

## Supporting Information

### Inversing Chirality and Boosting Circularly Polarized Luminescence of Pyrene Moieties in Supramolecular Gel Matrix

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## 1. Experimental

### 1.1 Instrument and material

UV/Vis absorption spectra were collected on a JASCO UV-550 spectrometer. Fluorescence spectra were measured on a Hitachi F-4600 spectrometer. Circular Dichroism (CD) spectra were recorded with a JASCO J-1500 spectrophotometer. Circularly Polarized Luminescence (CPL) measurements were performed with a JASCO CPL-200 spectrometer. XRD analysis was performed on a Rigaku D/Max-2500 X-ray diffractometer (Japan) with Cu K $\alpha$  radiation ( $\lambda = 1.5406 \text{ \AA}$ ), which was operated at a voltage of 40 kV and a current of 150 mA. <sup>1</sup>H NMR data was acquired with BrukerAvance 400MHz spectrometer. MALDI-ToF MS was recorded on Bruker Autoflex III machine. SEM images were recorded on a Hitachi S-4800 FE-SEM instrument with an accelerating voltage of 10 kV. All the reagents including ethylisocyanate, 1-pyrenecarboxylic acid, L/D-glutamic acid and octadecylamine were purchased from Innochem. 99.9% purify of DMSO was purchased from Merck. All the chemicals were analytical pure and used without further purification. *N,N'*-bis-octadecyl-*L/D*-glutamicdiamide (*L/DGAm*) was synthesized according to reported method.<sup>1, 2</sup>

### 1.2 Experimental Details

#### Gelation test and critical gel concentration (CGC)

**L-SG** or **D-SG** gelator (10.0 mg) was added into an appropriate solvent (1.0 mL) in a capped test tube. The mixture was heated until the solid was dissolved completely, which was subsequently cooled to room temperature. Gelation was determined by the absence of the flow of the solvent when the tube was inverted. To measure the critical gelation concentration, the solvent (100  $\mu$ L for every time) was further added to the gel sample and the CGC was

determined until the concentration is insufficient to form a stable gel after a heating-cooling cycle.

### **Py-LG/Py-DG gel in DMSO**

A certain amount of **Py-LG/Py-DG** solid was mixed with 1.0 mL DMSO in a capped sample glass bottle, and the mixture was heated up to 90 °C for 5 min to make a uniform transparent solution. After the solution had been spontaneously cooled down to room temperature (25 °C, the cooling rate was about 10 °C/min), and stable transparent gels were always obtained when the concentration was higher than 1 mg/mL.

### **Co-gel (Py-LG/Py-DG in L/D-SG)**

To study chiral packing and emission behaviors of pyrene derivatives (**Py-LG** and **Py-DG**) in the gel matrix, **Py-LG** or **Py-DG** in 1.0 mL DMSO was first prepared ( $1 \times 10^{-5}$ ,  $1 \times 10^{-4}$ ,  $2 \times 10^{-4}$ ,  $5 \times 10^{-4}$ ,  $1 \times 10^{-3}$  and  $1 \times 10^{-2}$  M), then 8.0 mg (10  $\mu$ M) of **L-SG** or **D-SG** was added into mixture solution (corresponding to  $1 \times 10^{-2}$  M in DMSO), the mixture solution was further heated until the solid was dissolved completely, which was subsequently cooled to room temperature to obtain co-gel (25 °C, the cooling rate was about 10 °C/min). Subsequently, all the samples were left standing for about 12 h under ambient condition before being measured. Thus, pyrene derivatives in **L-SG** or **D-SG** gel matrix with the mole contents of 0.1%, 1%, 2%, 5%, 10% and 100% were prepared, respectively.

### **SEM and XRD measurement**

**SEM:** Gel samples were cast onto single-crystal silica plates, the solvent was first dried for 10 hours under the ambient conditions, and then vacuum dried 48 h for complete removal of the solvent. The sample surface was coated with a thin layer of Pt before SEM observation.

**XRD:** Gel samples were cast onto single-crystal silica plates (1cm $\times$ 1cm), the solvent was first dried for 10 hours under the ambient conditions, and then vacuum dried 48 h for complete removal of the solvent before XRD measurement.

