

Supporting Information

## **Anthanthrene Dye-Sensitized Solar Cells: Influence of the Number of Anchoring Groups and Substitution Motif**

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**Table S1. Dye-1 M06-2X/6-31+G(d,p)**

State	Wavelength [nm]	Oscillator strength $f_{calc}$	Major contributions [%]M06-2X	$\mu$ [Debye]	Character	
S <sub>0</sub>				0.0009		
S <sub>1</sub>	439.84	0.0001	HOMO-1 → LUMO	3	0.0016	$\pi \rightarrow \pi^*$
			HOMO → LUMO+1	90		$\pi \rightarrow \pi^*$ CT
			HOMO → LUMO+4	7		$\pi \rightarrow \pi^*$
S <sub>2</sub>	438.83	0.6770	HOMO → LUMO	96	9.7808	$\pi \rightarrow \pi^*$ CT
			HOMO → LUMO+2	4		$\pi \rightarrow \pi^*$ CT
S <sub>3</sub>	397.43	0.3172	HOMO-1 → LUMO+1	7	4.1505	$\pi \rightarrow \pi^*$
			HOMO → LUMO	2		$\pi \rightarrow \pi^*$ CT
			HOMO → LUMO+2	85		$\pi \rightarrow \pi^*$ CT
			HOMO → LUMO+4	6		$\pi \rightarrow \pi^*$
S <sub>4</sub>	359.89	0.1320	HOMO-3 → LUMO	4	1.5650	$\pi \rightarrow \pi^*$
			HOMO-3 → LUMO+2	9		$\pi \rightarrow \pi^*$
			HOMO-2 → LUMO	25		$\pi \rightarrow \pi^*$
			HOMO-2 → LUMO+2	8		$\pi \rightarrow \pi^*$
			HOMO-1 → LUMO+1	5		$\pi \rightarrow \pi^*$
			HOMO-1 → LUMO+3	49		$\pi \rightarrow \pi^*$
S <sub>5</sub>	340.43	0.0000	HOMO-4 → LUMO+2	3	0.0011	$\pi \rightarrow \pi^*$
			HOMO-3 → LUMO+1	7		$\pi \rightarrow \pi^*$
			HOMO-2 → LUMO+1	21		$\pi \rightarrow \pi^*$ CT
			HOMO-1 → LUMO	69		$\pi \rightarrow \pi^*$ CT
S <sub>6</sub>	339.43	1.6266	HOMO-4 → LUMO+1	5	18.1774	$\pi \rightarrow \pi^*$
			HOMO-3 → LUMO	10		$\pi \rightarrow \pi^*$
			HOMO-2 → LUMO	16		$\pi \rightarrow \pi^*$
			HOMO-2 → LUMO+2	4		$\pi \rightarrow \pi^*$
			HOMO-1 → LUMO+1	40		$\pi \rightarrow \pi^*$ CT
			HOMO → LUMO	4		$\pi \rightarrow \pi^*$ CT
			HOMO → LUMO+2	9		$\pi \rightarrow \pi^*$ CT
			HOMO → LUMO+3	11		$\pi \rightarrow \pi^*$
S <sub>7</sub>	325.68	0.0000	HOMO-2 → LUMO+1	2	0.009	$\pi \rightarrow \pi^*$
			HOMO-1 → LUMO	3		$\pi \rightarrow \pi^*$ CT
			HOMO-1 → LUMO+2	22		$\pi \rightarrow \pi$
			HOMO → LUMO+1	4		$\pi \rightarrow \pi^*$ CT
			HOMO → LUMO+4	66		$\pi \rightarrow \pi^*$
			HOMO → LUMO+7	2		$\pi \rightarrow \pi^*$
S <sub>8</sub>	309.65	0.0000	HOMO-4 → LUMO	13	0.009	$\pi \rightarrow \pi^*$ CT
			HOMO-3 → LUMO+1	6		$\pi \rightarrow \pi^*$ CT
			HOMO-2 → LUMO+1	10		$\pi \rightarrow \pi^*$
			HOMO-2 → LUMO	3		$\pi \rightarrow \pi^*$
			HOMO-1 → LUMO+2	40		$\pi \rightarrow \pi^*$
			HOMO → LUMO+1	3		$\pi \rightarrow \pi^*$
S <sub>9</sub>	294.55	0.2999	HOMO → LUMO+4	25	2.9091	$\pi \rightarrow \pi^*$
			HOMO-3 → LUMO	6		$\pi \rightarrow \pi^*$ CT
			HOMO-2 → LUMO	34		$\pi \rightarrow \pi^*$
			HOMO-2 → LUMO+2	14		$\pi \rightarrow \pi^*$
			HOMO-1 → LUMO+1	19		$\pi \rightarrow \pi^*$ CT
S <sub>10</sub>	281.20	0.0000	HOMO → LUMO+3	27	0.0009	$\pi \rightarrow \pi^*$
			HOMO-7 → LUMO	3		$\pi \rightarrow \pi^*$
			HOMO-3 → LUMO+1	29		$\pi \rightarrow \pi^*$ CT
			HOMO-3 → LUMO+4	48		$\pi \rightarrow \pi^*$
			HOMO-2 → LUMO+1	7		$\pi \rightarrow \pi^*$
			HOMO-2 → LUMO+4	5		$\pi \rightarrow \pi^*$

