Supporting information for:

Nitrogen-enriched porous carbon fiber as a CO_2 adsorbent with superior CO_2 selectivity by air activation

Long Xiong,[ab] Xue-Fei Wang,*[b] Li Li,[b] Lu Jin,[b] Yong-Gang Zhang,[b] Shu-Lin Song,[b] Rong-Pei Liu[a]

[a] Faculty of Material Science and Engineering, Kunming University of Science and Technology, Kunming 650093, China

[b] Ningbo Institute of Industrial Technology, Chinese Academy of Sciences, Ningbo 315201, China

Correspondence to: FAX: +86 574 87911382. E-mail address: wangxf@nimte.ac.cn (Xue-Fei Wang)

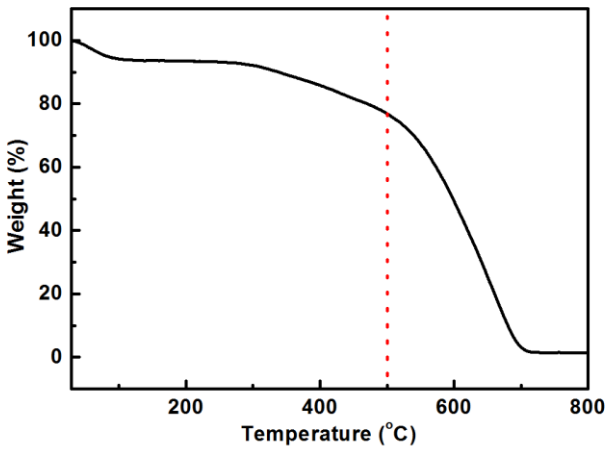

Figure S1. TG curve of oxidized polyacrylonitrile fiber under air atmosphere.

Table S1. Structure parameters of graphite-like crystallite of porous carbon fibers

Sample	2θ (°)	d_{002} (nm)	FWHM (°)	L_c (nm)	L_c/ d_{002}
PCF-400	25.763	0.3457	5.915	1.53	4-5
PCF-450	26.047	0.3420	6.559	1.38	4-5
PCF-500	26.177	0.3403	6.261	1.45	4-5
PCF-N	25.425	0.3502	4.943	1.83	5-6

