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Electronic Supplementary Information

Effect of Structural Manipulation in Hetero-tri-aryl Amine Donor Based

D-A'-π-A sensitizers in Dye Sensitized Solar Cells

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Figure S1. HOMO LUMO energy representation of the all sensitizer, parameters obtained at the B3LYP/6-31G(d) level in vacuum.



Figure S2. IPCE characteristics of DP devices





Figure S3. The optimized geometries of the DP1, DP2, DP3 and DP4 sensitizers, obtained at the B3LYP/6-31G(d) level in vacuum.



Figure S4: ¹H NMR spectrum of compound 1



Figure S5: ¹³C NMR spectrum of compound 1



Figure S6: ¹H NMR spectrum of compound 2a



Figure S7: ¹³C NMR spectrum of compound 2a



Figure S8: ¹H NMR spectrum of compound 2b



Figure S9: ¹³C NMR spectrum of compound 2b



Figure S10: ¹H NMR spectrum of compound 3a



Figure S11: ¹H NMR spectrum of compound 3b



Figure S12: ¹³C NMR spectrum of compound 3b



Figure S13: ¹H NMR spectrum of compound 4a



Figure S14: ¹³C NMR spectrum of compound 4a



Figure S15: ¹H NMR spectrum of compound 4b



Figure S16: ¹³C NMR spectrum of compound 4b



Figure S17: ¹H NMR spectrum of sensitizer DP1



Figure S18: ¹³C NMR spectrum of sensitizer DP1



Figure S19: ¹H NMR spectrum of sensitizer DP2



Figure S20: ¹³C NMR spectrum of sensitizer DP2



Figure S21: ¹H NMR spectrum of sensitizer DP3



Figure S22: ¹³C NMR spectrum of sensitizer DP3



Figure S23: ¹H NMR spectrum of sensitizer DP4



Figure S24: ¹³C NMR spectrum of sensitizer DP4

Sensitizer	НОМО	LUMO	LUMO+1	HL-gap	HL+1-gap
	(eV)	(eV)	(eV)		
DP1	-5.498	-3.0626	-1.958	2.435	3.539
DP2	-5.297	-2.9211	-1.866	2.372	3.426
DP3	-5.425	-3.058	-2.096	2.367	3.328
DP4	-5.211	-2.945	-2.053	2.266	3.158

Table S1. Electrochemical characterization of DP sensitizers by DFT calculations.

Table S2 Electronic transition data obtained by TD-B3LYP/6-311++G(d,p) level for each molecule in the DMF solution.

Sensi tizer s	State s	λ _{max} (nm)	f	LHE	Excite d energ y (eV)	Transition character
DP1	S_1 S_2 S_3	573 412 383	1.323 0.503 0.073	0.9525 0.6859 0.1547	2.16 3.01 3.24	H → L (99.56%) H-1 → L (84.53%), H → L+1 (15.13%) H-1 → L (14.66%) H → L+1 (80.46%)
DP2	S_1 S_2	594 452	1.644 0.441	0.9773 0.6377	2.08 2.74	H → L (99.34%) H-1 → L (91.32%), H → L (8.06%) H-2 → L (89.48%), H-2 → L+1 (7.54%), H-2 →
DP3	S_3 S_1 S_2 S_2	431 575 406	0.001 1.658 0.156	0.0023 0.9780 0.3017 0.0262	2.87 2.15 3.05 2.28	L+2 (2.79%). H → L (99.97%) H-1 → L (26.79%), H → L+1 (71.62%) H 1 → L (71.40%) H → L+1 (24.72%)
DP4	$ \begin{array}{c} \mathbf{S}_3\\ \mathbf{S}_1\\ \mathbf{S}_2\\ \mathbf{S}_3 \end{array} $	610 441 422	0.010 1.808 0.312 0.001	0.0362 0.9844 0.5124 0.0023	3.38 2.03 2.81 2.93	$\begin{array}{l} \text{H-1} \rightarrow \text{L} \ (71.49\%), \ \text{H} \rightarrow \text{L+1} \ (24.72\%). \\ \text{H} \rightarrow \text{L} \ (99.79\%) \\ \text{H-1} \rightarrow \text{L} \ (28.27\%), \ \text{H} \rightarrow \text{L+1} \ (70.47\%) \\ \text{H-2} \rightarrow \text{L} \ (87.51\%), \ \text{H-2} \rightarrow \text{L+1} \ (9.31\%). \end{array}$