HOMO-1 → LUMO	7	$\pi \rightarrow \pi^*$
HOMO-1 → LUMO+2	3	$\pi \rightarrow \pi^*$
HOMO-1 → LUMO+3	3	$\pi \rightarrow \pi^*$

**Table S2. Dye-2** M06-2X/6-31+G(d,p)

State	Wavelength [nm]	Oscillator strength $f_{calc}$	Major contributions [%]M06-2X	$\mu$ [Debye]	Character
S <sub>0</sub>				9.0788	
					$\pi \rightarrow \pi^*$
S <sub>1</sub>	449.47	0.3298	HOMO-2 → LUMO 2 HOMO-1 → LUMO 9 HOMO → LUMO 85 HOMO → LUMO+1 4	10.9990	$\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ CT
S <sub>2</sub>	414.47	0.2511	HOMO-2 → LUMO 3 HOMO-1 → LUMO+1 6 HOMO → LUMO+1 89 HOMO → LUMO+2 2	10.4267	$\pi \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ CT
S <sub>3</sub>	365.29	0.0143	HOMO-3 → LUMO 6 HOMO-3 → LUMO+1 21 HOMO-1 → LUMO 13 HOMO-1 → LUMO+1 24 HOMO-1 → LUMO+2 3 HOMO → LUMO 3 HOMO → LUMO+2 28 HOMO → LUMO+3 2	9.1465	$\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ CT
S <sub>4</sub>	360.08	0.0181	HOMO-4 → LUMO+1 3 HOMO-3 → LUMO+1 3 HOMO-2 → LUMO 6 HOMO-2 → LUMO+1 6 HOMO-1 → LUMO 23 HOMO-1 → LUMO+1 25 HOMO-1 → LUMO+2 2 HOMO → LUMO 3 HOMO → LUMO+2 17 HOMO → LUMO+3 12	9.2066	$\pi \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ CT

						$\pi \rightarrow \pi^*$
						CT
						$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
						CT
S <sub>5</sub>	344.84	1.5337	HOMO-4 $\rightarrow$ LUMO	10		$\pi \rightarrow \pi^*$
			HOMO-2 $\rightarrow$ LUMO	58		$\pi \rightarrow \pi^*$
			HOMO-1 $\rightarrow$ LUMO	5		CT
			HOMO-1 $\rightarrow$ LUMO+1	6	15.8728	$\pi \rightarrow \pi^*$
			HOMO $\rightarrow$ LUMO	3		CT
			HOMO $\rightarrow$ LUMO+1	3		$\pi \rightarrow \pi^*$
			HOMO $\rightarrow$ LUMO+3	15		CT
						$\pi \rightarrow \pi^*$
						CT
						$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
						CT
S <sub>6</sub>	332.73	0.1028	HOMO-2 $\rightarrow$ LUMO	10		$\pi \rightarrow \pi^*$
			HOMO-2 $\rightarrow$ LUMO+1	3		$\pi \rightarrow \pi^*$
			HOMO-1 $\rightarrow$ LUMO	8		$\pi \rightarrow \pi^*$
			HOMO-1 $\rightarrow$ LUMO+3	6	9.3997	CT
			HOMO $\rightarrow$ LUMO+2	18		$\pi \rightarrow \pi^*$
			HOMO $\rightarrow$ LUMO+3	54		CT
						$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
						CT
						$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
						CT
S <sub>7</sub>	329.94	0.0138	HOMO-2 $\rightarrow$ LUMO	11		$\pi \rightarrow \pi^*$
			HOMO-1 $\rightarrow$ LUMO	45		CT
			HOMO-1 $\rightarrow$ LUMO+1	28		$\pi \rightarrow \pi^*$
			HOMO-1 $\rightarrow$ LUMO+3	5	9.1948	CT
			HOMO $\rightarrow$ LUMO	5		$\pi \rightarrow \pi^*$
			HOMO $\rightarrow$ LUMO+1	2		$\pi \rightarrow \pi^*$
			HOMO $\rightarrow$ LUMO+3	4		CT
						$\pi \rightarrow \pi^*$
						CT
						$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
						CT
						$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
						CT
S <sub>8</sub>	309.35	0.0370	HOMO-4 $\rightarrow$ LUMO	11		$\pi \rightarrow \pi^*$
			HOMO-3 $\rightarrow$ LUMO	3		CT
			HOMO-3 $\rightarrow$ LUMO+1	7		$\pi \rightarrow \pi^*$
			HOMO-2 $\rightarrow$ LUMO+1	69	9.1001	$\pi \rightarrow \pi^*$
			HOMO-1 $\rightarrow$ LUMO+1	3		$\pi \rightarrow \pi^*$
			HOMO $\rightarrow$ LUMO+3	7		$\pi \rightarrow \pi^*$
						CT
						$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
						CT
						$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
						CT
S <sub>9</sub>	306.91	0.0216	HOMO-1 $\rightarrow$ LUMO+2	2		$\pi \rightarrow \pi^*$
			HOMO-1 $\rightarrow$ LUMO+4	73		$\pi \rightarrow \pi^*$
			HOMO-1 $\rightarrow$ LUMO+9	3	9.1495	$\pi \rightarrow \pi^*$
			HOMO $\rightarrow$ LUMO+4	22		CT
						$\pi \rightarrow \pi^*$
						CT
						$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
						CT
						$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
						CT
S <sub>10</sub>	299.59	0.8485	HOMO-3 $\rightarrow$ LUMO	10		$\pi \rightarrow \pi^*$
			HOMO-3 $\rightarrow$ LUMO+1	11		CT
			HOMO-1 $\rightarrow$ LUMO+1	9		$\pi \rightarrow \pi^*$
			HOMO-1 $\rightarrow$ LUMO+3	20	12.3383	$\pi \rightarrow \pi^*$
			HOMO-1 $\rightarrow$ LUMO+5	25		CT
			HOMO-1 $\rightarrow$ LUMO+7	4		$\pi \rightarrow \pi^*$