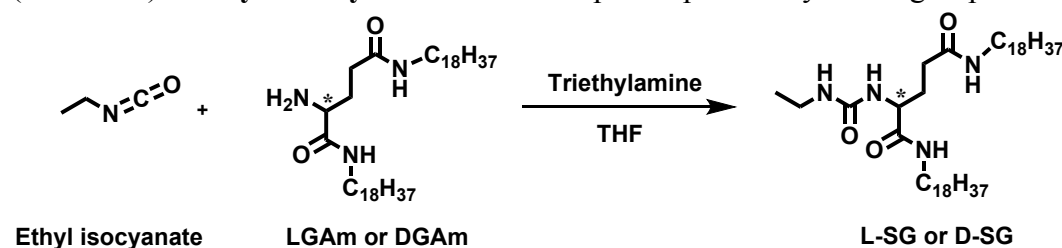
### **UV-vis, fluorescence, CD and CPL spectra measurement**

The gel was first prepared in a glass bottle, partial gel sample was taken out and placed in a 0.1mm quartz clip for testing (as shown below Fig. a). The quartz

clip was placed perpendicular to the light path spectral measurement. In the process of CD spectral measurement, the quartz clip was continuously rotated on a rotatable sample stage to get rid of the possible linear dichroism.<sup>3</sup> 0.2 cm quartz cells were used for the spectral measurements of **Py-LG/Py-DG** in DMSO solution and the UV-Vis spectra for 0.1% of **Py-LG/Py-DG** in **L/D-SG** gel matrix.

### 1.3 Experimental procedures

The synthesis and characterization of *N,N'*-bis-octadecyl-*L/D*-glutamicdiamide (**L/DGAm**) and **Py-LG/Py-DG** have been reported previously in our group.<sup>1,2</sup>



