Electronic Supplementary Information (ESI)

A new D-A-π-A type organic sensitizer based on substituted dihydroindolo [2, 3-b] carbazole and DPP unit with a bulky branched alkyl chain for highly efficient DSCs

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1. The frontier orbital plots of the HOMO and LUMO of **T1-T2(Table 3)**;
2. Computational analysis(**Table 4**), (**Fig. 4**);
3. Absorption curves of dyes **T1-T2** upon light irradiation of AM 1.5 solar light (30 min) with UV cutoff filter at 400 nm.
4. Normalized absorption and emission spectra of **T1-T2** in both solvent systems.
5. The absorption amounts of **T1-T2** in $CHCl_3$: EtOH (*v*/*v* 3:7) and CH_2Cl_2 were showed in **Table 5**.
6. The printout of elemental analysis of **T1-T2**.

1. The frontier orbital plots of the HOMO and LUMO of **T1-T2.**

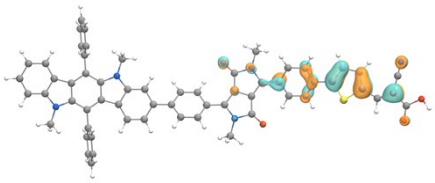
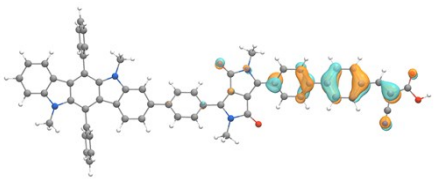
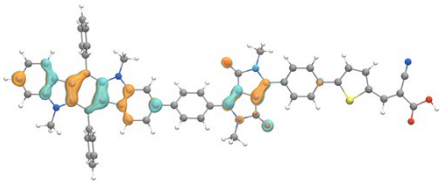
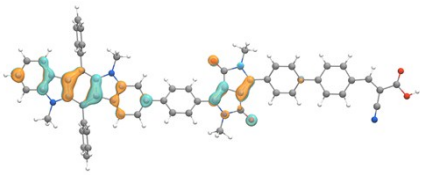
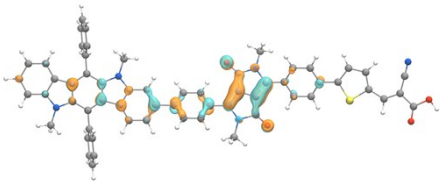
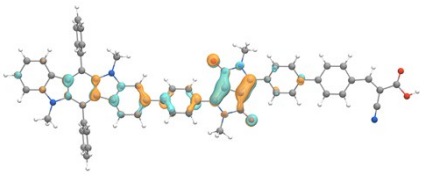
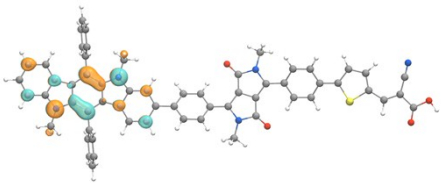
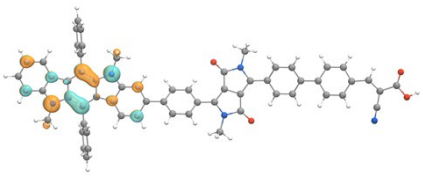
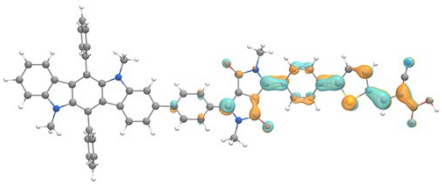
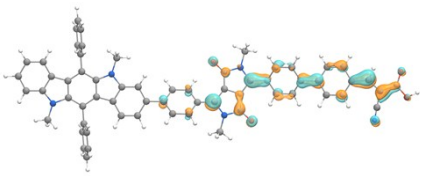
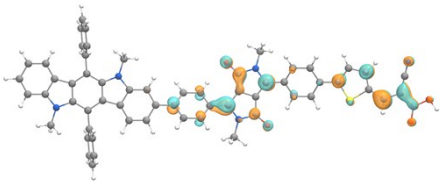
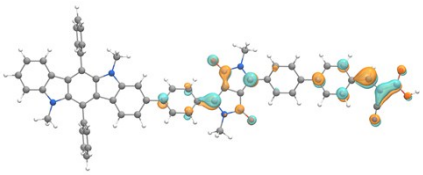
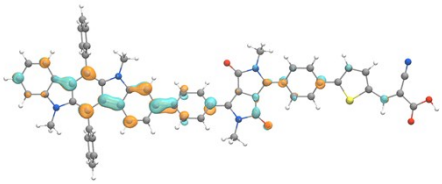
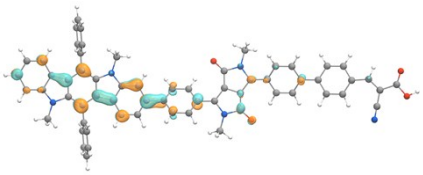
	T1	T2
HOMO-4		
HOMO-2		
HOMO-1		
HOMO		
LUMO		
LUMO+1		
LUMO+2		

