Supporting Information

Cigarette butt-derived carbons have ultra-high surface area and unprecedented hydrogen storage capacity

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Appendix 1

Excess and total hydrogen uptake

Our measurements provided the excess hydrogen uptake, which is the amount of hydrogen adsorbed in the carbons above that which would have been stored in the pores under similar conditions (temperature and pressure) assuming that there is zero energy of interaction between the hydrogen and the carbon pore walls. The total uptake is calculated from the excess storage by taking into account the amount of hydrogen compressed into the carbon pore volume space. Our gravimetric methods measured the excess hydrogen uptake (θ_{Exc}) from which the total storage (θ_T) was calculated from the equation:

$$\theta_T = \theta_{Exc} + \frac{100 \text{ x } d_{H2} \text{ x } V_T}{\left(1 + d_{H2} \text{ x } V_T\right)}$$

Where;

θ_T = total hydrogen uptake (wt%)

θ_{Exc} = excess hydrogen uptake (wt%)

d_{H2} = density (g cm^{-3}) of compressed hydrogen gas at the relevant temperature and pressure. The density was obtained from the National Institute of Standards and Technology (NIST) website (http://www.nist.gov/)

V_T = Pore volume (cm^3 g^{-1}) of the carbon from nitrogen or CO_2 sorption analysis

Table S1. Elemental analysis of hydrochar derived from fresh (FF-hydrochar) and smoked (SF-hydrochar) cigarette filters, and activated carbons derived from the hydrochars.

Sample	C [%]	H [%]	N [%]	O [%]	(O/C)[a]	(H/C)[a]
FF-hydrochar	63.6	4.2	0	32.2	0.380	0.793
SF-hydrochar	68.5	5.7	1.0	24.8	0.272	1.000
CA-hydrochar	66.2	3.9	0	29.9	0.339	0.707

[a]Atomic ratio

Table S2. Textural properties and H_2 uptake of O-rich (16.4 wt%) activated carbon (SF-4800) derived from cigarette butts compared to cellulose-derived activated carbon (C-4700) with lower O content (7.1 wt%).

Sample	Surface area[a] (m^2 g^{-1})	Pore volume[b] (cm^3 g^{-1})	H_2 uptake[c] (wt%)		
			1 bar	20 bar[d]	Reference
SF-4800	2393 (1810)	1.09 (0.70)	3.0	6.6 (5.9)	This work
C-4700	2370 (2201)	1.08 (0.96)	2.5	5.6 (4.9)	1

Values in the parenthesis refer to: [a]micropore surface area and [b]micropore volume. [c]Gravimetric (wt%) H_2 uptake at -196 ^oC and various pressures (i.e., 1 or 20 bar).[d]The values in parenthesis are excess H_2 uptake.

Reference

1. M. Sevilla, A. B. Fuertes and R. Mokaya R. *Energy Environ. Sci*., 2011, **3**, 1400.

Table S3. Surface area, pore volume hydrogen storage capacity (at -196 ^{o}C and 20 or 30 bar) for cigarette filter (FF-4800) or cigarette butt (SF-4600) derived carbons compared to the best benchmark metal organic frameworks (MOFs).

Sample	Surface area (m^2 g^{-1})	Pore Volume (cm^3 g^{-1})	Gravimetric (wt%) H_2 uptake @ 20 bar Excess	@ 20 bar Total	@ 30 bar Excess	@ 30 bar Total	Reference
SF-4600	4310	2.09	8.1	9.4	8.3	10.4	This work
FF-4800	4113	1.87	7.0	8.2	7.2	9.1	This work
NOTT-112	3800	1.62	6.8	7.8	7.0	8.6	1
NU-100	6143	2.82	6.9	8.5	7.8	10.0	2
MOF-210	6240	3.60	6.4	8.4	7.3	10.2	3

References

1. Y. Yan, X. Lin, S. Yang, A. J. Blake, A. Dailly, N. R. Champness, P. Hubberstey and M. Schroder, *Chem. Commun*. 2009, 1025–1027.
2. O. K. Farha, A. O. Yazaydın, I. Eryazici, C. D. Malliakas, B. G. Hauser, M. G. Kanatzidis, S. T. Nguyen, R. Q. Snurr and J. T. Hupp, *Nat. Chem*. 2010, **2**, 944–948.
3. H. Furukawa, N. Ko, Y. B. Go, N. Aratani, S. B. Choi, E. Choi, A. Ö. Yazaydin, R. Q. Snurr, M. O'Keeffe, J. Kim and O. M. Yaghi, *Science* 2010, **329**, 424–428.