HOMO  $\rightarrow$  LUMO+2 6  
HOMO  $\rightarrow$  LUMO+3 3  
HOMO  $\rightarrow$  LUMO+5 12

$\pi \rightarrow \pi^*$   
CT  
 $\pi \rightarrow \pi^*$   
CT  
 $\pi \rightarrow \pi^*$   
 $\pi \rightarrow \pi^*$   
 $\pi \rightarrow \pi^*$   
CT

Dye-2 CAM-B3LYP/6-31+G(d,p)

State	Wavelength [nm]	Oscillator strength $f_{calc}$	Major contributions [%]	$\mu$ [Debye]	Character
S <sub>0</sub>				9.3353	$\pi \rightarrow \pi^*$
S <sub>1</sub>	444.39	0.4310	HOMO-2 $\rightarrow$ LUMO 2 HOMO-1 $\rightarrow$ LUMO 7 HOMO $\rightarrow$ LUMO 75 HOMO $\rightarrow$ LUMO+1 16	11.8163	$\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ (CT)
S <sub>2</sub>	412.65	0.2136	HOMO-2 $\rightarrow$ LUMO 5 HOMO-1 $\rightarrow$ LUMO+1 5 HOMO $\rightarrow$ LUMO 10 HOMO $\rightarrow$ LUMO+1 76 HOMO $\rightarrow$ LUMO+2 4	10.4772	$\pi \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ (CT) $\pi \rightarrow \pi^*$
S <sub>3</sub>	364.59	0.0055	HOMO-3 $\rightarrow$ LUMO 6 HOMO-3 $\rightarrow$ LUMO+1 28 HOMO-2 $\rightarrow$ LUMO 3 HOMO-2 $\rightarrow$ LUMO+1 3 HOMO-1 $\rightarrow$ LUMO+1 3 HOMO-1 $\rightarrow$ LUMO+2 4 HOMO $\rightarrow$ LUMO+2 44 HOMO $\rightarrow$ LUMO+3 9	9.3611	$\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ $\pi \rightarrow \pi^*$
S <sub>4</sub>	348.49	0.0181	HOMO-4 $\rightarrow$ LUMO+1 4 HOMO-2 $\rightarrow$ LUMO 8 HOMO-2 $\rightarrow$ LUMO+1 8 HOMO-1 $\rightarrow$ LUMO 20 HOMO-1 $\rightarrow$ LUMO+1 44 HOMO $\rightarrow$ LUMO 7 HOMO $\rightarrow$ LUMO+3 9	9.4168	$\pi \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$
S <sub>5</sub>	343.92	1.5337	HOMO-4 $\rightarrow$ LUMO 17 HOMO-2 $\rightarrow$ LUMO 59 HOMO-1 $\rightarrow$ LUMO+1 2 HOMO $\rightarrow$ LUMO 3 HOMO $\rightarrow$ LUMO+3 19	16.1671	$\pi \rightarrow \pi^*$ (CT) $\pi \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$ CT $\pi \rightarrow \pi^*$
S <sub>6</sub>	328.32	0.1028	HOMO-2 $\rightarrow$ LUMO 4 HOMO-1 $\rightarrow$ LUMO 9 HOMO-1 $\rightarrow$ LUMO+1 8	9.7727	$\pi \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ CT



