Electronic Supplementary Information

Polydiacetylene–Embedded Supramolecular Electrospun Fibres for Colourimetric Sensor of Organic Amine Vapour

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Experimental Section

1. Materials

10,12-Pentacosadiynoic acid (DA) with a purity higher than 97% was purchased from Alfa Aesar and used after further purification according to the reported procedure.\(^\text{1}\) Polystyrene-co-poly(4-vinylpyridine) (PS-co-P4VP) was obtained from Sigma-Aldrich Co. Ltd. The molar ratio of PS to P4VP in the copolymer was 1:9. The molecular weight and the polydispersity were \(1 \times 10^6\) and 5.7, respectively. Propylamine (PA), dipropylamine (DPA), tripropylamine (TPA), diethylamine (DEA) triethylamine (TEA) and organic solvents involved in this work were purchased from Sinopharm Chemical Reagent Co..

2. Preparation of PDA-Embedded Supramolecular Electrospun Fibres

The precursor solution of the supramolecular electrospun fibres PSVP(DA)\(_x\), where the ‘\(x\)’ represents the molar ratio of DA molecules to the repeating pyridine units of PS-co-P4VP in the complex (\(x = 0.03, 0.06, 0.09, 0.12, 0.15\)), was obtained by dissolving DA and PS-co-P4VP in dimethylformamide. Before electrospinning, the solution was stirred at room temperature for 20 h and aged for another 24 h until it was clear and had no bubbles. The solution was drawn into a syringe and then expelled through the metal needle at rate of 3 mL h\(^{-1}\). The DA-embedded supramolecular electrospun fibres PSVP(DA)\(_x\) were collected on grounded aluminium foils by application of a direct working voltage of 15 kV to the metal syringe needle. The working distance between the tip of the needle and the receptor was 20 cm.
Electrospinning was carried out at 40 °C. The thickness of the obtained fiber mats was about 50-60 μm. Photopolymerization via 1,4-addition reaction of the self-assembled DA monomers in the fibre mats was carried out by irradiation of fibres with 254 nm UV light for 3 min to obtain the PDA-embedded PS-co-P4VP electrospun fibres.

3. Instruments and Measurements

Attenuated total reflectance (ATR) fourier transform infrared (FTIR) spectra of fibres were recorded on a PerkinElmer Paragon 1000 FTIR spectrometer with an ATR attachment. The PSVP(PDA)$_x$ on aluminium foil was directly used for the ATR FTIR measurement. Scanning electron microscopy (SEM) images was observed on a Hitachi S-2150. Diffuse reflectance UV–vis spectroscopy (DRUVS) was performed on a UV–vis spectrophotometer (PerkinElmer Lambda 750) equipped with an integrating sphere attachment. The optical images of the electrospun fibre mats were captured with a digital camera.

4. Detection of the Organic Amine and Solvent Vapours

Colorimetric detection of organic amine and solvent vapour was carried out in a closed glass chamber with a rubber stopper (400 mL). The blue electrospun fibre mats were placed in the centre of the chamber. A quantitative amount of volatile organic amine was injected into the chamber by a microsyringe. The amine vapour formed because of the rapid evaporation of the organic amine in the chamber. After exposure to the vapour of amine (20 s) or organic solvent (30 s), the fibre mats were removed from the chamber, and optical images of the mats were captured by a digital camera.
The amount of volatile organic amine was calculated as following:

\[ w = \frac{mVM}{22.4} \times 10^{-6} \]

where \( w \) (µg) is the weight of the organic amine, \( m \) (ppb) is the concentration, \( V \) (mL) is the volume of the chamber and \( M \) is the mol weight of the organic amine.

**Fig. S1** SEM image of PSVP(DA)\(_{0.12}\) supramolecular electrospun fibres with 50 mg mL\(^{-1}\) PS-\(co\)-P4VP in the precursor. The scale bar is 5 µm.

**Fig. S2** (a) DRUVS and (b) optical images of PSVP(PDA)\(_x\) fibre mats obtained by photopolymerization.
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