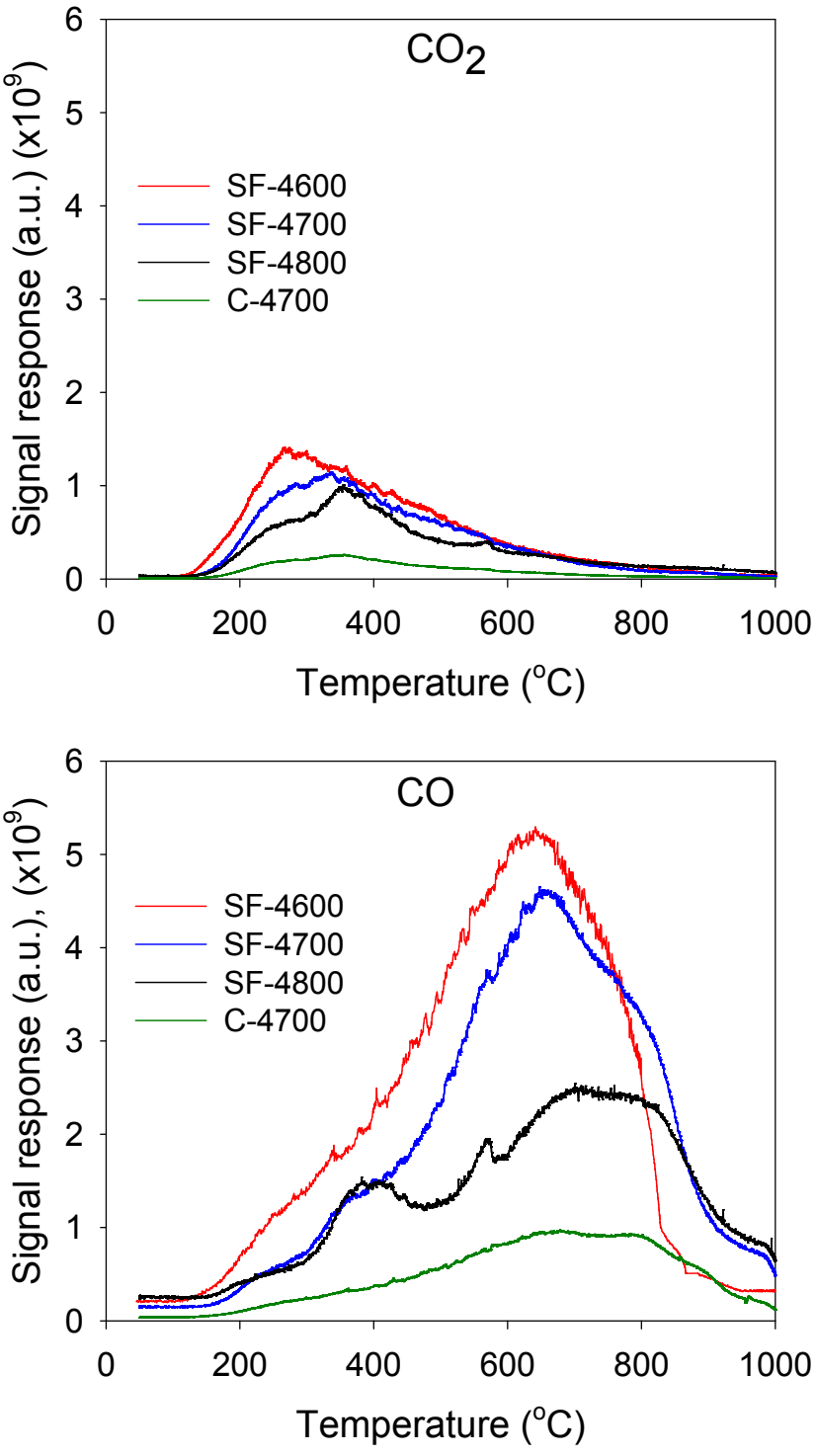

Figure S1. Evolution of CO_2 (top) and CO (bottom) under TPD conditions for activated carbons derived from smoked cigarette butts (SF-xT) compared to an activated carbon derived from cellulose (C-4700). SF-xT have O content of 16 – 31 wt%, and C-4700 has O content of 7.1 wt%.

