

Supporting Information

Electrospinning of Ultrafine Poly(1-trimethylsilyl-1-propyne) [PTMSP] Fibers: Highly Porous Fibrous Membranes for Volatile Organic Compound Removal

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1. Gel Permeation Chromatography

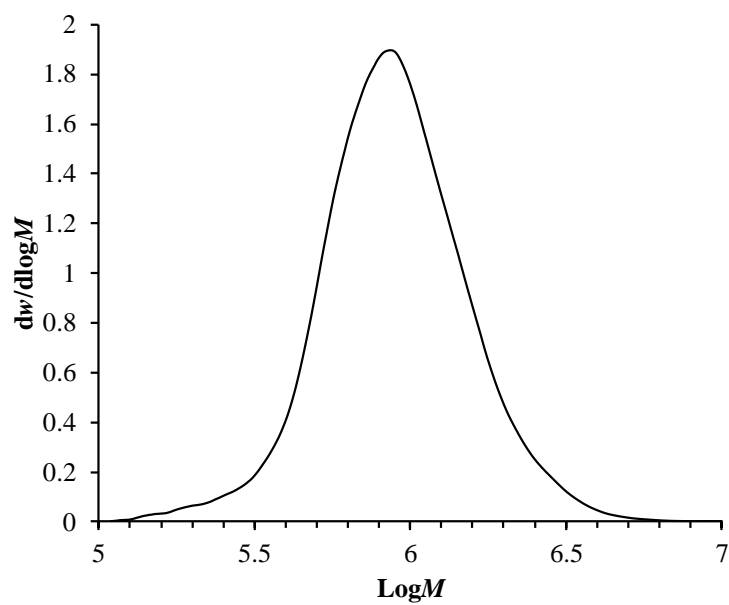


Figure S1: GPC curve of PTMSP powder.

2. Scanning Electron Microscopy

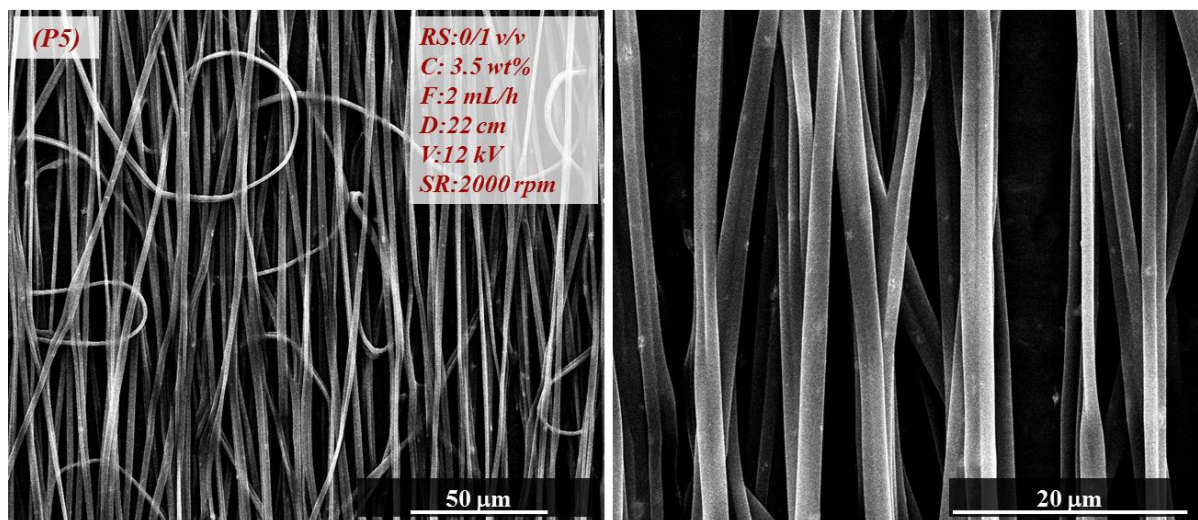


Figure S2: SEM images of sample P5 showing fused fibers (RS, ratio of the solution (THF/TCE); C, concentration; F, flow rate; D, distance; V, voltage; SR, spinning rate).

3. Viscosity data

Table S1: Viscosity data for selected samples in THF:TCE (1:2) solvent mixture.

