

Supporting information (SI):

Facile fabrication of porous carbon nanofibers by electrospun PAN/dimethylsulfone for capacitive deionization

Haojie Pan ^a, Jianmao Yang ^b, Shiping Wang ^a, Zhubiao Xiong ^a, Wenshu Cai ^a, Jianyun Liu ^a

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1. The proof-of-concept experiment for DMSO2 recovery:

The recovery experiment was done by a simple self-made setup. The electrospun PAN/DMSO2 pristine fiber with the ratio of 2:3 was placed on a bottom-up culture dish and caged by a beaker. After sealed by aluminum foil and tightened by an iron wire, the device was put on the hotplate (Talboys 7X7 CER, USA) and was heated at 80 °C for 2 h (room temperature at 15 °C). After cooling down, the white sample deposited on the top wall of the container was collected for characterization. For comparison, the control experiment about electrospun pure PAN pristine fiber was done using the same procedure.

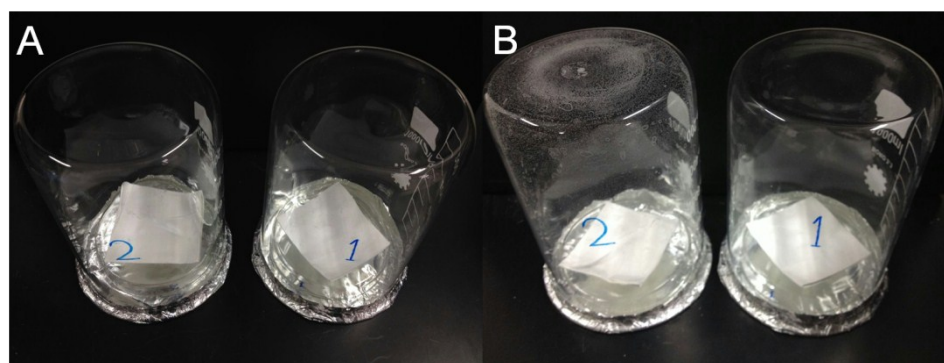


Fig S1. Digital photographs of (1) the pristine NF(1:0) and (2) the pristine NF (2:3) before (A) and after (B) heating at 80 °C

Fig. S 1 A and B showed the photographs of the samples before and after heating in the setup. Clearly, after heating, the white crystals can be deposited on the top wall of the container for the pristine NF (2:3) sample due to the evaporation of DMSO2.

While, there was nothing found as to the control experiment (pristine NF, 1:0). In order to confirm the components of the white solid, the FTIR experiment was conducted. Fig. S2 exhibited the FTIR spectrum of the collected white solid sample. The characteristic peaks at 1137 cm^{-1} and 1300 cm^{-1} corresponded to the typical O=S=O symmetric and asymmetric stretching vibration of DMSO₂. The absorption peaks were well consistent with that of pure DMSO₂. The result reveals that DMSO₂ in our electrospun fibers was sublimated and re-crystallized easily with good purity.

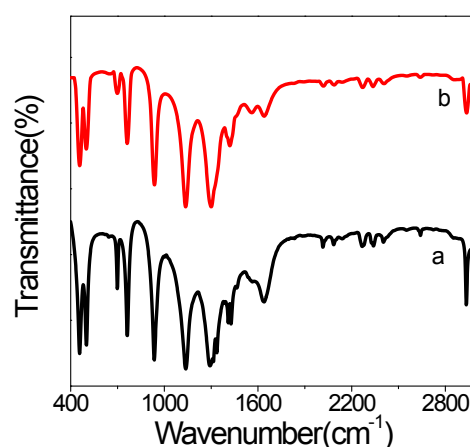


Fig S2. FTIR spectra of pure DMSO₂ (a) and the re-crystallized white sample (b).

