Supporting Information

New low bandgap near-IR conjugated D-A copolymers for BHJ polymers solar cell applications

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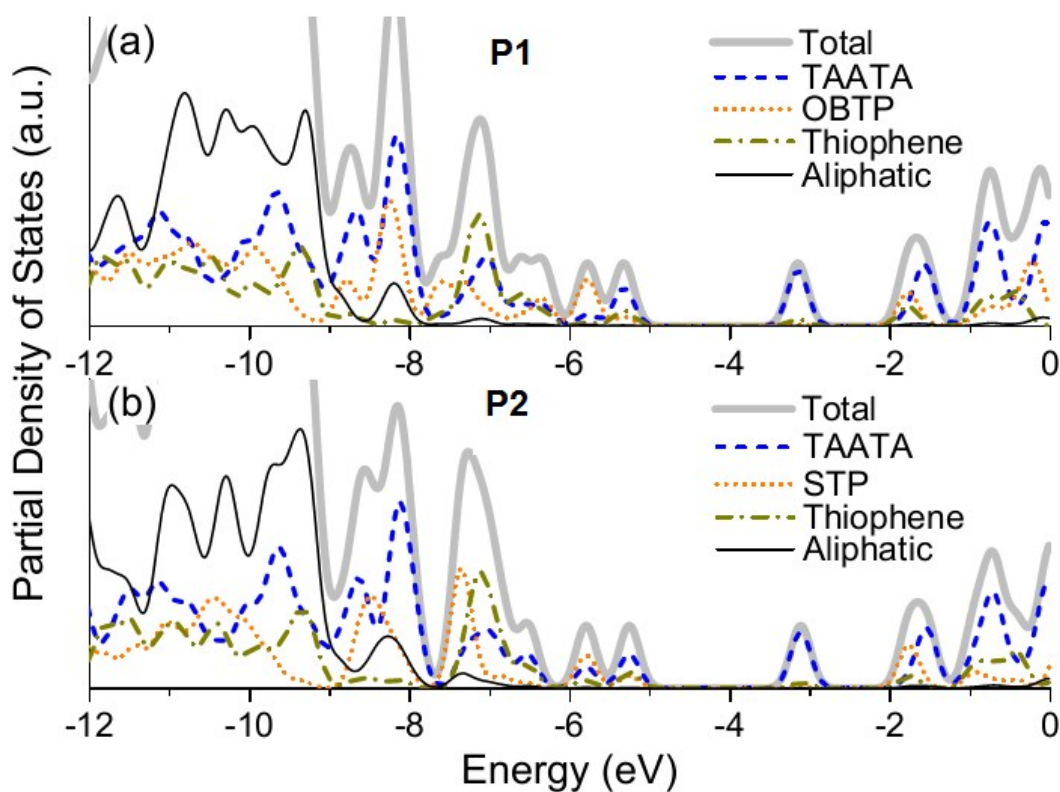
Figure S1Total and partial density of states of (a) **P1**, and (b) **P2** (calculated using the M06 functional).
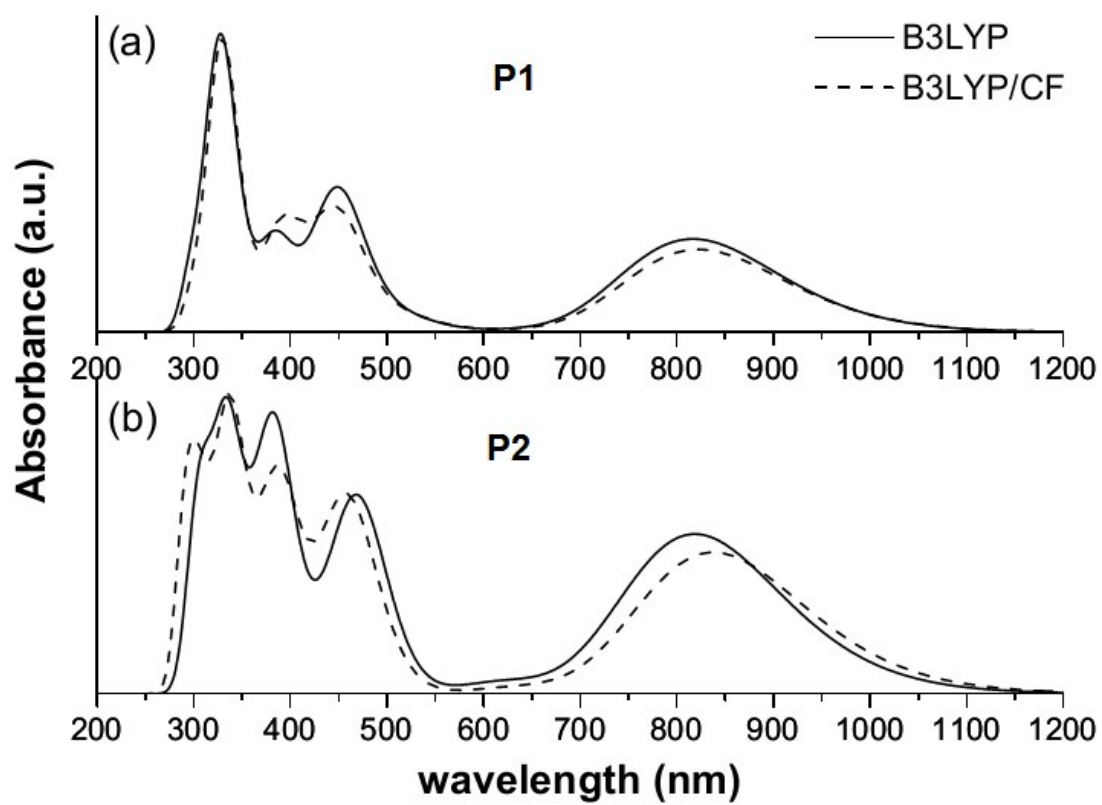
Figure S2 Theoretical UV/Vis absorption spectrum of (a) **P1**, and (b) **P2** (calculated using the B3LYP functional).