**Table S3. Dye-3** M06-2X/6-31+G(d,p)

State	Wavelength [nm]	Oscillator strength $f_{calc}$	Major contributions [%]		$\mu$ [Debye]	Character
S <sub>0</sub>					0.0001	
S <sub>1</sub>	430.60	0.6210	HOMO → LUMO+1	94	0.6211	$\pi \rightarrow \pi^*$
			HOMO → LUMO+2	6		CT
S <sub>2</sub>	410.58	0.0000	HOMO → LUMO+2	100	0.0001	$\pi \rightarrow \pi^*$
S <sub>3</sub>	405.59	0.1215	HOMO → LUMO+1	6	0.1216	$\pi \rightarrow \pi^*$
			HOMO → LUMO+2	94		CT
S <sub>4</sub>	356.76	0.0227			1.5650	$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
						CT
			HOMO-5 → LUMO	12		$\pi \rightarrow \pi^*$
			HOMO-5 → LUMO+2	11		$\pi \rightarrow \pi^*$
			HOMO-4 → LUMO	5		$\pi \rightarrow \pi^*$
			HOMO-4 → LUMO+2	2		CT
			HOMO-2 → LUMO	14		$\pi \rightarrow \pi^*$
			HOMO-2 → LUMO+2	10		$\pi \rightarrow \pi^*$
			HOMO → LUMO+3	45		CT
S <sub>5</sub>	348.14	0.0000			0.0011	$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
			HOMO-6 → LUMO	6		$\pi \rightarrow \pi^*$
			HOMO-6 → LUMO+2	5		$\pi \rightarrow \pi^*$
			HOMO-1 → LUMO	47		CT
			HOMO-1 → LUMO+2	32		$\pi \rightarrow \pi^*$
S <sub>6</sub>	323.03	0.0000			18.1774	CT
						$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
			HOMO-4 → LUMO+1	5		CT
			HOMO-3 → LUMO	5		$\pi \rightarrow \pi^*$
			HOMO-3 → LUMO+2	3		$\pi \rightarrow \pi^*$
			HOMO-1 → LUMO	8		CT
			HOMO-1 → LUMO+2	4		$\pi \rightarrow \pi^*$
S <sub>7</sub>	321.71	1.4585			0.009	CT
						$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
			HOMO-5 → LUMO	7		CT
			HOMO-5 → LUMO+2	6		$\pi \rightarrow \pi^*$
			HOMO-4 → LUMO	22		$\pi \rightarrow \pi^*$
S <sub>8</sub>	316.64	0.0000			0.009	CT
						$\pi \rightarrow \pi^*$
			HOMO-4 → LUMO+2	15		$\pi \rightarrow \pi^*$
			HOMO-3 → LUMO+1	50		CT
S <sub>8</sub>	316.64	0.0000			0.009	$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
			HOMO-5 → LUMO+1	10		$\pi \rightarrow \pi^*$
			HOMO-4 → LUMO+1	30		CT
					$\pi \rightarrow \pi^*$	
					$\pi \rightarrow \pi^*$	
					$\pi \rightarrow \pi^*$	
					CT	



			HOMO → LUMO+4	18		$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
			HOMO-2 → LUMO	48		CT
S <sub>9</sub>	303.08	0.6550	HOMO-2 → LUMO+2	26	2.9091	$\pi \rightarrow \pi^*$
			HOMO-1 → LUMO+4	5		CT
			HOMO → LUMO+3	21		$\pi \rightarrow \pi^*$
						(CT)
						$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
S <sub>10</sub>	293.88	0.0000	HOMO-2 → LUMO+1	11	0.0009	$\pi \rightarrow \pi^*$
			HOMO-1 → LUMO	36		$\pi \rightarrow \pi^*$
			HOMO-1 → LUMO+2	53		CT
						$\pi \rightarrow \pi^*$

**Table S4. Dye-4** M06-2X/6-31+G(d,p)

State	Wavelength [nm]	Oscillator strength $f_{calc}$	Major contributions [%]		$\mu$ [Debye]	Character
S <sub>0</sub>					10.1014	
S <sub>1</sub>	436.90	0.2390	HOMO-1 → LUMO	4	11.4537	$\pi \rightarrow \pi^*$
			HOMO → LUMO	85		CT
			HOMO → LUMO+1	11		$\pi \rightarrow \pi^*$
S <sub>2</sub>	421.96	0.5155	HOMO → LUMO	11	12.9188	$\pi \rightarrow \pi^*$
			HOMO → LUMO+1	89		CT
						$\pi \rightarrow \pi^*$
S <sub>3</sub>	363.39	0.0092			10.1448	$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
			HOMO-4 → LUMO+1	8		CT
			HOMO-3 → LUMO+1	10		$\pi \rightarrow \pi^*$
			HOMO-1 → LUMO	4		CT
			HOMO-1 → LUMO+1	58		$\pi \rightarrow \pi^*$
			HOMO → LUMO+2	17		CT
HOMO → LUMO+3	3	$\pi \rightarrow \pi^*$				
S <sub>4</sub>	358.29	0.0114			10.1541	$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
			HOMO-4 → LUMO+1	14		CT
			HOMO-3 → LUMO+1	16		$\pi \rightarrow \pi^*$
			HOMO-1 → LUMO	3		CT
			HOMO-1 → LUMO+1	34		$\pi \rightarrow \pi^*$
			HOMO → LUMO+2	19		CT
HOMO → LUMO+3	14	$\pi \rightarrow \pi^*$				
S <sub>5</sub>	341.98	0.0363			10.2624	$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
			HOMO-6 → LUMO+2	8		CT
			HOMO-5 → LUMO	6		$\pi \rightarrow \pi^*$
			HOMO-2 → LUMO	3		CT
			HOMO-2 → LUMO+1	58		$\pi \rightarrow \pi^*$
			HOMO-1 → LUMO+1	3		(CT)
HOMO → LUMO+2	7	$\pi \rightarrow \pi^*$				
HOMO → LUMO+3	15	CT				
S <sub>6</sub>	326.44	0.0158			10.1683	$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
			HOMO-6 → LUMO+2	3		CT
			HOMO-2 → LUMO+1	23		$\pi \rightarrow \pi^*$
S <sub>7</sub>	324.24	0.0003	HOMO → LUMO+2	21	10.1025	(CT)
			HOMO → LUMO+3	53		$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
					$\pi \rightarrow \pi^*$	
					CT	
					$\pi \rightarrow \pi^*$	
					CT	
					$\pi \rightarrow \pi^*$	

