

# SUPPLEMENTARY INFORMATION

Novel Porous Carbons derived from Coal Tar

Rejects: Assessment of the Role of Pore Texture in

CO<sub>2</sub> Capture under Realistic Post-combustion

Operating Temperatures

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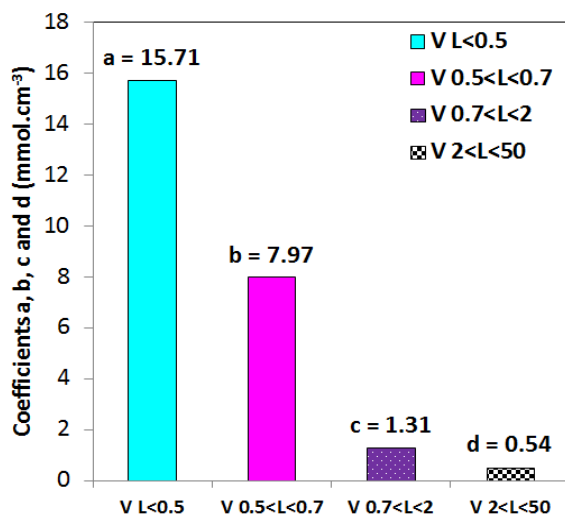
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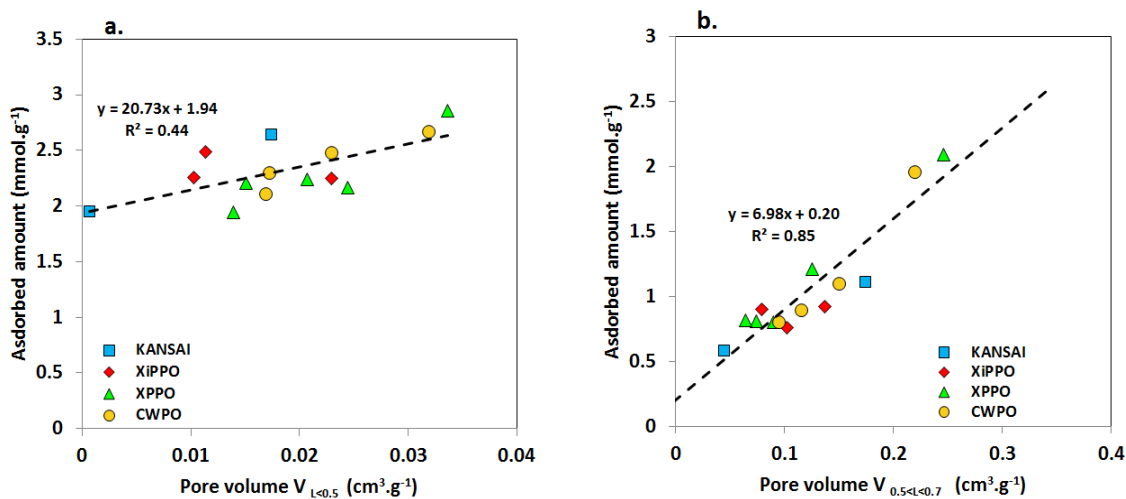
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**Table S1.** Reproducibility of CO<sub>2</sub> capture capacity values at 25°C and 1 bar under a 90% CO<sub>2</sub> atmosphere.

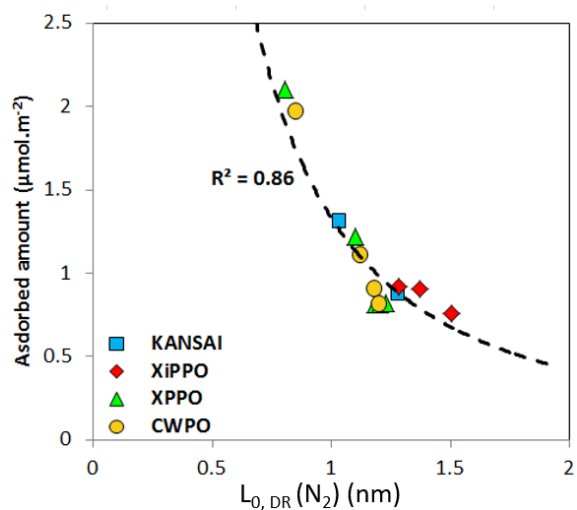
Sample	CO <sub>2</sub> capture capacity (mmol CO <sub>2</sub> / g AC)
MSP-20X	2.64 ± 0.04
MSC-30	1.95 ± 0.01
XiPPO_3	2.49 ± 0.02
XiPPO_4	2.26 ± 0.01
XiPPO_5	2.25 ± 0.06
XPPO_1	2.86 ± 0.03
XPPO_2	2.24 ± 0.02
XPPO_3	2.21 ± 0.03
XPPO_4	2.17 ± 0.03
XPPO_5	1.95 ± 0.03
CWPO_1	2.66 ± 0.07
CWPO_2	2.47 ± 0.07
CWPO_3	2.29 ± 0.01
CWPO_4	2.10 ± 0.02



