Electronic Supplementary Information

Accurate estimation on photoelectric conversion efficiency of a series of anthracene-based organic dyes for dye-sensitized solar cells

Panpan Heng, Lemin Mao, Xugeng Guo*, Li Wang* and Jinglai Zhang*

Institute of Upconversion Nanoscale Materials, Henan Provincial Engineering Research Center of Green Anticorrosion Technology for Magnesium Alloy, College of Chemistry and Chemical Engineering, Henan University, Kaifeng 475004, China

E-mail: xgguo@henu.edu.cn, chemwangl@henu.edu.cn, zhangjinglai@henu.edu.cn

Table S1 Calculated charge transfer (CT) and local excitation (LE) characteristics for the HOMO → LUMO transition of four molecules investigated in this work

Dye	CT	LE
1	0.900	0.100
2	0.836	0.164
3	0.991	0.009
4	0.899	0.101

Table S2 Calculated vertical excitation energy (E_v), absorption wavelength (λ), oscillator strength (f), and major composition of MOs for all dyes at the TD-CAM-B3LYP/6-31G(d,p) level in tetrahydrofuran solvent

Dye	State	E_v (eV)	λ (nm)	f	Main configuration
1	S_1	2.52	493	0.937	H → L (82%); H → L+1 (11%)
2	S_1	2.89	429	0.319	H → L (6%); H → L+1 (89%)
	S_2	3.50	355	1.167	H-2 → L+1 (47%); H-1 → L(44%)
3	S_1	2.25	552	1.751	H-1 → L (80%); H → L (13%)
	S_4	3.26	380	0.405	H-3 → L (45%); H-1 → L+1 (26%)
4	S_1	2.02	613	1.199	H → L (80%); H-1 → L (11%)
	S_3	2.98	417	0.595	H-2 → L (60%); H-3 → L (13%)

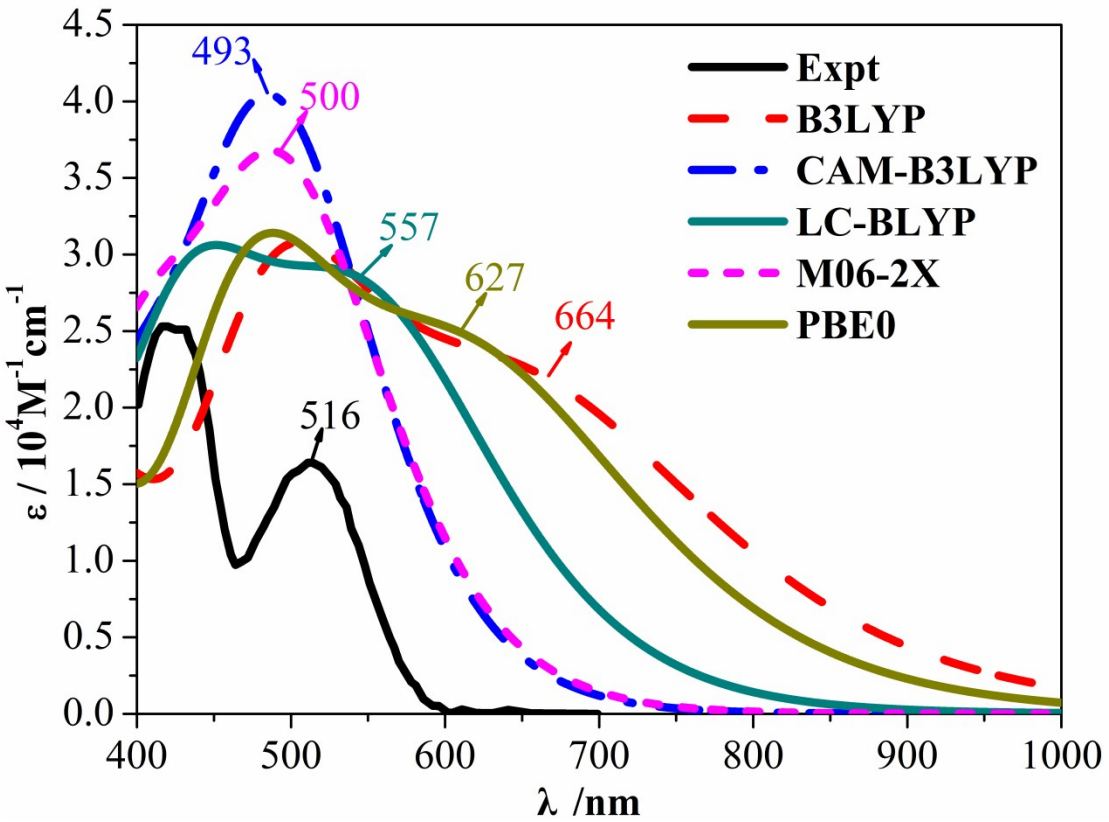

Fig. S1 The absorption spectra of dye **1** calculated by B3LYP, CAM-B3LYP, LC-BLYP, M06-2X, and PBE0 functionals and the 6-31G(d,p) basis set in tetrahydrofuran along with the experimental value.

Table S3 Calculated total energies of isolated dye (E_{dye}), pure TiO_2 (E_{TiO_2}), and dye@TiO_2 complex ($E_{dye+TiO_2}$), as well as the adsorption energy (E_{ads})

Dye	$E_{dye+TiO_2}$ (eV)	E_{dye} (eV)	E_{TiO_2} (eV)	E_{ads} (eV)[a]
1	-4443.30	-595.72	-3846.98	-0.60
2	-4565.61	-715.53	-3846.98	-3.10
3	-4649.14	-799.80	-3846.98	-2.36
4	-4689.27	-839.65	-3846.98	-2.64

[a] $E_{ads} = E_{dye+TiO_2} - (E_{dye} + E_{TiO_2})$.