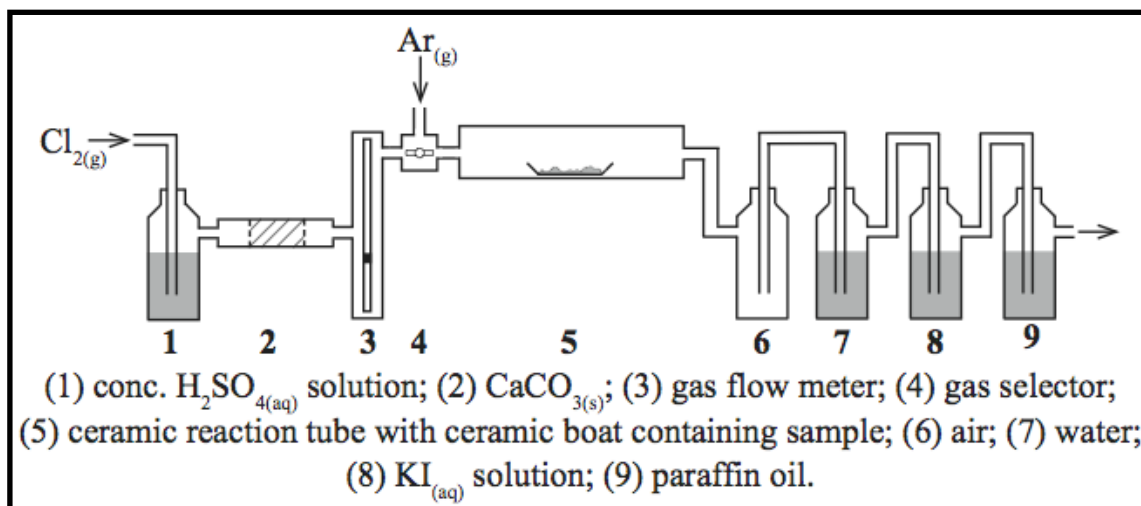


Supplementary Information

Superactivated carbide-derived carbons with high hydrogen storage capacity

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Scheme 1. Diagram showing the experimental setup for the synthesis of CDCs from Zirconium carbide.

The sulphuric acid (position 1) and calcium carbonate (position 2) are drying agents to remove water from the chlorine gas. The gas flow meter (position 3) measures the flow rate of chlorine gas. The gas selector (position 4) switches the gas flow between chlorine and argon. The ceramic reaction tube (position 5) is placed inside a furnace. The Dreschel bottle filled with air (position 6) prevents any liquids from being sucked back into the reaction tube. The water (position 7) reacts with the chloride compounds produced as by-product of the CDC synthesis. The potassium iodide solution (position 8) removes unreacted chlorine gas, and the paraffin oil (position 9) prevents air from accessing the system.

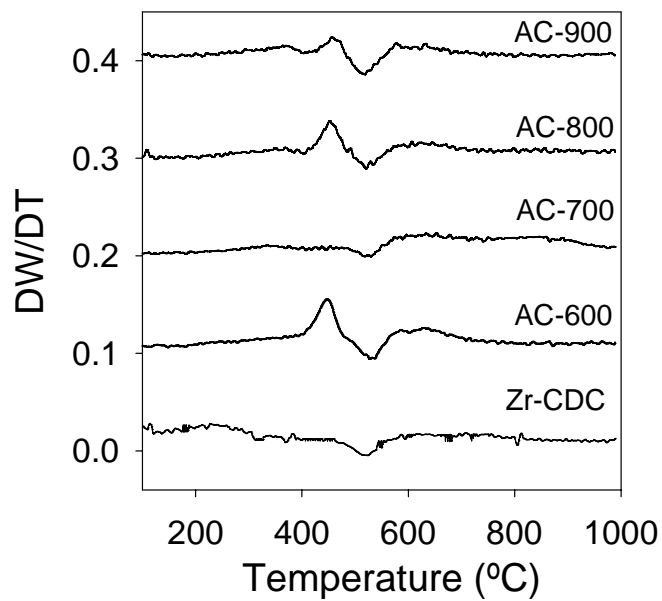
We investigated CDC samples that were chemically (KOH) activated at temperatures between 600 and 900°C. The activation process was very carefully controlled and reproducible given that the starting CDC material was the same for all activated samples. Prior to expanding the KOH activation temperature range, we prepared several samples at 800°C, which generated very similar activated carbons. Our study emphasises trends observed over a range of samples rather than on the data of any one sample. The total number of carbon samples investigated is six; two CDCs and four KOH activated (i.e., superactivated) carbons.

Supplementary Table 1. Hydrogen uptake at -196°C of various activated carbons.