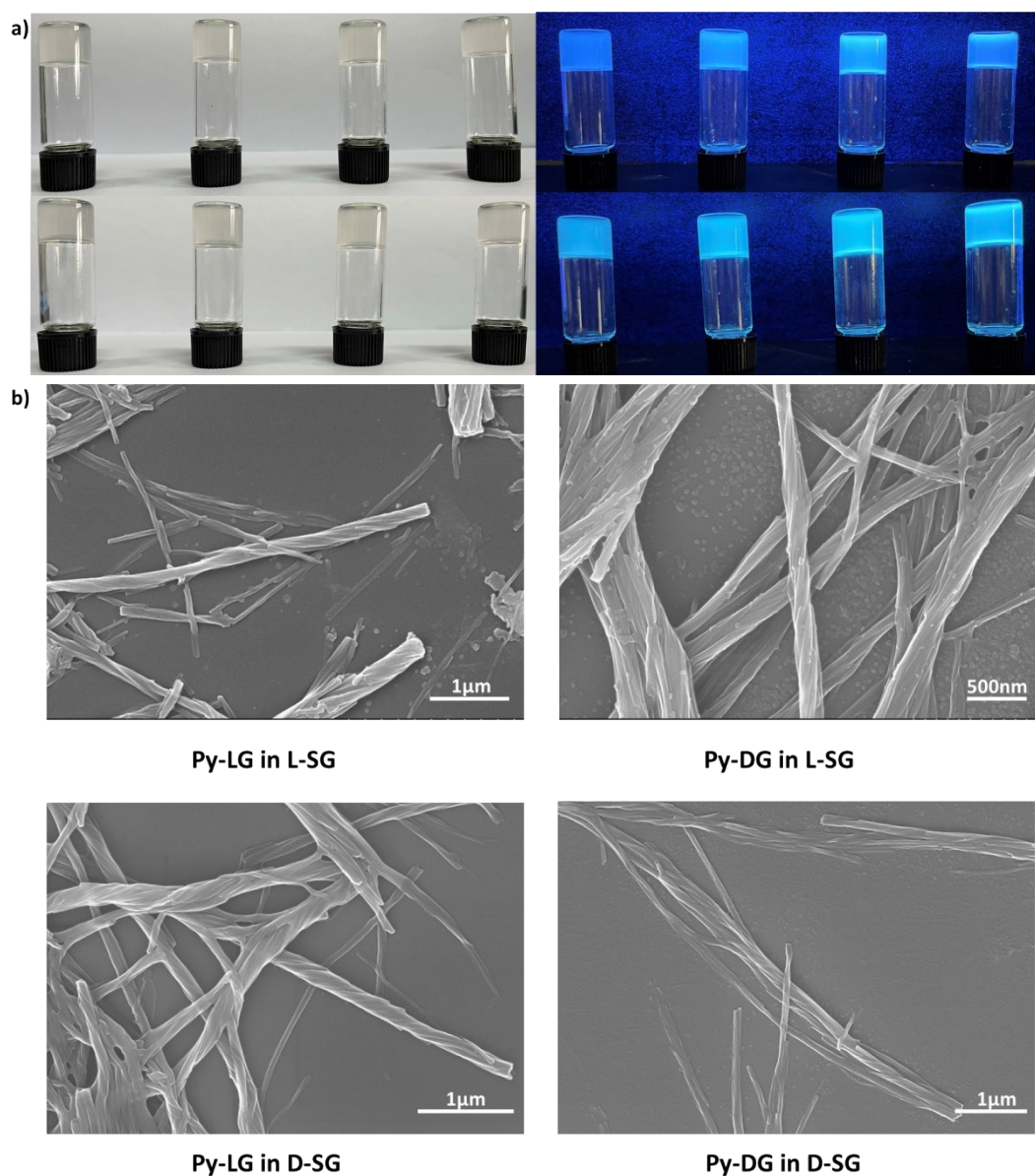
The mixture of *N,N'*-bis-octadecyl-*L/D*-glutamicdiamide<sup>12i</sup> (**L/DGAm**, 1.0 g, 1.54 mmol) and Ethyl isocyanate (0.3 g, 4.22 mmol) was firstly stirred for 30 min in THF (200 mL). Thereafter, triethylamine (10 mL) was added to the mixture, and then the mixture was stirred and heated to reflux for 2 days. The crude gel was formed upon cooling to room temperature, which was isolated by filtration and washed with cold THF for several times. After dried, the product was purified by recrystallization three times in THF to give the target compounds **L-SG** (0.72g, 65% yield) or **D-SG** (0.81g, 73% yield). **L-SG**: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 4.23-4.19 (m, 1H), 3.30-3.21 (m, 6H), 1.56-1.49 (m, 4H), 1.45-1.20 (m, 64H), 1.19-1.16 (t, J = 1.2 Hz, 3H), 0.90-0.86 (m, 6H). MS (MALDI-TOF): m/z for C<sub>44</sub>H<sub>88</sub>N<sub>4</sub>O<sub>3</sub>: 720.7 [M]<sup>+</sup>; found: 743.4 [M+Na]<sup>+</sup>; **D-SG**: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 4.25-4.21 (m, 1H), 3.27-3.21 (m, 6H), 1.56-1.49 (m, 4H), 1.34-1.22 (m, 64H), 1.18-1.15 (t, J = 1.2 Hz, 3H), 0.89-0.85 (m, 6H). MS (MALDI-TOF): m/z for C<sub>44</sub>H<sub>88</sub>N<sub>4</sub>O<sub>3</sub>: 720.7 [M]<sup>+</sup>; found: 743.8 [M+Na]<sup>+</sup>.

