

Supporting information

Chiral signs of TPPS co-assemblies with chiral gelators: Role of molecular and supramolecular chirality

Qiuling Wang^{a,b}, Li Zhang^{b*}, Dong Yang^b, Tiesheng Li^{a*}, Minghua Liu^{b,c*}

^a College of Chemistry and Molecular Engineering, Zhengzhou University, 100 Science Road, Zhengzhou, Henan 450001, China

^b Beijing National Laboratory for Molecular Science (BNLMS), CAS Key Laboratory of Colloid, Interface and Chemical Thermodynamics, Institute of Chemistry, Chinese Academy of Sciences, Beijing, 100190, China

^c Collaborative Innovation Centre of Chemical Science and Engineering, Tianjin, P. R. China.

1 .EXPERIMENTAL SECTION

Materials. All of the reagents and solvents were of the highest purity and used without further purification unless otherwise noted. Water-soluble porphyrin, meso-tetraphenylsulfonatoporphyrin (TPPS), was purchased from Dojindo Laboratories and used without further purification. A cationic amphiphile (abbreviated as PUDG or PULG) was synthesized according to a method in the literature.¹⁴

Gel formation. A stock solution of TPPS in ultrapure Milli-Q water was first prepared with the concentration of 10^{-3} mol/L, and the pH value at 2.0 or at 5.0, respectively. Then TPPS was diluted to final concentration of 1.0×10^{-4} mol/L, 1.25×10^{-4} mol/L, 2.0×10^{-4} mol/L, 2.5×10^{-4} mol/L, and 4×10^{-4} mol/L, respectively, in mixed DMSO /H₂O with a volume ratio of 2/1. And the pH value of TPPS solution was again adjusted to 2.0 and 5.0 by HCl and NaOH. The gelator (PUDG), 8.35 mg) mixed with 1 mL TPPS solution in a capped test tube and the mixture was heated until the solid was completely dissolved to prepare the complex of PUDG(PULG)/TPPS at various ratios. The hot solution was naturally cooled at room temperature and then the gel or suspension formed in a few minutes, which was confirmed by inverting the test tube. The xerogels obtained were used for SEM, UV-vis and CD spectral measurements.

Characterization. UV-Vis spectra were measured on a Hitachi U-3900 UV-Vis spectrophotometer, and CD spectra were performed on a JASCO-815 spectrometer. Scanning electron microscopy (SEM) was performed on a Hitachi S-4800 FE-SEM microscope. The fully aged gels were cast onto single-crystal silica plates (Pt coated), and the trapped solvents in gels were evaporated under ambient conditions first, then vacuum-dried for 12 hours for SEM measurements. 20 mL hydrochloric acid or ammonia was in a vessel (30mL), respectively, and xerogel on mica substrate was put above 5cm of liquid interface and exposed to hydrochloric acid or ammonia acid for 20s in room temperature. Another vessel containing 20mL boiling water was used to carry out the treatment of water vapor. The treatment of water vapor was also done in room temperature for 20s. The xerogels was initially exposed to NH₃ gas 20s, and the following exposure to HCl gas 20s, then exposing the treated films water vapor 20s.