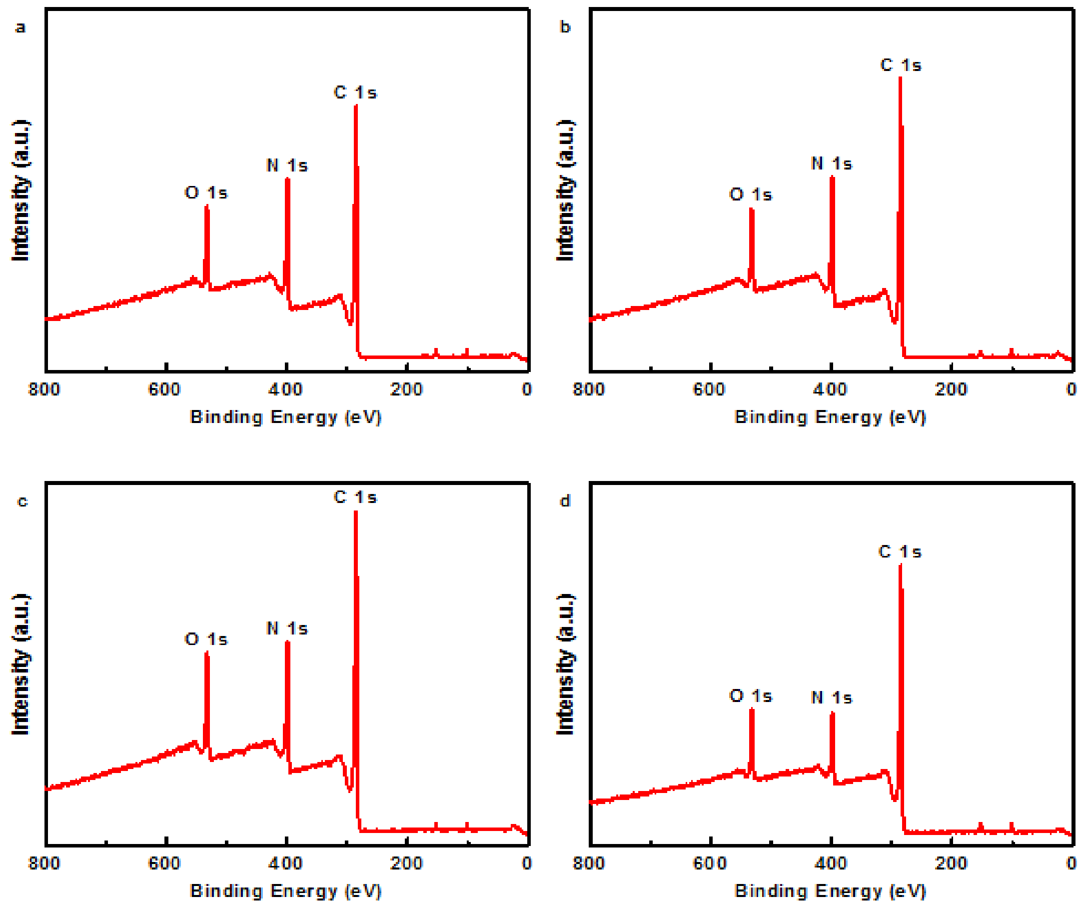

Figure S2. XPS spectra of (a) PCF-400, (b) PCF-450, (c) PCF-500, and (d) PCF-N.

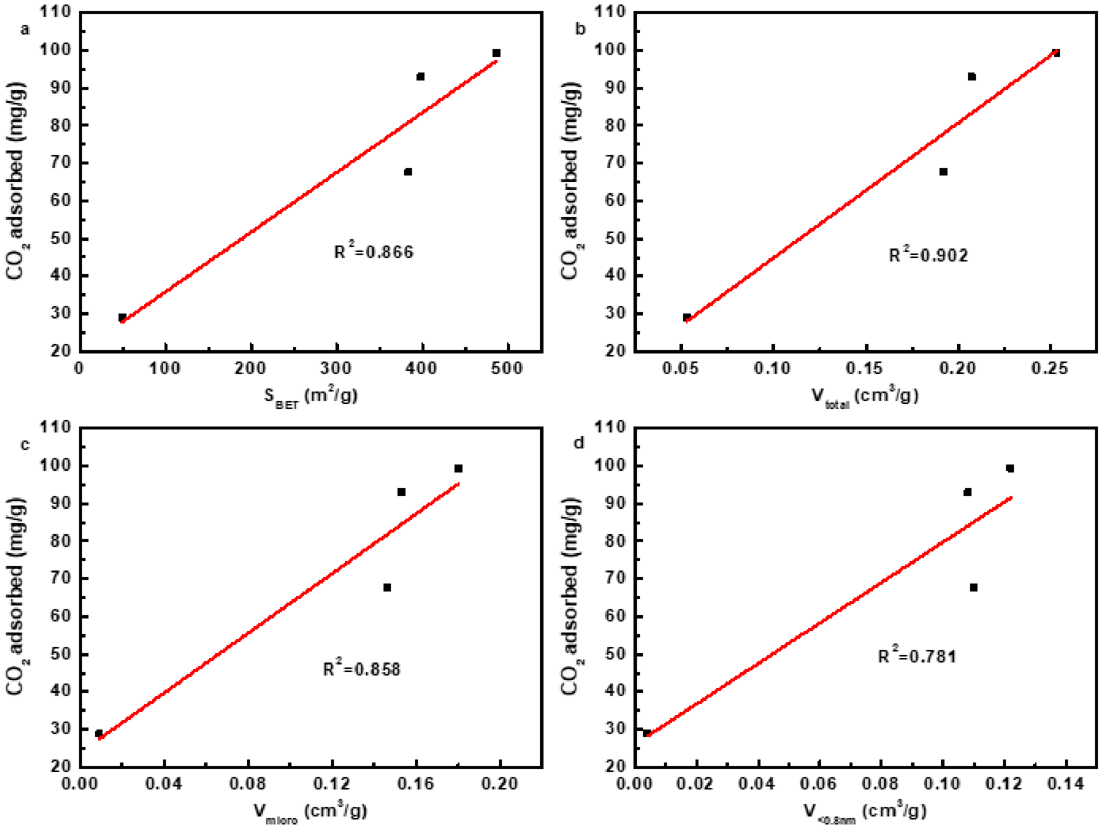

Figure S3. Correlation between adsorption capacity (1 bar, 25 °C) and (a) specific surface area, (b) total pore volume, (c) micropore volume, and (d) volume of pores with a size below 0.8 nm.