Table S1 Weight loss of NF after heating at 80°C

Pristine NF	PAN/DMSO ₂ in solution	Mass loss in NF (%)	DMSO ₂ Recovery (%)
NF(1:0)	1:0	2.0	-
NF(3:2)	3:2	9.8	25
NF(1:1)	1:1	18	36
NF(2:3)	2:3	28	47

The recovery of DMSO₂ could be roughly estimated from the weight loss of the sample before and after heating at 80°C. The results were shown in Table S1. It was found that with the increase of DMSO₂ ratio in the sample, the weight loss increased, indicating that more DMSO₂ could be recovered at this stage. If ignoring the weight loss from the possible adsorbed water, the recovery could be roughly estimated from weight loss. For the pristine NF(2:3) that we used, the 47% recovery of DMSO₂ could be obtained. It is reasonable that there may be some loss together with DMF solvent during electrospinning, and that some DMSO₂ trapped inside the electrospun fiber

could not release until arriving at the boiling points (238°C), which has been demonstrated from TG analysis in Fig.3.

2. CDI cell setup:

For CDI cell assembly, the PCNF web was cut into a 60 mm × 40 mm size and used as the CDI electrode. Fig. S3 gave the schematic structure of the CDI cell.

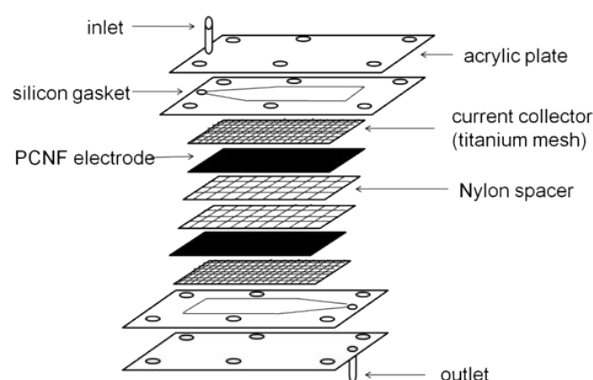


Fig S3. Schematic representation of the CDI cell structure

3. Morphology characterization of pristine fibers

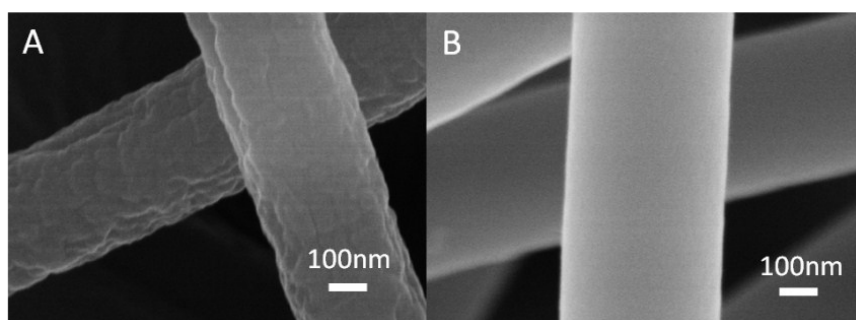


Fig S4. SEM images of (A) the pristine NF (2:3) and (B) pristine NF(1:0)

4. CV characterization of different PCNF electrodes

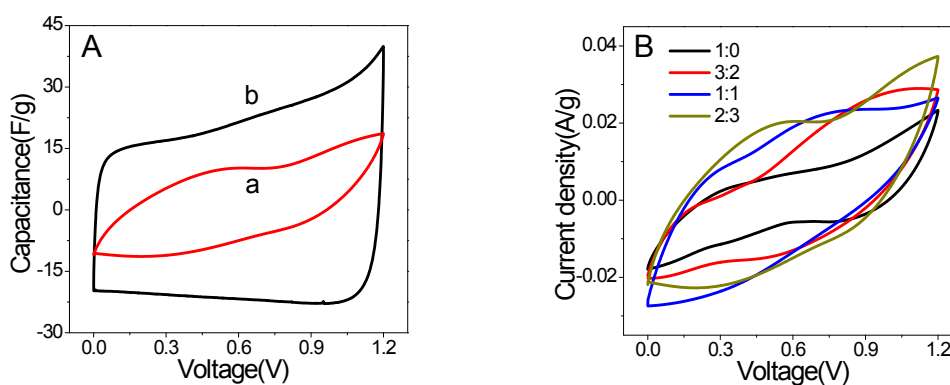


Fig S5. (A) CV curves of PCNF(2:3) electrodes in (a) 58.5 g/L and (b) 0.5 g/L NaCl solution at scan rate of 2 mV/s; (B) CV curves of the PCNF (1:0, 3:2, 1:1, 2:3) electrodes in 0.5 g/L NaCl solution at scan rate of 2 mV/s.

