Tuning the Properties of Iron-doped Porous Graphitic Carbon Synthesized by Hydrothermal Carbonization of Cellulose and Subsequent Pyrolysis

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Supporting Information

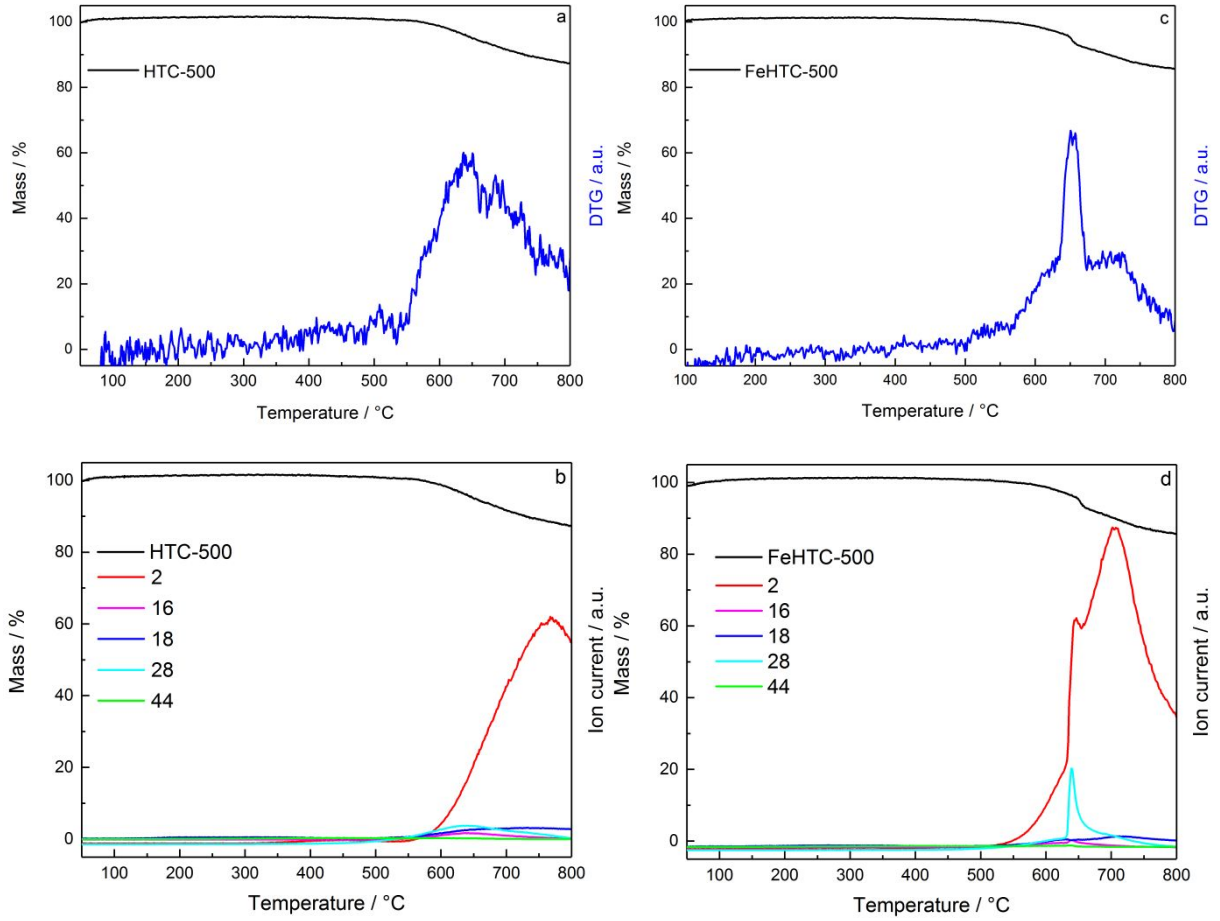

Figure S1. Relative mass losses, DTG curves (a,c) and QMS profiles (b,d) of the undoped (a,b) and the iron-loaded carbon materials (c,d) pre-treated at 500 °C during temperature-programmed desorption in He in a thermobalance applying a heating rate of 5 K min^{-1}.

