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Electronic Supplementary Information

Graphitic Sulphur Functionalized Carbon Sheets as an Efficient "Turn-Off" Absorption Probe for the Optical Sensing of Mercury Ions in Aqueous Solutions

Vishal Bharati Jaryal[a], Dilbag Singh[b], and Neeraj Gupta [a]*

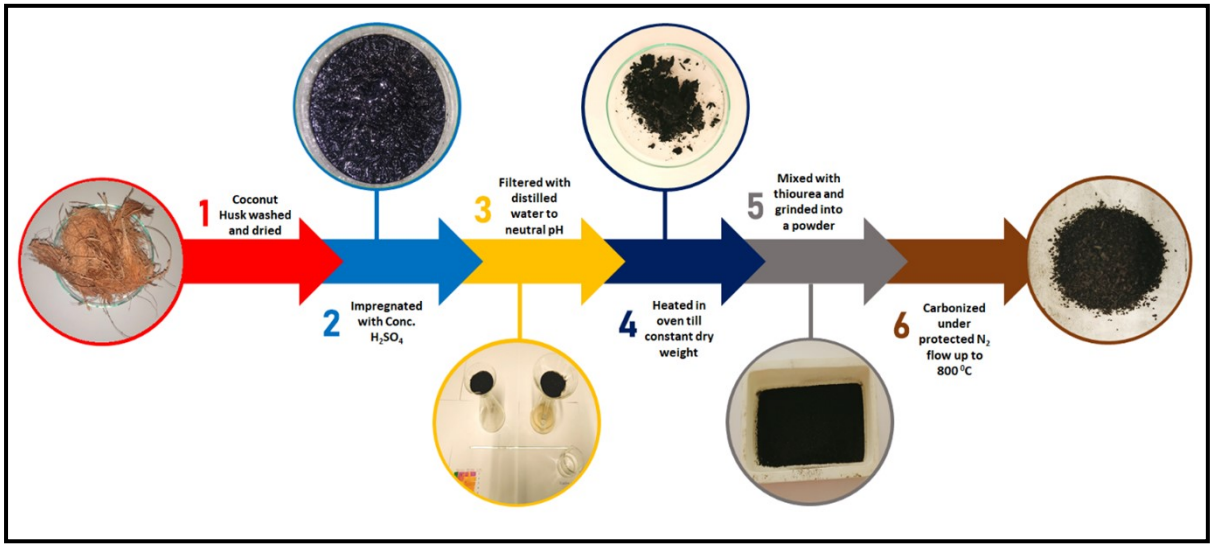

Fig. S-1 The schematic representation of preparation of g-SFCSs.

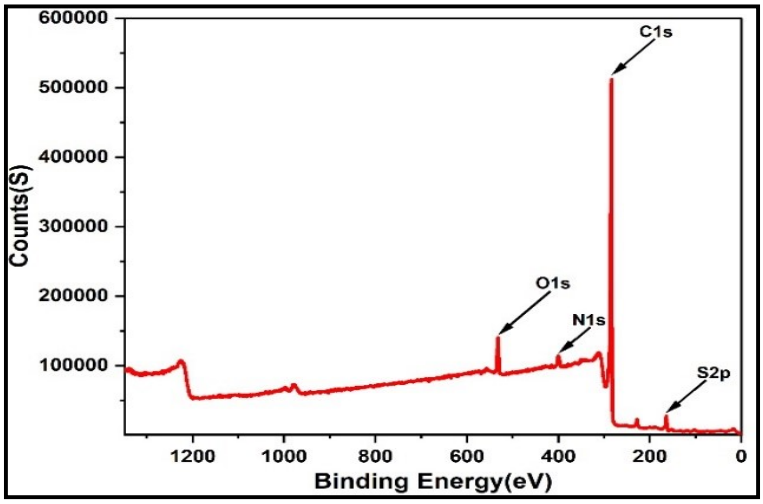

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Fig. S-2 XPS Survey spectrum of g-SFCSs.

Table S-1 Elemental peak table of XPS analysis of g-SFCSs.