From the CV curves in Fig. S5A, we can see clearly that the capacitance of the PCNF(2:3) electrode is much smaller in NaCl solution at low concentration (0.5 g/L), comparing to that at high concentration (58.5 g/L). And the redox current was observed obviously owing to the low capacitance current. These redox peaks were probably from the redox reaction of the oxygen-containing or nitrogen-containing group on the carbon fiber surface. In contrast, the capacitance current is predominant in 58.5 g/L NaCl solution, and the curve is close to ideal rectangle shape.

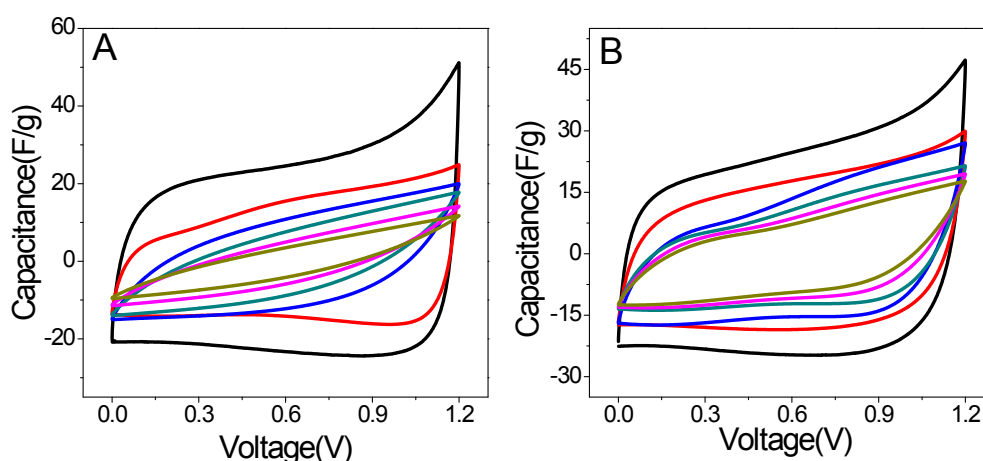


Fig. S6. Normalized CV curves of (A) PCNF(3:2) and (B) PCNF(1:1) electrodes in 58.5 g/L NaCl at different scan rates (from outside to inside: 1, 5, 10, 20, 30 and 40 mV/s)

5. galvanostatic characterization of different electrodes

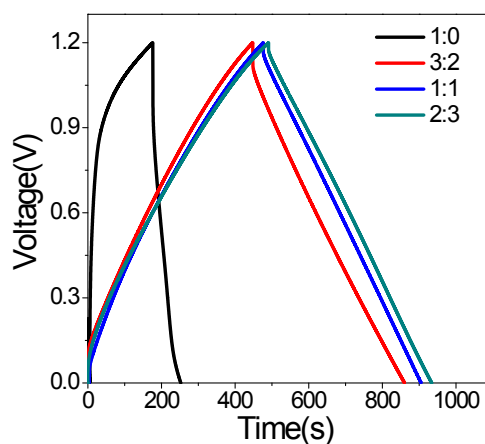


Fig S7. Galvanostatic charge–discharge curves of different PCNF electrodes with the charging current density of 0.06A/g.

The galvanostatic charging and discharging curve also easily shows the capacitance behavior. It was conducted in the range of 0 – 1.2 V in 58.5 g/L NaCl solution. The control PCNF (1:0) electrode showed a fast discharge process, indicating a pretty low specific capacitance. While the near linear discharge curves were obtained on the PCNF (3:2, 1:1, 2:3) electrodes (Fig. S7), and discharge time was longer with more DMSO2 addition. Based on the discharging curve, the corresponding specific capacitance could be calculated to be 3.2, 31.7, 34.3 and 37.8 F/g for PCNF with PAN/DMSO2 ratio of 1:0, 3:2, 1:1 and 2:3, respectively. The capacitance values were similar to those from CV curves. It indicates that both CV scan and galvanostatic measurement are suitable for specific capacitance estimation. It has also been demonstrated in literatures (*Electrochimica Acta*, 2005, 50, 2499-2506).