Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
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Water-induced the expression of supramolecular chirality for phenylalanine derivative

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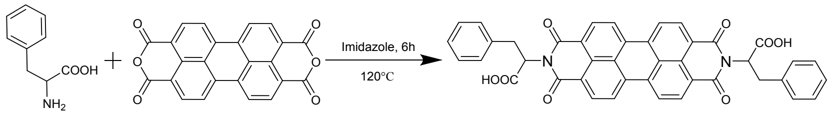
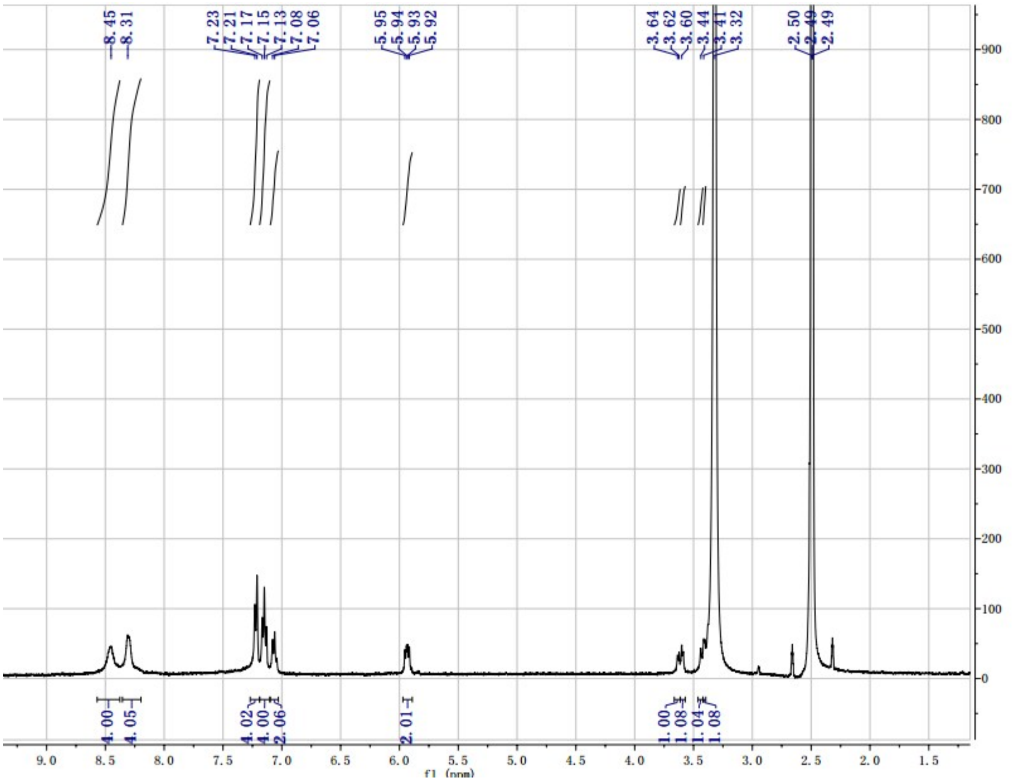
1. Synthesis of PBI-Phe



0.392 g (1 mmol) of perylene -3, 4, 9, 10-tetracarboxylic dianhydride, 0.330 g (2 mmol) phenylalanine and 2.0 g of imidazole were heated at 120 ℃for 6 hrs under nitrogen atmosphere. Then 100 mL of ethanol was poured into the hot mixture, refluxed for 6 hrs and kept for overnight to precipitate out. The resulting light yellow precipitate was concentrated by decompression filters after being acidified with dilute HCl, then washed with deionized water to neutral, filtrated and dried at room temperature under atmospheric pressure oven to get 0.665g light yellow powder (Yield: 97%). IR (KBr): 1252.4, 1396.4, 1501.2 cm-1 (C=C), 1344.9, 1432.5 cm-1 (-CH2-), 1656.6, 1697.0, 1737.9 cm-1 (C=O), 2934.8 cm-1 (C-H), 3439.3 cm-1 (O-H); MALDI-TOF-MS: calcd for C42H28N2O8, 686.1.



