

Supporting Information

Preparation and characterization of exfoliated graphene oxide-L-cystine as an effective adsorbent of Hg(II) adsorption

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Materials

The starting material, graphite used in the preparation of GO was procured from Sigma Aldrich. A stock solution of 1000 mg L⁻¹ Hg(II) solution was prepared using A. R. grade mercuric chloride and a working solution of 10 mg L⁻¹ for batch adsorption was prepared by appropriate dilution with Milli Q water, L-cystine was purchased from Fluka. The other required reagents were procured from Merck chemicals respectively.

Instruments and characterizations

Raman spectra were recorded on a WITec Confocal Raman Microscope Alpha 300R using a 532 nm He-Ne laser with 5 mW. Cross Polarization Magic Angle Spinning Nuclear Magnetic Resonance (¹³CPMAS-NMR) was analyzed Varian Innova Unity 500 MHz Solid State NMR Spectrometer by superconducting magnet 11.4 Tesla (Proton operating frequency : 500MHz). A Perkin Elmer Fourier Transform Infrared Spectroscopy (FT-IR) spectrum100 spectrometer was used to characterize the material functional groups identifications in the range 400–4000 cm⁻¹ by mixing 0.01g of the material with 0.1g KBr (spectroscopy grade). Kratos Axis Ultra X-ray Photoelectron

Spectroscopy (XPS) instruments were used to record samples, X-Ray Sources: 500 mm Rowland Circle Monochromator Al Mg/Al achromatic Source 450W max power. The spectra were recorded using a monochromatic Al K α X-ray source (15 mA, 14 KV). The pressure in the analyzer chamber was 1×10^{-8} Torr. The conditions applied for the survey scans includes an energy range 0-1200 eV and the survey spectra were collected at pass energy of 160 eV and a step size of 0.7 eV. High resolution spectra were collected using 40 eV pass energy, spot size of 300 x 700 μm slot and 0.05 eV step size. Ultraviolet visible spectroscopy (UV-visible) was taken out by the use Jasco V-630 UV-visible spectrometer (Jasco, Japan). X-ray diffraction (Pwder-XRD) was carried out on a D8 Discover X-ray diffractometer with Cu Ka radiation ($\lambda = 0.1541$ nm, Bruker, Germany) was utilized to record the characteristic changes in the diffraction pattern of the adsorbent material. A JEOL JSM-6330TF analyzer were used to observe the morphological changes scanning electron microscope(SEM) were recorded and the energy dispersive X-ray analysis spectrum (EDX) was recorded adsorbent and after the adsorption of Hg(II). The concentration of mercury in the aqueous solution was measured using inductively coupled plasma mass spectrometry (ICP-MS) Perkin-Elmer, Sciex- Elan DRC Plus, Software which we used Elan-6100 DRC PLUS respectively. The pH adjustments of the aqueous solutions were done using METTLER TOLEDO pH meter S20.

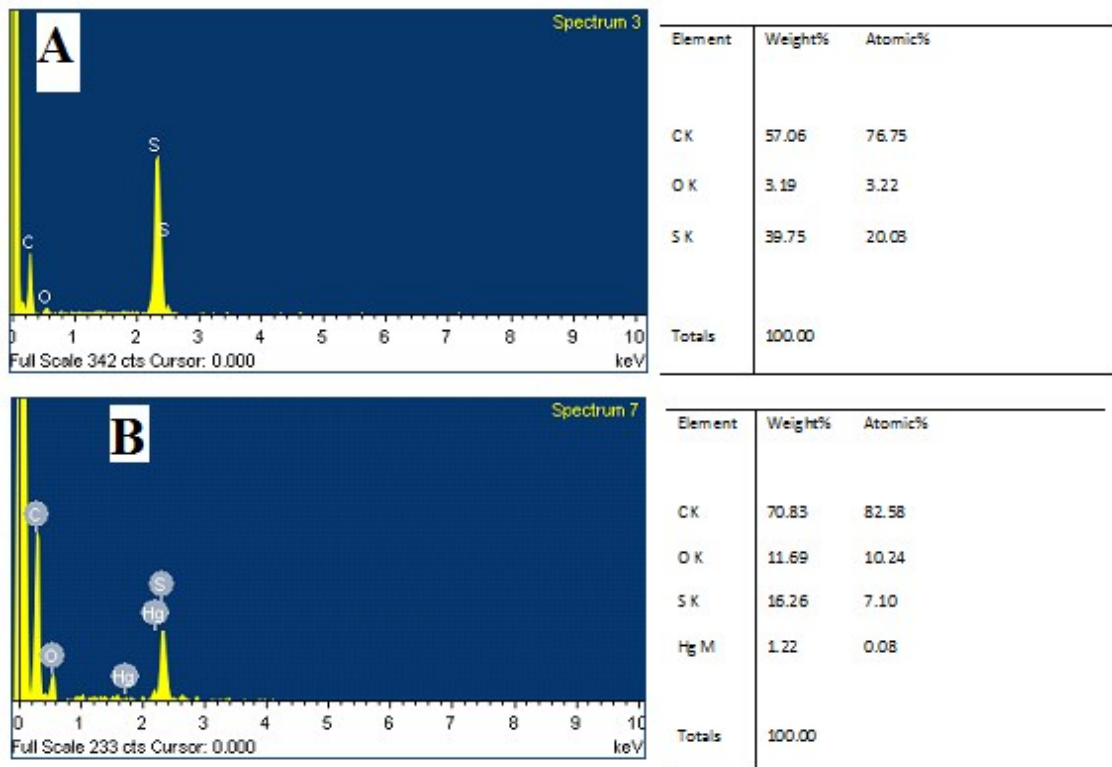


Fig. S1. EDX spectrum of the A) L-cysteine functionalized- EGO adsorbent (B) after adsorption of Hg(II) onto the adsorbent.