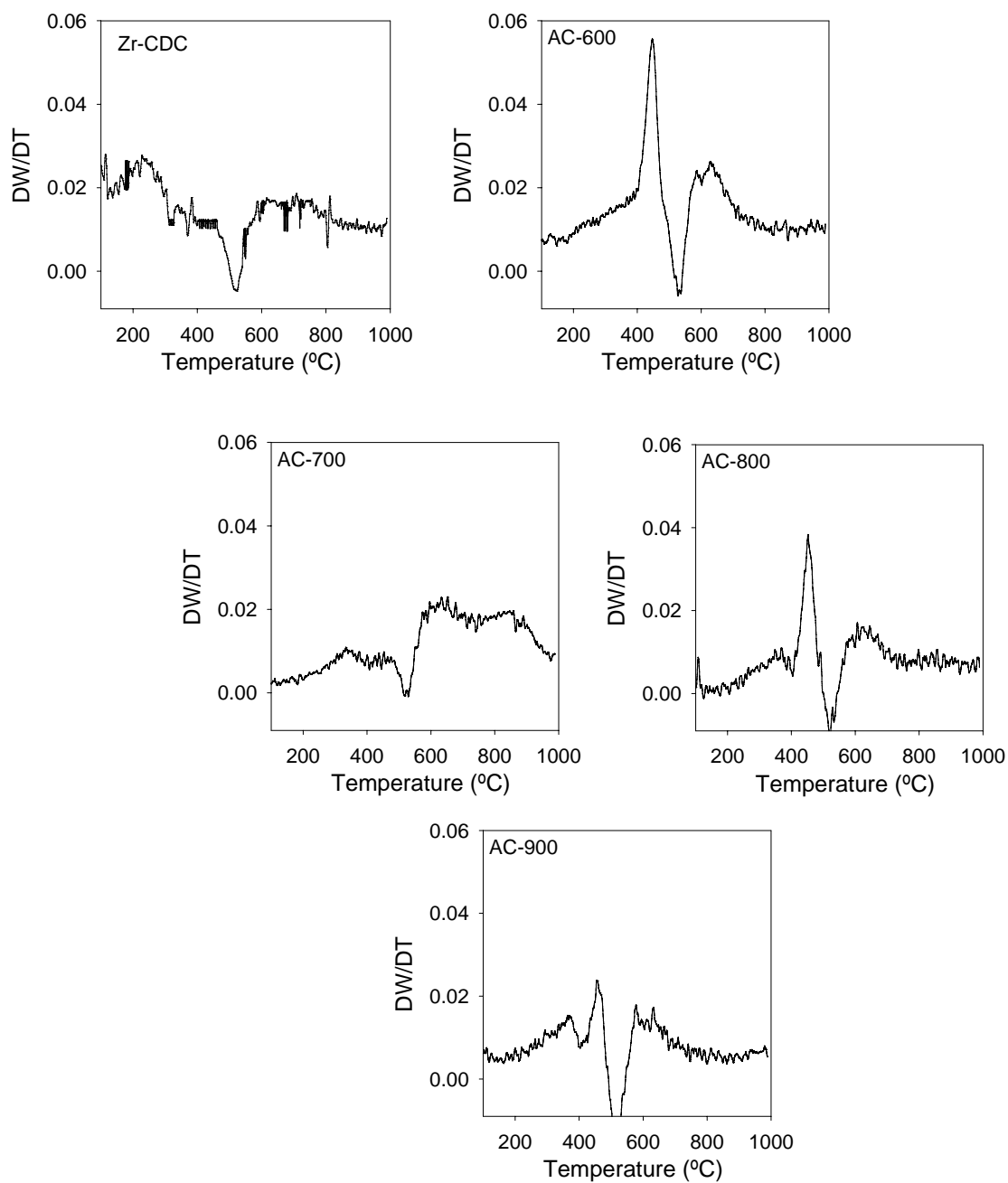
Activated carbon	Surface area (m ² g ⁻¹)	Hydrogen uptake at 20 bar (wt%)	Hydrogen uptake at 1 bar (wt%)	Reference
AC I	2560	4.0	~ 2.4	[1]
M30	3220	5.0	-	[2]
KUA3	1694	3.0	~ 1.8	[3]
KUA4	1953	3.5	~ 2.0	[3]
KUA5	3183	4.8	~ 2.5	[3]
KUA6	3808	5.2	~ 2.2	[3]
Carbon A	2330	-	2.3	[4]
AX-21	2421	-	2.4	[4]
Carbon B	3000	-	2.5	[4]
PK775C	2680	5.6	-	[5]
MK725	1800	~ 4.5	-	[5]
APOR8	2550	~ 5.0	-	[6]
PC76	2468	-	2.3	[6]

References

1. B. Panella, M. Hirscher and S. Roth, *Carbon* 2005, **43**, 2209.
2. Y. Kojima, Y. Kawai, A. Koiwai, N. Suzuki, T. Haga, T. Hioki and K. Tange, *J. Alloys Compd.* 2006, **421**, 204.
3. M. Jordá-Beneyto, F. Suárez-García, D. Lozano-Castelló, D. Cazorla-Amorós and A. Linares-Solano, *Carbon* 2007, **45**, 293.
4. N. Texier-Mandoki, J. Dentzer, T. Piquero, S. Saadallah, P. David and C. Vix-Guterl, *Carbon* 2004, **42**, 2744.
5. I. Cabasso and Y. Yuan, *Nanostructured activated carbons for hydrogen storage*.
http://www.hydrogen.energy.gov/pdfs/progress08/iv_c_3_cabasso.pdf.
 Accessed in May 2009.
6. J. B. Parra, C. O. Ania, A. Arenillas, F. Rubiera, J. M. Palacios, and J. J. Pis, *J. Alloys Compd.* 2004, **379**, 280.



Supporting Figure 1. Differential thermogravimetric profiles of pristine CDC (Zr-CDC) and activated CDC carbons. TGA analysis was performed under helium flow (100 ml/min) and heating rate of 20°C/min.



Supporting Figure 2. Differential thermogravimetric profiles of pristine CDC (Zr-CDC) and activated CDC carbons. TGA analysis was performed under helium flow (100 ml/min) and heating rate of 20°C/min.