Table 3. Contour plots of frontier molecular orbitals of compounds **T1** and **T2.**

2. Computational analysis

Compound	State	λ_{abs}	f	MO composition
T1	S_1	2.46 eV, 503 nm	1.631	H-2 -> L+0 (15%) H-1 -> L+0 (59%) H-1 -> L+1 (15%)
	S_2	3.19 eV, 388 nm	0.450	H-4 -> L+0 (46%) H-1 -> L+1 (30%)
	S_5	3.54 eV, 349 nm	1.145	H-2 -> L+0 (30%) H-2 -> L+1 (16%) H-1 -> L+2 (11%)
T2	S_1	2.56 eV, 485 nm	1.366	H-2 -> L+0 (15%) H-1 -> L+0 (58%) H-1 -> L+1 (18%)
	S_5	3.60 eV, 344 nm	1.810	H-2 -> L+0 (18%) H-2 -> L+1 (25%) H-1 -> L+0 (10%)

Table 4. Computed excitation energies, oscillator strengths and molecular orbital (MO) compositions of important low-lying excited states of **T1** and **T2.**

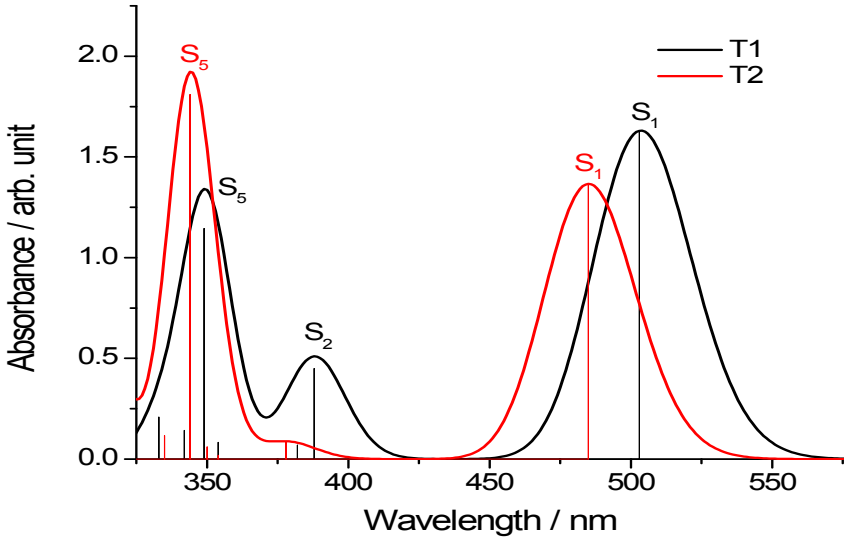
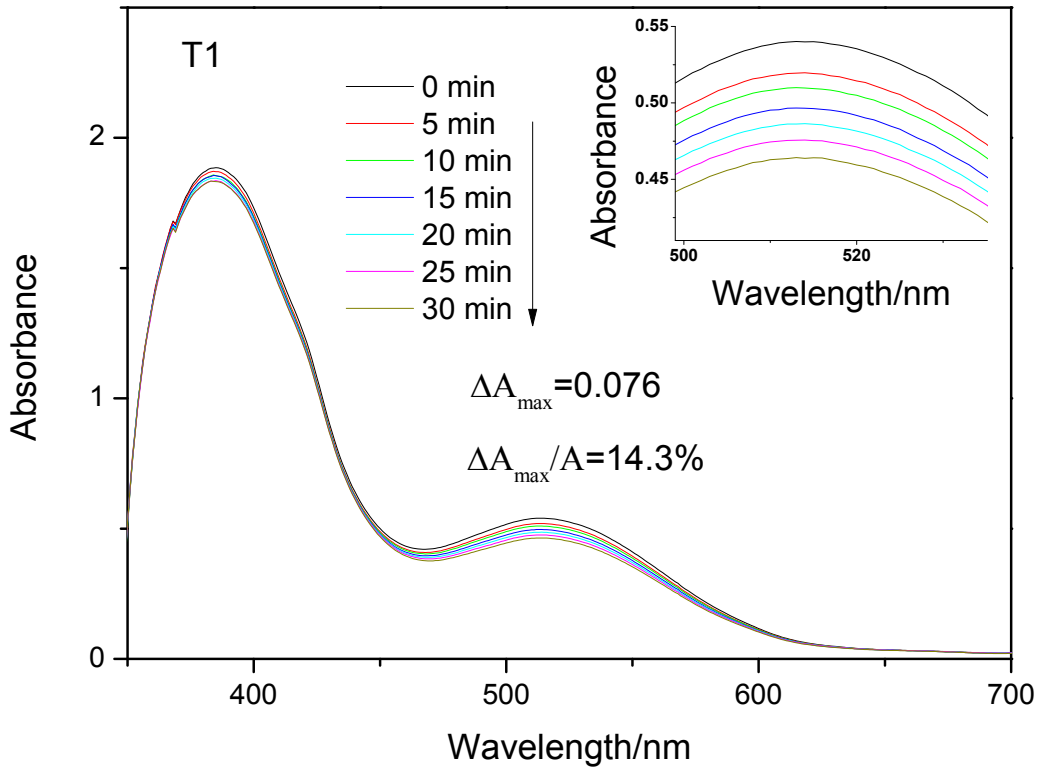
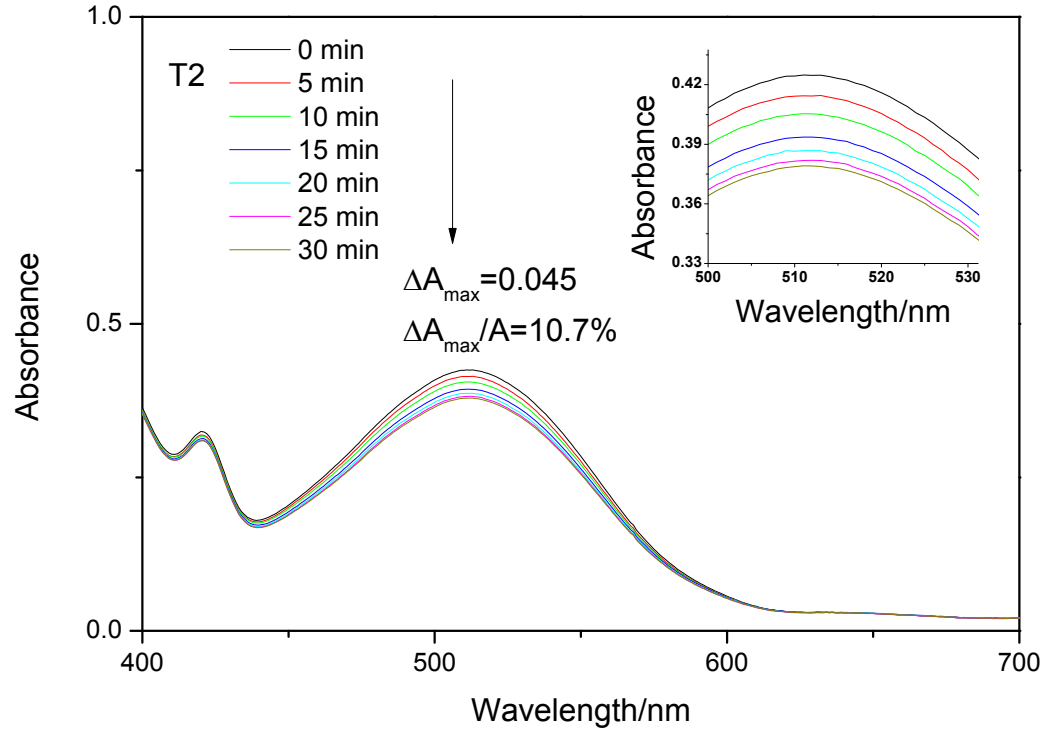


Fig. 4 Simulated absorption spectra of **T1** and **T2**.