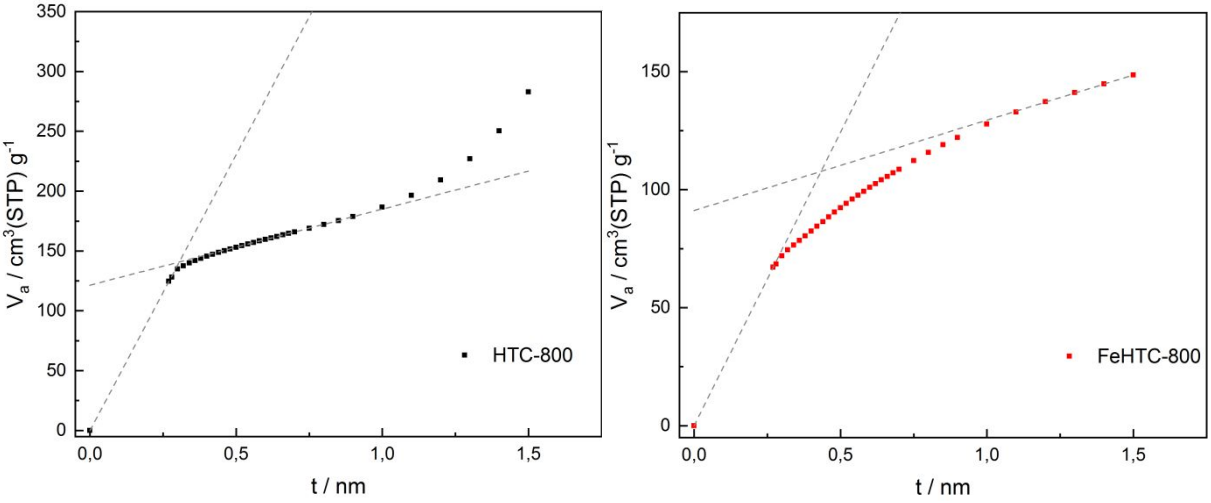

Figure S2. t-plots based on the N_2 physisorption measurements of the pure (left) and iron-loaded (right) porous carbon materials pyrolyzed at 800 °C.

