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芴基张力半导体结构和光电性质的理论研究

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Theoretical Studies on the Structures and Opto-Electronic Properties of Fluorene-Based Strained Semiconductors

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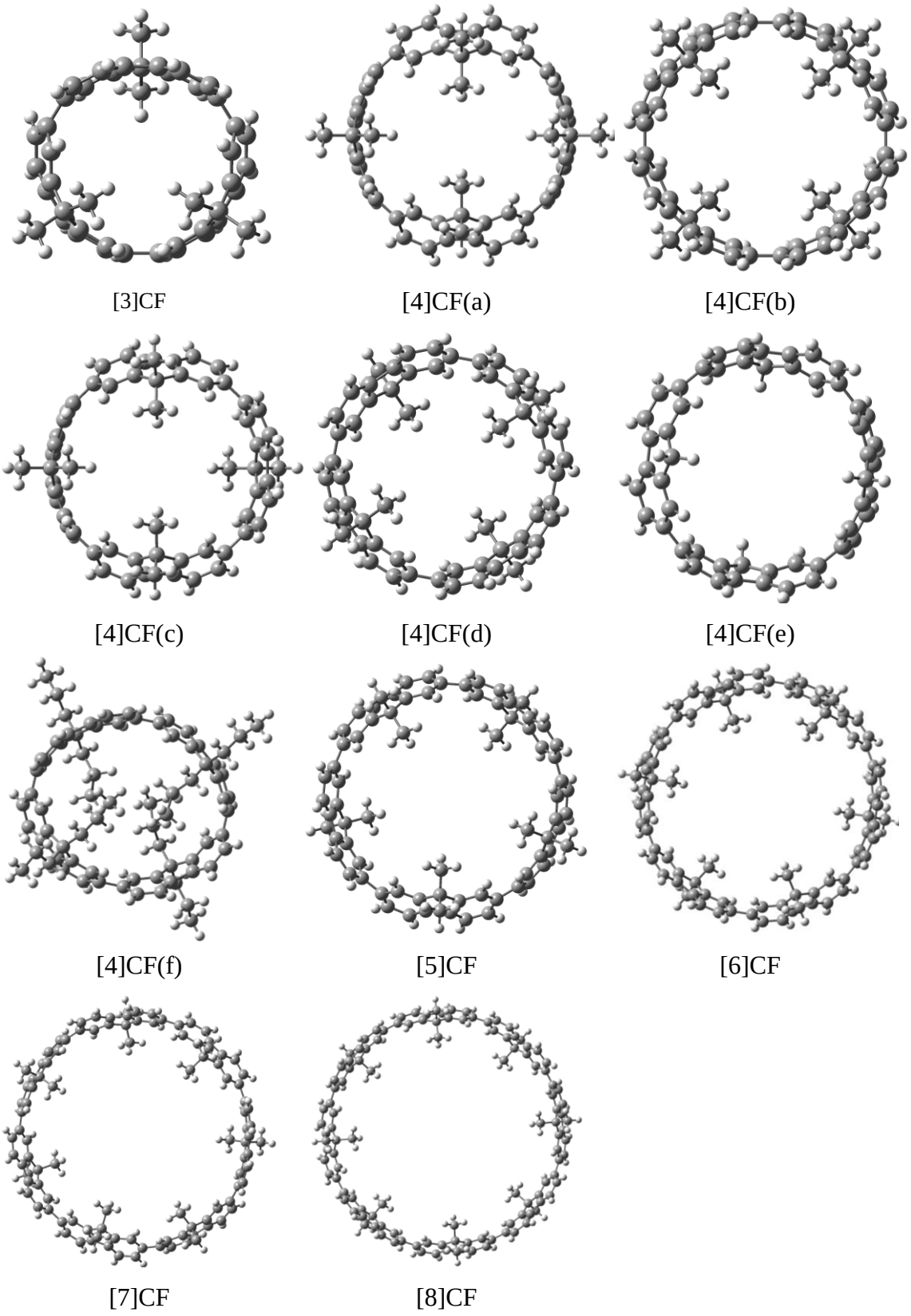
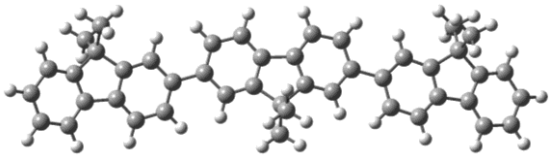


Fig.S1 Optimized structures of [*n*]CFs.



