Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

# *Supporting information*

## Heterocycle Containing Different Atoms as π-bridge effect on the Performance of Dye-Sensitized Solar Cells

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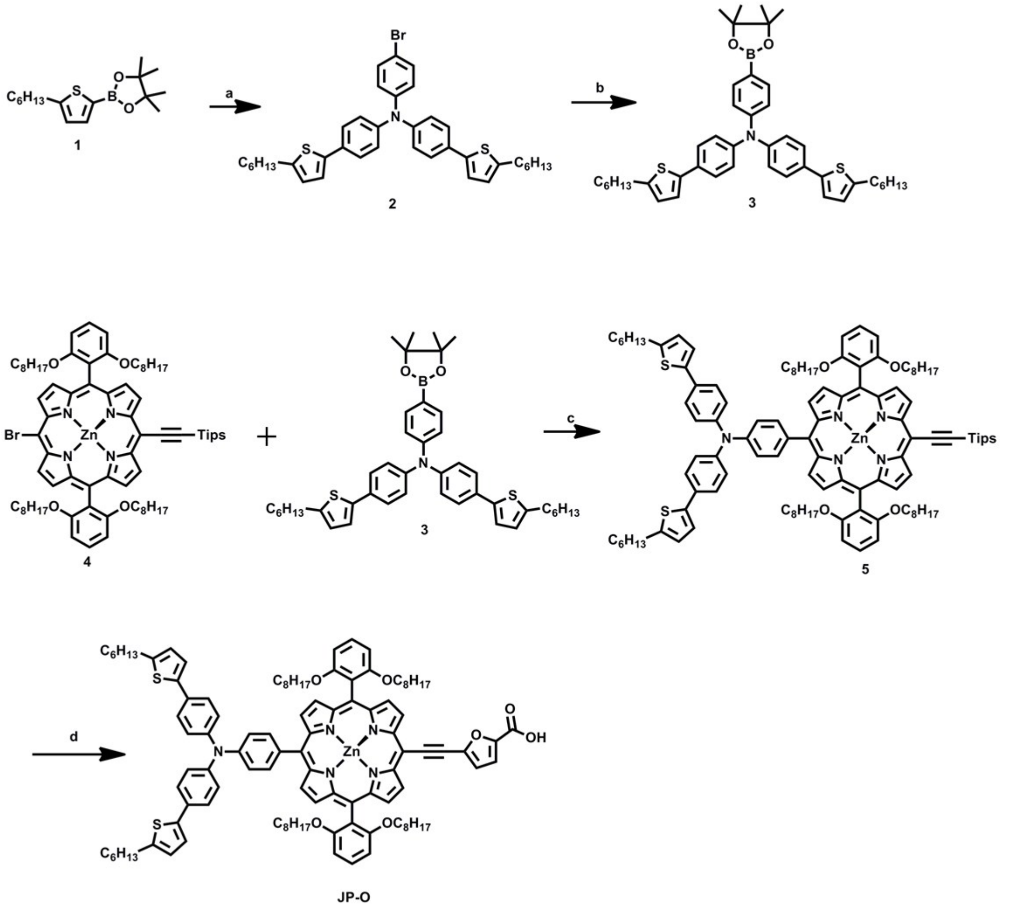
## General information

All solvents were treated by standard methods before use and all chemicals were purchased from commercial suppliers and used without further purification unless indicated otherwise. *N*, *N*-Dimethylformamide, toluene and tetrahydrofuran were dried and distilled from $CaH_2$.

The $^1$H NMR and $^{13}$C NMR spectra were recorded on a Bruker DRX (500 MHz) NMR spectrometer with tetramethylsilane (TMS) as the internal standard. The mass spectra were measured in ESI Mass Spectrometer (LCQ Fleet).

# Synthesis of the dye JP-O



**Scheme S1** Reagents and conditions: a) Tris(4-bromophenyl)amine, $Pd(PPh_3)_4$, $K_2CO_3$, $H_2O$, 1, 4-dioxane, 90℃; b) Bis(pinacolato)diboron, $Pd(dppf)Cl_2$, KOAc, DMF, 80℃; c) $Pd(PPh_3)_4$, $K_2CO_3$, $H_2O$, 1, 4-dioxane, 90℃; d) i: TBAF, THF, rt; ii: 5-bromofuroic acid, $Pd_2(dba)_3$, $AsPh_3$, TEA, THF, reflux.