3. Absorption curves of dyes **T1-T2** upon light irradiation of AM 1.5 solar light (30 min) with UV cutoff filter at 400 nm.

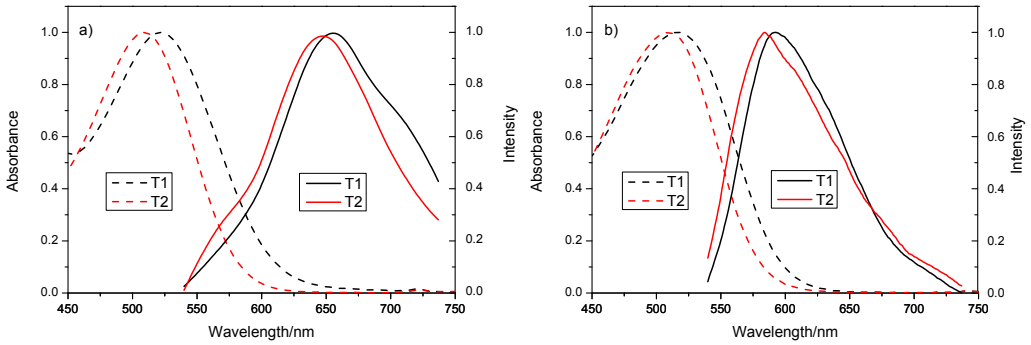


Absorption curves of dyes **T1** upon light irradiation of AM 1.5 solar light (30 min) with UV cutoff filter at 400 nm.



Absorption curves of dyes **T2** upon light irradiation of AM 1.5 solar light (30 min) with UV cutoff filter at 400 nm.

4. Normalized absorption and emission spectra of **T1-T2** in both solvent systems.

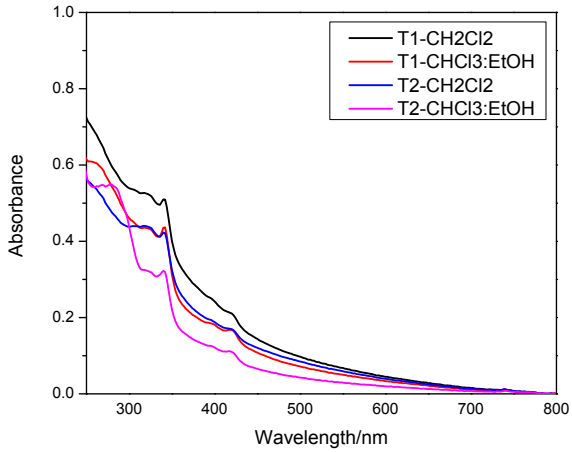


Normalized absorption and emission spectra of **T1-T2** in both solvent systems: a) was in CH2Cl2; b) was in $CHCl_3$: EtOH (*v*/*v* 3:7).

5. The absorption amounts of **T1-T2** in $CHCl_3$: EtOH (*v*/*v* 3:7) and CH_2Cl_2 were showed in Table 5.

T1-$CHCl_3$:EtOH	T2-$CHCl_3$:EtOH	T1-CH_2Cl_2	T2-CH_2Cl_2
2.32×10^{-8}(molcm^{-2})	1.94×10^{-8}(molcm^{-2})	2.68×10^{-8}(molcm^{-2})	2.34×10^{-8}(molcm^{-2})

Table 5. The absorption amounts of **T1-T2** in $CHCl_3$: EtOH (*v*/*v* 3:7) and CH_2Cl_2. The corresponding absorption spectra were below:



6. The printout of elemental analysis of **T1-T2**.

The analysis and test center in East China university of science and technology

The data of element analysis

Number:20140220

Department	Fine chemical institution
Name	TH-TGJ-(1-2)
Content	N, C, H
Instrument	Germany elementar vario EL III

Results:

Sampling name	Sampling weight (mg)	N%	C%	H%
TH-TGJ-1	2.070	5.19	79.83	7.29
	2.107	5.18	79.80	7.30
TH-TGJ-2	2.115	5.15	82.20	7.38
	2.006	5.14	82.19	7.39

	Date	13/6 2014