## 2. Supplementary Figures and Tables

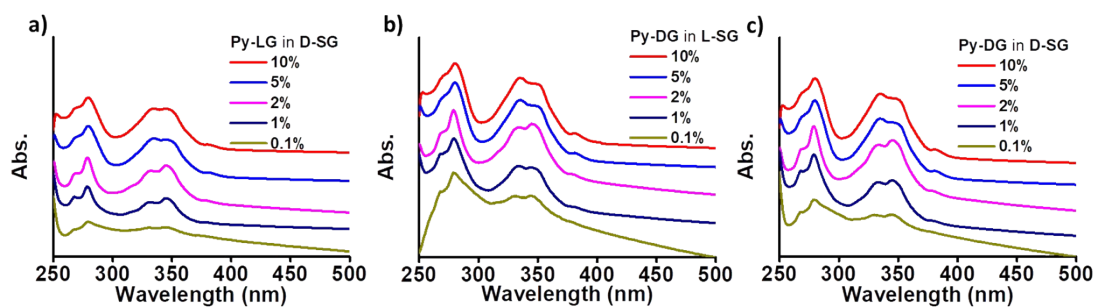
Table S1. The gelation properties of L-SG and racemic SG (L-SG:D-SG=1:1) in various solvents

Solvents	Property <sup>a</sup>	CGC for L-SG (mg/mL)	CGC for SG (mg/mL)
Toluene	TG	0.9	2.5
Chloroform	TG	0.9	3.3
Dichloromethane	TG	0.7	1.4
Ethyl acetate	TG	1.1	3.8
THF	TG	0.9	2.5
Acetone	TG	1.3	4.0
Ethanol	TG	2.0	4.0
Acetonitrile	G	2.0	3.8
DMF	TG	1.0	3.0
DMSO	TG	1.0	2.0

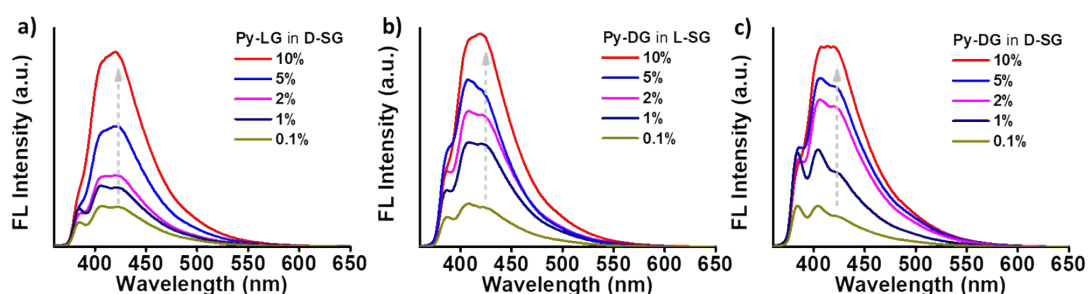
<sup>a</sup> G = white gel; TG = transparent gel.



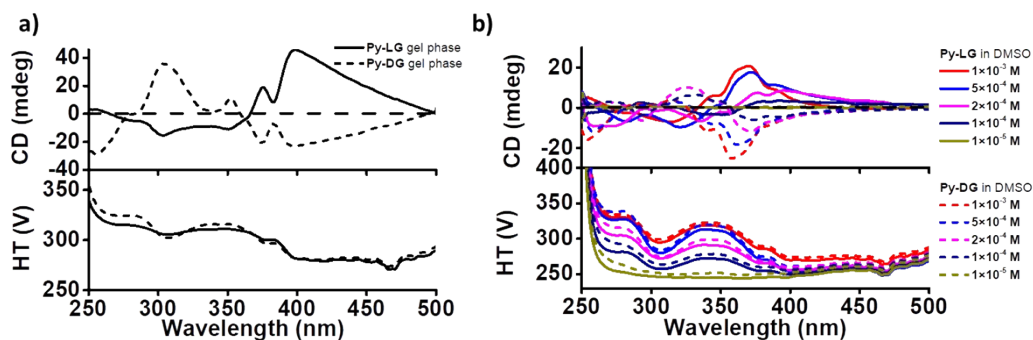
**Figure S1.** a) Pyrene derivatives co-assembling with **L-SG** (The mole concentrations from left to right are 0.1%, 1%, 2%, 5% (up), 10%, 20%, 50%, 100% (down); b) SEM image of **Py-LG/Py-DG** in **L/D-SG** (10%).