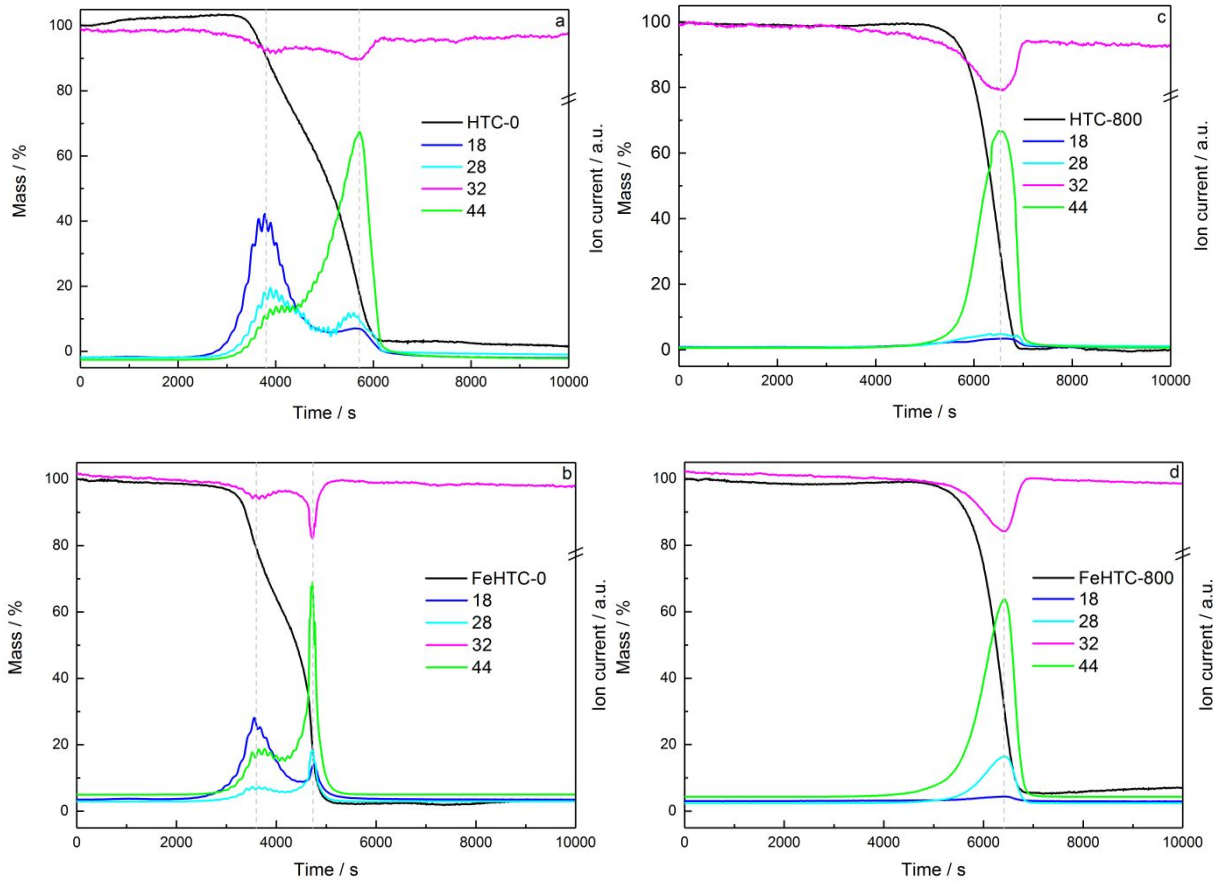

Figure S3. Relative mass losses and the QMS profiles of the undoped (a,c) and iron-loaded (b,d) hydrochar (a,b) and the corresponding carbon materials pyrolyzed at 800 °C (c,d) during TPO in 20 % O_2 in He in a thermobalance applying a heating rate of 5 K min^{-1}.

