Supporting Information

Quadrupolar (Donor)$_2$Acceptor-Acid Chromophores for Dye-sensitized Solar Cells: Influence of the Core Acceptor

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Table of Contents

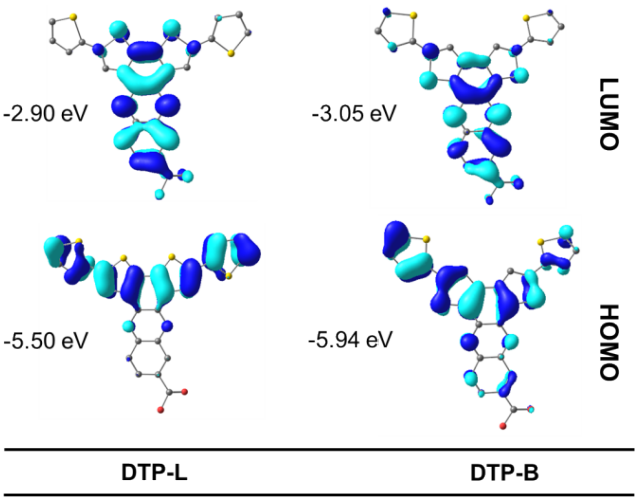

Figure S1. Illustration of the computed molecular orbitals for compounds **DTP-L** (left) and **DTP-B** (right).

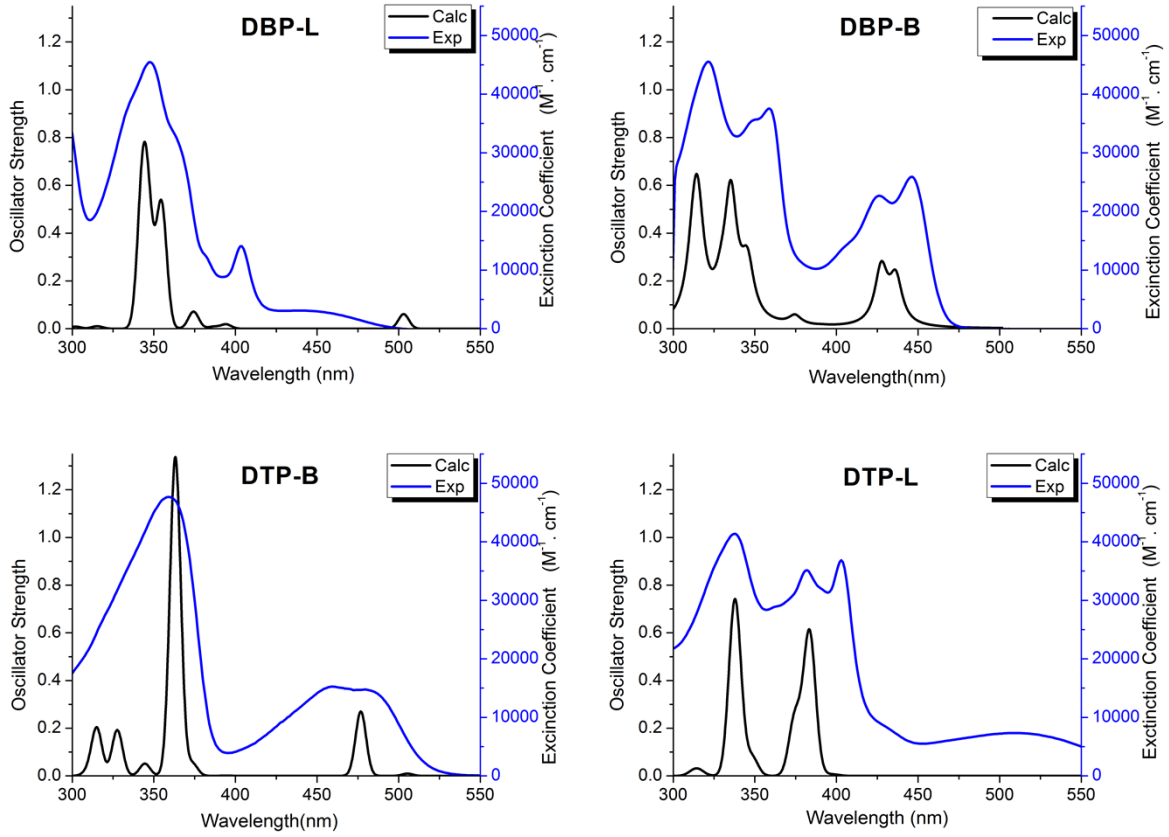

Figure S2. UV-visible absorption spectra in toluene (blue) and simulated absorption spectra determined with TD-DFT at the B3PW91/6-31G* level of theory (black) of **DBP-L, DBP-B, DTP-L** and **DTP-B.**