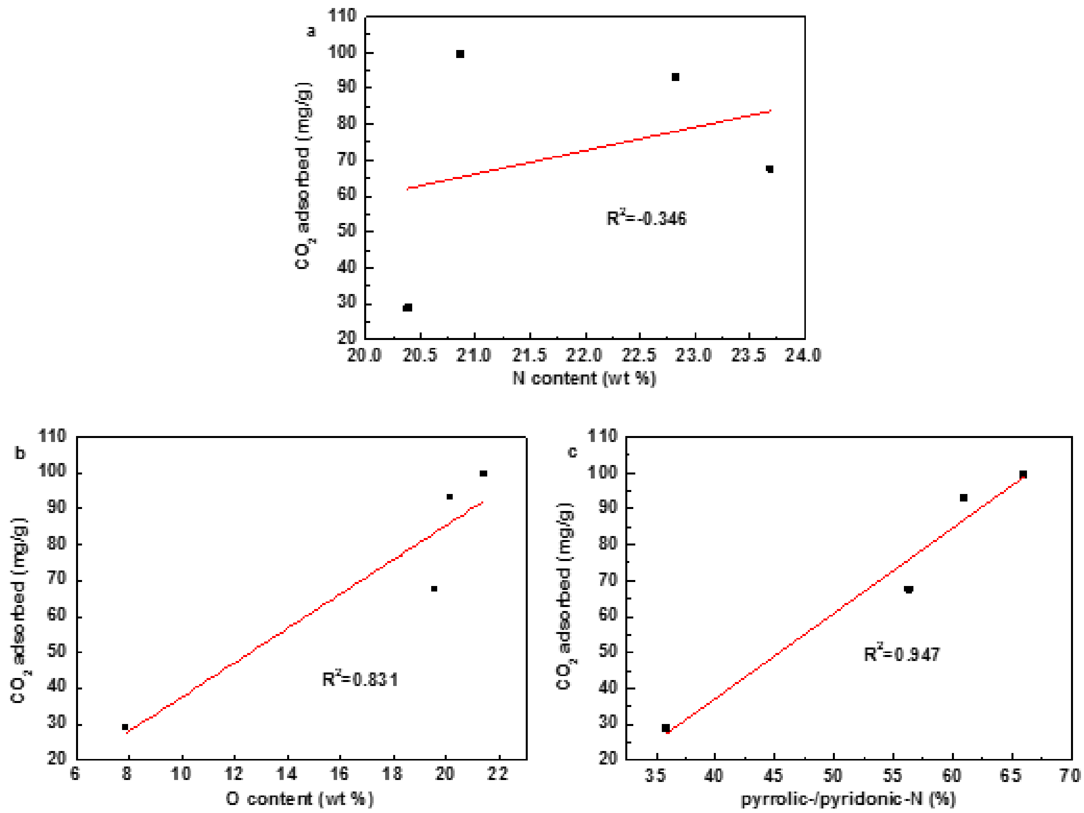

Figure S4. Correlation between adsorption capacity (1 bar, 25 °C) and (a) nitrogen content, (b) oxygen content, and (c) pyrrolic-/pyridonic-N content.

