

## Supporting Information

for

### Excitonic Coupling Interactions in the Self-Assembly of Perylene-Bridged Bis( $\beta$ -cyclodextrin)s and Porphyrin

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## Experiment Section

**Materials.** The synthesis and the characteristic data of compound **1** were reported in our previous paper.<sup>1</sup> Compound **2** was obtained from 5,10,15,20-Tetrakis(4-sulfonatophenyl)porphyrin (purchased from Sigma–Aldrich) reacting with zinc oxide by the reported methods.<sup>2</sup>

**Measurements.** 2D NOESY spectrum was recorded on a Varian 300 Spectrometer. UV–Vis spectra were recorded in a conventional quartz cell (light path 10 mm) on a Shimadzu UV-3600 spectrophotometer equipped with a PTC-348WI temperature controller to keep the temperature at 25 °C. The fluorescence spectra were recorded in a conventional quartz cell on a VARIAN CARY Eclipse equipped with a VARIAN CARY single cell peltier accessory to keep the temperature at 25 °C. Circular dichroism spectra were performed on J-715-150S (JASCO). The dynamic light scattering (DLS) was performed on a laser light scattering spectrometer (BI-200SM) equipped with a digital correlator (BI-9000AT) at 636 nm.

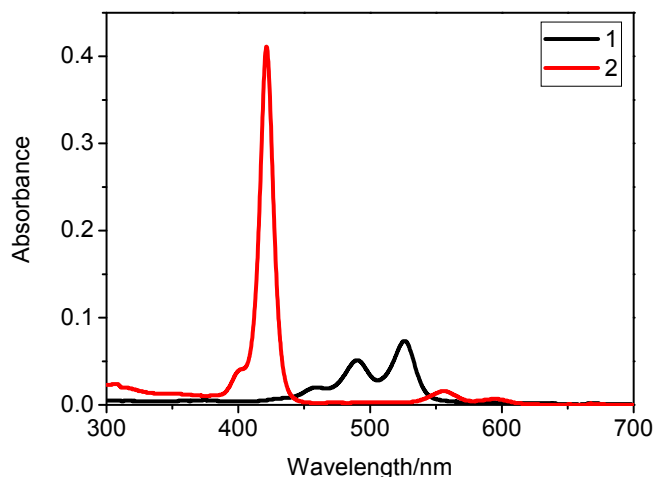


Fig. S1. UV–Vis spectra of **1** ( $1.0 \times 10^{-6}$  M) and **2** ( $1.0 \times 10^{-6}$  M) in phosphate buffer (pH 7.0, 0.05 M) at 25 °C.

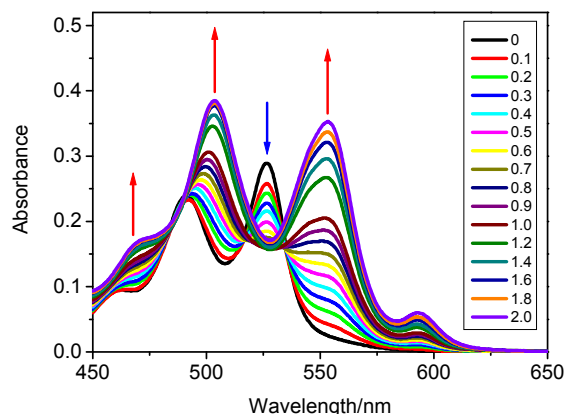


Fig. S2. UV–Vis spectral changes of **1** ( $5.0 \times 10^{-6}$  M) upon addition of **2** (0–2 equiv.) in phosphate buffer (pH 7.0, 0.05 M) at 25 °C.

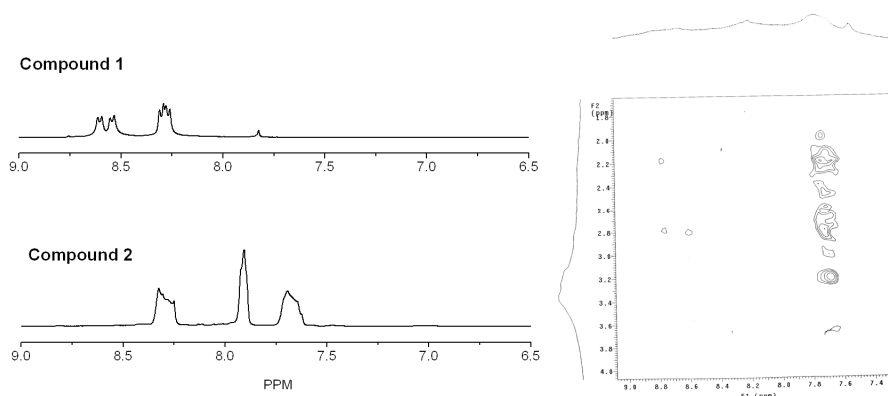


Fig. S3.  $^1\text{H}$  NMR spectra of **1** and **2**, and 2D NOESY spectra of **1** with **2** in  $\text{D}_2\text{O}$  at 25 °C.