Sample	Concentration (% w/v)	Viscosity (Pa s)
P8	1	0.01
P9	2	0.05
P6	3.5	0.32

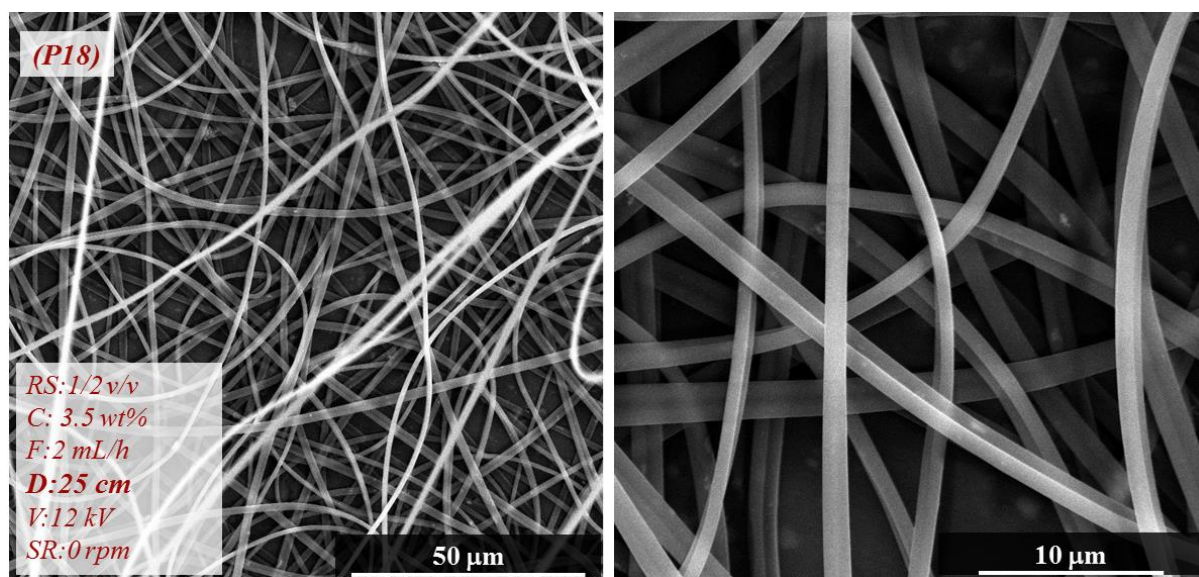


Figure S3: SEM images of P18 (RS, ratio of the solution (THF/TCE); C, concentration; F, flow rate; D, distance; V, voltage; SR, spinning rate).

4. FT-IR Spectroscopy

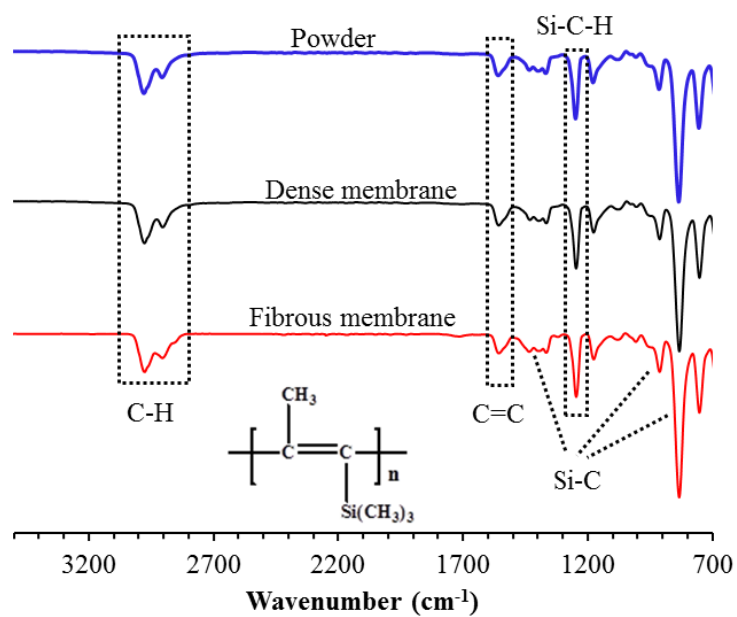


Figure S4: FT-IR spectra of PTMSP powder, dense and fibrous membranes.