S <sub>8</sub>	322.77	1.0124	HOMO-5 → LUMO	97	14.3337	CT
			HOMO-2 → LUMO+1	3		π → π*
						π → π*
						(CT)
						π → π*
						CT
S <sub>9</sub>	307.42	0.0230	HOMO-1 → LUMO+2	20	10.1930	π → π*
			HOMO-1 → LUMO+3	4		CT
			HOMO-1 → LUMO+4	52		π → π*
			HOMO-1 → LUMO+6	5		π → π*
			HOMO-1 → LUMO+7	8		CT
			HOMO-1 → LUMO+8	3		π → π*
			HOMO → LUMO+4	8		π → π*
						π → π*
						CT
						π → π*
S <sub>10</sub>	299.35	0.7436	HOMO-3 → LUMO	10	12.9843	CT
			HOMO-3 → LUMO+1	43		π → π*
			HOMO-2 → LUMO	23		CT
			HOMO-1 → LUMO+5	2		π → π*
			HOMO → LUMO+2	15		CT
			HOMO → LUMO+3	7		π → π*
						π → π*

Dye-4 CAM-B3LYP/6-31+G(d,p)

State	Wavelength [nm]	Oscillator strength $f_{calc}$	Major contributions [%]	$\mu$ [Debye]	Character	
S <sub>0</sub>				10.4030		
S <sub>1</sub>	433.29	0.5852	HOMO → LUMO	45	11.8904	$\pi \rightarrow \pi^*$
			HOMO → LUMO+1	55		CT
					$\pi \rightarrow \pi^*$	
S <sub>2</sub>	419.28	0.1924	HOMO → LUMO	54	10.8920	$\pi \rightarrow \pi^*$
			HOMO → LUMO+1	46		CT
					$\pi \rightarrow \pi^*$	
S <sub>3</sub>	361.89	0.0076	HOMO-4 → LUMO+1	24	10.4223	$\pi \rightarrow \pi^*$
			HOMO-2 → LUMO+1	26		$\pi \rightarrow \pi^*$
			HOMO → LUMO+2	41		(CT)
			HOMO → LUMO+3	9		$\pi \rightarrow \pi^*$
					$\pi \rightarrow \pi^*$	
					$\pi \rightarrow \pi^*$	
					$\pi \rightarrow \pi^*$	
					(CT)	
S <sub>4</sub>	347.09	0.0096	HOMO-6 → LUMO+1	7	10.4274	$\pi \rightarrow \pi^*$
			HOMO-5 → LUMO	3		(CT)
			HOMO-2 → LUMO+1	25		$\pi \rightarrow \pi^*$
			HOMO-1 → LUMO	2		CT
			HOMO-1 → LUMO+1	50		$\pi \rightarrow \pi^*$
			HOMO → LUMO+4	13		CT
					$\pi \rightarrow \pi^*$	
					CT	
					$\pi \rightarrow \pi^*$	
					$\pi \rightarrow \pi^*$	
					$\pi \rightarrow \pi^*$	
					(CT)	
S <sub>5</sub>	339.42	0.0866	HOMO-6 → LUMO+2	5	10.6231	$\pi \rightarrow \pi^*$
			HOMO-5 → LUMO	7		$\pi \rightarrow \pi^*$
			HOMO-2 → LUMO+1	30		(CT)
			HOMO-1 → LUMO	2		$\pi \rightarrow \pi^*$
			HOMO-1 → LUMO+1	43		CT
			HOMO → LUMO+2	5		$\pi \rightarrow \pi^*$
					CT	
					$\pi \rightarrow \pi^*$	
					$\pi \rightarrow \pi^*$	
S <sub>6</sub>	325.59	0.9266	HOMO-5 → LUMO	92	12.7582	$\pi \rightarrow \pi^*$
			HOMO-2 → LUMO+1	5		$\pi \rightarrow \pi^*$
			HOMO → LUMO+3	3		CT
					$\pi \rightarrow \pi^*$	
S <sub>7</sub>	323.12	0.0147	HOMO-6 → LUMO+1	5	10.4404	$\pi \rightarrow \pi^*$
			HOMO-2 → LUMO+1	23		$\pi \rightarrow \pi^*$
			HOMO → LUMO+2	15		$\pi \rightarrow \pi^*$
			HOMO → LUMO+3	57		$\pi \rightarrow \pi^*$
					$\pi \rightarrow \pi^*$	
					CT	
S <sub>8</sub>	305.24	0.0003	HOMO-2 → LUMO	2	10.4038	$\pi \rightarrow \pi^*$
			HOMO-1 → LUMO	90		CT
			HOMO-1 → LUMO+1	4		$\pi \rightarrow \pi^*$
			HOMO → LUMO	4		CT
					$\pi \rightarrow \pi^*$	
					CT	