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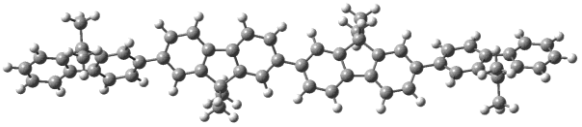

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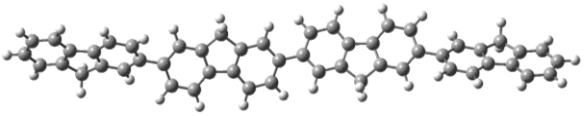

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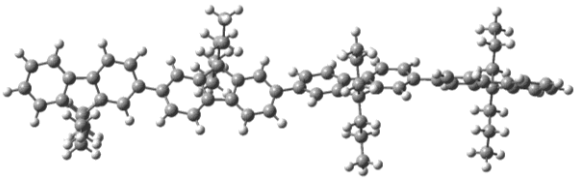

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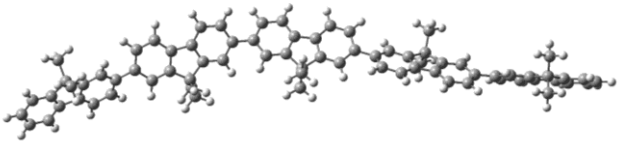
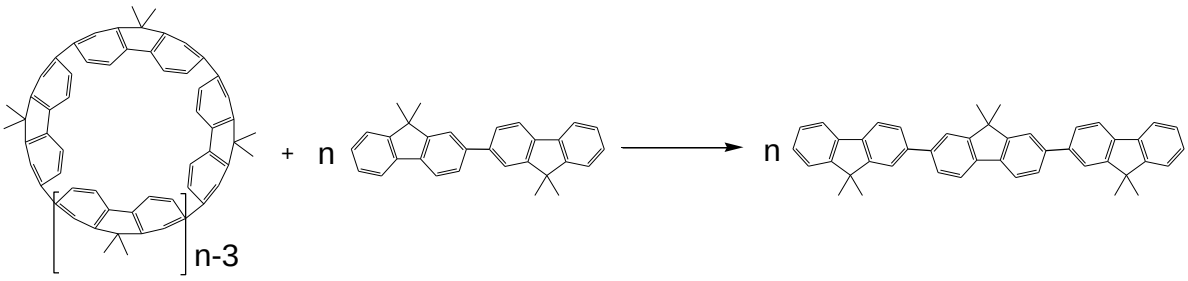


Fig.S2 Optimized structures of [*n*]LFs

Table S1 Computed total energies (*E*, in Hartree) and imaginary frequencies (in cm^{-1}) of stationary points

COMPD	*E*	Imaginary frequency
TS_{ac}	2315.292274	33.38 *i*
TS_{ac}'	2315.234041	37.25 *i*
TS_{bc}'	2315.235223	31.60 *i*
TS_{bc}	2315.294698	29.36 *i*
TS_{cd}	2315.297306	28.75 *i*
TS_{cd}'	2315.235787	36.94 *i*



n = 3-8

Scheme S1 Hypothetical homodesmotic reactions for the calculation of strain energies of [*n*]CFs.

Table S2 Strain energies and diameters of [*n*]CFs based on homodesmotic reactions (ΔH in kJ mol^{-1}).