1H NMR (DMSO, 400MHz, ppm): 8.31-8.45 (q, 8H), 7.13-7.23 (m, 8H), 7.04-7.08 (t, 2H), 5.92-5.95 (q, 2H), 3.59-3.64 (q, 2H), 3.40-3.44 (t, 2H), 3.32 (s, 2H);

2. Characterization

Nuclear Magnetic Resonance (NMR) spectra were measured on a Bruker ULTRASHIELD 400(1H NMR 400 MHz) spectrometer. CD spectra were measured on a Chirascan. Ultraviolet (UV) absorption spectra were obtained using a UV-2700 UV-Vis spectrophotometer. The luminescence spectra were measured on a LS55 fluorescence spectrophotometer. The path length of the quartz cell is 1 cm, while the emission band-width was 5 nm. AFM measurements were performed by using a Nanoscope III a (Bruker, Germany), Samples were obtained through dropping the solution on these samples with same concentrations were prepared for following experiment. Molecular self-assembly was accomplished by using the pipette to drop dilute solution droplets onto a freshly cleaved mica surface and allowing the solvent to a freshly cleaved mica surface and allowing the solvent to evaporate in air at room temperature. A prart of SEM images were recorded using FEI QUANTA 450 with accelerating voltage 15.0 kV. Samples were obtained through dropping the gels on a flat surface of a cylindrical aluminum substrate and allowed to dry at room temperature, then the samples were coated with gold using a MSP-1S magnetron sputter (Japan) coater and the high-resolution images were recorded using TESCAN MIR3. IR spectra were recorded on a Nicolet IS50 instrument with the KBr disk technique. STM measurements were performed using a NanoscopeIIIa instrument (Bruker, Germany) under ambient conditions. All STM images presented were recorded in constant current mode using a mechanically cut Pt/Ir (80/20) tip. The sample with the concentration (1×10^{-5} M) was prepared. After a droplet (3μL) of the solution was deposited onto a freshly cleaved HOPG surface, the STM investigation was performed.

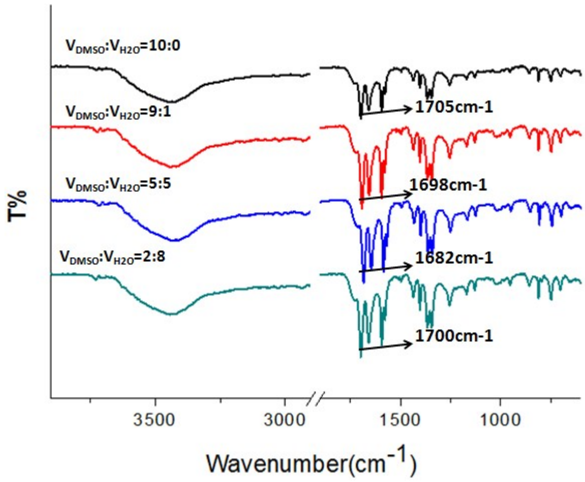


Figure S1. FTIR spectra of PBI-Phe in DMSO/water mixtures with different water contents (v/v %)