						$\pi \rightarrow \pi^*$
						CT
			HOMO-1 $\rightarrow$ LUMO+2	14		$\pi \rightarrow \pi^*$
			HOMO-1 $\rightarrow$ LUMO+3	5		CT
S <sub>9</sub>	303.68	0.0228	HOMO-1 $\rightarrow$ LUMO+4	70	10.4610	$\pi \rightarrow \pi^*$
			HOMO-1 $\rightarrow$ LUMO+9	3		$\pi \rightarrow \pi^*$
			HOMO $\rightarrow$ LUMO+4	8		CT
						$\pi \rightarrow \pi^*$
						CT
						$\pi \rightarrow \pi^*$
						CT
			HOMO-3 $\rightarrow$ LUMO	3		$\pi \rightarrow \pi^*$
			HOMO-3 $\rightarrow$ LUMO+1	56		CT
S <sub>10</sub>	295.48	1.2210	HOMO-1 $\rightarrow$ LUMO+5	7	13.5065	$\pi \rightarrow \pi^*$
			HOMO $\rightarrow$ LUMO+2	27		(CT)
			HOMO $\rightarrow$ LUMO+3	7		$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$
						$\pi \rightarrow \pi^*$

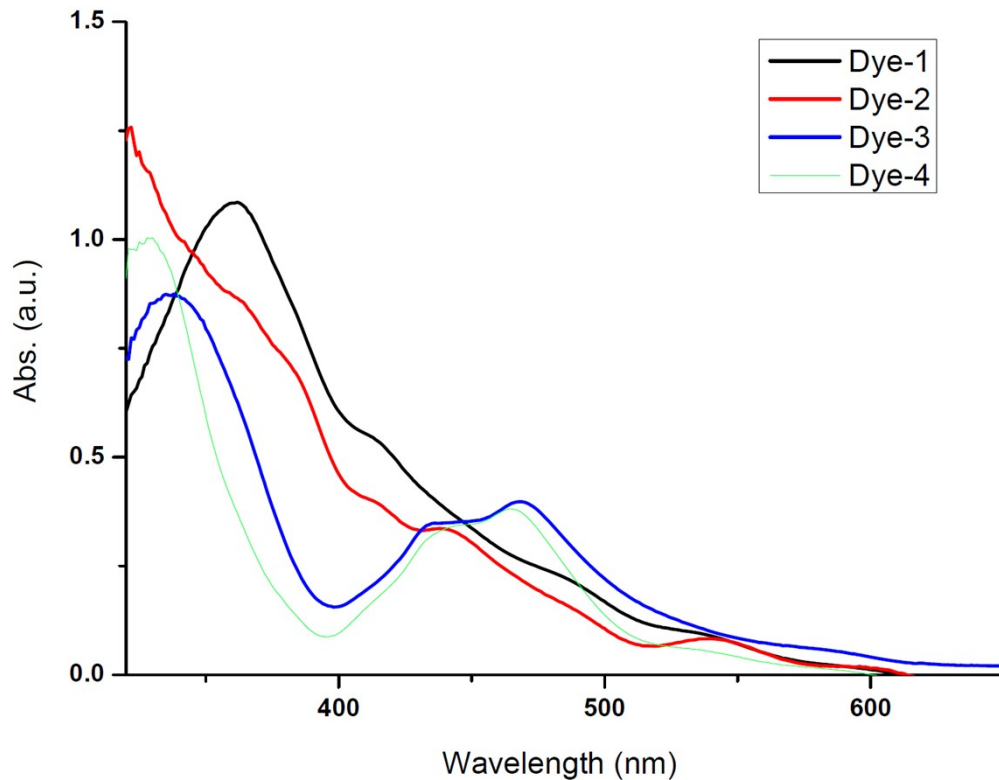
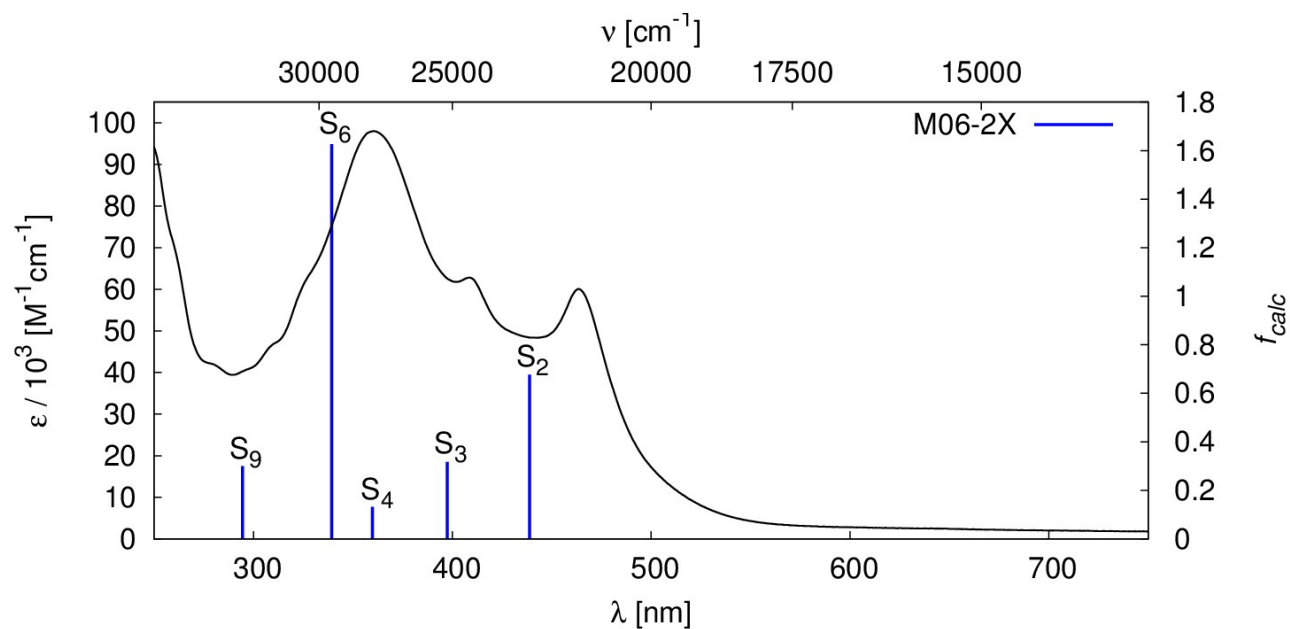
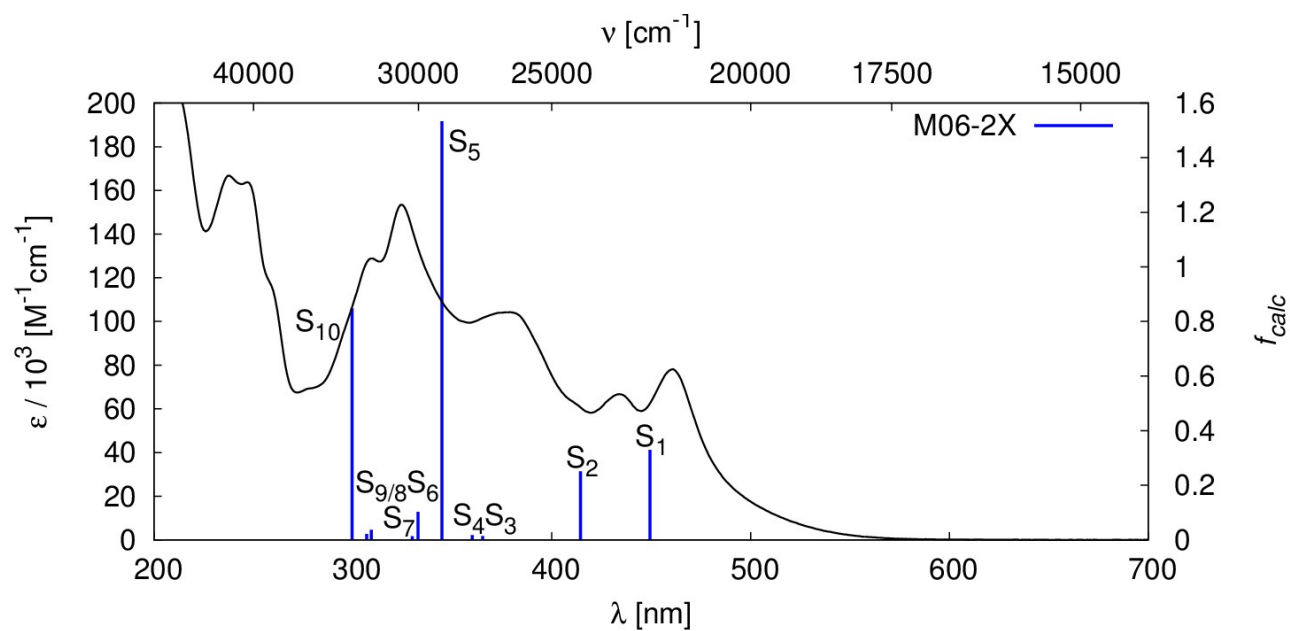