5. ^1H -NMR Spectroscopy

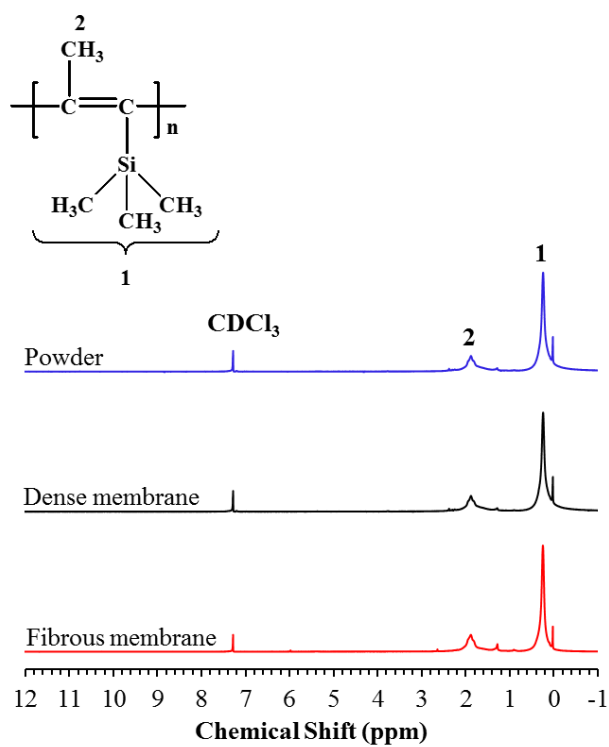


Figure S5: ^1H NMR spectra of spectra of PTMSP powder, dense and fibrous membranes dissolved in CDCl_3 .

6. XPS Spectroscopy

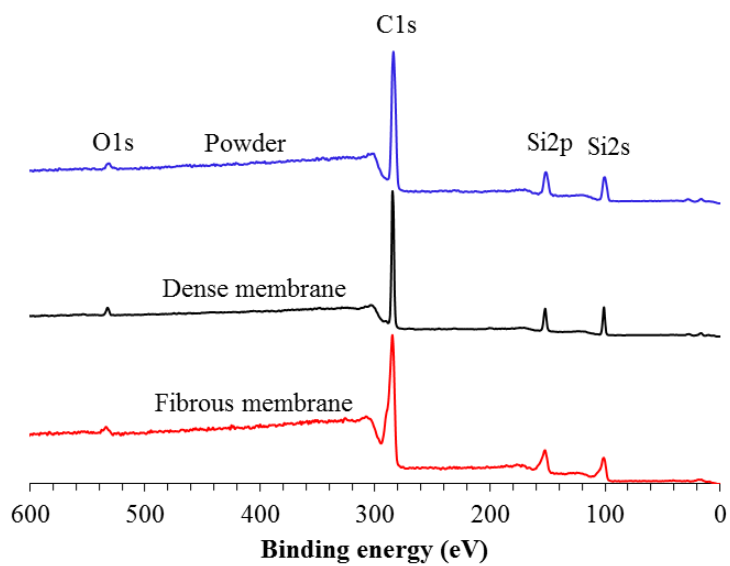


Figure S6: XPS spectra of PTMSP powder, dense and fibrous membranes.

Table S2: Surface elemental composition of PTMSP powder, dense and fibrous membranes by XPS.

Sample	% Atoms		
	C	Si	O
Powder	82.8	14.7	2.5
Dense membrane	82.0	15.3	2.7
Fibrous membrane	83.1	14.3	2.6

7. Thermal Gravimetric Analysis

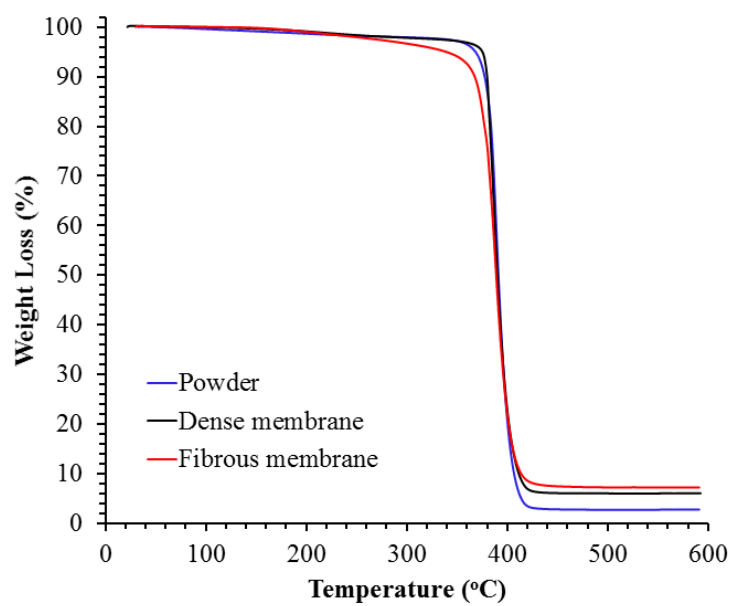


Figure S7: TGA curves of PTMSP powder, dense and fibrous membranes.

