

Supporting materials

Table S1. Calculated transition energy and oscillator strength of the CA2/TiO₂ and CA3/TiO₂.

Dye/method		CA2						CA3	
Cam-B3LYP 6-311G(d,p)	S1	2.61	475	(0.48225)H→L+4	1.8005	2.31	536	(0.42382)H→L+1	2.3603
	S2	3.14	395	(0.67784)H→L	0.0092	3.39	366	(0.50988)H→L	0.0410
	S3	3.27	379	(0.69743)H→L+1	0.0000	3.40	365	(0.47243)H→L+1	0.0302
	S4	3.33	373	(0.69218)H→L+2	0.0001	3.61	343	(0.66379)H→L+2	0.0000
	S5	3.44	360	(0.50535)H→L+3	0.0022	3.65	340	(0.66635)H-1→L+3	0.0001
	S6	3.55	350	(0.45369)H→L+3	0.0001	3.71	335	(0.50961)H→L+4	0.0040

Table S2.Calculated transition properties and excited state lifetime of CA2 and CA3.

Dye	E(eV)	Strength f	T (ns)
CA2	3.38	1.3837	1.46
CA3	2.25	1.7643	2.58

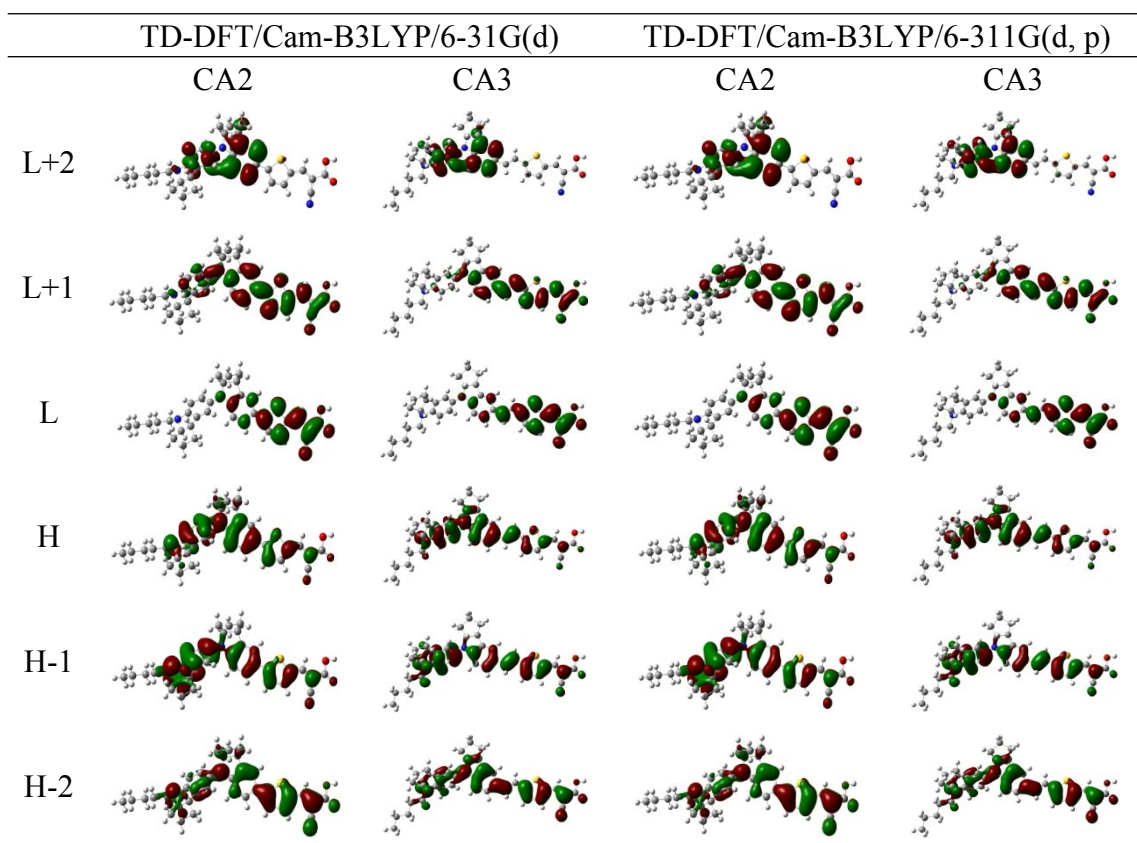


Figure S1. Electron densities of the selected HOMO and LUMO of the CA2 and CA3 in TD-DFT/Cam-B3LYP/6-31G(d) and TD-DFT/Cam-B3LYP/6-311G(d, p).