Electronic Supplementary Material (ESI) for Energy & Environmental Science

Supplementary information

2,6-Conjugated anthracene sensitizers for high-performance dye-sensitized solar cells

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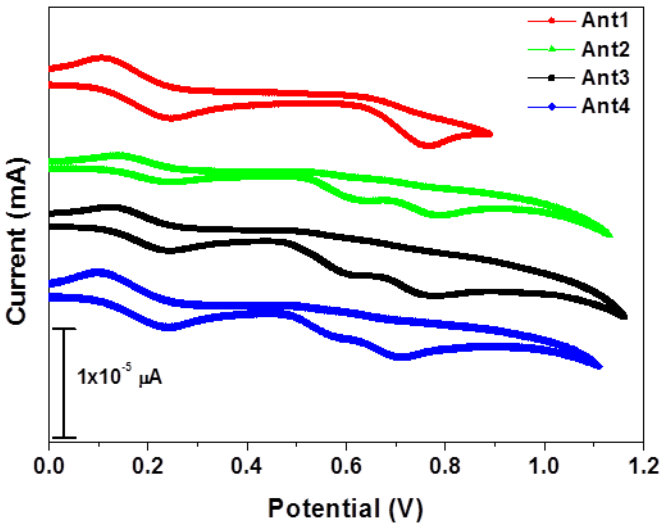

Fig. S1 Cyclic voltammograms of **Ant** dyes recorded in THF.