S.No.	Element	Peak B.E. (eV)	Atomic%
1.	C1s	284.48	90.44
2.	O1s	532.41	4.91
3.	N1s	399.81	2.57
4.	S2p	164.19	2.08

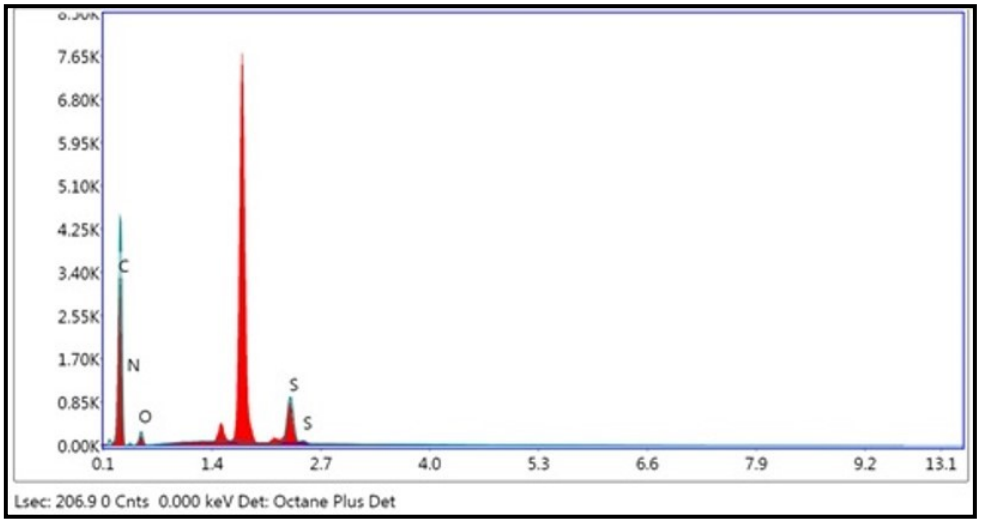

Fig. S-3 EDX analysis of g-SFCSs.

Table S-2 Elemental peak table of EDX analysis of g-SFCSs.

Element	Weight %	Atomic %	Net Int.	Error %	K ratio	Z	R	A	F
C K	78.76	84.40	177.20	6.81	0.37	1.01	0.99	0.46	1
N K	5.67	5.21	1.93	20.09	0.00	0.99	1	0.07	1
O K	10.27	8.26	12.54	13.09	0.01	0.97	1.01	0.11	1

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S K	5.29	2.13	77.32	2.22	0.05	0.86	1.06	1.01	1

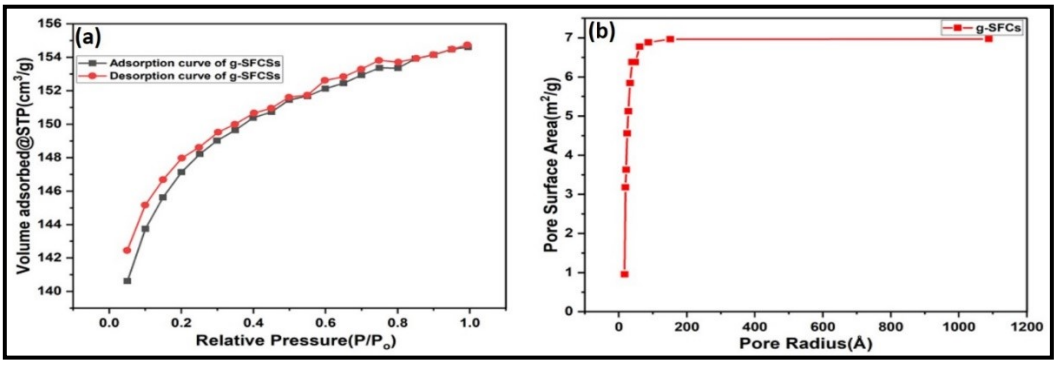

Fig. S-4 (a) Nitrogen adsorption – desorption isotherm of g-SFCSs, (b) Pore size distribution of g-SFCSs

Experimental

Materials and Chemicals Used

The raw material (coconut husk) required for the preparation of activated carbon was purchased from market near the campus area of Central University of Himachal Pradesh, Dharamshala, Himachal Pradesh – 176215, India. All the chemicals used in the whole process of synthesis of AC were of analytical grade. Low ash content present in coconut husk serves as the best precursor for preparing activated carbon. Coconut husk was chemically activated using concentrated sulfuric acid (analytical grade) purchased from Thermo Fischer Scientific India Pvt. Ltd. 403 - 404, B - Wing, Delphi, Hiranandani, Business Park, Powai, Mumbai - 400 076.

