Electronic Supplementary Material (ESI) for RSC Advances.

Table S1 Excitation energies (E_{ex}), oscillator strengths (f), and transition compositions in CH_2Cl_2 solution, obtained by applying TD-CAM-B3LYP/6-31G(d,p) using C-PCM model.

Dyes	State	E_{ex}, eV (nm)	f	Transition composition
An1	$S_0 \rightarrow S_1$	3.31 (374)	0.8596	(+0.62) H-1→L+1 (-0.21) H-2→L+1
	$S_0 \rightarrow S_3$	3.74 (331)	0.6376	(+0.66) H-5→L (-0.18) H-1→L+1
	$S_0 \rightarrow S_7$	4.25 (292)	0.5290	(+0.53) H→L (+0.24) H-1→L+3 (-0.21) H-2→L+3 (+0.19) H→L+4
An2	$S_0 \rightarrow S_1$	2.75 (450)	1.6038	(+0.63) H→L+1 (+ 0.22) H-1→L+1
	$S_0 \rightarrow S_4$	3.74 (331)	1.0348	(+0.64) H-5→L (-0.17) H-2→L+1
An3	$S_0 \rightarrow S_1$	2.53 (490)	1.6325	(+0.51) H-1→L (-0.40) H→L
	$S_0 \rightarrow S_8$	4.24 (292)	0.8582	(+0.42) H→L+3 (+0.35) H-2→L+3
An4	$S_0 \rightarrow S_1$	2.21 (562)	2.2861	(+0.64) H→L (-0.17) H→L+1
	$S_0 \rightarrow S_4$	3.67 (337)	0.6031	(+0.53) H-5→L (+0.27) H-5→L (+0.23) H→L+1

NOTE: H = HOMMO, H-1 = HOMO-1, H-2 = HOMO-2, …
L = LUMO, L+1 = LUMO+1, L+2 = LUMO+2, …

Figure S1 Schematic energy diagram of the free dyes, bare TiO_2 and dye@TiO_2 system at the optimized structures by Dmol^3.