COMPD	Strain energy	Minor axis/nm	Major axis/nm
[3]CF	418.3	0.78	0.82
[4]CF (a)	322.0	1.08	1.08
[4]CF (b)	313.6	1.08	1.11
[4]CF (c)	309.8	1.09	1.10
[4]CF (d)	291.4	1.09	1.09
[4]CF (e)	285.5	1.02	1.02
[5]CF	232.4	1.33	1.35
[6]CF	175.0	1.63	1.63
[7]CF	147.8	1.87	1.89
[8]CF	116.8	2.16	2.16

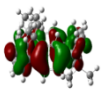
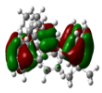
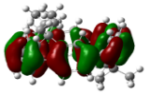
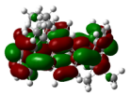
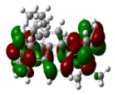
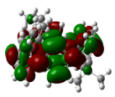
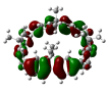
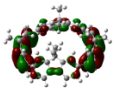
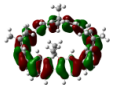
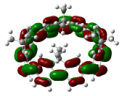
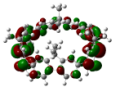
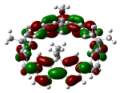
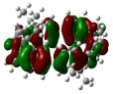
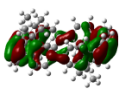
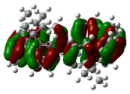
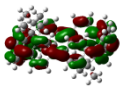
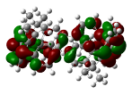
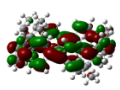
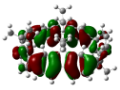
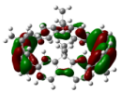
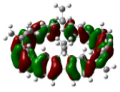
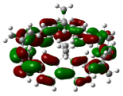
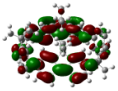
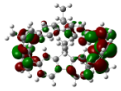
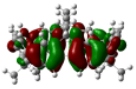
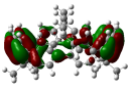
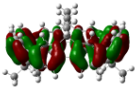
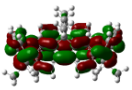
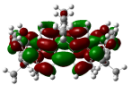
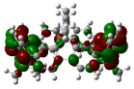
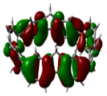
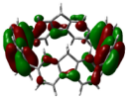
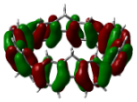
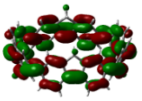
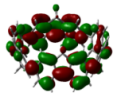
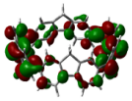
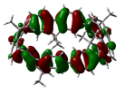
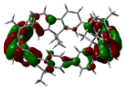
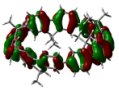
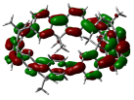
COMPD	HOMO - 2	HOMO - 1	HOMO	LUMO	LUMO + 1	LUMO + 2
[3]CF						
[4]CF (a)						
[4]CF (b)						
[4]CF (c)						
[4]CF (d)						
[4]CF (e)						
[5]CF						
[6]CF						
[7] CF						
[8]CF						

Fig.S3 HOMO and LUMO of [*n*]CFs at the B3LYP/6-31G(*d*) level.

