Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.

Supporting Information

Control the Physical and Electrochemical Properties of Block Copolymer-based Porous Carbon Fibers by pyrolysis temperature

Zhengping Zhou,[†] Tianyu Liu,[†] Assad U. Khan,[†] Guoliang Liu[*,†,‡,§]

[†]Department of Chemistry, [‡]Macromolecules Innovation Institute, and [§]Division of Nanoscience, Virginia Tech, Blacksburg, Virginia 24061, United States

* Corresponding Author: gliu1@vt.edu

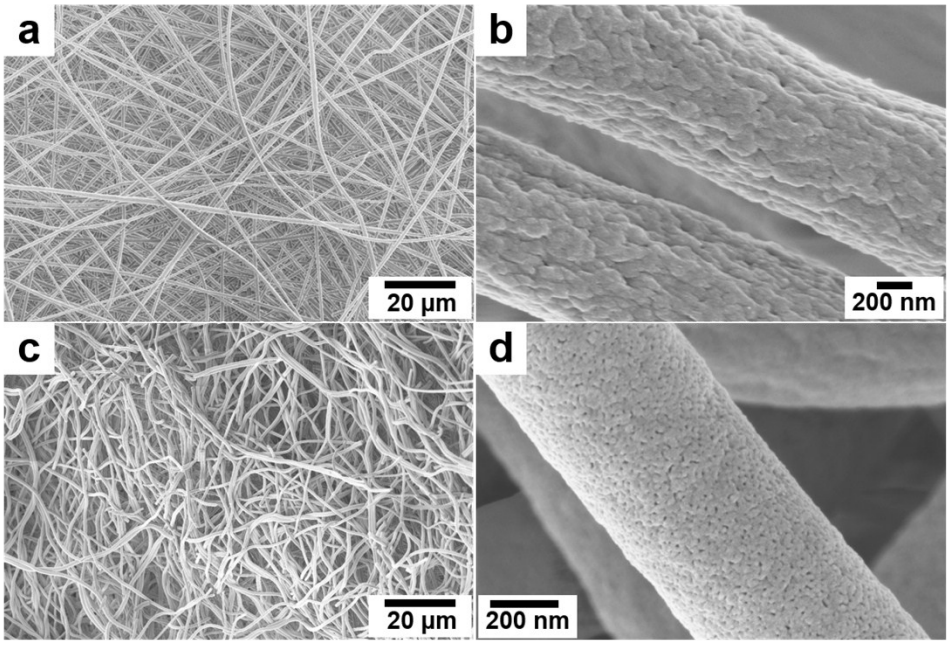

Figure S1. SEM images of (a-b) as-electrospun PAN-*b*-PMMA block copolymer fibers and (c-d) PAN-*b*-PMMA fibers after oxidation at 280 °C in air.