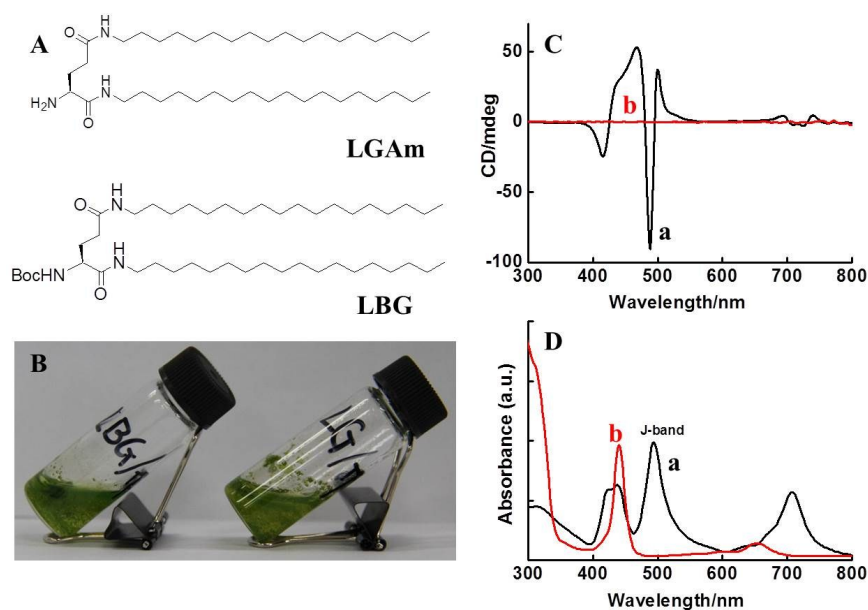


Fig. S1 (A) molecular structure of amine precursor of PULG (abbreviated as LGAm) and Boc protected glutamic acid derivative (LBG); (B) Photo pictures of LBG/TPPS and LGAm/TPPS; (C) and (D) CD and UV spectra of LGAm /TPPS and LBG /TPPS, in which curve a is LGAm/TPPS, and curve b is LBG/TPPS

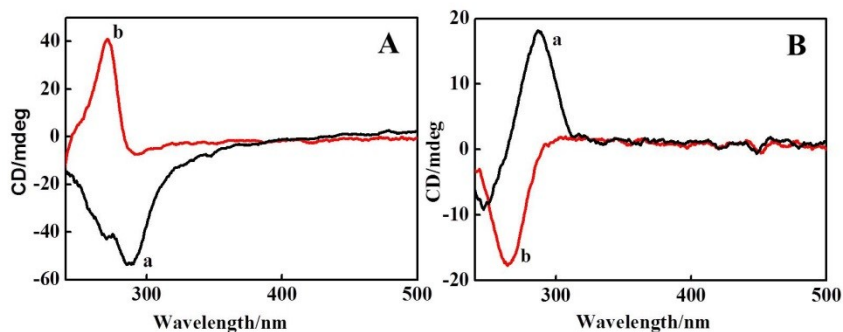


Fig. S2 CD spectra of PUDG xerogel obtained (A) (a) from cyclohexane/water (H_2O wt% =1%); b) after exposed to the water vapor 20s and (B) (a) from DMF/water (H_2O wt% =15 %); b) after exposed to the water vapor 20s.

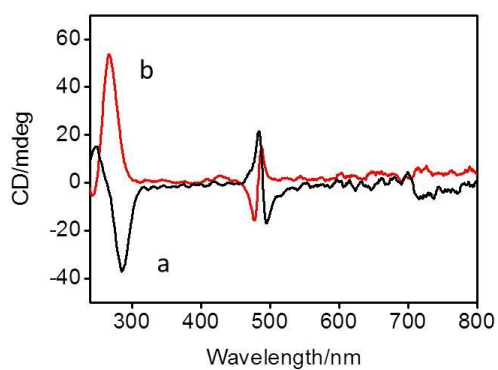


Fig. S3 CD spectra of PULG/TPPS as-prepared xerogel (a) and after treatment by NH_3-HCl -water vapor (b).

