

**Electrochemical performance of activated carbon fiber with hydrogen bond-induced high sulphur/nitrogen doping**

Chaohui Ruan, Yibing Xie\*

School of Chemistry and Chemical Engineering, Southeast University, Nanjing 211189, China

**Table S1** Elemental contents in S/N-CF, S/N-CF-O and S/N-ACF.

Samples	Surface element (at. %)				Surface content (at.%) of different N functionalities				Surface content (at.%) of different S functionalities		
	C	O	N	S	N-6	N-5	N-Q	N-O	S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>
S/N-CF	98.14	—	1.25	0.61	0.54	0.18	0.53	—	0.38	0.23	—
S/N-CF-O	90.40	7.37	1.45	0.78	0.43	0.55	0.09	0.38	0.17	0.46	0.15
S/N-ACF	88.77	3.71	4.36	3.16	1.26	1.75	0.67	0.68	1.30	1.28	0.58

Note: N-6 is pyridinic nitrogen; N-5 is pyrrolic nitrogen; N-Q is graphitic nitrogen; S<sub>1</sub> is thiophene-S<sub>2</sub>p<sub>3/2</sub>; S<sub>2</sub> is thiophene-S<sub>2</sub>p<sub>1/2</sub>; S<sub>3</sub> is the sulfur oxide.

**Table S2** Comparison of nitrogen and sulfur content of recently reported carbons with S/N co-doping.

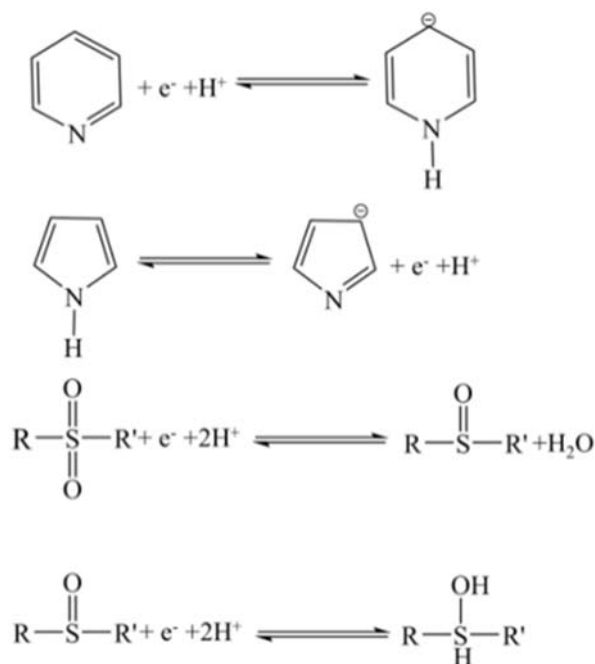
Samples	methods	N (At. %)	S (At. %)	Ref.
N/S Co-Doped Graphene Hydrogel	Graphene, (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> and melamine at 600 °C	2.86	0.07	<sup>1</sup>
N/S Self-Doped Activated Carbon	Pretreated elm flowers at 700 °C for 1h	2.61	0.8	<sup>2</sup>
N/S Co-Doped Graphene Hydrogel	Hydrothermal treatment of TU and GO	2.5	1.2	<sup>3</sup>
Porous Carbon	Glucose, NaHCO <sub>3</sub> and TU at 700 °C for 2h	3.42	0.2	<sup>4</sup>
S-RGO	H <sub>2</sub> SO <sub>4</sub> , H <sub>2</sub> O <sub>2</sub> and graphite at 1000 °C for 2h	-	1.47	<sup>5</sup>
CFC-750-N-S	LiNO <sub>3</sub> , Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub> and CFC at 1000 °C for 2h	2.72	1.84	<sup>6</sup>
N/S co-doped carbon nanosheets	C15 powders and TU at 800 °C for 3h	1.7	2.6	<sup>7</sup>
S/N-ACF	TU and CF-OH at 1000 °C for 2h	<b>4.36</b>	<b>3.16</b>	This work

**Table S3** Summary of calculated results: the binding energy ( $E_b$ ), the distance of TU to C<sub>32</sub> or hydrogen bond (d).

Configurations	Binding site	$E_b$ (eV)	d (Å)
TU/C <sub>32</sub>	N	0.73	3.08
TU/C <sub>32</sub> -O	H	0.79	1.78
TU/C <sub>32</sub> -OH	H	1.46	1.86
	S		1.40

**Table S4** Fitting values of the equivalent circuit elements for S/N-CF, S/N-CF-O and S/N-ACF.

Samples	$R_o$ ( $\Omega$ )	$R_{ct}$ ( $\Omega$ )	CPE			$W_o$	
			$CPE_T$	$CPE_P$	$W_R$	$W_T$	$W_P$
S/N-CF	2.36	0.82	0.33	0.83	2.97	2.01	0.48
S/N-CF-O	4.15	4.83	0.35	0.81	1.94	1.32	0.47
S/N-ACF	1.36	0.72	0.51	0.97	1.35	1.20	0.49

**Fig. S1** Redox reaction of S, N compounds.

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