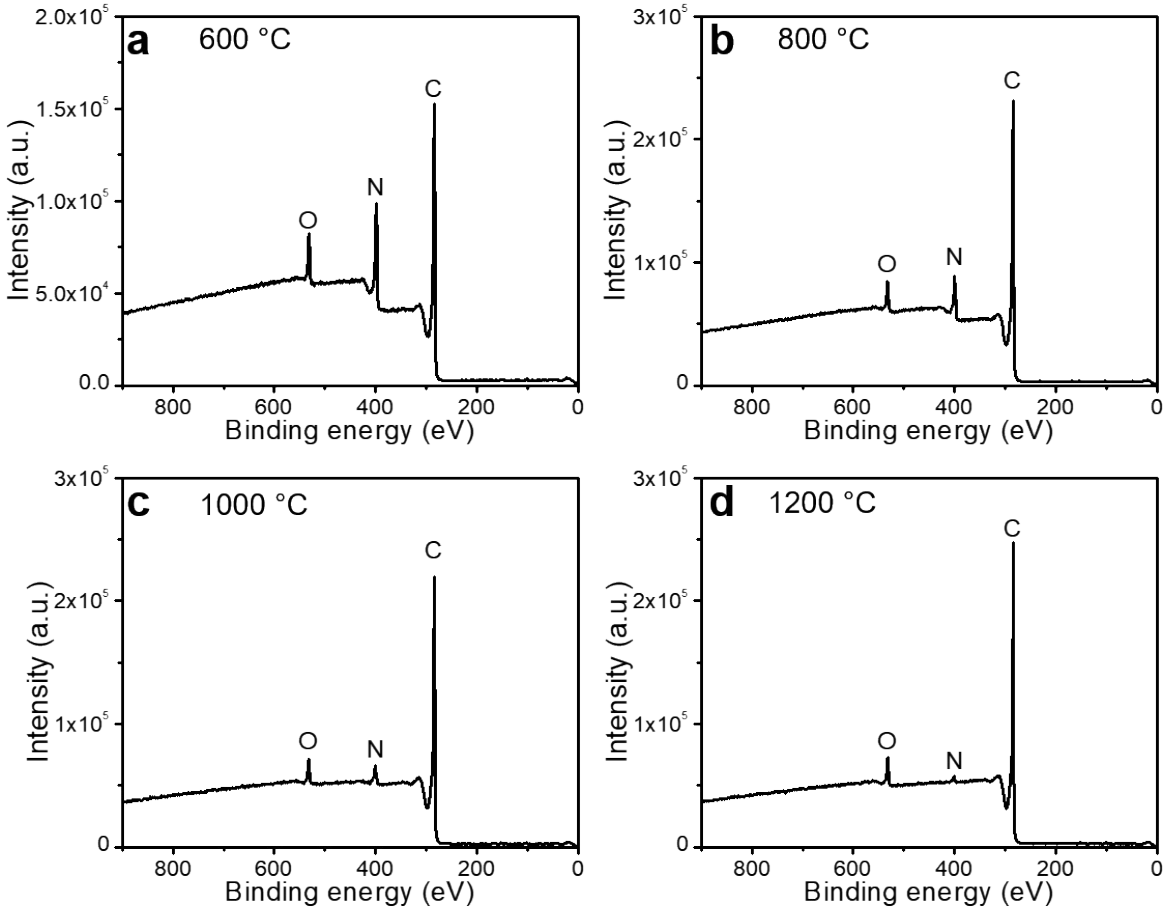

Figure S2. XPS survey spectra of the porous carbon fibers. The porous carbon fibers were obtained after pyrolysis at (a) 600 °C, (b) 800 °C, (c) 1000 °C and (d) 1200 °C.