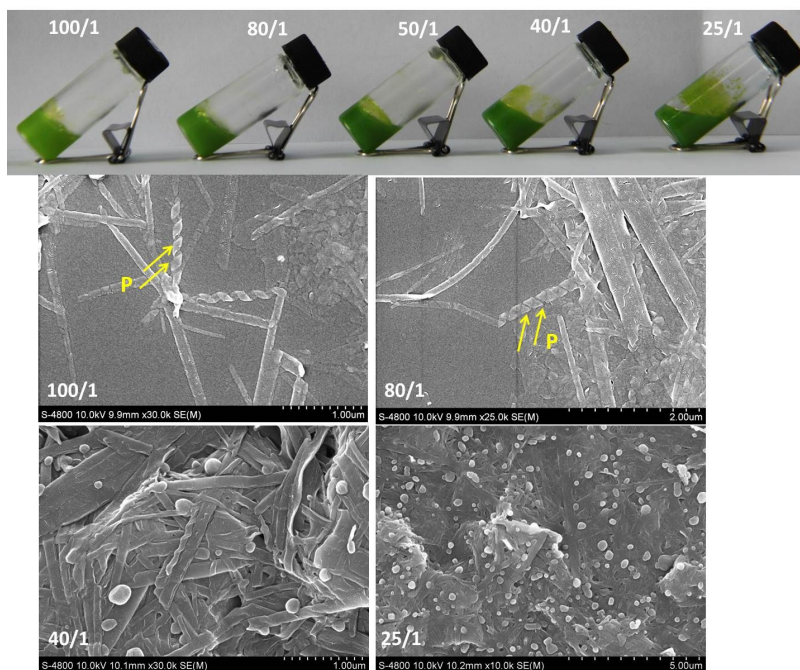


Fig. S4 Photo pictures and SEM images of complex of PUDG/TPPS at various molar ratios.

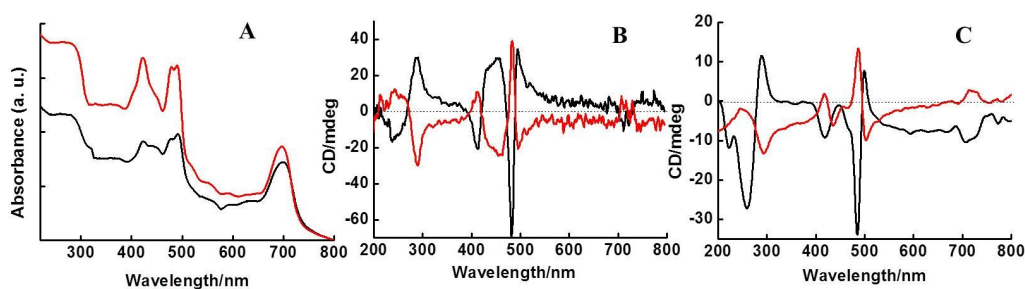


Fig. S5 (A) UV spectra of PUDG/TPPS xerogels; black line represents PUDG/TPPS at ratio of 100/1; red line represents PUDG/TPPS at 80/1. (B) CD spectra of PUDG/TPPS xerogels at ratio of 100/1; black line is as-prepared xerogels and red line is xerogels after treatment by $\text{NH}_3\text{-HCl}$ -water vapor. (C) CD spectra of PUDG/TPPS xerogels at ratio of 80/1; black line is as-prepared xerogels and red line is xerogels after treatment by $\text{NH}_3\text{-HCl}$ -water vapor.

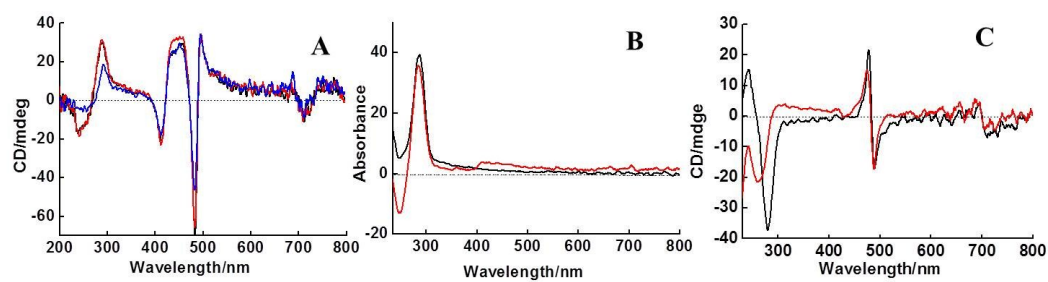


Fig. S6 (A) CD spectra of PUDG/TPPS (ratio at 100/1) as-prepared xerogels (black line); after treated by acetone vapors (red line) and after treated by cyclohexane (red line). (B) CD spectra of PUDG/TPPS xerogels (ratio at 50/1) treated by NH₃-HCl (black line) and following treated by acetone vapors (red line). (C) CD spectra of PUDG/TPPS xerogels (ratio at 50/1) treated by NH₃-HCl-water vapor (black line) and further treated by acetone vapors (red line).