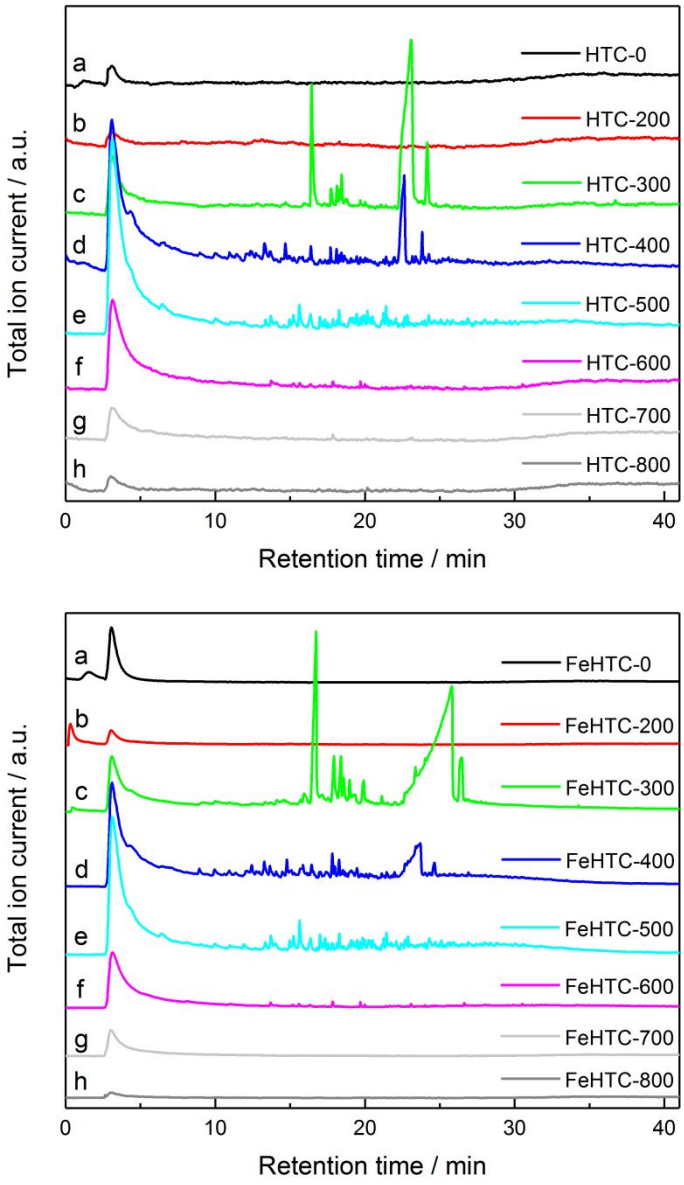

Figure S4. Chromatograms of the evolved species of the pure (top) and the iron oxide- loaded hydrochars (bottom) as a function of the pyrolysis temperature during sequential flash pyrolysis in the pyrolysis-GC/MS set-up.

Table S1. Compounds evolving during the stepwise pyrolysis of the undoped carbon material at 300 °C.

Similarity	Compound name	Molar mass [g/mol]	Sum formula	Retention time [min]
	CO, H_2O, CO_2	18, 28, 44		3.06
94	Levoglucosenone	126	$C_6H_6O_3$	16.41
92	1,4:3,6-Dianhydro-α-d-glucopyranose	144	$C_6H_8O_4$	18.11
80	2-Heptanol, 5-ethyl-	144	$C_9H_{20}O$	18.31
89	β-D-Glucopyranose, 1,6-anhydro-	162	$C_6H_{10}O_5$	23.11
92	1,6-Anhydro-β-D-glucofuranose	162	$C_6H_{10}O_5$	24.16

Table S2. Compounds evolving during the stepwise pyrolysis of the undoped carbon material at 400 °C.

Similarity	Compound name	Molar mass [g/mol]	Sum formula	Retention time [min]
	CO, H_2O, CO_2	18, 28, 44		3.06
82	Furan, 2-methyl-	82	C_5H_6O	4.35
87	Furan, 2,5-dimethyl-	96	C_6H_8O	6.57
91	2(3H)-Furanone, 5-methyl-	98	$C_5H_6O_2$	10.96
87	1,2-Cyclopentanedione	98	$C_5H_6O_2$	12.36

93	2-Furancarboxaldehyde, 5-methyl-	110	$C_6H_6O_2$	13.30
94	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	112	$C_6H_8O_2$	14.68
83	Phenol, 2-methyl-	108	C_7H_8O	15.60
80	2-Furanmethanol	98	$C_5H_6O_2$	16.38
82	2-Pentanol, 5-(2-propynyloxy)-	142	$C_8H_{14}O_2$	17.70
91	1,4:3,6-Dianhydro-α-d-glucopyranose	144	$C_6H_8O_4$	18.10
82	2-Coumaranone	134	$C_8H_6O_2$	18.60
87	1H-Inden-1-one, 2,3-dihydro-	132	C_9H_8O	19.40
84	2-Methyl-5-hydroxybenzofuran	148	$C_9H_8O_2$	21.41
91	β-D-Glucopyranose, 1,6-anhydro-	162	$C_6H_{10}O_5$	22.60
88	1,6-Anhydro-β-D-glucofuranose	162	$C_6H_{10}O_5$	23.83

Table S3. Compounds evolving during the stepwise pyrolysis of the undoped carbon material at 500 °C.

Similarity	Compound name	Molar mass [g/mol]	Sum formula	Retention time [min]
	CO, H_2O, CO_2	18, 28, 44		3.06
93	Furan, 2,5-dimethyl-	96	C_6H_8O	6.46
80	2-Cyclopenten-1-one	82	C_5H_6O	10.01
92	2-Cyclopenten-1-one, 3-methyl-	96	C_6H_8O	13.38
92	Phenol	94	C_6H_6O	13.70
93	2-Cyclopenten-1-one, 2,3-dimethyl-	110	$C_7H_{10}O$	14.96
94	Phenol, 3-methyl-	108	C_7H_8O	15.23
94	Phenol, 2-methyl-	108	C_7H_8O	15.61

