Electronic supplementary information

Theoretical investigation of the donor group related electronic structure properties in push-pull organic sensitizers

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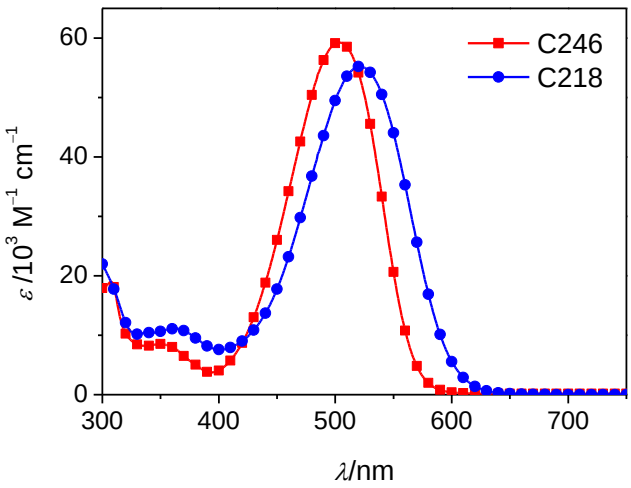

Fig. S1 Electronic absorption spectra of C246 and C218 in THF recorded on an Agilent G1103A spectrometer. The synthesis of C246 and C218 was reported in our previous papers.[S1,S2]

Table S1. The calculated lowest excitation energies (E_{exi}>200 nm) with inclusion of larger transtion oscillator strengths (*f*>0.1).

Dye	Vacuum		THF solution	
	E_{exi}/eV	*f*	E_{exi}/eV	*f*
C246	2.77	1.4883	2.58	1.6907
	3.92	0.1064	3.78	0.1772
	4.07	0.1829	4.03	0.1758
	4.58	0.1070	4.44	0.1713
	4.80	0.1329	4.72	0.1623
	5.53	0.7015	5.36	0.1188
	6.09	0.2351	5.44	0.8189
			5.93	0.1161
			6.08	0.1905
C218	2.59	1.5893	2.37	1.7780
	3.40	0.1303	3.24	0.1199
	3.93	0.2724	3.85	0.2953
	4.56	0.1078	4.45	0.1685
	4.66	0.2615	4.64	0.1577
	4.72	0.1184	4.65	0.4344
	4.73	0.1619	5.91	0.1108
	5.94	0.1079		
K201	2.57	1.6897	2.37	1.8569
	3.27	0.1879	3.12	0.1500
	3.83	0.3937	3.75	0.3147
	3.86	0.7733	3.76	0.4050
	4.41	0.1505	3.84	0.6915
	4.87	0.3144	4.34	0.1945
	5.16	0.1283	4.47	0.1482
			4.72	0.1042
			4.84	0.1368
			4.85	0.1646
			5.15	0.1210

Reference:

[S1] M. Xu, D. Zhou, N. Cai, J. Liu, R. Li and P. Wang, *Energy Environ. Sci.*, 2011, **4**, 4735.

[S2] R. Li, J. Liu, N. Cai, M. Zhang and P. Wang, *J. Phys. Chem. B*, 2010, **114**, 4461.