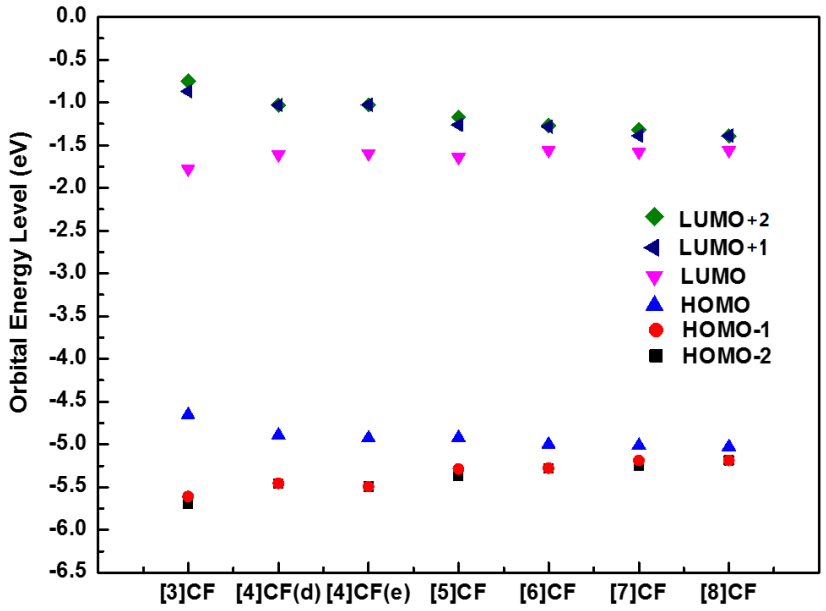


Fig.S4 Calculated energy levels of LUMO, LUMO + 1, LUMO + 2 and HOMO, HOMO - 1, HOMO - 2 orbitals for [*n*]CFs at the B3LYP/6-31G(*d*) level.

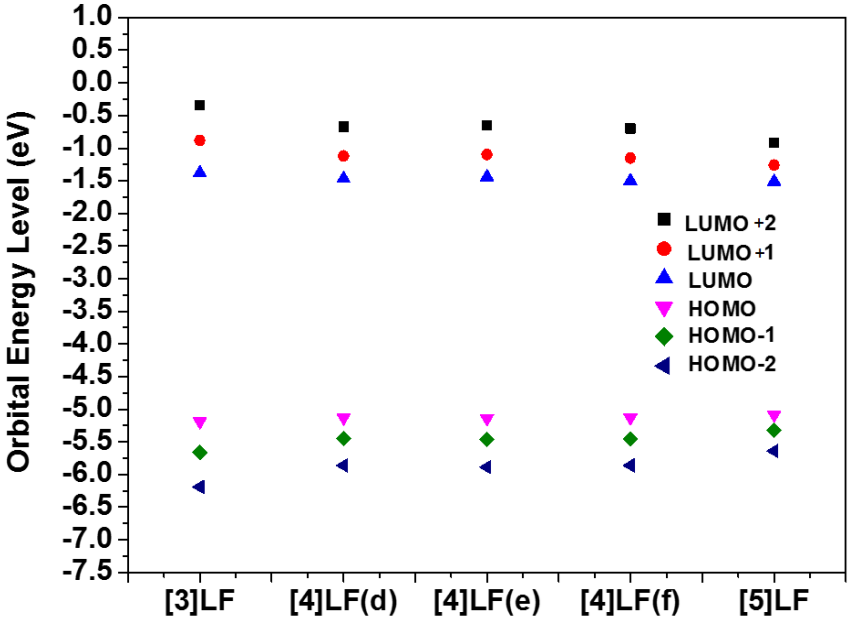


Fig.S5 Calculated energy levels of LUMO, LUMO + 1, LUMO + 2 and HOMO, HOMO- 1, HOMO - 2 orbitals for [*n*]LFs at the B3LYP/6-31G(*d*) level.

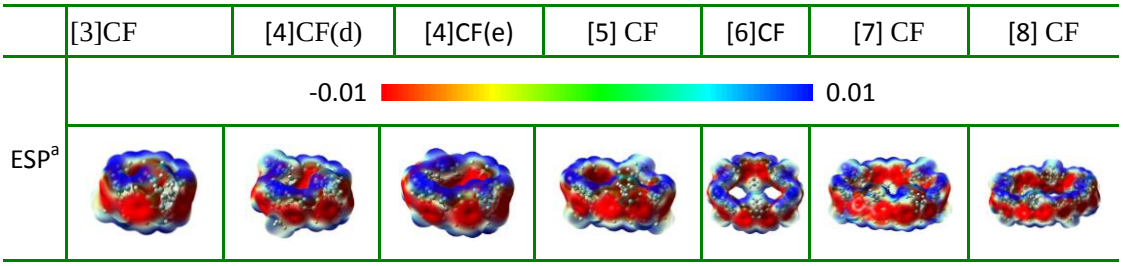


Fig.S6 ESPs of [*n*]CFs at the B3LYP/6-31G(*d*) level.
The color code ranges from -0.01 eV (red) to 0.01 eV (blue).