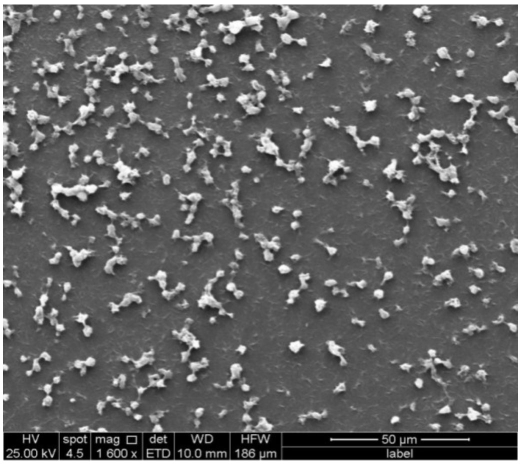


Figure S2.SEM image of the PBI-Phe molecules in pure DMSO solutions

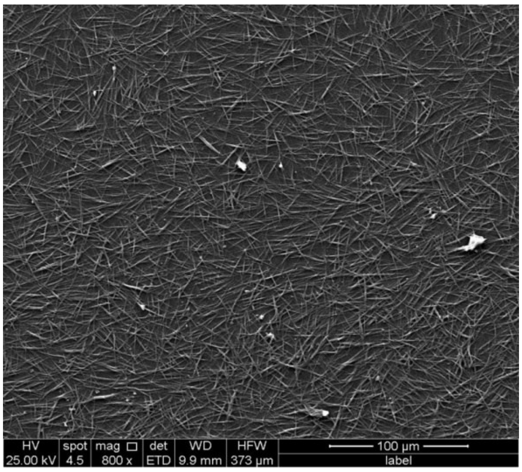


Figure S3.SEM image of PBI-Phe in the DMSO/water (90/10) solutions

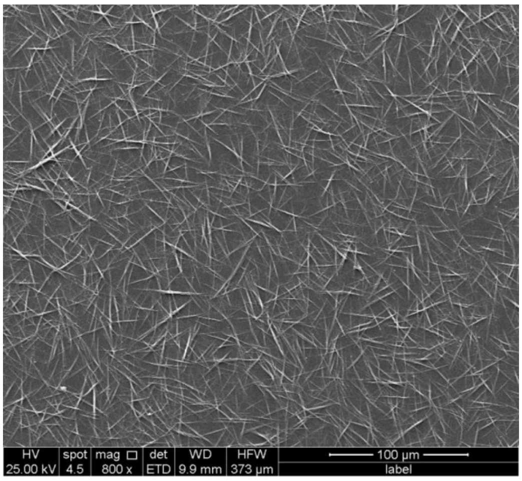


Figure S4.SEM image of PBI-Phe in the DMSO/water (50/50) solutions

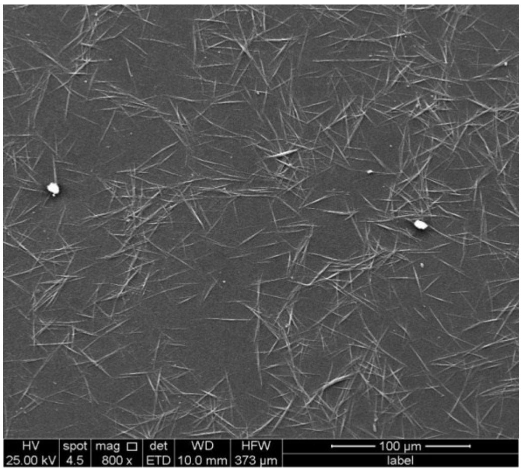


Figure S5.SEM image of PBI-Phe in the DMSO/water (20/80) solutions

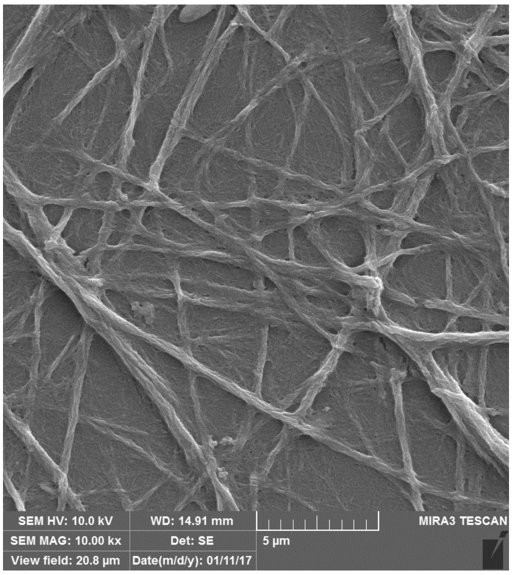


Figure S6. High resolution SEM image of PBI-Phe in the DMSO/water (90/10) solutions