8. BET Surface area and pore parameters

Table S3: BET surface area, Micropore volume, Micropore area, Total pore volume and Average pore diameter of PTMSP powder dense and fibrous membranes.

Sample	BET surface area (m ² g ⁻¹)	Micropore volume (cm ³ g ⁻¹)	Micropore area (m ² g ⁻¹)	Total pore volume* (cm ³ g ⁻¹)	Average pore diameter* (nm)
Powder	826	0.182	400	0.88	4.2
Dense membrane	780	0.198	463	0.51	2.6
Fibrous membrane	852	0.211	466	0.63	2.9

*: Calculated at P/P_0 : 0.99

9. VOC removal

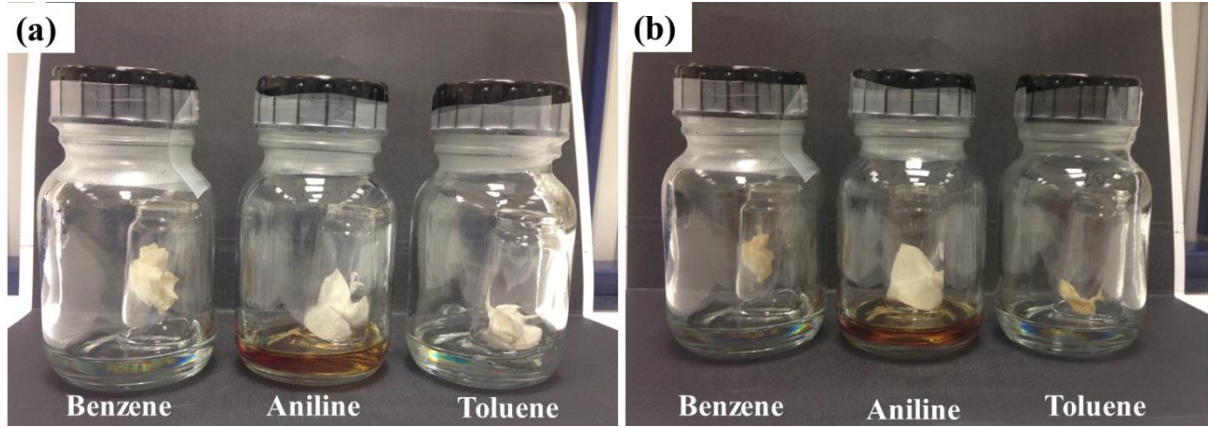


Figure S8: Digital images of VOC removal by PTMSP fibrous membrane (a) at the beginning and (b) at the end of the adsorption experiments

Calculations of VOC contents by TGA

$$m_{total} = m_{PTMSP} + m_{VOC} = 1 \quad \text{Eq.(S1)}$$

Where m_{PTMSP} and m_{VOC} represent the amount of PTMSP and VOC (m_A for aniline, m_B benzene or m_i for toluene) respectively. The total amount of sample is assigned as 1 according to Eq. (S1).

The ratio of the amount of VOC to the amount of PTMSP can be found from TGA chromatogram directly. As can be seen from **Fig. 10a**, first weight loss continues up to 190 °C. thus, this temperature was taken as reference. The % weight loss at 190 °C ($wt\%_{190}$) represents the % weight of PTMSP in the samples and the rest should belong to VOC mass. Thus,

$$\frac{m_{VOC}}{m_{PTMSP}} = \frac{100 - wt\%_{190}}{wt\%_{190}} \quad \text{Eq.(S2)}$$

Combination of Eq. (S1) and Eq. (S2) gives Eq. (S3).

$$m_{total} = 1 = m_{PTMSP} \left(\frac{100 - wt\%_{190}}{wt\%_{190}} + 1 \right) \quad \text{Eq.(S3)}$$

Calculations of VOC contents by ¹HNMR Spectroscopy

Similar to TGA approach;

$$m_{total} = m_{PTMSP} + m_{VOC} = 1 \quad \text{Eq. (S1)}$$

Where m_{PTMSP} and m_{VOC} represent the amount of PTMSP and VOC (m_A for aniline, m_B benzene or m_T for toluene) respectively. The total amount of sample is assigned as 1 according to Eq. (S1).