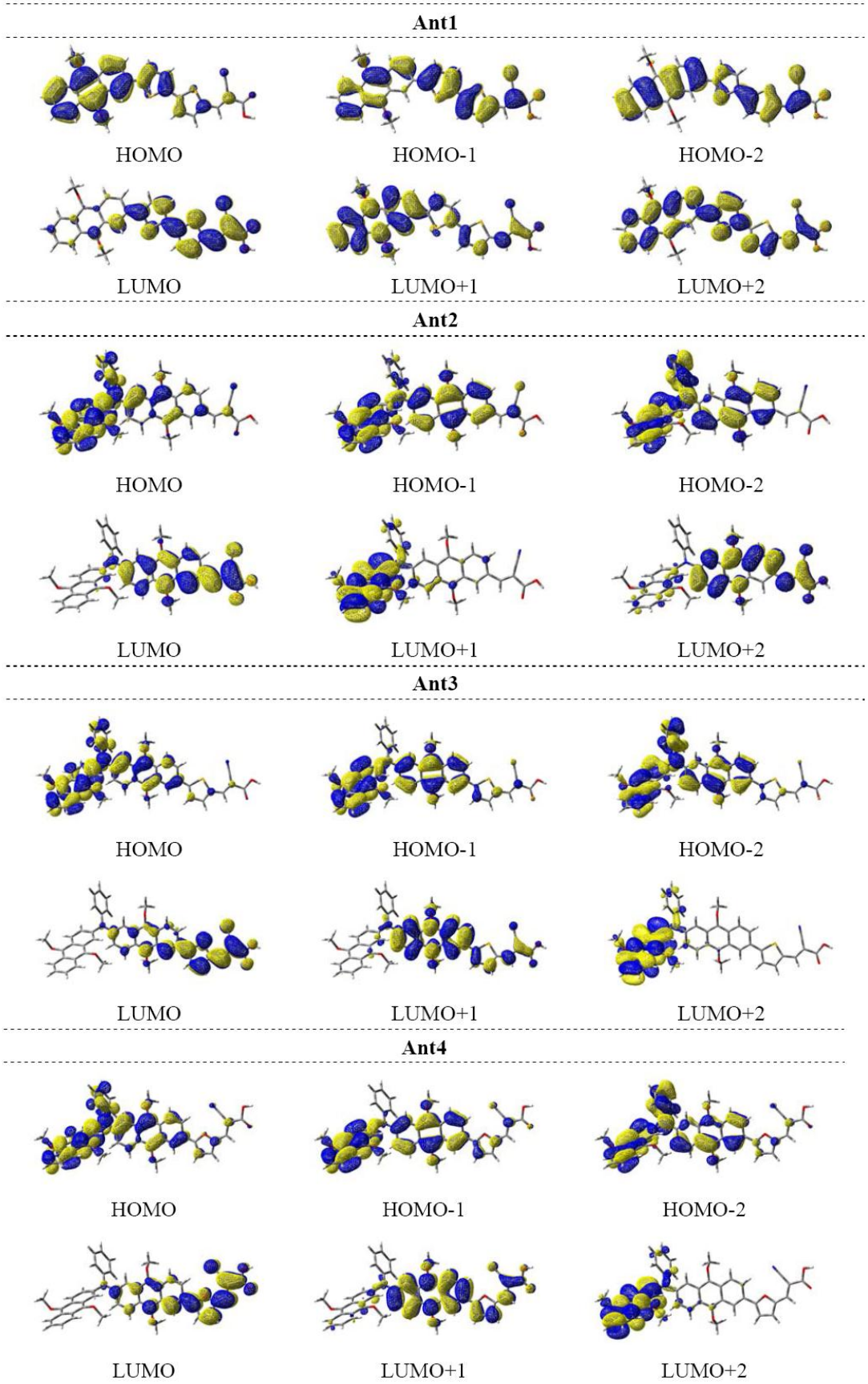

Fig. S2 Selected frontier orbitals of the dyes

Table S1 Calculated lower-lying transitions of the dyes[a]

dye	State	excitation[a]	λ_{cal}, eV	f [b]	Δ(Mulliken charge),[c] |e|	$f \times \Delta q$	dye	State	excitation[a]	λ_{cal}, eV	f [b]	Δ(Mulliken charge),[c] |e|	$f \times \Delta q$
Ant1	S_1	H → L (98%)	2.16	0.39	Ant: 0.77 T1: -0.12 T2: -0.30 Ac: -0.35	-0.13	**Ant2**	S_1	H → L (99%)	2.12	0.38	AntN: 0.73 Ant: -0.35 Ac: -0.38	-0.14
	S_2	H1 → L (92%) H → L1 (5%)	2.76	1.08	Ant: 0.11 T1: 0.14 T2: -0.06 Ac: -0.19	-0.21		S_2	H1 → L (97%)	2.46	0.17	AntN: 0.36 Ant: 0.04 Ac: -0.40	-0.07
	S_6	H → L1 (93%)	2.94	0.11	Ant: 0.07 T1: 0.03 T2: -0.03 Ac: -0.08	-0.01		S_6	H → L1 (84%) H → L2 (9%)	2.78	0.04	AntN: 0.00 Ant: 0.02 Ac: -0.02	0.00
Ant3	S_1	H → L (99%)	1.99	0.43	AntN: 0.63 Ant: 0.07 T: -0.32 Ac: -0.38	-0.17	**Ant4**	S_1	H → L (99%)	2.02	0.45	AntN: 0.60 Ant: 0.06 F: -0.25 Ac: -0.41	-0.19
	S_2	H1 → L (97%)	2.33	0.15	AntN: 0.46 Ant: 0.26 T: -0.33 Ac: -0.39	-0.06		S_2	H1 → L (96%)	2.35	0.12	AntN: 0.48 Ant: 0.21 F: -0.26 Ac: -0.43	-0.05
	S_3	H→ L1 (85%) H → L2 (7%)	2.63	0.08	AntN: 0.60 Ant: -0.45 T: -0.06 Ac: -0.09	-0.01		S_3	H → L1 (77%) H → L2 (12%)	2.65	0.08	AntN: 0.53 Ant: -0.36 F: -0.06 Ac: -0.11	-0.01

[a] Results are based on gas-phase TD-DFT calculation. [b] H = HOMO, L = LUMO, H1 = The next highest occupied molecular orbital, or HOMO – 1, H2 = HOMO – 2, L1 = LUMO + 1, L2 = LUMO + 2. In parentheses is the population of a pair of MO excitations. [c] Oscillator strength. [d] The difference of the Mulliken charge between the ground state and excited state.