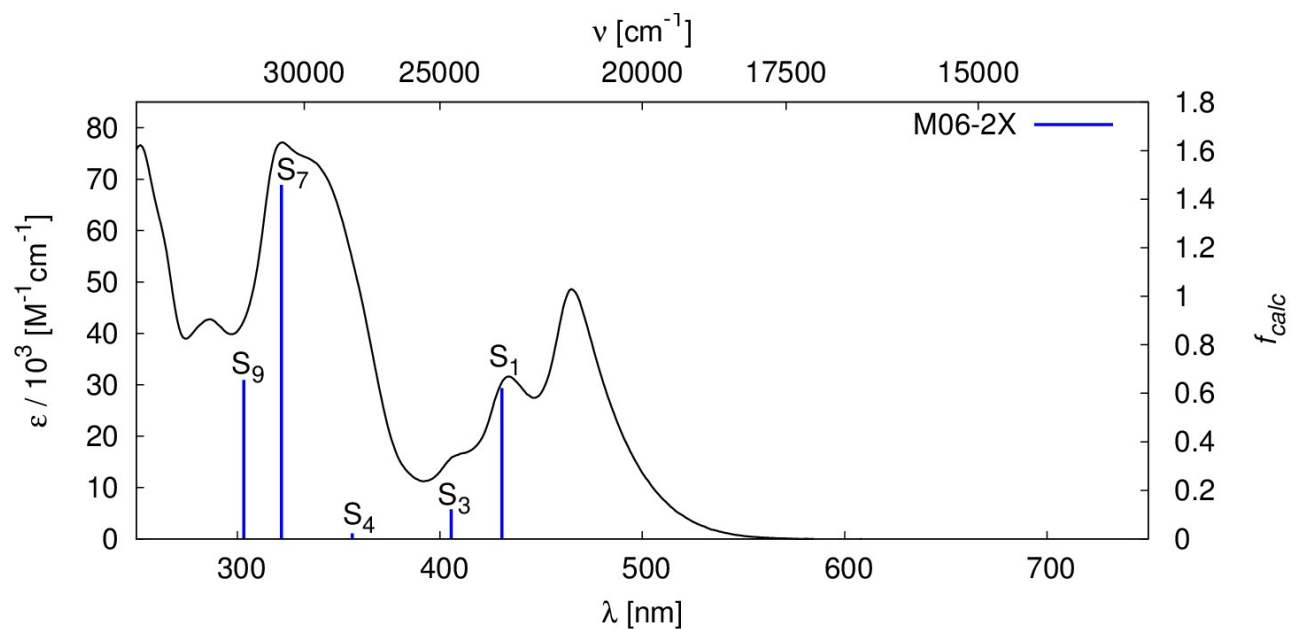
Figure S1 Optical absorption spectra of **Dye-1** to **Dye-4** adsorbed on TiO<sub>2</sub> films.



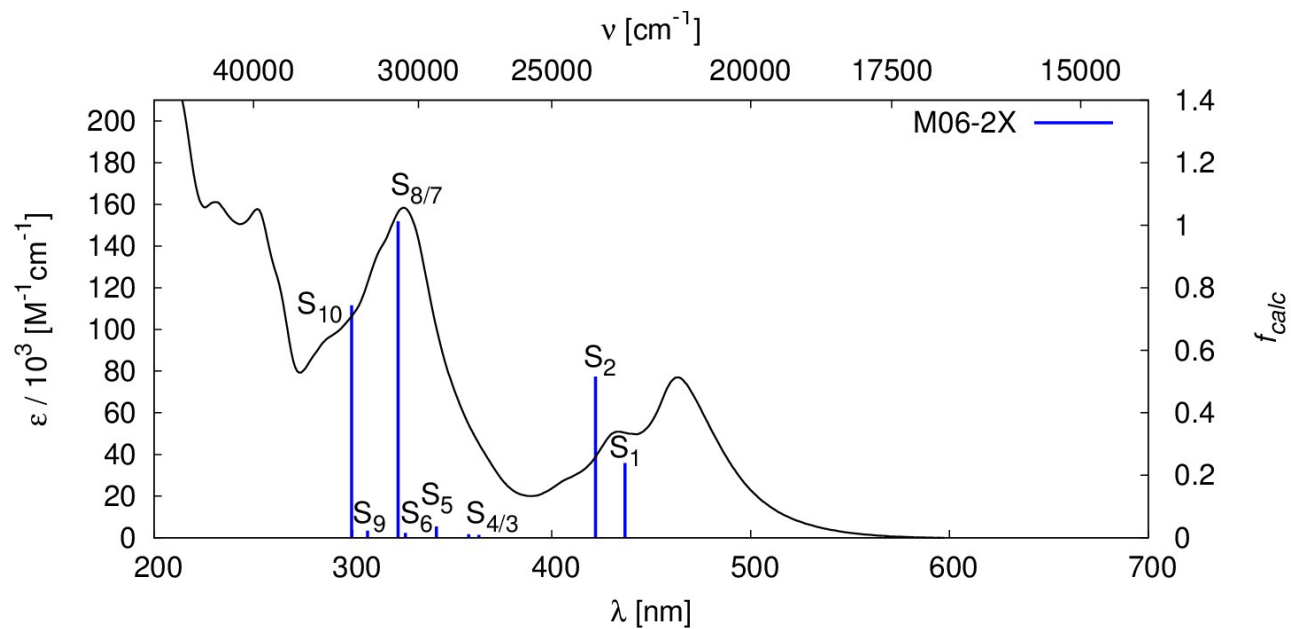
**Figure S2** Optical absorption spectrum of **Dye-1** together with the calculated electronic excitations (stick plot).



**Figure S3** Optical absorption spectrum of **Dye-2** together with the calculated electronic excitations (stick plot).



**Figure S4** Optical absorption spectrum of **Dye-3** together with the calculated electronic excitations (stick plot).



**Figure S5** Optical absorption spectrum of **Dye-4** together with the calculated electronic excitations (stick plot).