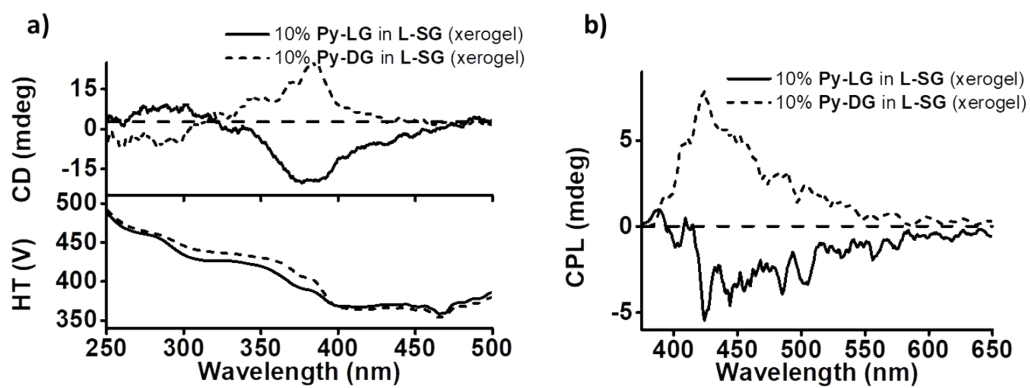
**Figure S2.** UV-Vis spectra of Py-LG in D-SG gel, Py-DG in L-SG gel and Py-DG in D-SG gel under different content: 0.1%, 1%, 2%, 5% and 10%.



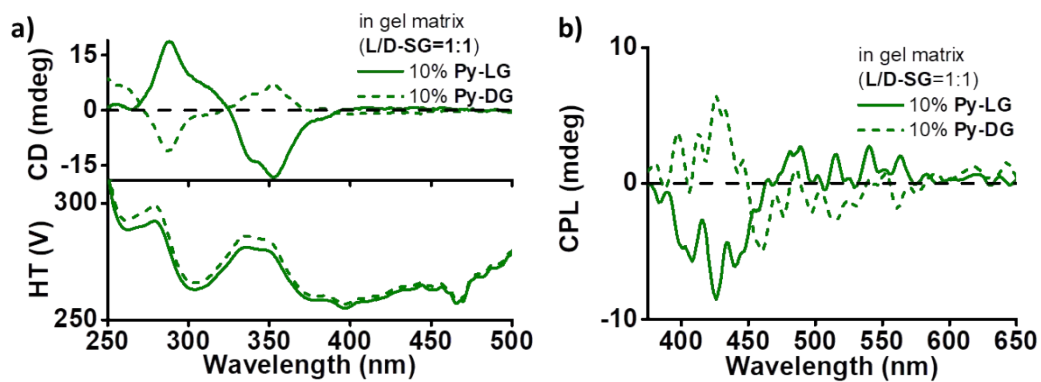
**Figure S3.** Fluorescent spectra of Py-LG in D-SG gel, Py-DG in L-SG gel and Py-DG in D-SG gel under different content: 0.1%, 1%, 2%, 5% and 10%,  $\lambda_{\text{ex}} = 340 \text{ nm}$ .