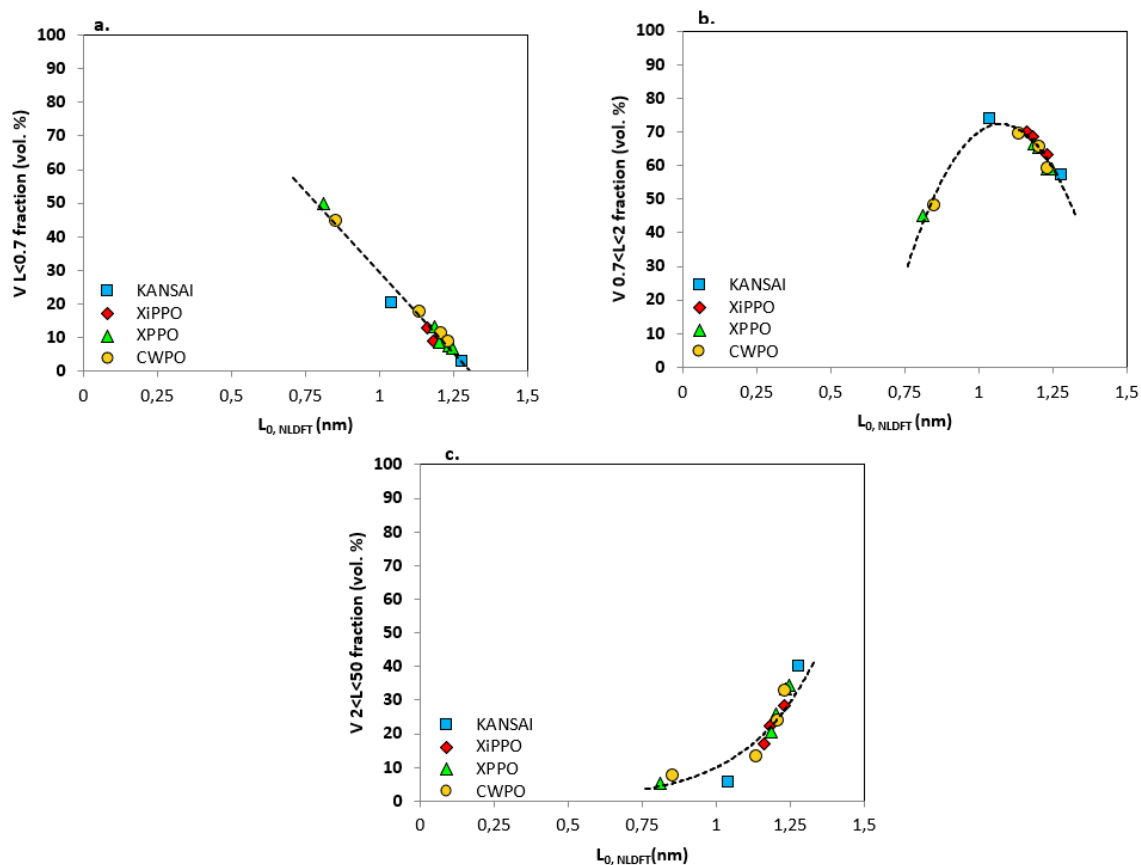
**Figure S1.** Coefficients of multiple linear regressions for CO<sub>2</sub> adsorption at 25°C for four different pore classes (below 0.5 nm, and in the ranges 0.5-0.7 nm, 0.7-2 nm and 2-50 nm) ( $R^2 = 0.891$ ).



**Figure S2.** Simple linear regression between adsorbed amounts of CO<sub>2</sub> at 25°C and pore volumes: a)  $V_{L<0.5}$ , or b)  $V_{0.5<L<0.7}$ .



**Figure S3.** Adsorbed amount of CO<sub>2</sub> per unit of BET surface area as a function of the average micropore size calculated by application of the Dubinin-Radushkevich method.



**Figure S4.** a) Ultramicropore fraction, b) supermicropore fraction, and c) mesopore fraction, as a function of the average micropore size according to the NLDFT.

As the temperature is at least 25°C for all experiments and the pressure is constant and low, the CO<sub>2</sub> concentration (in molecules per nm<sup>2</sup>) in the micropores is assumed low. Under those conditions, it can be assumed that adsorption only forms a monolayer and that CO<sub>2</sub> behaves like an ideal gas. In these conditions, the equilibrium constant can be identified with Henry's constant (eq. S1)<sup>13</sup>:

$$K_{mono}^H = \frac{C_{mono}^s}{P} \quad (\text{eq. S1})$$

with  $C_{mono}^s$  the concentration of adsorbed gas in mol per m<sup>2</sup> and  $P$  the pressure (Pa).