94	Benzofuran, 2-methyl-	132	C_9H_8O	16.36
95	Phenol, 2,5-dimethyl-	122	$C_8H_{10}O$	17.00
89	1H-Indene, 3-methyl-	130	$C_{10}H_{10}$	17.13
90	Phenol, 3,4-dimethyl-	122	$C_8H_{10}O$	17.31
83	Phenol, 2,3-dimethyl-	122	$C_8H_{10}O$	17.53
86	Phenol, 2,4-dimethyl-	122	$C_8H_{10}O$	17.78
80	Catechol	110	$C_6H_6O_2$	17.86
89	Benzofuran, 4,7-dimethyl-	146	$C_{10}H_{10}O$	18.26
83	Hydroquinone	110	$C_6H_6O_2$	19.01
90	Resorcinol	110	$C_6H_6O_2$	19.18
92	1H-Inden-1-one, 2,3-dihydro-	132	C_9H_8O	19.45
84	1,4-Benzenediol, 2-methyl-	124	$C_7H_8O_2$	20.16
84	2-Methyl-5-hydroxybenzofuran	148	$C_9H_8O_2$	21.23
81	Benzaldehyde, 2,4,5-trimethyl-	148	$C_{10}H_{12}O$	21.40
80	1,4-Benzenedicarboxaldehyde, 2,5-dimethyl-	162	$C_{10}H_{10}O_2$	22.68
82	1-Naphthalenol, 2-methyl-	158	$C_{11}H_{10}O$	24.25

Table S4. Compounds evolving during the stepwise pyrolysis of the iron-loaded carbon material at 300 °C.

Similarity	Compound name	Molar mass [g/mol]	Sum formula	Retention time [min]
	CO, H_2O, CO_2	18, 28, 44		3.06
81	2,5-Dimethyl-4-hydroxy-3(2H)-furanone	128	$C_6H_8O_3$	15.96
92	Levoglucosenone	126	$C_6H_6O_3$	16.73
84	Heptanal	114	$C_7H_{14}O$	17.93

94	1,4:3,6-Dianhydro-α-d-glucopyranose	144	$C_6H_8O_4$	18.38
91	5-Hydroxymethylfurfural	126	$C_6H_6O_3$	18.56
80	2-Butene-1,4-diol	88	$C_4H_8O_2$	18.96
80	β-d-Ribopyranoside, methyl, 3-acetate	206	$C_8H_{14}O_6$	23.36
80	β-D-Glucopyranose, 1,6-anhydro-	162	$C_6H_{10}O_5$	25.76
91	1,6-Anhydro-β-D-glucofuranose	162	$C_6H_{10}O_5$	26.45

Table S5. Compounds evolving during the stepwise pyrolysis of the iron-loaded carbon material at 400 °C.

Similarity	Compound name	Molar mass [g/mol]	Sum formula	Retention time [min]
	CO, H_2O, CO_2	18, 28, 44		3.06
82	Furan, 2-methyl-	82	C_5H_6O	4.33
89	Furan, 2,5-dimethyl-	96	C_6H_8O	6.48
80	2(5H)-Furanone	84	$C_4H_4O_2$	8.93
82	2-Heptanone, 3-methyl-	128	$C_8H_{16}O$	10.61
88	2(3H)-Furanone, 5-methyl-	98	$C_5H_6O_2$	10.93
85	4-Cyclopentene-1,3-dione	96	$C_5H_4O_2$	11.37
91	Ethanone, 1-(2-furanyl)-	110	$C_6H_6O_2$	12.06
88	1,2-Cyclopentanedione	98	$C_5H_6O_2$	12.41
89	2(5H)-Furanone, 5-methyl-	98	$C_5H_6O_2$	12.71
90	2-Furancarboxaldehyde, 5-methyl-	110	$C_6H_6O_2$	13.23
85	1,4-Cyclohexanedione	112	$C_6H_8O_2$	14.47
94	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	112	$C_6H_8O_2$	14.78
83	2-Cyclopenten-1-one, 2,3-dimethyl-	110	$C_7H_{10}O$	15.00