Table S3 Ionization potential (IP), electronic affinity (EA), and reorganization energy (λ) of [*n*]CFs and [*n*]LFs (in eV).

Molecule	IP(v)	IP(a)	HEP[a]	EA(v)	EA(a)	EEP[b]	λ_{hole}	$\lambda_{electron}$
[3]CF[c]	-	-	-	-	-	-	-	-
[3]LF	6.20	6.08	5.98	0.39	0.54	0.68	0.22	0.29
[4]CF(a)	5.73	5.63	5.53	0.81	0.91	1.00	0.20	0.20
[4]CF(b)	5.74	5.65	5.55	0.80	0.88	0.96	0.19	0.17
[4]CF(c)	5.79	5.68	5.57	0.74	0.85	0.97	0.22	0.22
[4]CF(d)	5.85	5.74	5.63	0.66	0.77	0.87	0.22	0.21
[4]LF(d)	5.99	5.90	5.81	0.61	0.72	0.84	0.17	0.23
[4]CF(e)	5.90	5.79	5.69	0.63	0.73	0.84	0.22	0.21
[4]LF(e)	6.02	5.94	5.85	0.56	0.68	0.80	0.17	0.24
[5]CF	5.77	5.68	5.59	0.80	0.88	0.98	0.18	0.18
[5]LF	5.85	5.78	5.71	0.75	0.85	0.94	0.14	0.19

[a] Hole extraction potential (HEP) is the energy difference from M+ (cationic) to M (neutral molecule) using the M+ geometric structure. [b] Electron extraction potential (EEP) is the energy difference from M-(anionic) to M using the M- geometric structure. [c] the calculation of [3]CF is not converged

Table S4 Electronic transition data obtained by TDDFT methods (TD-B3LYP/6-31G(*d*)//B3LYP/6-31G(*d*)) for [*n*]CFs and [*n*]LFs (in eV).

COMPD	Electronic transitions	Wavelength /nm	*f*	Main configurations
[3]CF	$S_1 \leftarrow S_0$	548	0.0035	HOMO → LUMO (99%)
	$S_6 \leftarrow S_0$	336	0.6893	HOMO - 2 → LUMO (49%), HOMO → LUMO + 2 (47%)
[3]LF	$S_1 \leftarrow S_0$	363	2.0213	HOMO → LUMO (98%)
[4]CF(a)	$S_1 \leftarrow S_0$	499	0.00	HOMO → LUMO (98%)
	$S_4 \leftarrow S_0$	363	1.21	HOMO - 1 → LUMO (44%) HOMO → LUMO + 1 (55%)
	$S_5 \leftarrow S_0$	358	1.30	HOMO - 2 → LUMO (45%) HOMO → LUMO + 2(54%)
[4]CF(b)	$S_1 \leftarrow S_0$	492	0.00	HOMO → LUMO (98%)
	$S_3 \leftarrow S_0$	366	1.35	HOMO - 1 → LUMO (50%)
	$S_5 \leftarrow S_0$	353	1.10	HOMO → LUMO + 1 (49%)
[4]CF(c)	$S_1 \leftarrow S_0$	475	0.04	HOMO → LUMO (97%)
	$S_4 \leftarrow S_0$	356	1.01	HOMO - 1 → LUMO (36%) HOMO →LUMO + 2 (62%)
	$S_5 \leftarrow S_0$	353	1.22	HOMO - 2 → LUMO (44%), HOMO → LUMO + 1 (54%)
[4]CF(d)	$S_1 \leftarrow S_0$	450	0.00	HOMO - 2 → LUMO (41%), HOMO → LUMO + 2 (58%)
	$S_4 \leftarrow S_0$	347	1.12	HOMO → LUMO (97%)
	$S_5 \leftarrow S_0$	347	1.12	HOMO → LUMO + 1 (53%)
[4]LF(d)	$S_1 \leftarrow S_0$	381	2.84	HOMO → LUMO (29%)
[4]CF(e)	$S_1 \leftarrow S_0$	444	0.00	HOMO → LUMO + 2 (53%)
	$S_4 \leftarrow S_0$	342	1.21	HOMO → LUMO (28%)
[4]LF(e)	$S_1 \leftarrow S_0$	376	2.93	HOMO → LUMO (96%)
[5]CF	$S_1 \leftarrow S_0$	439	0.0441	HOMO → LUMO (94%)
	$S_3 \leftarrow S_0$	366	0.8423	HOMO → LUMO + 1 (98%)
[5]LF	$S_1 \leftarrow S_0$	391	3.4591	HOMO → LUMO (93%)

