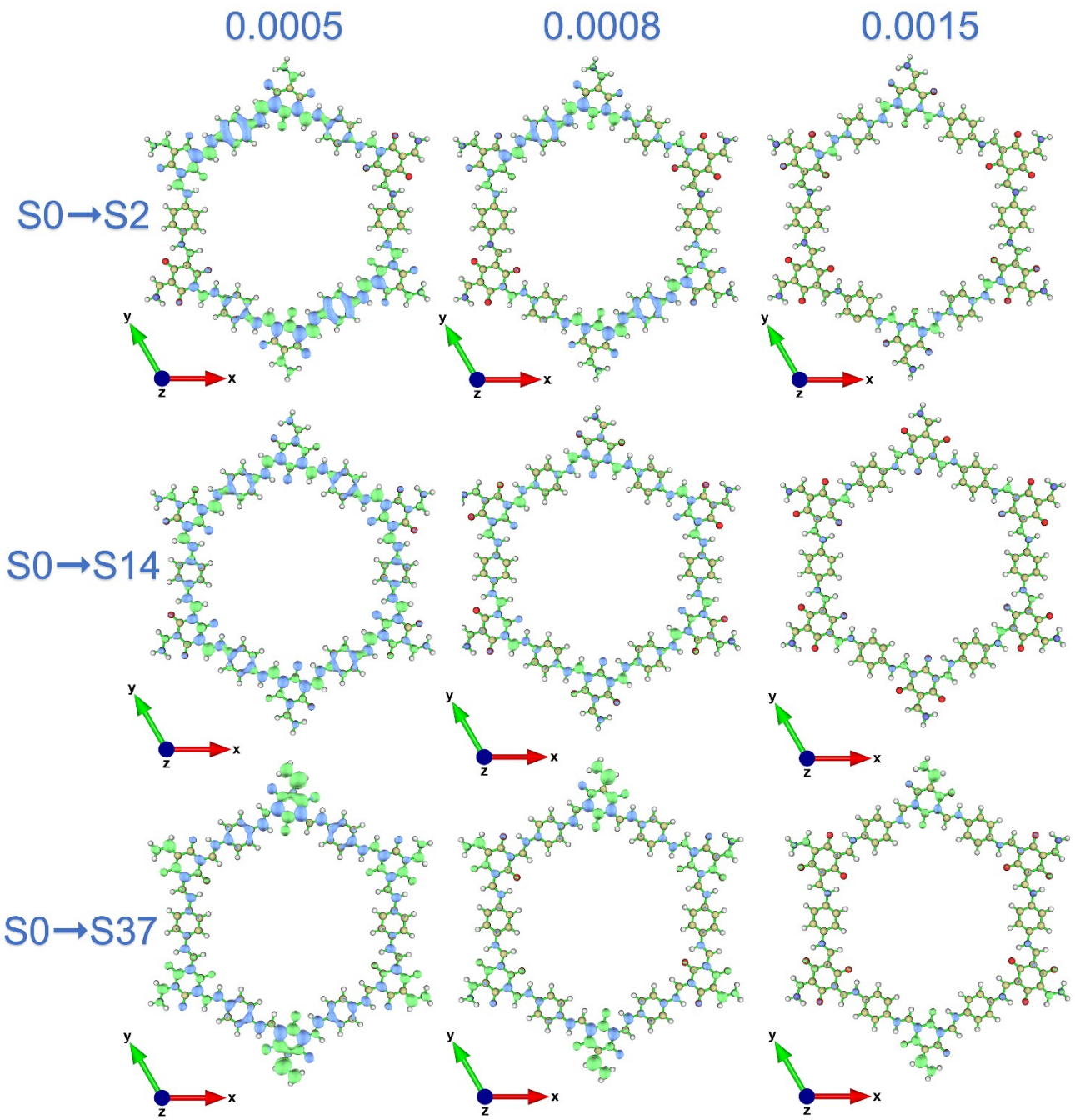


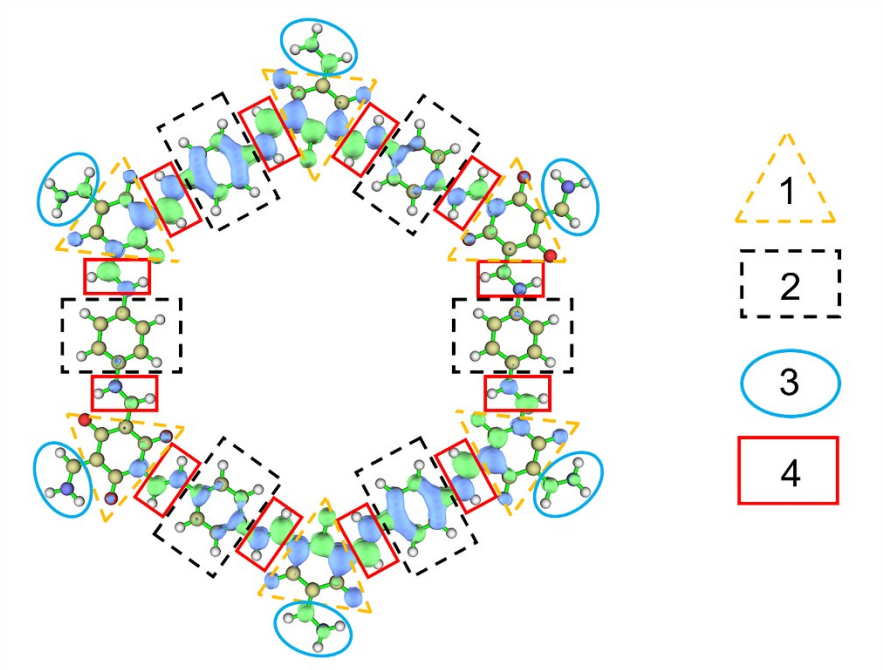
S1. The oscillator strength of TPPA-COF monolayer.



S2. Electron-hole distribution of excitations S0→S3, S0→S15, S0→S18, S0→S19, S0→S30, S0→S31and S0→S38 of TPPA-COF monolaye.



S3. Excitations S0→S2, S0→S14 and S0→S37 electron hole distributions under different isosurface (0.0005, 0.0008 and 0.0015).



S4. The fragments definition diagram of the TPPA-COF monolayer.

Table S1. Excitation energy, corresponding wavelength for light absorption, and relevant orbital contribution of each excited state of TPPA-COF monolayer.

Materital	TPPA-COF									
The excitation energy	#2	#3	#14	#15	#18	#19	#30	#31	#37	#38
The Excitation energy/eV	2.6956	2.6963	3.2175	3.2176	3.2814	3.2816	3.5307	3.5310	3.6430	3.6434
Corresponding wavelength/nm	459.95	459.83	385.34	385.33	377.84	377.82	351.16	351.13	340.34	340.30
Orbital contribution	H-1-> L	H-2-> L	H-3->L+1	H-4->L+1	H-1->L+4	H-1->L+3	H-5->L+4	H-5->L+3	H->L+9	H->L+10
	43.5%	43.4%	22.8%	22.8%	34.5%	34.6%	26.7%	26.7%	22.6%	22.5%
	H->L+1	H->L+2	H-4->L+2	H-3->L+2	H2->L+3	H-2->L+4	H-4->L+5	H-3->L+5	H-1->L+11	H-2->L+11