**Figure S4.** CD spectra for Py-LG/ Py-DG with different concentrations including in its gel phase in DMSO.



**Figure S5.** a) CD and b) CPL spectra of Py-LG /Py-DG (10%) in L-SG (xerogel).



**Figure S6.** a) CD and b) CPL spectra of Py-LG /Py-DG (10%) in a racemic gel matrix (L-SG: D-SG=1:1).

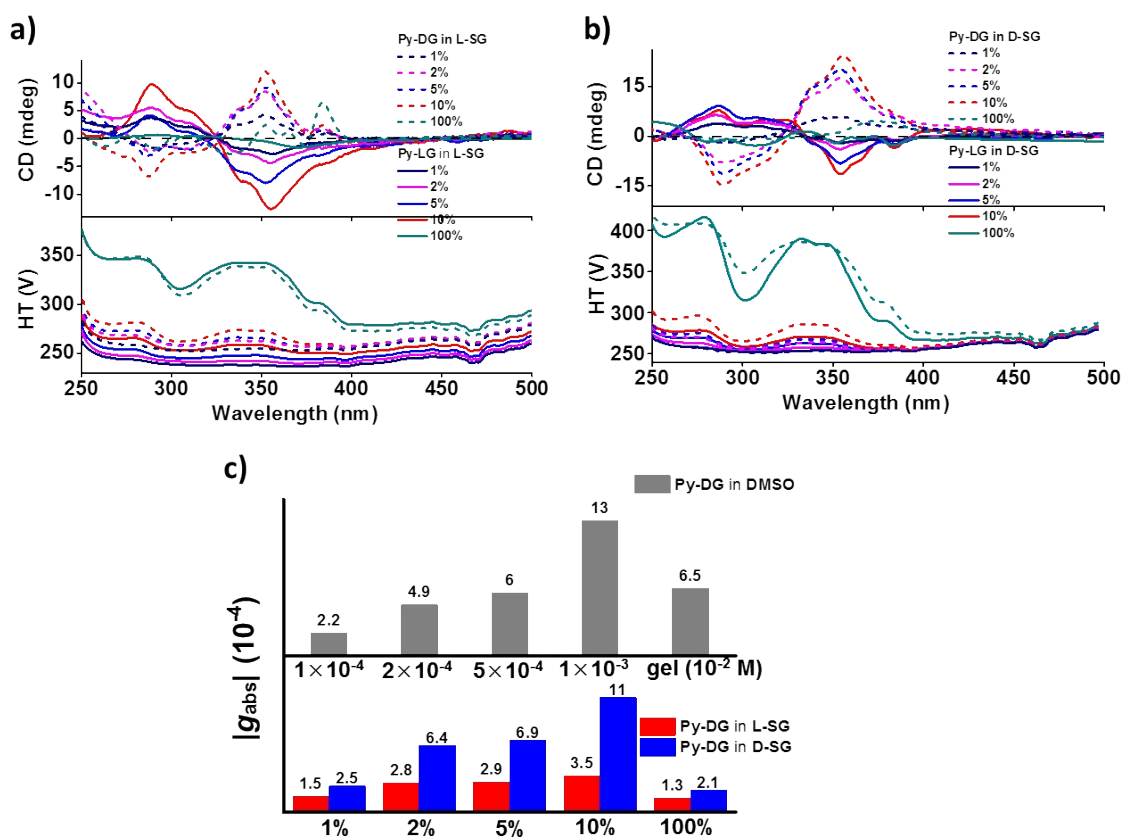


Figure S7. CD spectra for Py-LG/ Py-DG with different concentrations in L/D-SG.