Table S1. Orbital energies for oligomers **DBP-L**, **DBP-B**, **DTP-L**, **DTP-B,** empirical and obtained via DFT calculations with different hybrids functional (B3LYP, B3PW91, B3PW91-SCRF and B3LYP-CAM). All energies are in eV.

Cpd	Empirical		B3LYP		B3PW91		B3PW91-SCRF		B3LYP-CAM	
	HOMO	LUMO	HOMO	LUMO	HOMO	LUMO	HOMO	LUMO	HOMO	LUMO
DBP-L	-6.22	-3.30	-5.52	-2.58	-5.55	-3.00	-5.74	-2.84	-6.75	-1.49
DBP-B	-6.23	-3.54	-5.76	-2.56	-5.90	-2.68	-5.98	-2.84	-7.00	-1.49
DTP-L	-5.63	-3.53	-5.37	-2.82	-5.50	-2.90	-5.50	-2.97	-6.56	-1.77
DTP-B	-6.06	-3.70	-5.62	-2.72	-5.94	-3.01			-6.86	-1.70

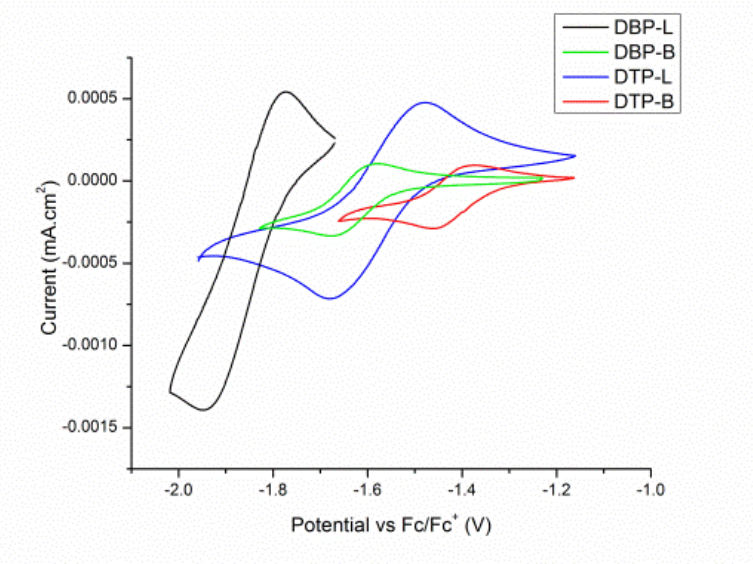

Figure S3. Cyclic Voltammetry (CV) data for compounds **DBP-L** (black), **DBP-B** (green), **DTP-L** (blue) and **DTP-B** (red). The data were obtained in benzonitrile solution using 0.1M tetrabutylammonium hexafluorophosphate as the supporting electrolyte, a platinum button working electrode, a non-aqueous $Ag/AgNO_3$ reference electrode, and a platinum flag counter electrode.

Table S2. Open circuit voltage (Voc), short circuit current (Jsc), fill factor (FF) and efficiency (PCE) for studied sensitizers, for 3 or more devices

Cpd	Voc(V)	Jsc(mA.cm^{-2})	FF	PCE
DBP-L	0.52 ± 0.01	2.24 ± 0.2	0.62 ± 0.02	0.73 ± 0.02
DBP-B	0.49 ± 0.02	2.61 ± 0.1	0.53 ± 0.03	0.66 ± 0.02
DTP-L	0.43 ± 0.02	2.23 ± 0.2	0.54 ± 0.04	0.53 ± 0.05
DTP-B	0.44 ± 0.01	2.85 ± 0.3	0.53 ± 0.07	0.66 ± 0.06
N3	0.69	11.4	0.42	3.29

Computations Citations

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B3PW91: Becke A.D., *J.Chem.Phys,* **1993**, *98*, 5648. Perdew J.P.; Burke K.; Wang Y., *Phys. Rev. B*, **1996**, *54,* 16533