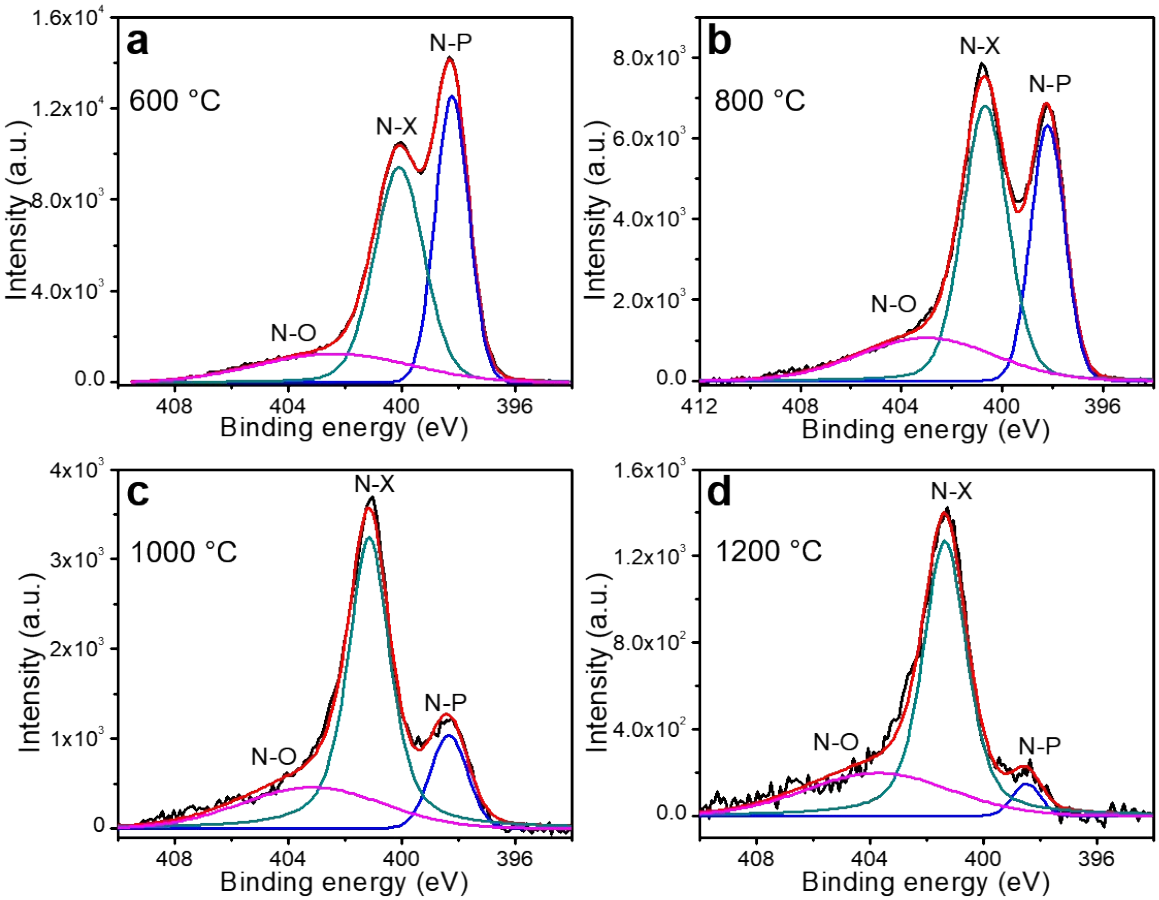

Figure S3. XPS N 1s peaks of porous carbon fibers and the corresponding fittings. The porous carbon fibers were obtained after pyrolysis at (a) 600 °C, (b) 800 °C, (c) 1000 °C and (d) 1200 °C.