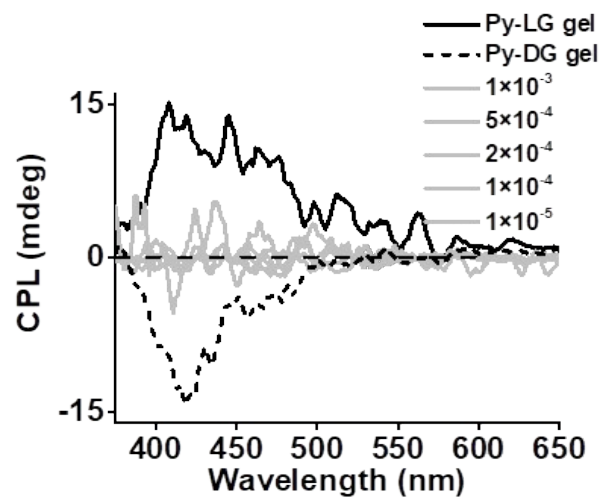
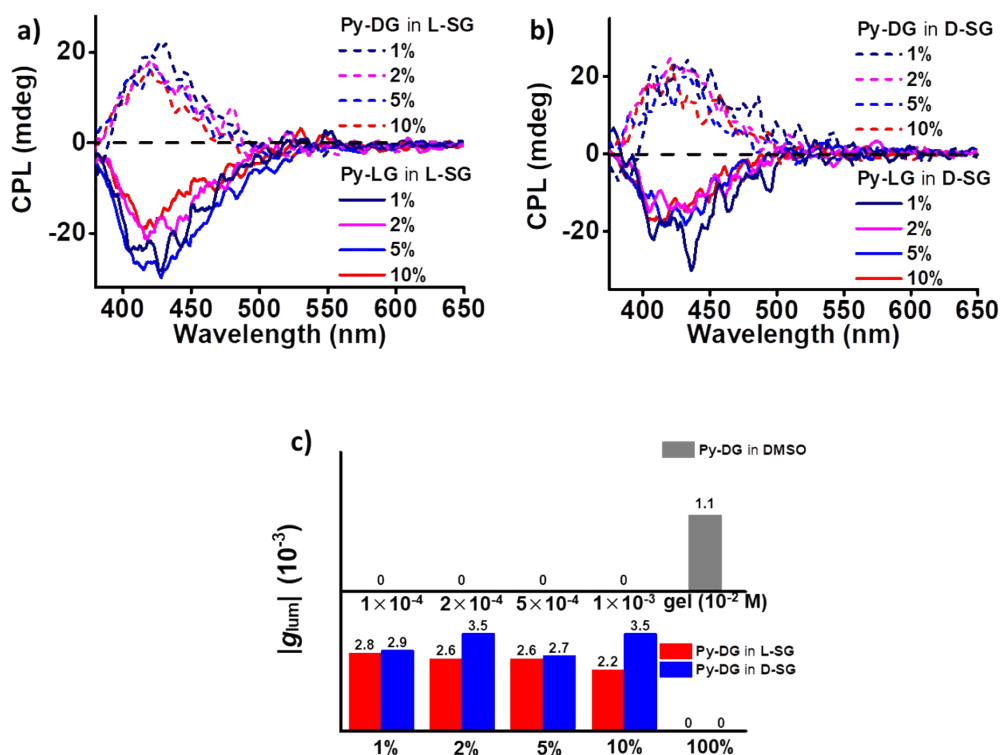
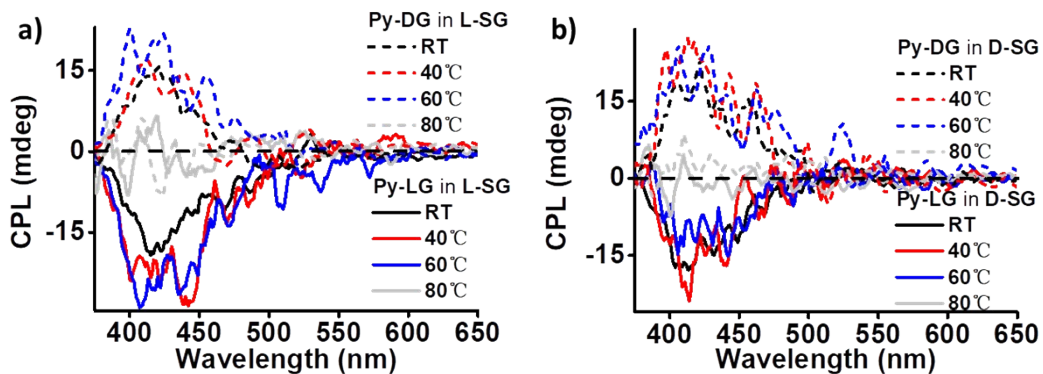


Figure S8. CPL spectra of Py-LG/ Py-DG including in its gel phase in DMSO.





**Figure S9.** CPL spectra for Py-LG/ Py-DG with different concentrations in L/D-SG,  $\lambda_{ex}$  = 340 nm.



**Figure S10.** CPL spectra for 10% Of Py-LG/Py-DG in L/D-SG under different temperatures (room temperature, 40 °C, 60 °C and 80 °C),  $\lambda_{ex}$  = 340 nm.

## References

1. X. Zhu, Y. Li, P. Duan and M. Liu. *Chem. Eur. J.*, 2010, **16**, 8034-8040.
2. L. Zhang, C. Liu, Q. Jin, X. Zhu and M. Liu. *Soft matter*, 2013, **9**, 7966-7973.
3. L. Zhang, Q. Lu, M. Liu, *J. Phys. Chem. B*, 2003, **107**, 2565-2569.