88	Phenol, 2-methyl-	108	C_7H_8O	15.26
88	Phenol, 3-methyl-	108	C_7H_8O	15.66
80	2,5-Dimethyl-4-hydroxy-3(2H)-furanone	128	$C_6H_8O_3$	15.86
88	Levoglucosenone	126	$C_6H_6O_3$	16.41
83	But-1-ene-3-yne, 1-ethoxy-	96	C_6H_8O	16.93
81	Heptanal	114	$C_7H_{14}O$	17.80
93	Catechol	110	$C_6H_6O_2$	17.96
89	1,4:3,6-Dianhydro-α-d-glucopyranose	144	$C_6H_8O_4$	18.25
92	2-Coumaranone	134	$C_8H_6O_2$	18.63
82	1H-Inden-1-one, 2,3-dihydro-	132	C_9H_8O	19.46
85	Ethanone, 1-(3-hydroxyphenyl)-	136	$C_8H_8O_2$	21.11
85	2-Methyl-5-hydroxybenzofuran	148	$C_9H_8O_2$	21.45
80	β-D-Glucopyranose, 1,6-anhydro-	162	$C_6H_{10}O_5$	23.70
80	1,6-Anhydro-β-D-glucofuranose	162	$C_6H_{10}O_5$	24.63

Table S6. Compounds evolving during the stepwise pyrolysis of the iron-loaded carbon material at 500 °C.

Similarity	Compound name	Molar mass [g/mol]	Sum formula	Retention time [min]
	CO, H_2O, CO_2	18, 28, 44		3.06
95	Furan, 2,5-dimethyl-	96	C_6H_8O	6.46
89	2-Cyclopenten-1-one	82	C_5H_6O	9.96
92	p-Xylene	106	C_8H_{10}	11.00
96	2-Cyclopenten-1-one, 2-methyl-	96	C_6H_8O	11.91
87	2-Cyclopenten-1-one, 3-methyl-	96	C_6H_8O	13.38

97	Phenol	94	C_6H_6O	13.73
80	Benzene, 1,2,4-trimethyl-	120	C_9H_{12}	14.00
92	2-Cyclopenten-1-one, 2,3-dimethyl-	110	$C_7H_{10}O$	14.96
95	Phenol, 3-methyl- Methylphenol	108	C_7H_8O	15.23
89	Phenol, 2-methyl-	108	C_7H_8O	15.61
94	Benzofuran, 2-methyl-	132	C_9H_8O	16.35
95	Phenol, 2,5-dimethyl-	122	$C_8H_{10}O$	16.98
90	1H-Indene, 3-methyl-	130	$C_{10}H_{10}$	17.13
94	Phenol, 3,4-dimethyl-	122	$C_8H_{10}O$	17.31
84	Phenol, 2,3-dimethyl-	122	$C_8H_{10}O$	17.55
88	Phenol, 2,4-dimethyl-	122	$C_8H_{10}O$	17.80
90	Catechol	110	$C_6H_6O_2$	17.86
91	Benzofuran, 4,7-dimethyl-	146	$C_{10}H_{10}O$	18.28
83	1,2-Benzenediol, 3-methyl-	124	$C_7H_8O_2$	18.93
93	Resorcinol	110	$C_6H_6O_2$	19.25
95	1H-Inden-1-one, 2,3-dihydro-	132	C_9H_8O	19.46
82	Naphthalene, 1-methyl-	142	$C_{11}H_{10}$	19.70
80	1H-Inden-1-one, 2,3-dihydro-3,3-dimethyl-	160	$C_{11}H_{12}O$	19.85
87	1,4-Benzenediol, 2-methyl-	124	$C_7H_8O_2$	20.23
82	2-Methyl-5-hydroxybenzofuran	148	$C_9H_8O_2$	21.26
84	1,4-Benzenedicarboxaldehyde, 2-methyl-	148	$C_9H_8O_2$	21.45
86	1-Naphthalenol, 2-methyl-	158	$C_{11}H_{10}O$	24.28