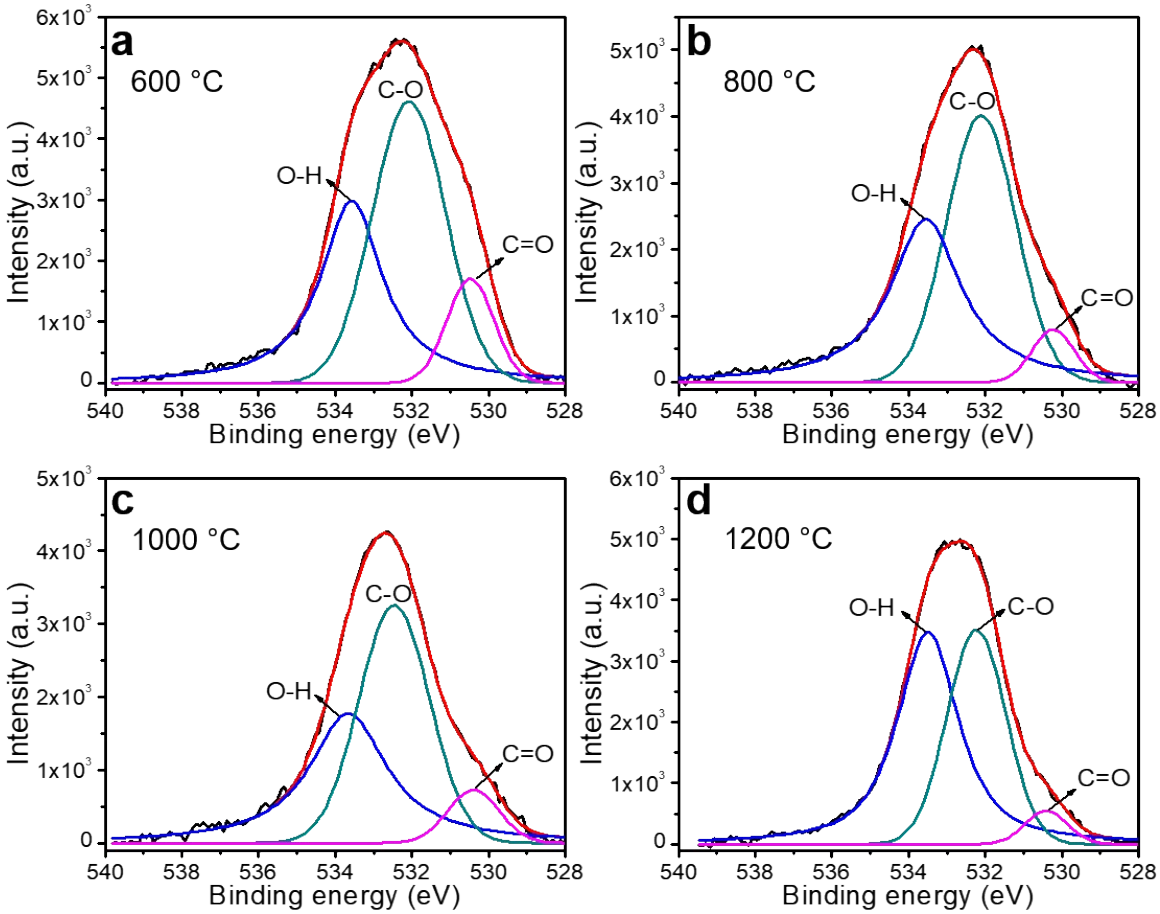

Figure S4. XPS O 1s peaks of porous carbon fibers and the corresponding fittings. The porous carbon fibers were obtained after pyrolysis at (a) 600 °C, (b) 800 °C, (c) 1000 °C and (d) 1200 °C.