	37.8%	37.8%	22.8%	22.70%	33.50%	33.4%	19.80%	19.80%	13.3%	13.1%
			H-17->L	H-2-> L	H->L+1	H->L+2	H-5->L+3	H-5->L+4	H->L+10	H->L+9
			13.7%	11.0%	10.90%	10.9%	18.7%	18.70%	9.30%	9.20%
			H-4->L+1	H-4->L+2					H-2->L+7	H-2->L+8
			11.1%	10.90%					8.90%	8.90%
			H-3->L+2	H-5->L+4				H-1->L+8	H-1->L+7	
			10.8%	7.2%					8.9%	8.80%
			H-5->L+3							
			7.2%							

Table S2. Some theoretically evaluated parameters attained from electron-hole method for excited states of TPPA-COF monolayer.

Type	N0	Excitation energy	Sm index	Sr index	D index	t index	H index	Hole delocalization index	Electron delocalization index
□	□	eV	a.u.	a.u.	Angstrom	Angstrom	Angstrom	/	/
TPPA-COF	2	2.69	0.39	0.68	0.002	-8.696	12.226	3.43	3.06
	3	2.69	0.39	0.68	0.004	-8.691	12.267	3.44	3.05
	14	3.22	0.46	0.74	0.002	-8.732	12.396	2.71	2.65
	15	3.22	0.46	0.74	0.001	-8.640	12.396	2.71	2.65
	18	3.28	0.47	0.75	0.002	-8.780	12.405	2.89	2.53
	19	3.28	0.47	0.75	0.002	-8.640	12.405	2.89	2.53
	30	3.53	0.43	0.73	0.004	-8.888	12.590	2.75	2.66
	31	3.53	0.43	0.73	0.003	-8.943	12.589	2.76	2.65
	37	3.64	0.31	0.62	0.004	-9.594	13.328	3.00	3.91
	38	3.64	0.31	0.62	0.006	-8.559	13.326	3.00	3.91