The mole of PTMSP, can be found by dividing the amount of PTMSP (g) to molecular weight of repeating unit of PTMSP (g mol^{-1}). The PTMSP possesses 2 aliphatic protons and they display two distinct signals at 0.2 and 1.8 ppm which were annotated as signals (1) and (2). Thus, the mole of methyl proton of PTMSP at 1.8 ppm (2) can be obtained by multiplying the mole of PTMSP by “three”, Eq. (S4).

$$n_{PTMSP} = \frac{m_{PTMSP}}{M_{PTMSP}} = \frac{n_{CH3(2)}}{3} \quad \text{Eq. (S4)}$$

Similar approach for VOC content, the mole of **aniline** can be found by dividing the amount of aniline to molecular weight of aniline. Thus, the mole of amine protons can be found by multiplying the mole number of aniline by two, Eq. (S5)

$$n_A = \frac{m_A}{M_A} = \frac{n_{NH2}}{2} \quad \text{Eq. (S5)}$$

The mole of **benzene** can be found by dividing the amount of benzene to molecular weight of benzene. Thus, the mole of aromatic protons can be found by multiplying the mole number of benzene by “six”, Eq. (S6)

$$n_B = \frac{m_B}{M_B} = \frac{n_{Ar-H}}{6} \quad \text{Eq. (S6)}$$

The mole of **toluene** can be found by dividing the amount of toluene to molecular weight of toluene. Thus, the mole of methyl protons can be found by multiplying the mole number of toluene by “three”, Eq. (S7)

$$n_T = \frac{m_T}{M_T} = \frac{n_{CH3(T)}}{3} \quad \text{Eq. (S7)}$$

Hence, the ratio of the mole of PTMSP to the mole of **aniline** is equal to the ratio methyl protons (2) to amine protons (NH₂), Eq. (S8)

$$\frac{n_{CH3(2)}}{n_{NH2}} = \frac{3m_{PTMSP}/M_{PTMSP}}{2m_A/M_A} = \frac{0.83 m_{PTMSP}}{m_A} \quad \text{Eq. (S8)}$$

Rearranging the Eq. (S8) gives Eq. (S9);

$$m_A = \frac{1.245 m_{PTMSP} n_{NH2}}{n_{CH3(2)}} \quad \text{Eq. (S9)}$$

Combining Eq. (S1) and Eq. (S9) gives Eq. (S10).

$$m_{total} = 1 = m_{PTMSP} \left(\frac{1.245 n_{NH2}}{n_{CH3(2)}} + 1 \right) \quad \text{Eq. (S10)}$$

With the same approach for **benzene** content; the ratio of the mole of PTMSP to the mole of benzene is equal to the ratio methyl protons (2) to aromatic protons (Ar-H), Eq. (S11)

$$\frac{n_{CH3(2)}}{n_{Ar-H}} = \frac{m_{PTMSP}/M_{PTMSP}}{2m_B/M_B} = \frac{0.696 m_{PTMSP}}{m_B} \quad \text{Eq. (S11)}$$

Rearranging the Eq. (S11) gives Eq. (S12);

$$m_T = \frac{0.35 m_{PTMSP} n_{CH3(T)}}{n_{CH3(2)}} \quad \text{Eq. (S12)}$$

Combining Eq. (S1) and Eq. (S12) gives Eq. (S13).

$$m_{total} = 1 = m_{PTMSP} \left(\frac{0.35 n_{CH3(T)}}{n_{CH3(2)}} + 1 \right) \quad \text{Eq. (S13)}$$

For **toluene** content; the ratio of the mole of PTMSP to the mole of toluene is equal to the ratio methyl protons (2) to methyl protons (CH_{3(T)}), Eq. (S14)

$$\frac{n_{CH3(2)}}{n_{CH3(T)}} = \frac{m_{PTMSP}/M_{PTMSP}}{m_T/M_T} = \frac{0.82 m_{PTMSP}}{m_T} \quad \text{Eq. (S14)}$$

Rearranging the Eq. (S14) gives Eq. (S15);

$$m_T = \frac{0.82 m_{PTMSP} n_{CH3(T)}}{n_{CH3(2)}} \quad \text{Eq. (S15)}$$

Combining Eq. (S1) and Eq. (S15) gives Eq. (S16).

$$m_{total} = 1 = m_{PTMSP} \left(\frac{0.82 n_{CH3(T)}}{n_{CH3(2)}} + 1 \right) \quad \text{Eq. (S16)}$$