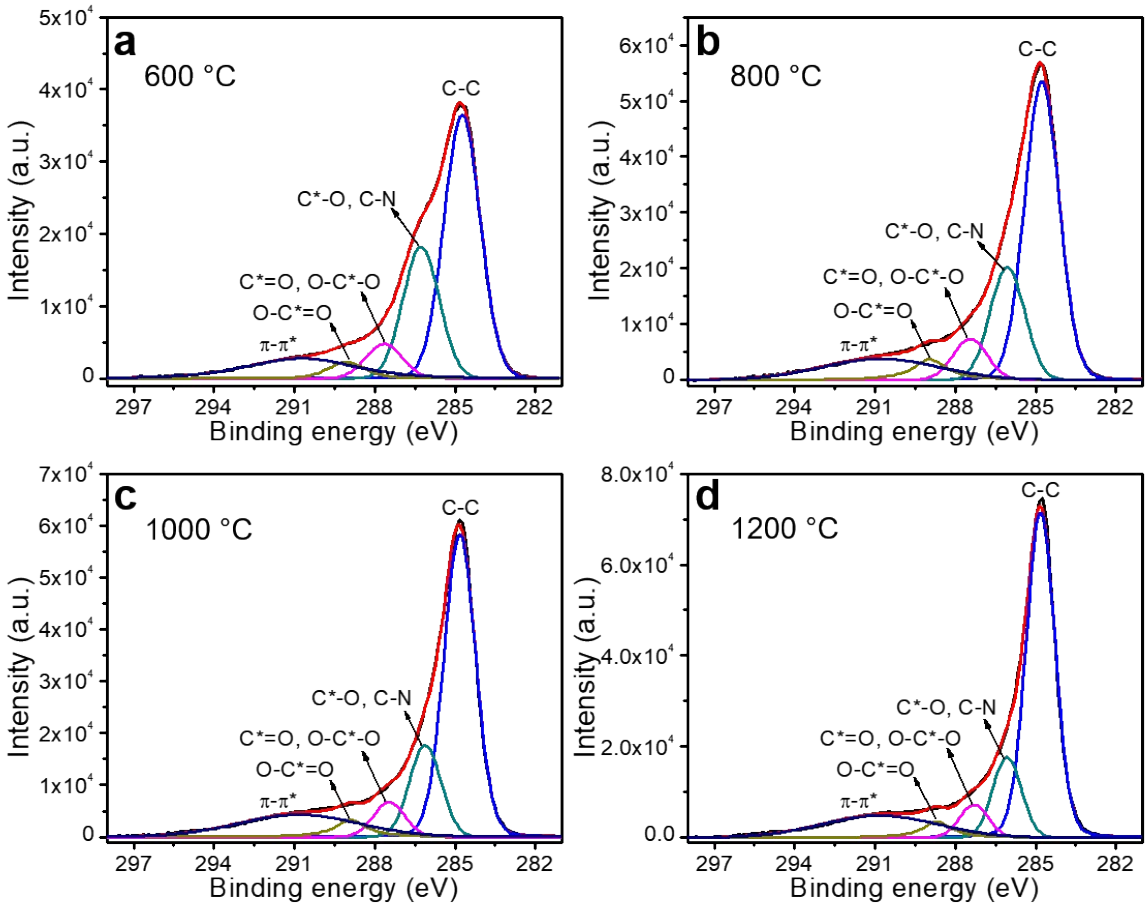

Figure S5. XPS C 1s peaks of porous carbon fibers and the corresponding fittings. The porous carbon fibers were obtained after pyrolysis at (a) 600 °C, (b) 800 °C, (c) 1000 °C and (d) 1200 °C.

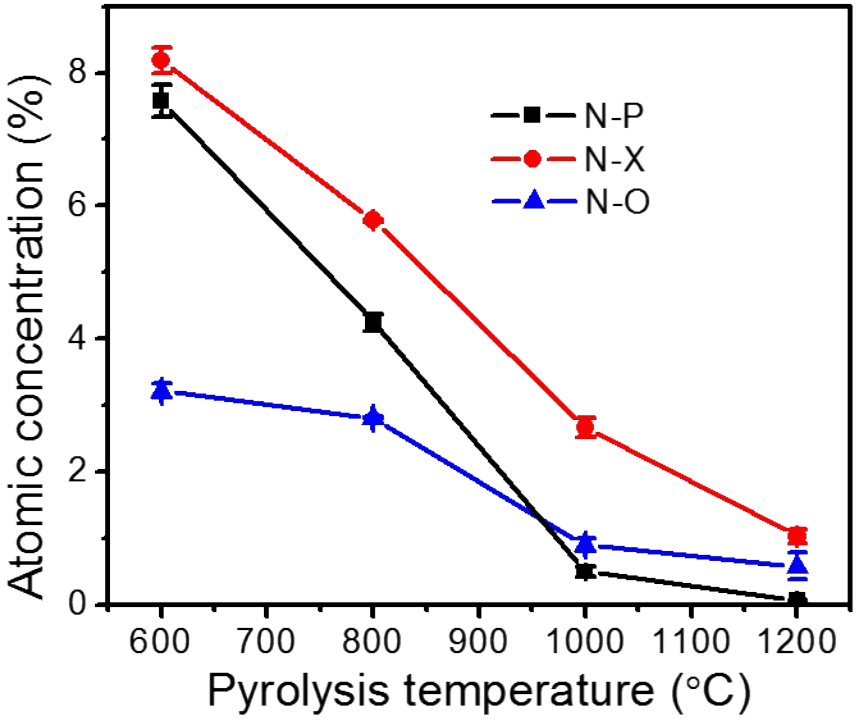

Figure S6. Atomic concentrations of pyridinic (N-P), pyridonic/pyrrolic (N-X), and pyridine oxide (N-O) groups in porous carbon fibers from PAN-*b*-PMMA after carbonization at various temperatures. The atomic concentrations were determined by XPS analysis and summarized in Table S5.