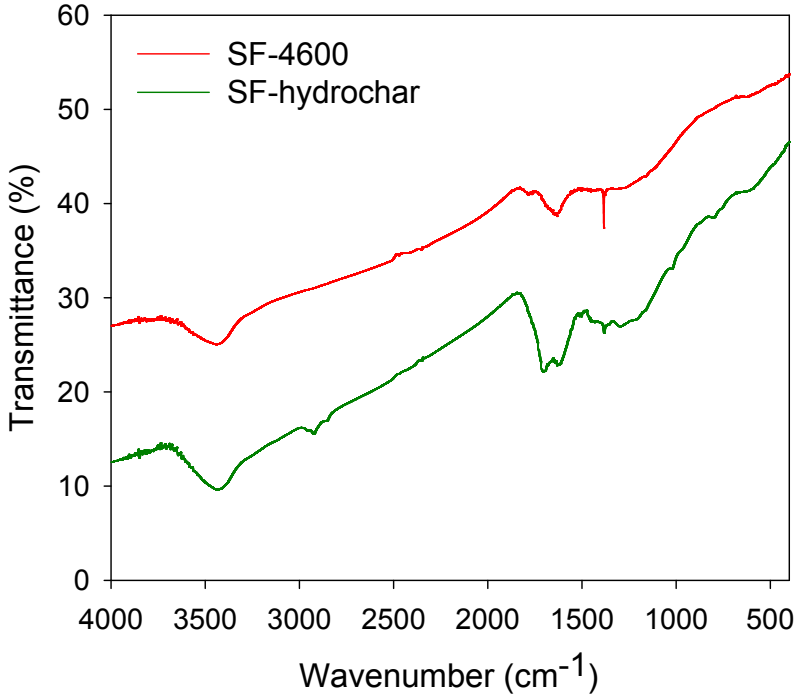

Figure S2. IR spectra of SF-hydrochar derived from smoked cigarette butts, and an activated carbon, SF-4600, prepared from the SF-hydrochar.

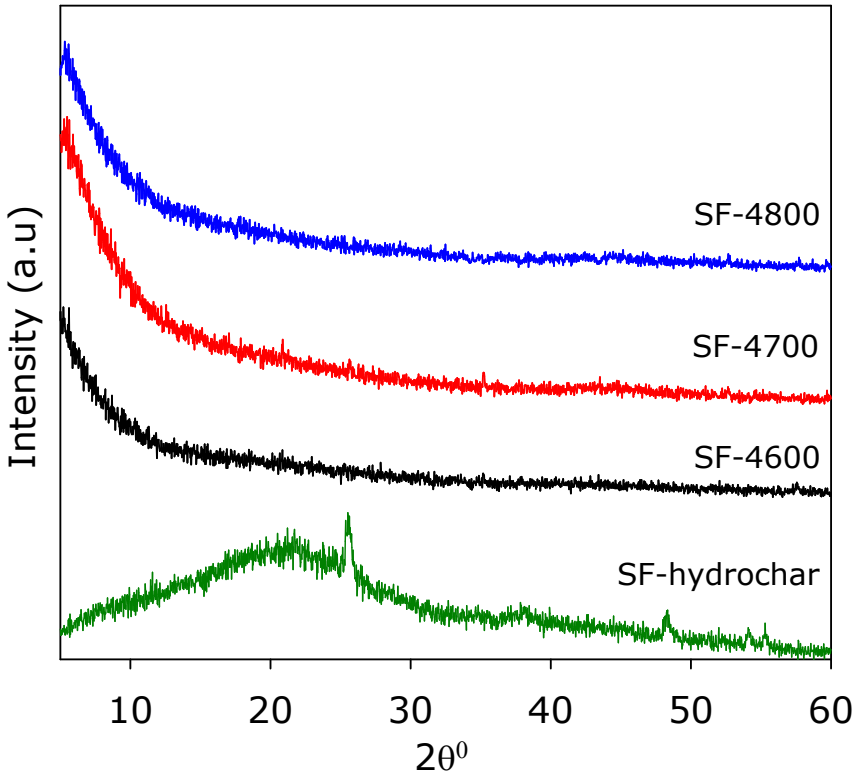

Figure S3. Powder XRD patterns of SF-hydrochar and SF-xT activated carbons prepared from SF-hydrochar.