At constant pressure, the Van't Hoff equation can be written as (eq. S2):

$$\frac{d \ln(K)}{dT} = \frac{\Delta H_{ads}}{R.T^2} \quad (\text{eq. S2})$$

where  $\Delta H_{ads}$  stands for the standard enthalpy of adsorption,  $K$  the equilibrium constant,  $R$  the ideal gas constant (8.314 J/mol/K) and  $T$  the temperature (K). After integration, the Van't Hoff equation becomes (eq. S3):

$$\ln(K) = A - \frac{\Delta H_{ads}}{R.T} \quad (\text{eq. S3})$$

with  $A$  a constant. Thus, by representing  $\ln(K)$  with respect to  $1/T$ , the slope gives the enthalpy of adsorption ( $\Delta H_{ads}$ ). Figure S5 gives the Van't Hoff plot for the four materials.

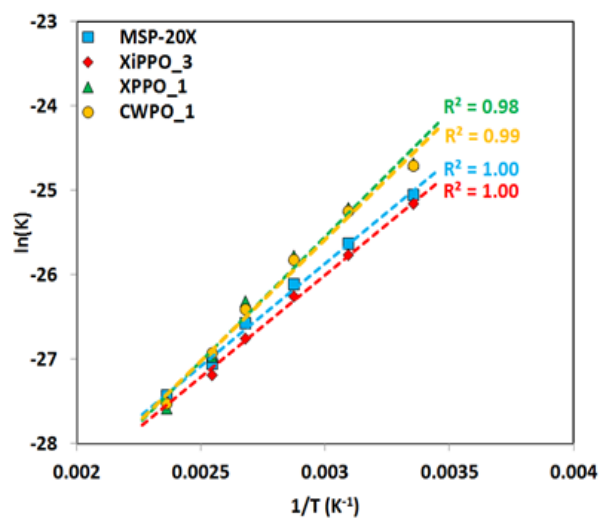
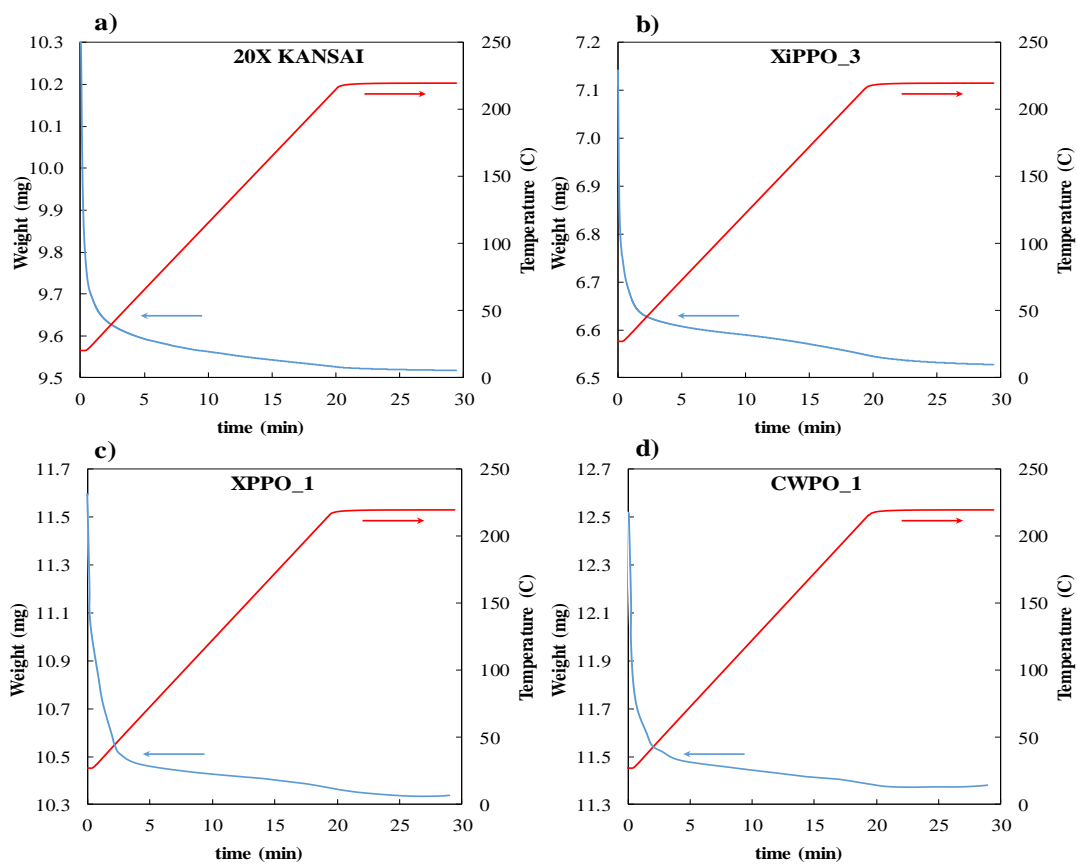


Figure S5. Van't Hoff plot for CO<sub>2</sub> adsorption at a pressure of 10<sup>5</sup> Pa.



**Figure S6.** Thermal stability of ACs from room temperature to 220°C: a) MSP-20X, b) XiPPO\_3, c) XPPO\_1, and d) CWPO\_1.