

# Water Adsorption in Nanoporous Carbon

## Characterized by in-situ NMR: Measurements of Pore Size and Pore Size Distribution

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### SUPPORTING INFORMATION

**Water adsorption isotherm.** Talu and Meunier suggested a semi-empirical model based on the association theory of water molecules in micropores (pore size < 2 nm), given by:<sup>1-2</sup>

$$P = \frac{H_0 \Psi}{1 + K \Psi} \exp(\Psi/N_m), \quad (\text{S1})$$

where  $K$  is a parameter related to the equilibrium constant for dimer formation,  $N_m$  is the saturation capacity of the pore (and thus varies with pore width),  $H_0 = \lim_{P \rightarrow 0} (dP/dN)$  is the inverse of the Henry's law constant, and

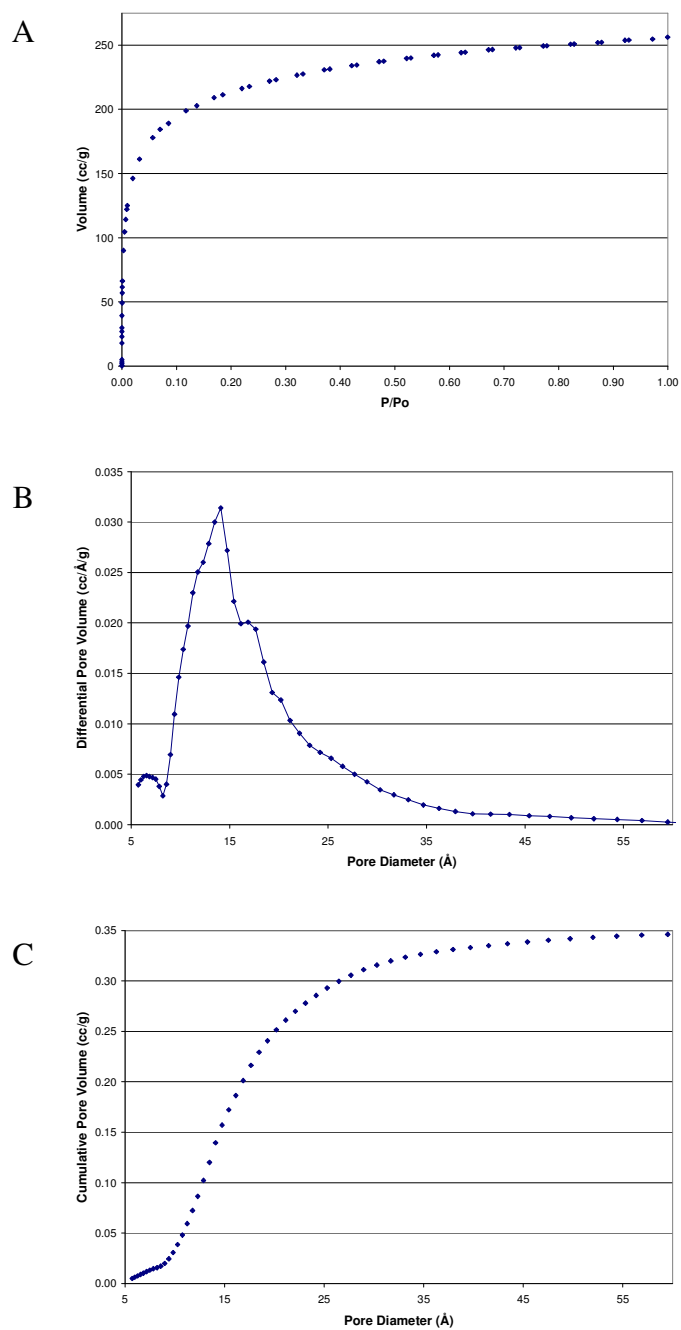
$$\Psi = \frac{-1 + (1 + 4K\xi)^{1/2}}{2K}, \text{ and } \xi = \frac{N_m N}{N_m - N}, \quad (\text{S2})$$

where  $N$  is the amount of adsorbed water in the unit of mmol/g at pressure  $P$ . The fitted isotherms based on Eq. 1 (solid lines in Fig. 2a) reproduce the measured isotherms (scattered data in Fig. 2a) very well, with the fitting parameters listed in Table I. The low  $H_0$  and  $K$  values ( $<3$ ) suggest that these nanoporous carbon samples have high affinity for water molecules, and that the PAS are in widely varying pore environment, respectively.<sup>1</sup> Although these parameters can be loosely connected to surface properties of activated carbon, they are implicitly related to the shape of the isotherm, such as the pore filling pressure and the steepness of the isotherm. It is difficult to interpret those parameters in terms of the pore size and its distribution.