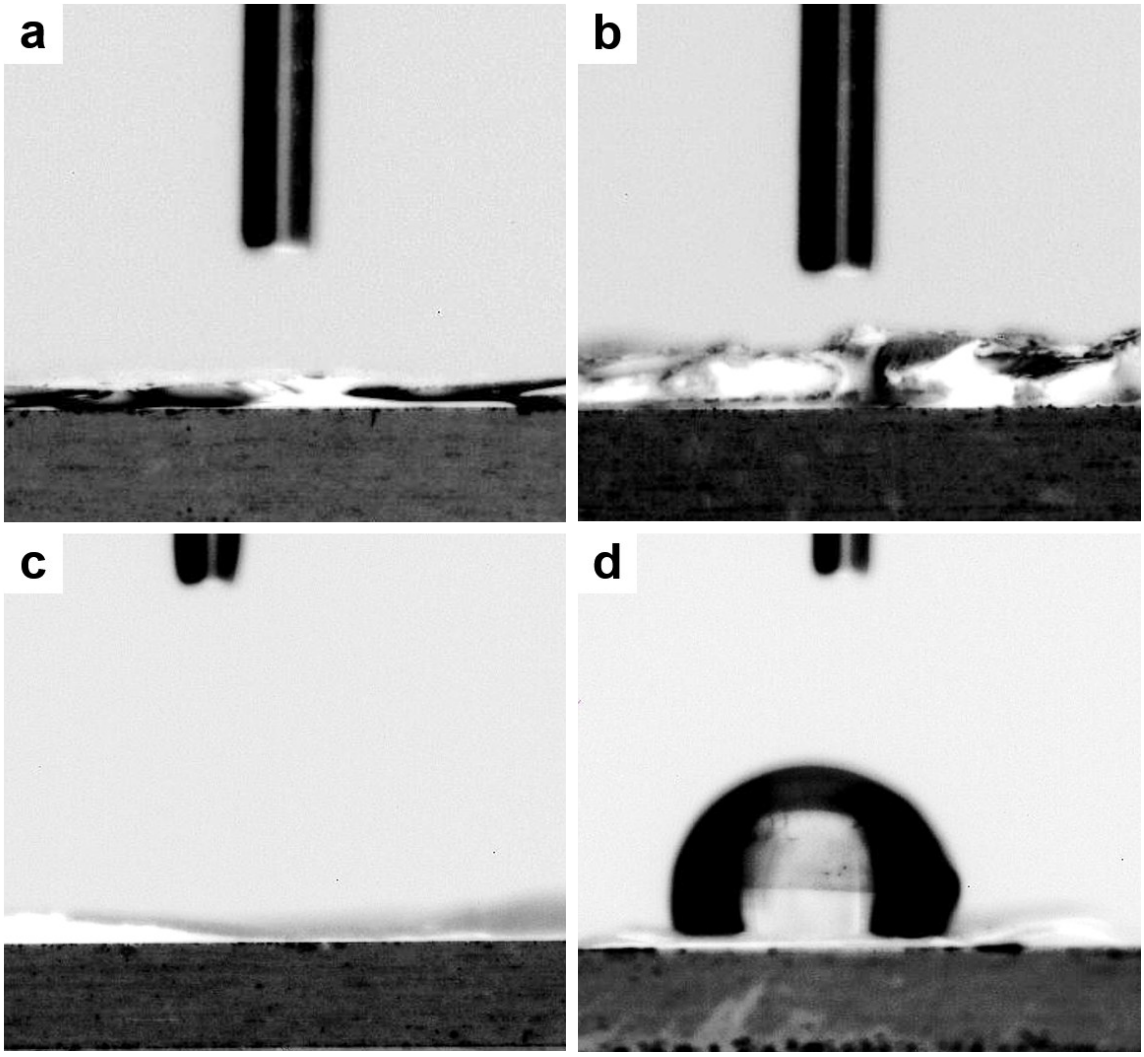

Figure S7. Contact angles of the porous carbon fiber mats from PAN-*b*-PMMA after pyrolysis at (a) 600 °C, (b) 800 °C, (c) 1000 °C, and (d) 1200 °C.

