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Supporting Information

New D-D-π-A type organic dyes having carbazol-N-yl phenothiazine moiety as a donor (D-D) unit for efficient dye-sensitized solar cells: Experimental and theoretical studies

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Quantum chemical calculation



Figure S1. Optimized structures of the dyes calculated by B3LYP/6-31G(d,p) in CH₂Cl₂ solvent.

Table S1 Excitation energy (eV), oscillator strength (*f*) and transition composition of the dyes at the 20 lowest transitions (f > 0.200) were calculated by TD CAM-B3LYP/6-31G(d,p) in CH₂Cl₂ (C-PCM model).

Dye		E _{ex} [eV, nm]	f	Transition contribution
CPhPA	$S_0 \rightarrow S_1$	3.04 (407)	0.9708	0.61 (H→L) + 0.25 (H→L+1)
	$S_0 \rightarrow S_2$	3.82 (324)	0.2670	$0.54 (H \rightarrow L+1) + 0.24 (H-3 \rightarrow L)$
	$S_0 \rightarrow S_3$	4.06 (305)	0.3284	$0.52 (H-3 \rightarrow L+2) + 0.21 (H \rightarrow L)$
CPhTPA	$S_0 \rightarrow S_1$	3.00 (413)	1.7595	$0.52 (H \rightarrow L) + 0.27 (H - 3 \rightarrow L)$
	$S_0 \rightarrow S_4$	4.31 (287)	0.2981	0.35 (H→L+3)
	$S_0 \rightarrow S_{10}$	4.81 (257)	0.2607	0.64 (H-2→L+2)
CPhT2PA	$S_0 \rightarrow S_1$	2.82 (440)	2.1499	$0.51 (H \rightarrow L) + 0.24 (H \rightarrow L+1)$
	$S_0 \rightarrow S_{13}$	4.81 (257)	0.2505	0.57 (H-3→L+2)
Note: $H = HOMO$, $L = LUMO$, $L+1 = LUMO+1$,				



Figure S2. DPV curves measured in CH_2Cl_2 with *n*-Bu₄NPF₆ as a supporting electrolyte at a scan rate of 50 mV s⁻¹.

¹H and ¹³C-NMR spectra Compound 3











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Compound 6





Compound 7





Compound 8











Actows





CPhPA



CPhTPA



CIMIT



CPhT2PA



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