

Supporting Information

Donor-Acceptor Dyes with Fluorine Substituted Phenylene Spacer for Dye-Sensitized Solar Cells

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Table S1. Calculated details of electronic transitions with the relative oscillator strengths of the **LJB** dyes.

Dye	State	Excitation single excited state	E _{cal} (eV)	λ _{cal} (nm)	(f)
LJB-F_o	S1	HOMO→LUMO(+90%)	2.16	574.9	0.7411
	S2	HOMO-1→LUMO(+80%), HOMO→LUMO+1(8%)	3.00	413.8	0.8111
	S3	HOMO-2→LUMO(+79%), HOMO→LUMO+1(15%)	3.28	377.5	0.0492
LJB-H	S1	HOMO→LUMO(+90%)	2.23	555.3	0.7703
	S2	HOMO-1→LUMO(+81%), HOMO→LUMO+1(7%)	3.04	408.5	0.7833
	S3	HOMO-2→LUMO(+66%), HOMO→LUMO+1(26%)	3.34	371.8	0.0756
LJB-F_m	S1	HOMO→LUMO(+93%)	2.05	603.7	0.4669
	S2	HOMO-1→LUMO(+87%)	2.91	426.7	0.5799
	S3	HOMO-2→LUMO(+95%)	3.09	400.9	0.0074