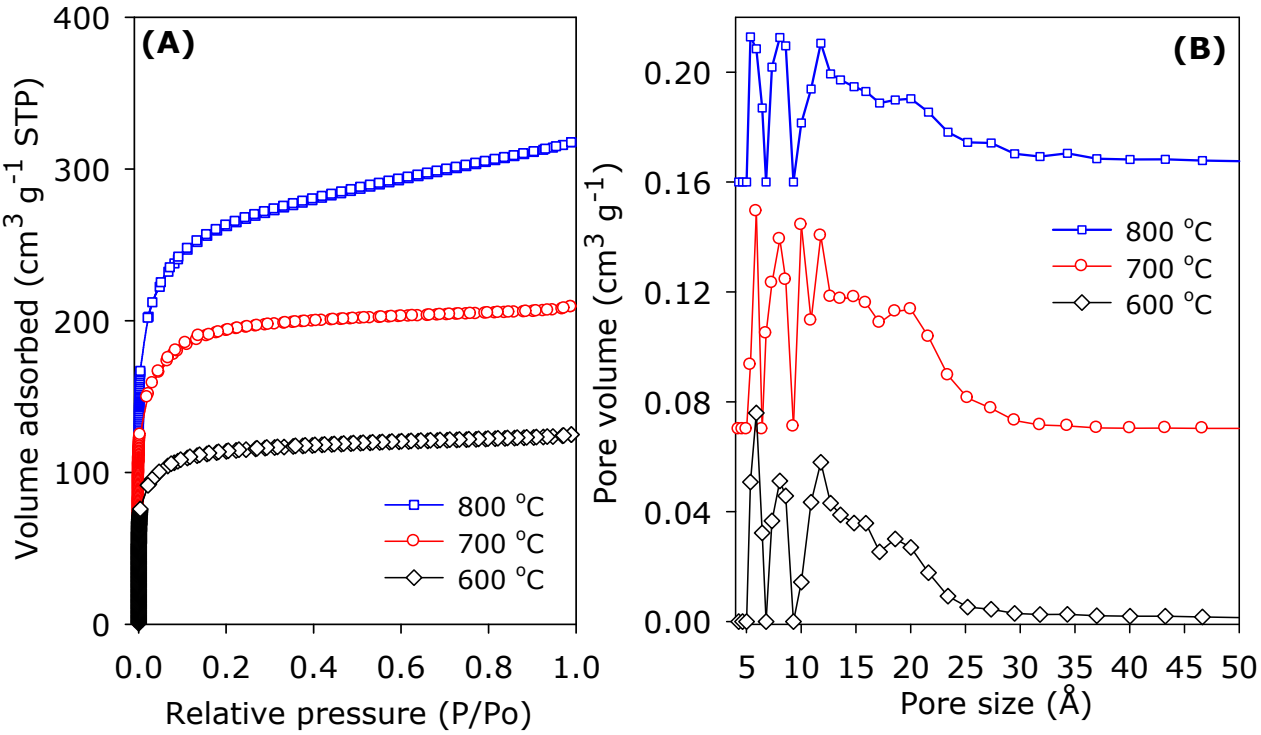

Figure S4. (A) Nitrogen sorption isotherms and (B) pore size distribution curves of carbon generated by heating the SF-hydrochar at various temperatures (600, 700 or 800 °C) for 1 h in the absence of KOH.