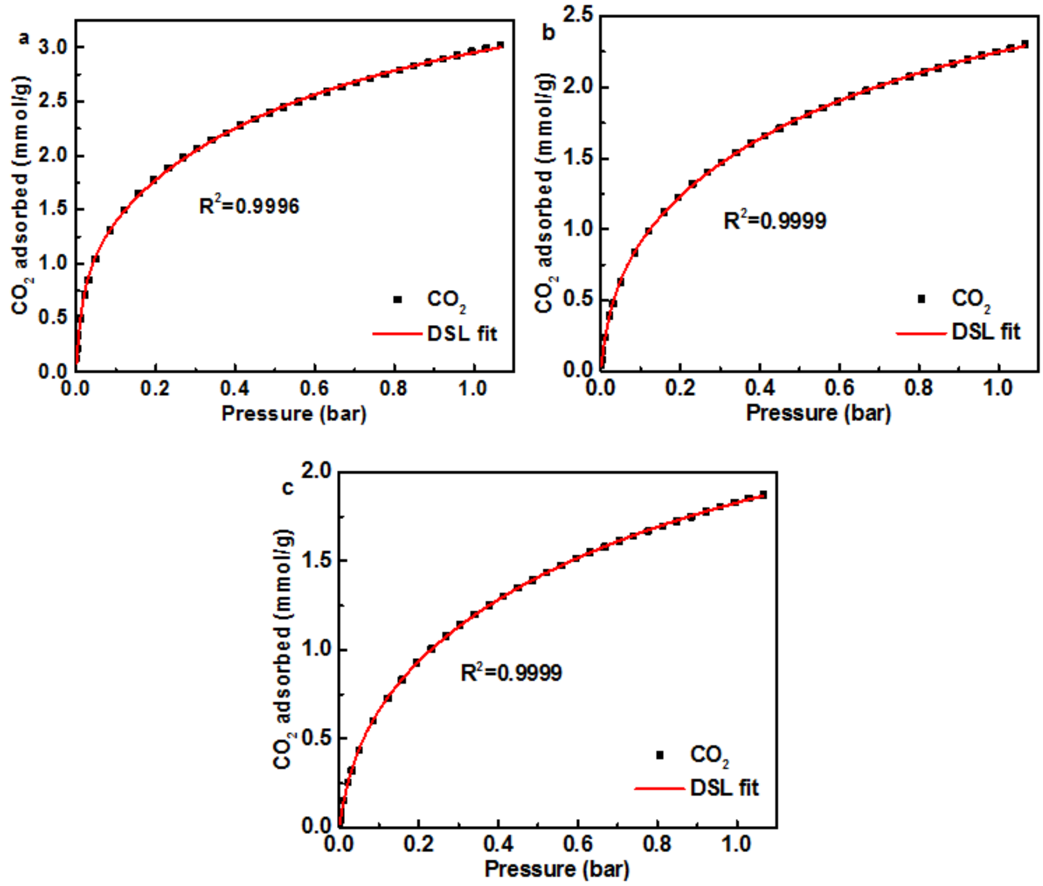

Figure S5. CO_2 adsorption isotherms of PCF-500 measured at (a) 0 °C, (b) 25 °C, and (c) 40 °C and curves fitted by the dual-site Langmuir model.

Calculation of Henry's law selectivity

To calculate the Henry's law selectivity of CO_2 over N_2 at 0, 25, and 40 °C for PCF-500, the CO_2 and N_2 adsorption isotherms were fitted with a virial-type equation:

$$\ln(n/p) = A_0 + A_1 n + A_2 n^2 + \cdots$$

where p (in Pa) is the pressure and n (in mol/g) is the gas adsorbed amount, A_i (i=1,2,3⋯) is virial coefficient which is required to sufficiently describe the isotherms. A_0 is in relation to the interaction between adsorbent and adsorbate, A_1 is in relation to the interaction between the adsorbate and the adsorbate. Under the condition of low surface coverage, A_i (i=2,3,4···) could be ignored, so this equation could be simplified to:

$$\ln(n/p) = A_0 + A_1 n$$

There is a linear relationship between $\ln(n/p)$ and the gas adsorbed amount n in the case of low surface coverage. The values of A_0 and A_1 could thus be obtained from the slop and the intercept.

The Henry's constants $K_H(i)$ for CO_2 and N_2 could then be obtained by the following equation:

$$K_H(i) = e^{A_0}$$

Finally, the Henry's law CO_2/N_2 selectivity was calculated via exploiting the following equation:

$$S_{ij} = K_H(i)/K_H(j)$$

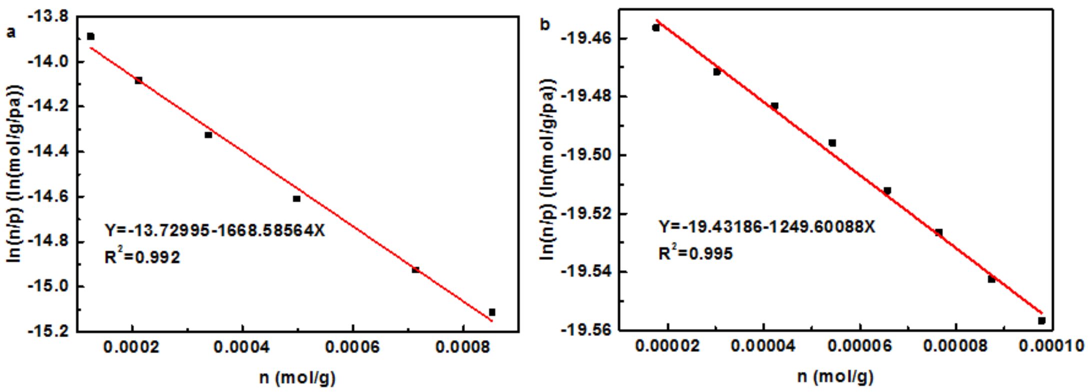

Figure S6. The virial characteristic curves of (a) CO_2 and (b) N_2 for PCF-500 at 0 °C.

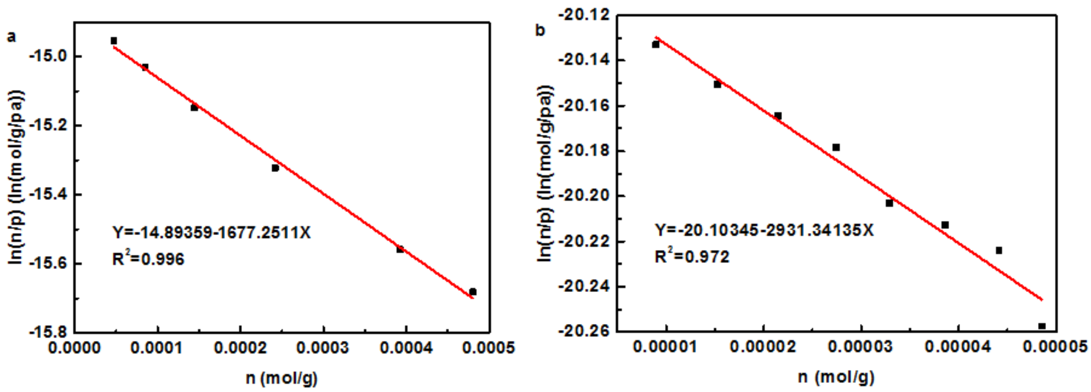

Figure S7. The virial characteristic curves of (a) CO_2 and (b) N_2 for PCF-500 at 25 °C.

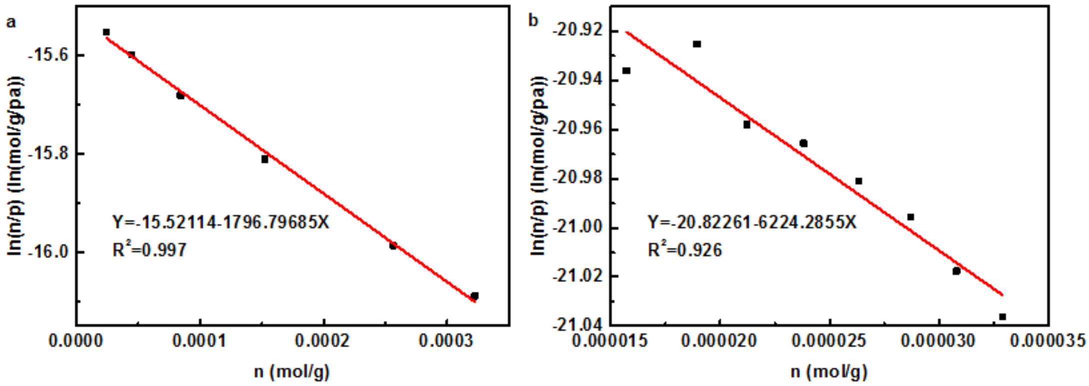

Figure S7. The virial characteristic curves of (a) CO_2 and (b) N_2 for PCF-500 at 40 °C.

Table S2. Henry's constants and virial fitting results for PCF-500 at 0, 25, and 40 °C.

Gas, Temperature (°C)	K_H	**Fitting R^2**
CO_2, 0 °C	1.09×10^{-6}	0.992
N_2, 0 °C	3.64×10^{-9}	0.995
CO_2, 25 °C	3.40×10^{-7}	0.996
N_2, 25 °C	1.86×10^{-9}	0.972
CO_2, 40 °C	1.82×10^{-7}	0.997
N_2, 40 °C	9.05×10^{-10}	0.926