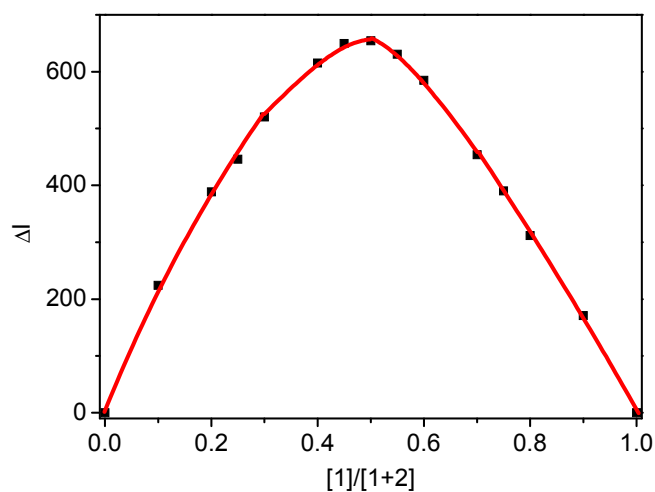


Fig. S4. The Job' plot for **1** upon complexation with **2**, fluorescence changes recorded at 535 nm for **1**, and the sum of the total concentrations of hosts and guests is constant ( $1.0 \times 10^{-6}$  M).

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First Delay:	5.0 $\mu$ sec	Samples:	5.8360e+07
Last Delay:	10.0 msec	Atot:	3.5169e+06
Elapsed Time:	00:07:52	A CR (avg.):	12.1 kcps
Wavelength:	636.0 nm	M. Base:	2.1395e+05
Angle:	90.0	C. Base:	2.1194e+05
Temp:	24.2 deg C (GTE)	Base diff:	0.948%
Liquid:	Water	Dust Cutoff:	10.00
Viscosity:	0.907 cP	Eff Dia:	124.0 nm
Ref Index:	1.331	Poly:	0.396

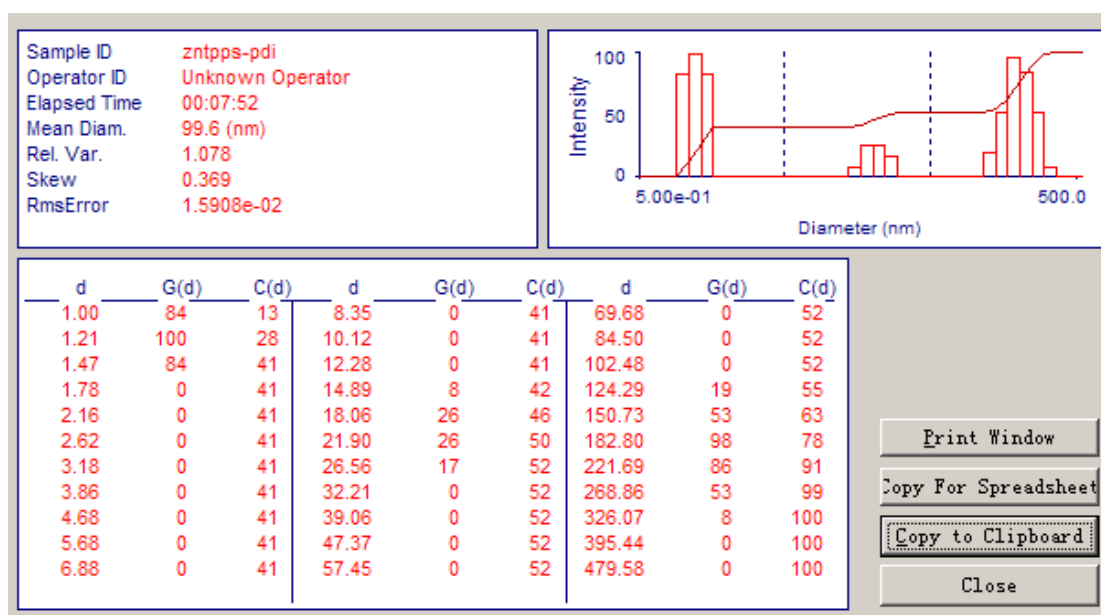


Fig. S5. Size distribution of **1** ( $5.0 \times 10^{-6}$ M) with **2** ( $5.0 \times 10^{-6}$ M) obtained from dynamic light scattering (DLS) in phosphate buffer (pH 7.0, 0.05 M).