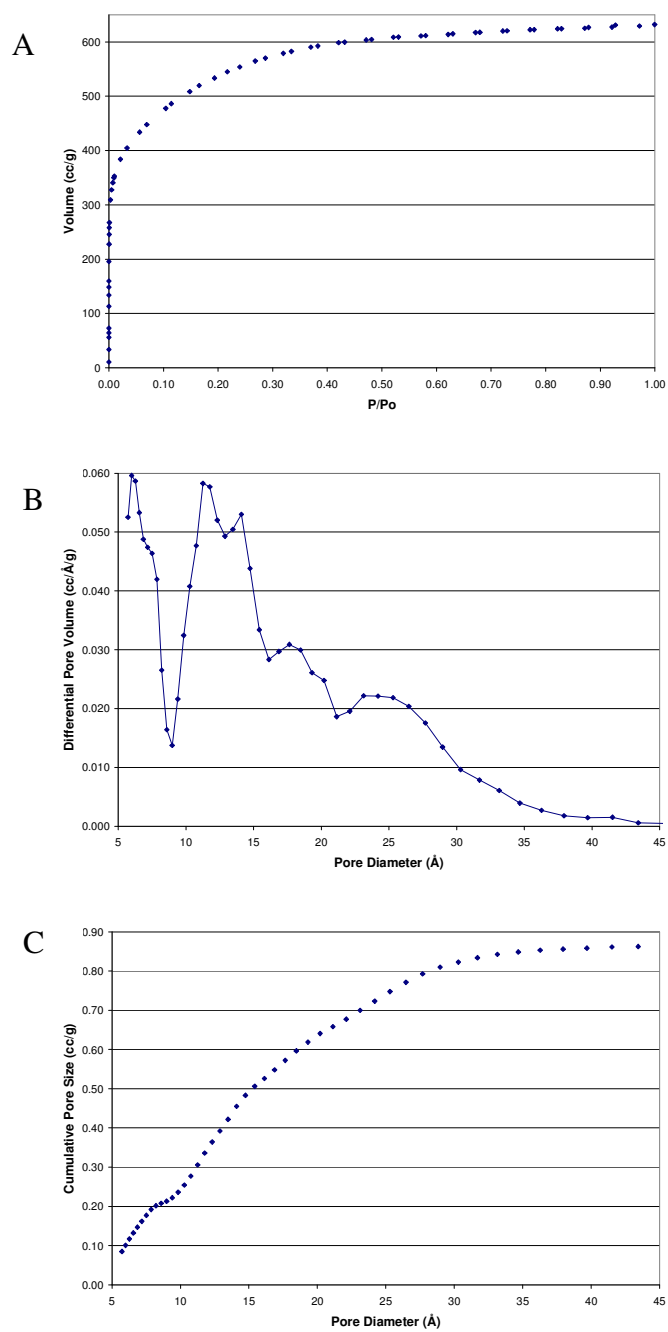
**Table SI.** Parameters characterizing three activated carbons derived from PEEK with different BO using Talu-Meunier model:  $H_0$ ,  $K$ , and  $N_m$  are used to fit the water adsorption isotherms to Eq. S1.

BO	$H_0$	$K$	$N_m$	$d$	SA
(wt %)	$(P/P_0)$	$(P/P_0)$	(mmol/g)	(nm)	(m <sup>2</sup> /g)
20	0.52(8)	0.9(1)	33.0(5)	1.2	1294
35	1.5(2)	2.5(3)	27.6(3)	1.4	981
91	2.1(2)	2.6(3)	49(1)	2.5	2368

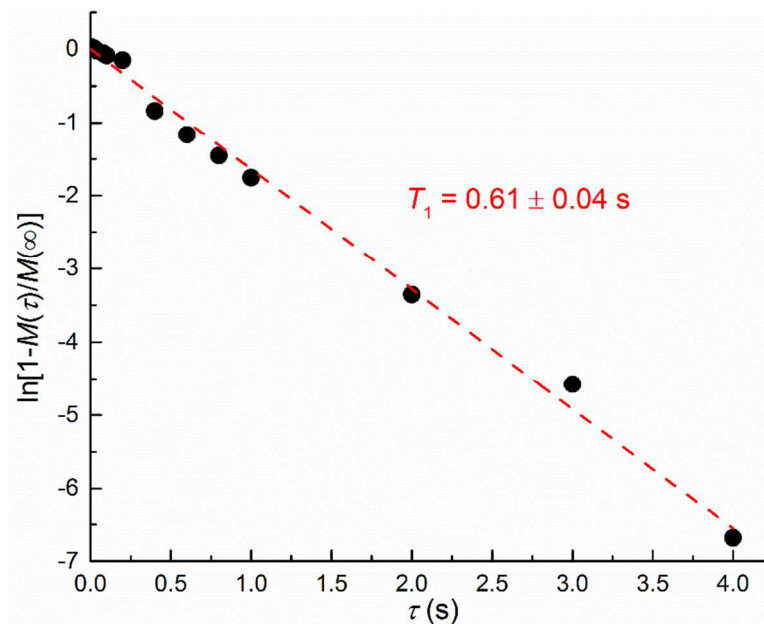
**Figure S1.** The N<sub>2</sub> adsorption measurement and analysis on 35 wt% BO sample. (A) Adsorption isotherm N<sub>2</sub> at 77K, (B) differential pore volume distribution via DFT method, (C) cumulative pore volume distribution via DFT Method.



**Figure S2.** The N<sub>2</sub> adsorption measurement and analysis on 70 wt% BO sample. (A) Adsorption isotherm N<sub>2</sub> at 77K, (B) differential pore volume distribution via DFT method, (C) cumulative pore volume distribution via DFT Method.



**Figure S3.** A representative fitting curve based on a mono-exponential function for the saturation recovery data to obtain the  $T_1$  at  $P/P_0 = 0.6$  for the 35 wt% BO sample. The magnetization (y-axis) is plotted in a normalized logarithm scale as the function of saturation recovery time ( $\tau$ ), such that the  $T_1$  is inversely proportional to the absolute value of the slope from a linear fitting. The standard deviation of the fitting parameter is used to determine the standard deviation of the  $T_1$ .



## References

1. Talu, O.; Meunier, F., Adsorption of associating molecules in micropores and application to water on carbon. *AIChE J.* **1996**, *42*, 809-819.
2. McCallum, C. L.; Bandosz, T. J.; McGrother, S. C.; Muller, E. A.; Gubbins, K. E., A molecular model for adsorption of water on activated carbon: Comparison of simulation and experiment. *Langmuir* **1999**, *15*, 533-544.