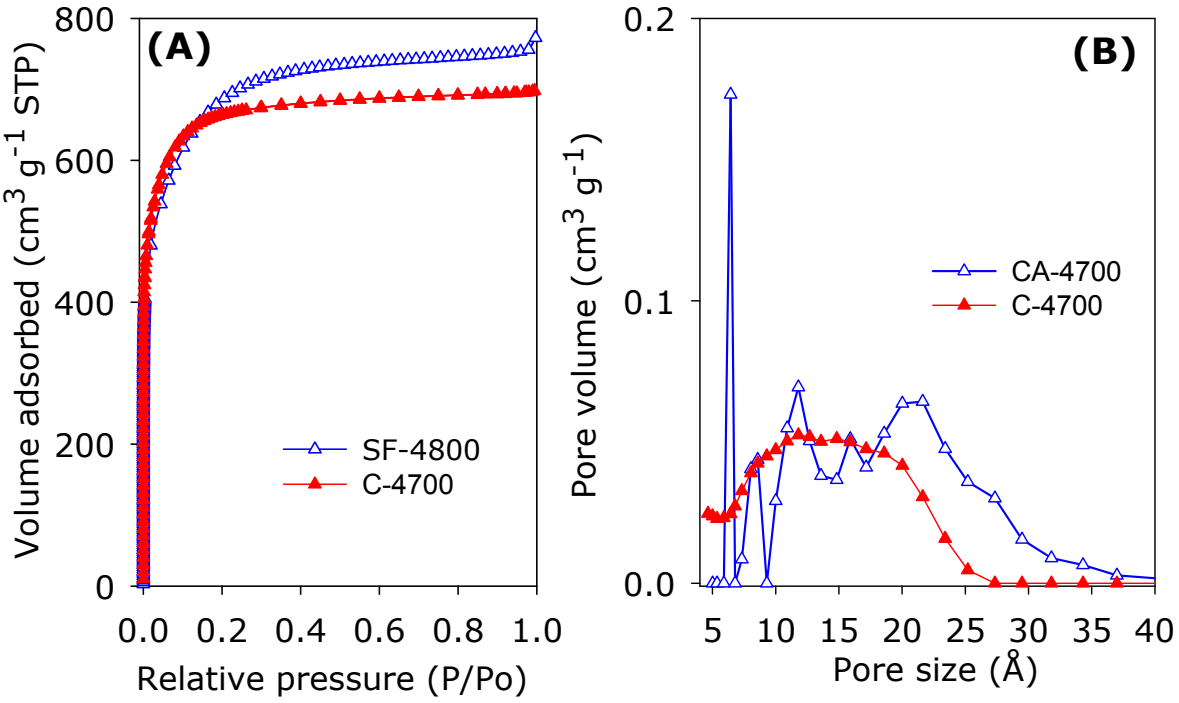

Figure S5. (A) Nitrogen sorption isotherms and (B) pore size distribution curves of carbon generated from cigarette butts (SF-4800) cellulose (C-4700).

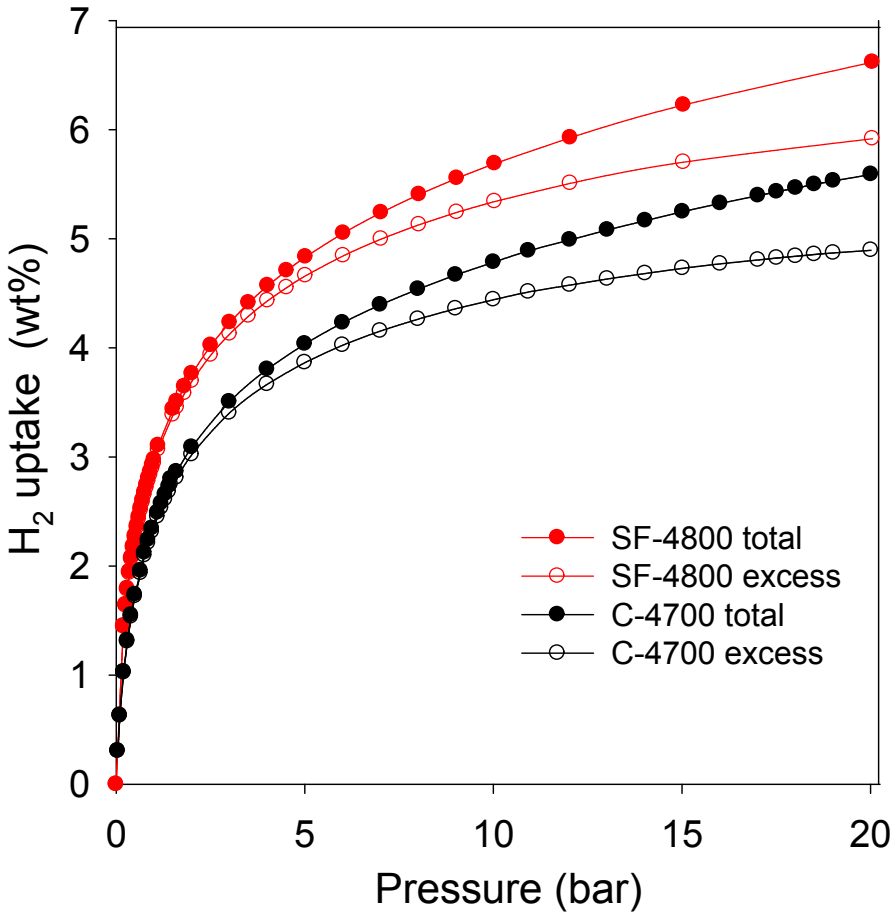

Figure S6. Excess and total hydrogen uptake at -196 °C of activated carbon derived from smoked cigarette filters/butts (SF-4800) and pure cellulose (C-4700). The samples have similar porosity (Figure S5) but SF-4800 has higher oxygen content.