Characterization

X–ray photoelectron spectroscopy was performed on Thermofischer Scientific Nexsa Base model. X–ray diffraction pattern was analyzed by using Powdered X – ray diffractometer, Smart Lab model (Rigaku) in the angular range from 5.00^0 to 79.98^0. The Bragg's equation (1) was used to calculate interlayer spacing (d), the degree of graphitization (g) was calculated with the help of Franklin equation (2) and the crystallite size (D) was evaluated using Scherrer equation (3).(Cameán et al., 2010)

$$d = \frac{n\lambda}{2\,Sin\theta} \quad (1)$$

$$g = \frac{0.3440 - d}{0.3440 - 0.3354} \times 100\% \quad (2)$$

$$D = \frac{k\lambda}{\beta\,Cos\theta} \quad (3)$$

Where; n=1 (Order of diffraction), λ=0.15406 nm (Wavelength of incident X-rays), Θ = Bragg's angle analogous to the diffraction peak, ƙ=0.9 (Scherrer constant), β = Full Width at Half Maximum (FWMH) of the diffraction peak.

The average pore diameter, specific surface area and total pore volume of adsorbent were evaluated with the help of nitrogen adsorption – desorption isotherm method using an Autosorb IQ, Quatachrome instrument, version 5.21. The BET method was adopted for calculating the specific surface area. The surface characteristics were elucidated by using a Fourier

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transform infrared spectrometer, Bruker ALPHA ECO – ATR 24 V & 2.0 A, Made in Germany. The spectra were scanned 10 – 15 times within the 400 – 4000 cm^{-1} range at room temperature. UV-Vis absorption spectra were recorded using Analytik Jena (Made in Germany) SPECORD 200 PLUS UV-Vis Spectrometer using 3.5 mL quartz cuvette of 10 mm path length with 1 mm resolution in wavelength range of 200-800 nm. The investigation of material size, morphology and topography were done using FE-SEM and EDS. The prepared sample of g-SFCSs was place in the specimen chamber and SEM images were captured using Nova Nano SEM-450, JFEI Company of USA (S.E.A.) PTE LTD at an accelerating voltage of 20 kV. The analysis of SEM images obtained was performed using the software image J. The instrumentation facility at IIT Mandi was used for the analysis purpose.

"Turn-Off" detection of Mercury (II)

Different concentrations of Hg^{2+} ions (49 µM) were added into 3 mL of g-SFCSs dispersion prepared in a 1:1 mixture of EtOH and de-ionized water. After that, the mixture solutions were left undisturbed at RT for about 1 minute to ensure maximum complexation of Hg^{2+} ions with the active sites of g-SFCSs. UV-Vis Spectrophotometer was used to record the absorption spectra within UV-Vis range of 200-800 nm at a speed of 20 nm/sec and an integration time of 0.05 sec.

Selectivity study of g-SFCSs towards Hg^{2+}

To investigate the interference of Ca^{2+}, Mg^{2+} and Fe^{2+} ions during the absorption of Hg^{2+} by g-SFCSs, 3 mL of g-SFCSs dispersion was taken and its absorbance was noted after the addition of 700 µL (9.27 µM) Hg^{2+} metal ion solution. Afterwards, the absorption intensity of g-SFCSs was observed on the addition of 700 µL of equimolar (9.27 µM) concentration of different metal ions solutions (Ca^{2+}, Mg^{2+}) at the same conditions. The solution mixtures after the addition of different metal ions were left undisturbed for 1-2 minutes to ensure maximum complexation. All these experiments were performed at RT.

References

Cameán, I., Lavela, P., Tirado, J. L., & García, A. B. (2010). On the electrochemical performance of anthracite-based graphite materials as anodes in lithium-ion batteries. *Fuel*, *89*(5), 986–991. https://doi.org/10.1016/j.fuel.2009.06.034