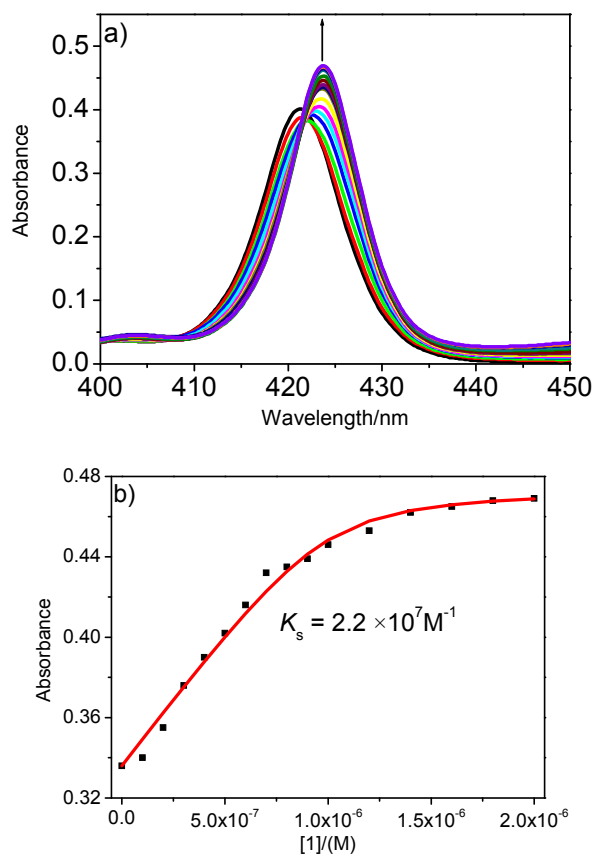


Fig. S6. (a) Soret band spectral changes of **2** ( $1.0 \times 10^{-6}$  M) upon addition of **1** (0–2 equiv.) in phosphate buffer (pH 7.0, 0.05 M) at 25 °C; (b) the curve of the complexation stability constants fitting at the 424 nm.

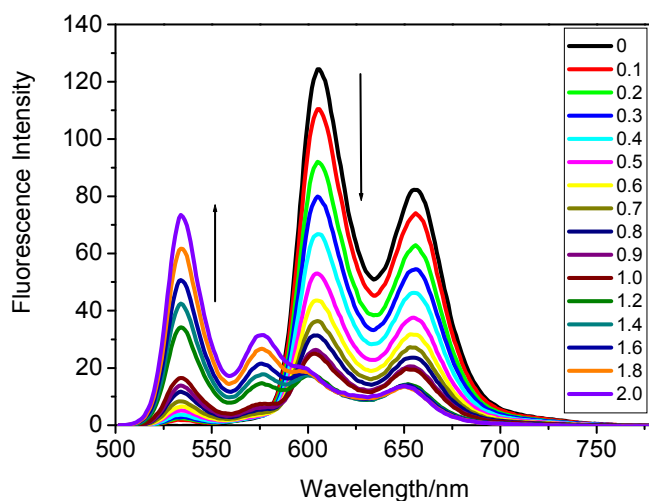


Fig. S7. Fluorescence spectral changes of **2** ( $\lambda_{ex} = 421$  nm,  $1.0 \times 10^{-6}$  M, emission slit width of 5 nm) with addition of **1** (0–2 equiv.) in phosphate buffer (pH = 7.0, 0.05 M) and 25 °C.

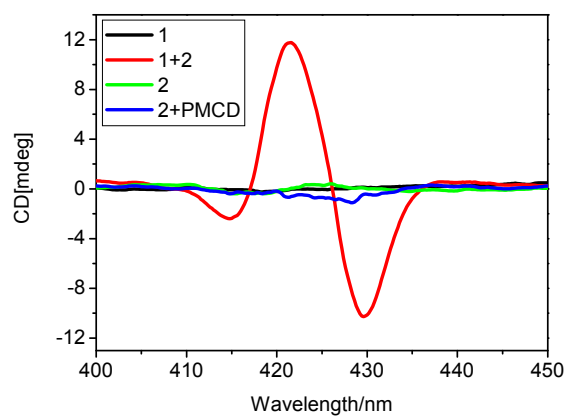


Fig. S8. Circular dichroism spectra of **1** (Black,  $5.0 \times 10^{-6}$  M), **1** (Red,  $5.0 \times 10^{-6}$  M) with addition of 1 equiv. **2**, **2** (Green,  $5.0 \times 10^{-6}$  M), and **2** (Blue,  $5.0 \times 10^{-6}$  M) with addition of 2 equiv. PMCD in phosphate buffer (pH 7.0, 0.05 M).

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- 1 Y. Liu, K. R. Wang, D. S. Guo, B. P. Jiang, *Adv. Funct. Mater.*, 2009, **19**, 2230.
  - 2 K. Kano, S. Kobayashi, *Bull. Chem. Soc. Jpn.*, 2003, **76**, 2027.