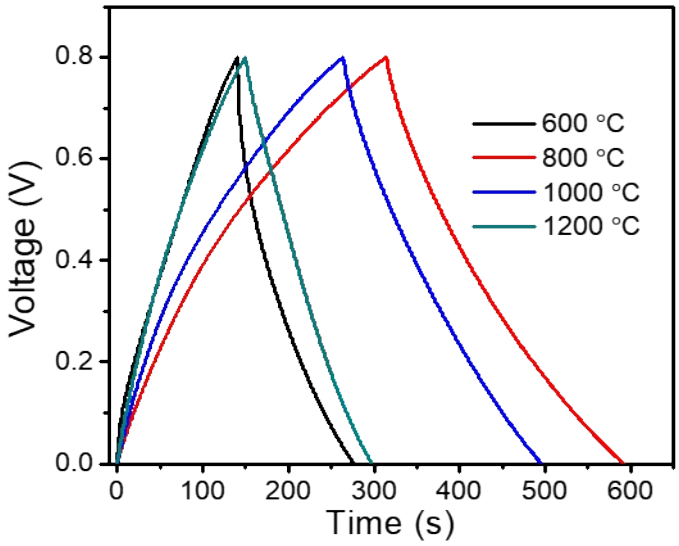

Figure S8. Galvanostatic charge and discharge (GCD) curves of porous carbon fibers after pyrolysis at various temperatures at a current density of 1 A g^{-1}.

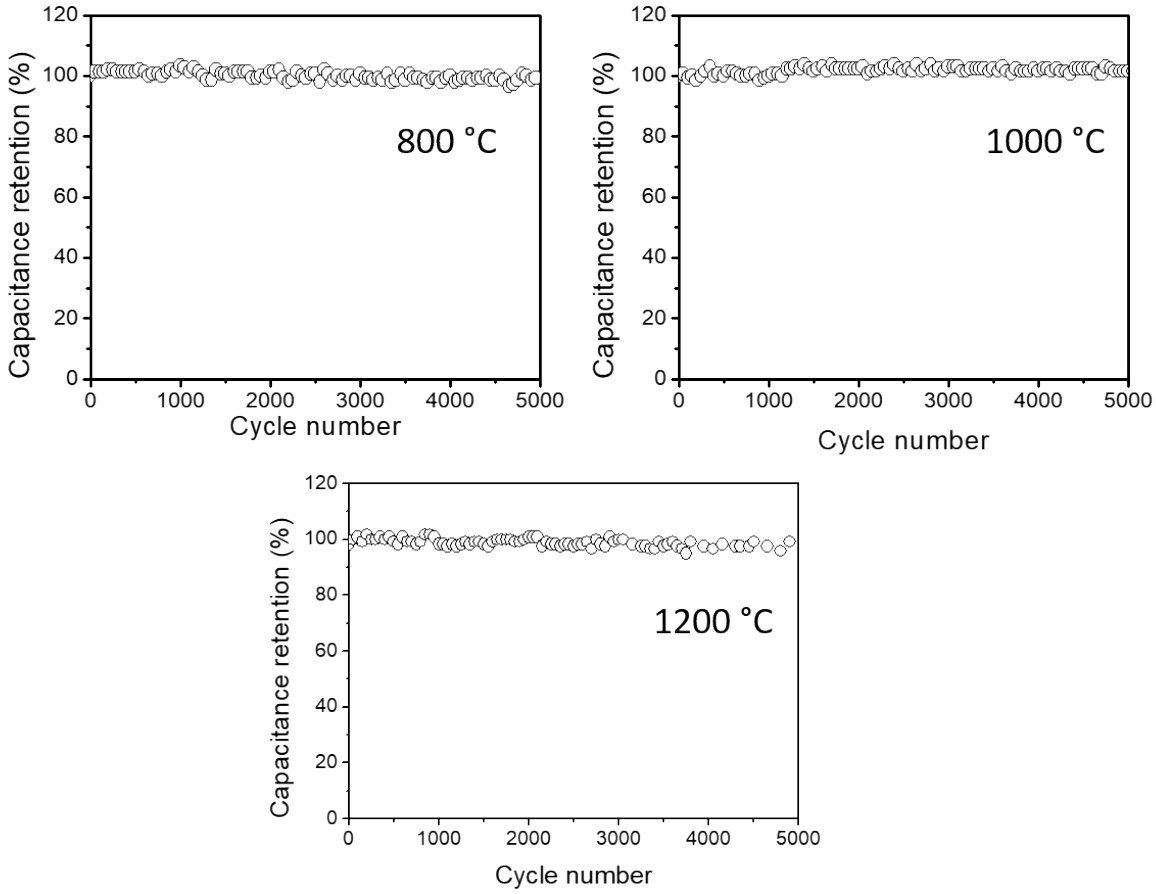

Figure S9. Cyclic stability of porous carbon fibers after pyrolysis at 800, 1000, and 1200 °C at a current density of 100 A/g. All these porous carbon fibers retained at least 98% of their initial capacitances after 5000 charge-discharge cycles.