Table S5 Electronic transition data obtained by TDDFT methods (TD-B3LYP/6-31G(*d*) //B3LYP/6-31G(*d*)) for the PL spectra of [*n*]CFs and [*n*]LFs (in eV).

COMPD	Electronic transitions	Wavelength /nm	*f*	Main configurations
[3]CF	$S_0 \leftarrow S_1$	827	0.0012	HOMO → LUMO (99%)
	$S_0 \leftarrow S_5$	374	0.848	HOMO - 2 → LUMO (51%) HOMO → LUMO + 2 (47%)
[3]LF	$S_0 \leftarrow S_1$	436	2.3407	HOMO → LUMO (99%)
[4]CF(**a**)	$S_0 \leftarrow S_1$	670	0	HOMO → LUMO (99%)
	$S_0 \leftarrow S_4$	404	1.4375	HOMO - 1 → LUMO (50%) HOMO → LUMO + 1 (50%)
	$S_0 \leftarrow S_5$	401	1.4991	HOMO - 2 → LUMO (48%) HOMO → LUMO + 2 (51%)
[4]CF(**b**)	$S_0 \leftarrow S_1$	639	0	HOMO → LUMO (99%)
	$S_0 \leftarrow S_4$	405	1.4943	HOMO - 1 → LUMO (50%) HOMO → LUMO + 1 (50%)
	$S_0 \leftarrow S_5$	391	1.3605	HOMO - 2 → LUMO (47%) HOMO → LUMO + 2 (52%)
[4]CF(**c**)	$S_0 \leftarrow S_1$	645	0.0068	HOMO → LUMO (99%)
	$S_0 \leftarrow S_4$	399	1.4089	HOMO - 2 → LUMO (47%) HOMO → LUMO + 2 (50%)
	$S_0 \leftarrow S_5$	399	1.4289	HOMO - 1 → LUMO (47%) HOMO → LUMO + 1 (50%)
[4]CF(**d**)	$S_0 \leftarrow S_1$	606	0	HOMO → LUMO (98%)
	$S_0 \leftarrow S_4$	392	1.3731	HOMO - 1 → LUMO (47%) HOMO → LUMO + 1 (48%)
	$S_0 \leftarrow S_5$	392	1.3816	HOMO - 2 → LUMO (48%) HOMO → LUMO + 2 (48%)
[4]LF(**d**)	$S_0 \leftarrow S_1$	457	3.1592	HOMO → LUMO (98%)
[4]CF(**e**)	$S_0 \leftarrow S_1$	595	0	HOMO → LUMO (98%)
	$S_0 \leftarrow S_4$	385	1.45	HOMO - 1 → LUMO (49%) HOMO → LUMO + 1 (41%)
	$S_0 \leftarrow S_5$	385	1.45	HOMO - 2 → LUMO (49%) HOMO → LUMO + 2 (41%)
[4]LF(**e**)	$S_0 \leftarrow S_1$	450	3.2483	HOMO → LUMO (98%)
[5]CF	$S_0 \leftarrow S_1$	542	0.023	HOMO → LUMO (96%)
	$S_0 \leftarrow S_4$	410	1.8424	HOMO - 1 → LUMO (45%) HOMO → LUMO + 1 (54%)
[5]LF	$S_0 \leftarrow S_1$	466	3.6758	HOMO → LUMO (97%)