## Experimental Details:

### Synthesis of compound 2 to compound 5

The compounds 2-5 were synthesized according to ref. 1.

### Synthesis of dye JP-O

To a solution of compound **5** (300 mg, 0.167 mmol) in anhydrous THF (20 mL) was added TBAF (0.6 mL, 1 M in THF). The solution was stirred at room temperature for 30 min under dinitrogen. The mixture was quenched with $H_2O$ and then extracted with $CH_2Cl_2$. The organic layer was dried over anhydrous $MgSO_4$ and the solvent was removed under reduced pressure. The residue and 5-bromofuroic acid (127 mg, 0.668 mmol) were dissolved in a mixture of anhydrous THF (40 mL) and TEA (10 mL) underdinitrogen, then $Pd_2(dba)_3$ (46 mg, 0.050 mmol) and $AsPh_3$ (102 mg, 0.334 mmol) were added to the mixture. The solution was refluxed for 6 h. The solvent was removed under reduced pressure. The residue was purified by silica gel column chromatography ($CH_2Cl_2$/MeOH = 20/1), recrystallization from MeOH/Ether to give dye **JP-O** (200 mg, 67%) as a green solid. $^1$HNMR ($CDCl_3$, 500Hz) $\delta_H$ 9.67 (d, *J* = 4.5Hz, 2H), 8.96 (d, *J* = 4.5Hz, 2H), 8.93 (d, *J* = 4.5Hz, 2H), 8.85 (d, *J* = 4.5Hz, 2H), 8.07 (d, *J* = 8.0Hz, 2H), 7.73 (t, *J* = 8.5Hz, 2H), 7.61 (d, *J* = 8.0Hz, 4H), 7.48 (d, *J* = 8.0Hz, 2H), 7.41 (d, *J* = 8.0Hz, 4H), 7.13 (d, *J* = 3.0Hz, 2H), 7.05 (d, *J* = 8.5Hz, 6H), 6.77 (d, *J* = 3.5Hz, 2H), 3.88 (s, 8H), 2.86 (t, *J* = 7.5Hz, 4H), 1.72-1.78 (m, 4H), 1.42-1.48 (m, 4H), 1.31-1.38 (m, 8H), 0.83-1.01 (m, 30H), 0.64-0.71 (m, 8H), 0.53-0.57 (m, 20H), 0.45-0.49 (m, 8H). $^{13}$CNMR ($CDCl_3$, 125Hz) $\delta_C$ 160.0, 152.0, 151.2, 150.3, 149.4, 146.6, 146.5, 145.2, 143.8, 141.5, 137.8, 135.6, 135.4, 132.5, 131.8, 130.9, 130.0, 129.7, 126.5, 125.0, 124.7, 122.0, 121.6, 116.1, 114.8, 105.2, 68.6, 31.6, 31.4, 30.3, 29.7, 28.7, 25.3, 22.6, 22.3, 14.1, 13.8. MS (ESI): Calcd for $C_{109}H_{127}N_5O_7S_2Zn$, 1748.71; found, 1746.75.