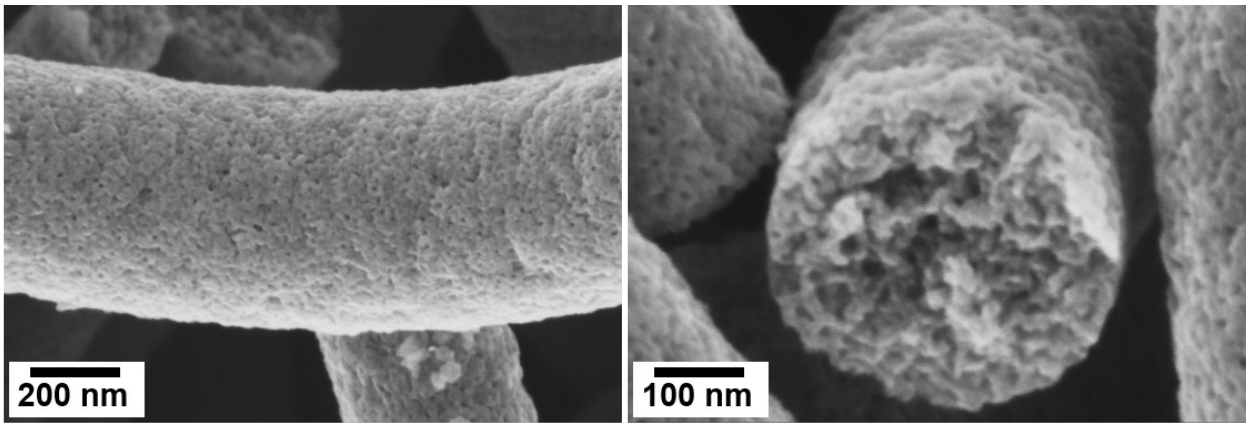

Figure S10. SEM images of porous carbon fibers after 5000 charge-discharge cycles at 100 A/g. The porous carbon fibers were pyrolyzed at 800 °C.

Table S1. XRD and Raman analyses of porous carbon fibers after pyrolysis at various temperatures.

Pyrolysis temperature	2θ (002)	2θ (100)	D band center (nm)	G band center (nm)	I_D/I_G
600 °C	24.9°	43.6°	1327	1567	1.20
800 °C	24.0°	43.5°	1327	1568	1.16
1000 °C	23.3°	42.7°	1334	1581	1.14
1200 °C	23.6°	43.3°	1336	1577	1.13

Table S2. XPS analyses of the porous carbon fibers derived after pyrolysis at various temperatures.

Pyrolysis temperature		**600 °C**	**800 °C**	**1000 °C**	**1200 °C**
C (%)		75.1±0.1	82.1±0.6	91.5±0.2	94.0±0.4
N (%)		19.0±0.1	12.8±0.1	4.1±0.2	1.7±0.3
O (%)		6.0±0.2	5.0±0.6	4.5±0.4	4.3±0.6
N-P	BE (eV)	398.2	398.2	398.3	398.5
	N-P (%)	7.6±0.2	4.3±0.1	0.5±0.1	< 0.1
N-X	BE (eV)	400.1	400.7	401.2	401.4
	N-X (%)	8.2±0.2	5.8±0.1	2.7±0.1	1.0±0.1
N-O	BE (eV)	402.4	403.0	403.2	403.7
	N-O (%)	3.2±0.1	2.8±0.1	0.9±0.1	0.6±0.2
C=O	BE (eV)	530.5	530.3	530.4	530.4
	C=O (%)	0.7±0.1	0.4±0.1	0.3±0.1	~ 0.1
C-O	BE (eV)	532.1	532.1	532.5	532.2
	C-O (%)	2.8±0.2	2.8±0.5	2.0±0.2	1.5±0.3
O-H	BE (eV)	533.6	533.6	533.7	533.5
	O-H (%)	2.4±0.1	1.8±0.1	2.2±0.3	2.7±0.4