Supporting Information

Octathienyl/phenyl-substituted zinc phthalocyanines J-aggregated through conformational planarization

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Fig. S1 (a) The TLC experiment of 4,5-dibromophthalic acid dimethyl ester (left) and the product obtained from the Suzuki cross-coupling reaction (right), with a 2:1(volume ratio) mixed solvents of petroleum and ether ethyl acetate as the eluent. (b) $^1$HNMR spectra of the product in CDCl$_3$.

Fig. S2 The TLC experiments in the synthesis of phthalonitrile 7 from the mixture obtained from the Suzuki cross-coupling reaction. In each TLC experiment, the left is reagent and the right is the product. (1) 2→3; (2) 3→4; (3) 4→5; (4) 5→6; (5) 6→7; The eluent is a 2:1(volume ratio) mixed solvents of petroleum and ether ethyl acetate.
Fig. S3 The UV-Vis spectrum of Cu-TPc and Ni-TPc in THF ($c = 1 \times 10^{-4}$ mol L$^{-1}$). The sample is placed in a standard 1-mm quartz cuvette.

Fig. S4 $^1$H NMR spectra of (A) Ni-TPc ($1.5 \times 10^{-3}$ mol L$^{-1}$) in CDCl$_3$; (B) Zn-TPc ($1.5 \times 10^{-3}$ mol L$^{-1}$) in the 5:1 mixed solvents of CDCl$_3$ and $d_5$-pyridine; (C) 5:1 mixed solvents of CDCl$_3$ and $d_5$-pyridine.
**Fig. S5** The UV-Vis spectrum of Zn-TPc in THF (c = 2 × 10⁻⁵ mol. L⁻¹)

**Fig. S6** The UV-Vis spectral changes of Zn-TPc (c = 2 × 10⁻⁵ mol. L⁻¹) in chloroform upon the addition of a drop of pyridine.

**Fig. S7** The plot of lg(c⁻A₇₀₀/ε₇₀₀) versus lg(A₇₀₀/ε₇₀₀) of Zn-TPc in the concentration range of 1.25 × 10⁻⁶ to 2 × 10⁻⁵ mol. L⁻¹.
Fig. S8  Computer optimized conformation of Zn-Pc by energy minimization method. Left: side view; right: top view