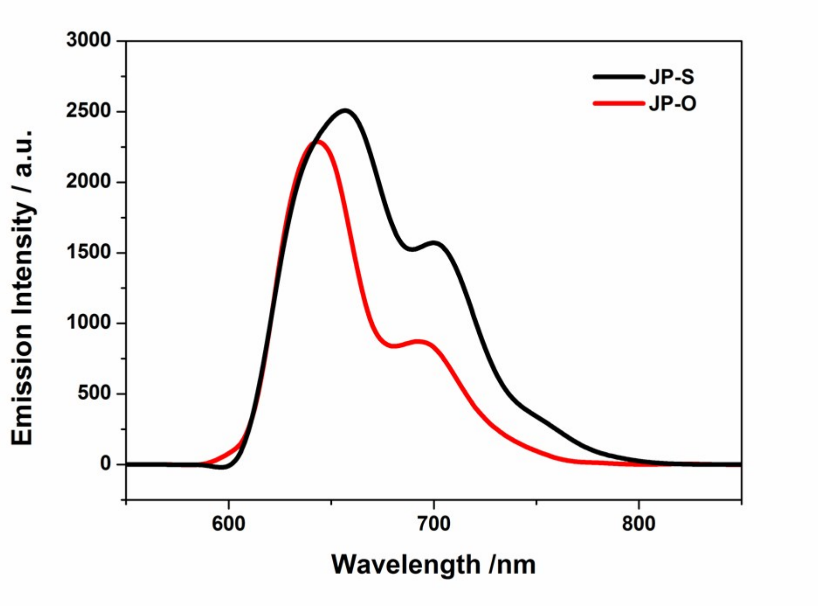


**Fig. S1** Emission spectra of **JP-S** and **JP-O** in DCM

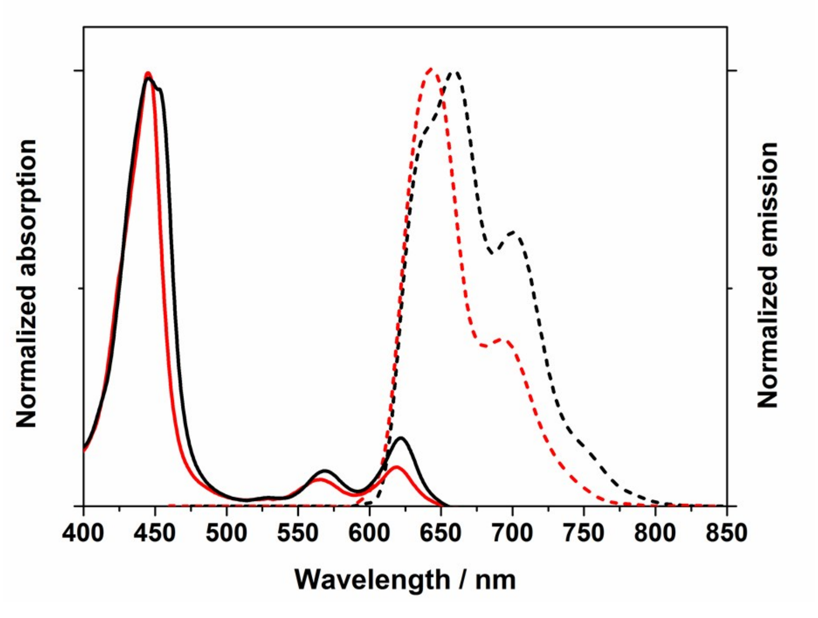


**Fig. S2** The normalized absorption spectra (solid lines) and emission spectra (broken lines) of **JP-S** (black) and **JP-O** (red) in DCM (the intersection of JP-S and JP-O is 613 nm and 601 mm, respectively, $E_{o-o} = 1240 / \lambda$).