Table S1 Electronic excitations of **P1** (with non-negligible oscillator strengths, *f*), and the corresponding major contributions. Calculated using the M06 functional (and CF for solvent).

No.	Wavelength (nm)	*f*	Main Contributions
1	788	0.350	H→L (99%)
2	584	0.029	H–1→L (93%)
3	485	0.053	H–3→L (10%)
			H–2→L (83%)
4	447	0.036	H–3→L (86%)
5	434	0.339	H→L+1 (95%)
6	407	0.162	H→L+2 (93%)
8	390	0.125	H–4→L (66%)
9	385	0.093	H–6→L (73%)
10	372	0.081	H–8→L (10%)
			H–7→L (55%)
			H–1→L+1 (23%)
11	370	0.157	H–7→L (15%)
			H–1→L+1 (70%)
12	341	0.025	H–8→L (61%)
13	337	0.036	H–1→L+2 (17%)
			H→L+3 (62%)
14	333	0.143	H–1→L+2 (68%)
			H→L+3 (20%)
15	327	0.253	H–2→L+1 (40%)
			H→L+4 (35%)
16	323	0.595	H–2→L+1 (42%)
			H→L+4 (27%)
			H–>L+5 (15%)
17	315	0.566	H→L+4 (13%)
			H→L+5 (61%)
19	302	0.026	H–18→L (43%)
			H–17→L (11%)
			H–10→L (11%)
20	298	0.026	H–10→L (69%)
			H–2→L+2 (12%)
21	298	0.151	H–10→L (14%)
			H–2→L+2 (53%)
26	285	0.121	H–15→L (39%)
			H–13→L (36%)
27	283	0.296	H–15→L (28%)
			H–14→L (27%)
			H–13→L (23%)
28	281	0.040	H–3→L+2 (14%)
			H–1→L+3 (24%)
			H→L+7 (12%)

Table S2 Electronic excitations of **P2** (with non-negligible oscillator strengths, f), and the corresponding major contributions. Calculated using the M06 functional (and CF for solvent).

No.	Wavelength (nm)	f	Main Contributions
1	800	0.381	H→L (99%)
2	588	0.037	H–1→L (96%)
3	463	0.037	H–2→L (94%)
4	440	0.462	H→L+1 (92%)
5	412	0.130	H→L+2 (89%)
6	407	0.081	H–3→L (85%)
7	396	0.047	H–5→L (26%)
			H–4→L (65%)
8	385	0.100	H–6→L (20%)
			H–5→L (54%)
			H–4→L (17%)
9	377	0.042	H–6→L (73%)
10	370	0.193	H–1→L+1 (87%)
12	347	0.124	H→L+3 (89%)
13	336	0.158	H–1→L+2 (77%)
			H→L+4 (11%)
14	329	0.228	H–9→L (59%)
			H→L+4 (24%)
15	328	0.513	H–9→L (35%)
			H→L+4 (38%)
16	325	0.064	H→L+5 (78%)
18	304	0.127	H–19→L (21%)
			H–10→L (13%)
			H–1→L+3 (17%)
			H→L+6 (18%)
19	302	0.139	H–19→L (15%)
			H–10→L (21%)
			H–1→L+3 (15%)
			H→L+6 (27%)
21	296	0.145	H–2→L+1 (48%)
			H–2→L+2 (11%)
			H–1→L+3 (10%)
			H→L+6 (11%)
22	294	0.031	H–2→L+1 (20%)
			H–1→L+3 (37%)
			H→L+6 (25%)
24	288	0.084	H–2→L+2 (65%)
26	284	0.034	H–12→L (20%)
			H–1→L+4 (15%)
			H→L+9 (13%)
27	283	0.339	H–14→L (15%)
			H–13→L (10%)
			H–12→L (21%)
			H–1→L+4 (19%)