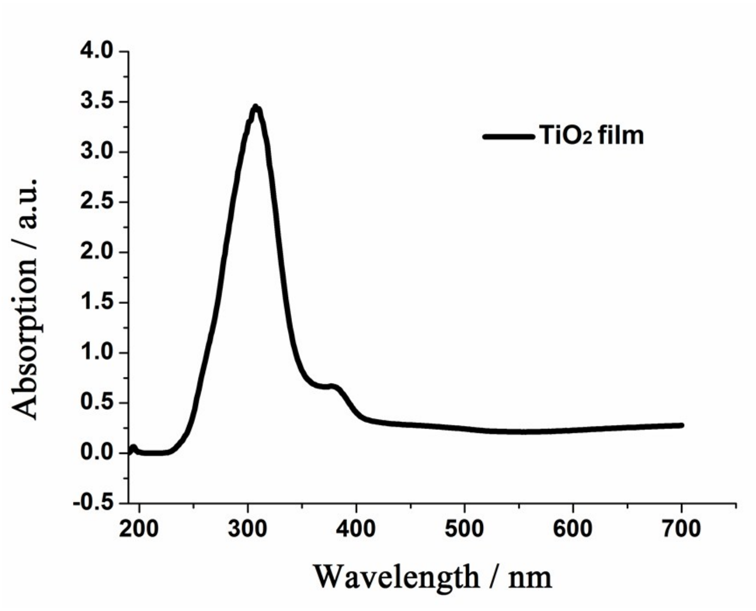


**Fig. S3** Absorption spectrum of $TiO_2$ film.

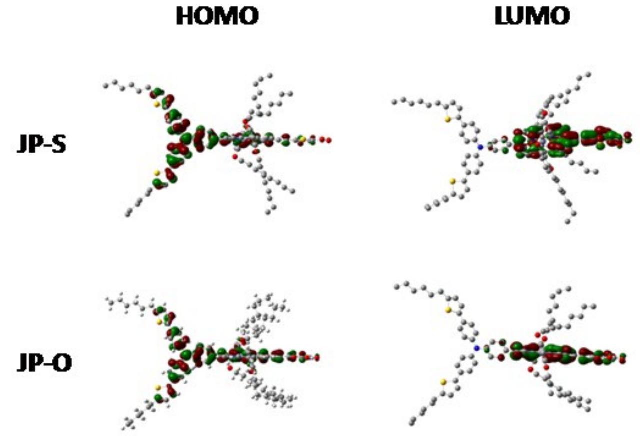


**Fig. S4** HOMO and LUMO frontier molecular orbitals of **JP-S** and **JP-O** calculated by density-functional theory (DFT) at the DFT-B3LYP/LanL2MB level with Gaussian 09 suite of programs.

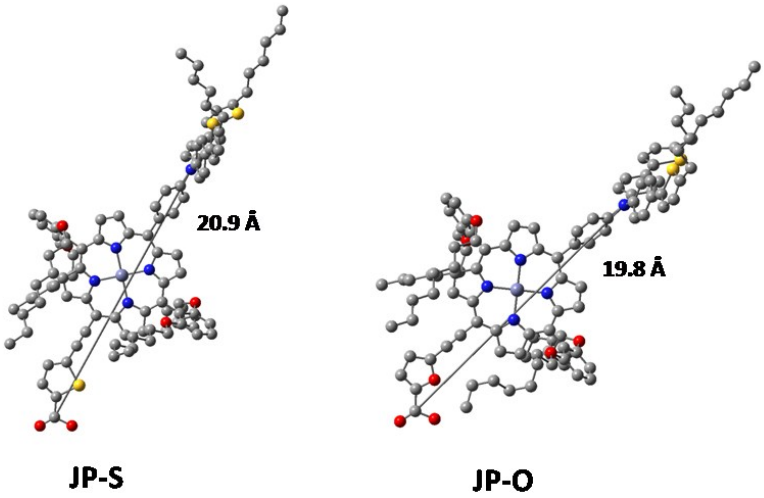


**Fig. S5** The geometry optimized ground state molecular structures of **JP-S** and **JP-O**.

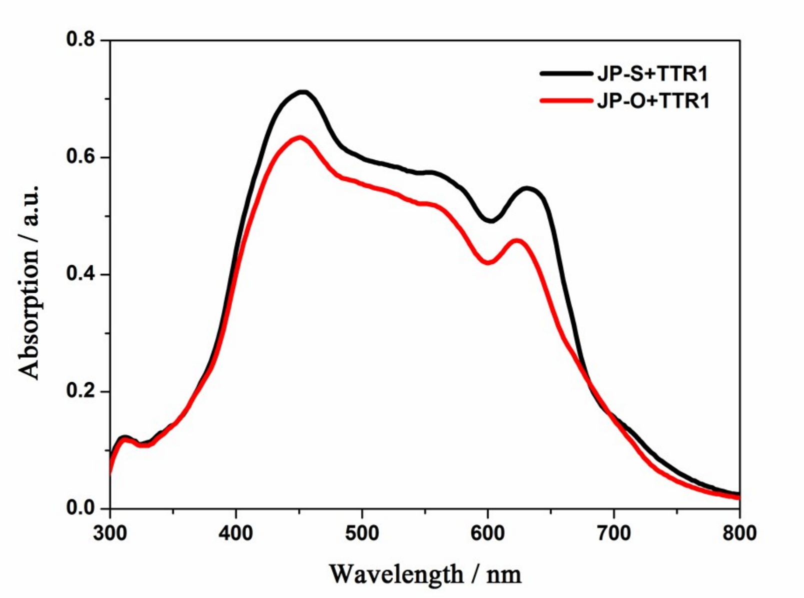


**Fig. S6** Absorption spectra of **JP-S+TTR1** and **JP-O+TTR1** anchoring on the 14 μm porous $TiO_2$ nanoparticle films.

## References

1 H. L. Jia, Z. M. Ju, H. X. Sun, X. H. Ju, M. D. Zhang, X. F. Zhou and H, G. Zheng, *J. Mater. Chem. A*, 2014, **2**, 20841.