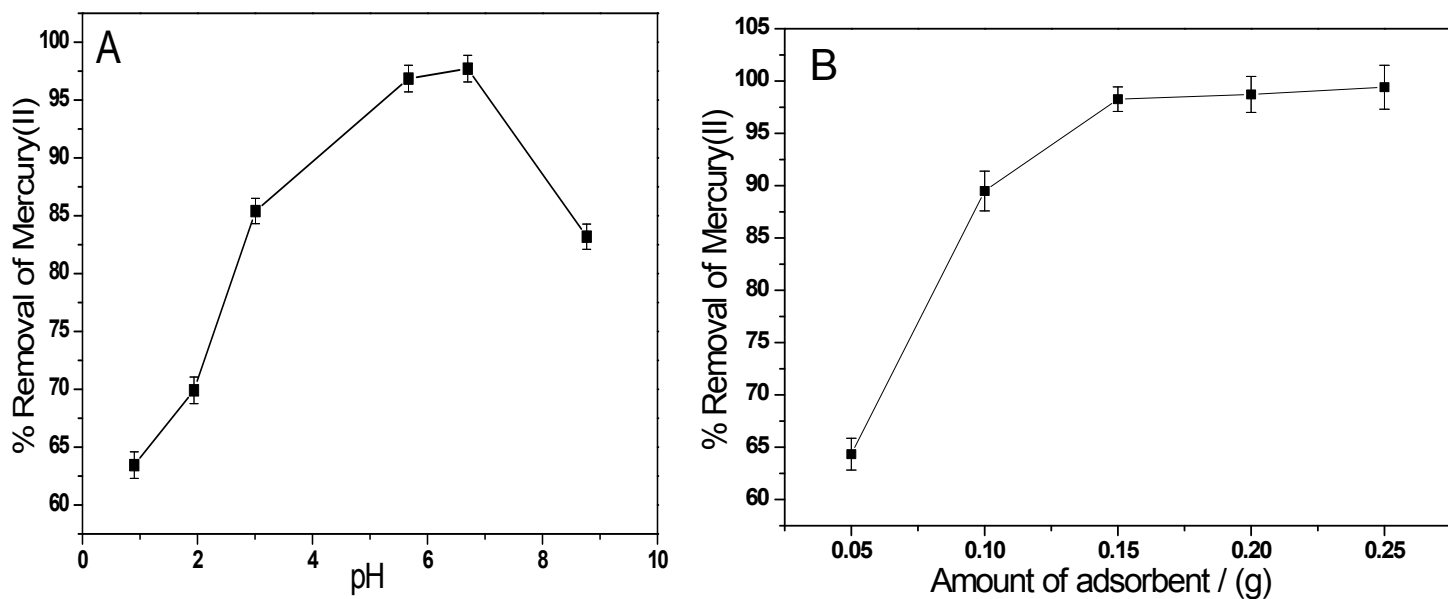


Fig. S2A. Effect of pH.

B) Amount of adsorbent

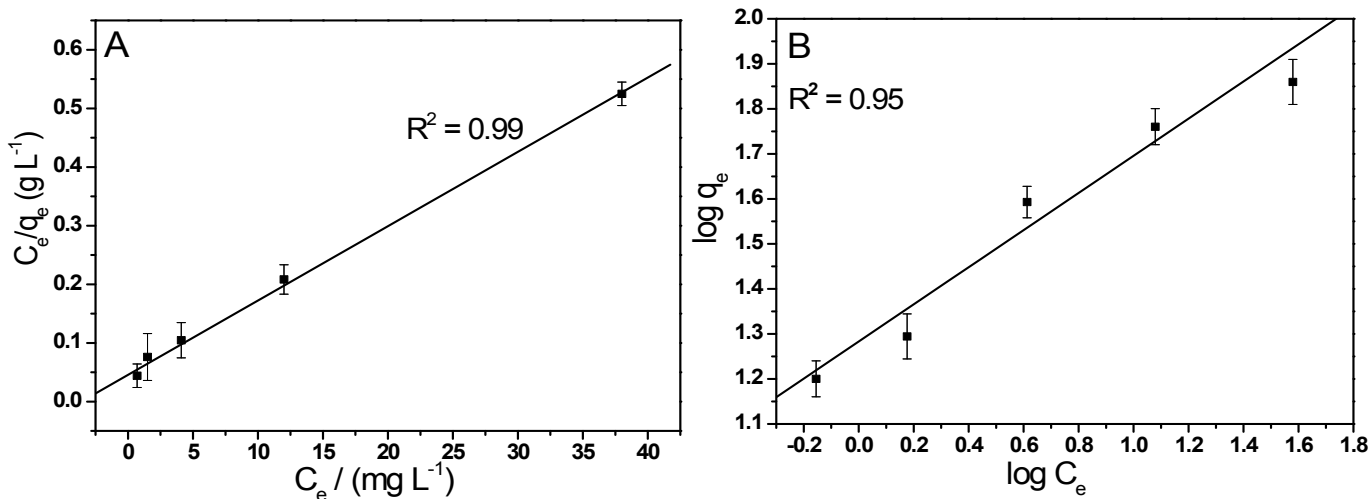


Fig. S3. A) Langmuir isotherm

B) Freundlich isotherm.

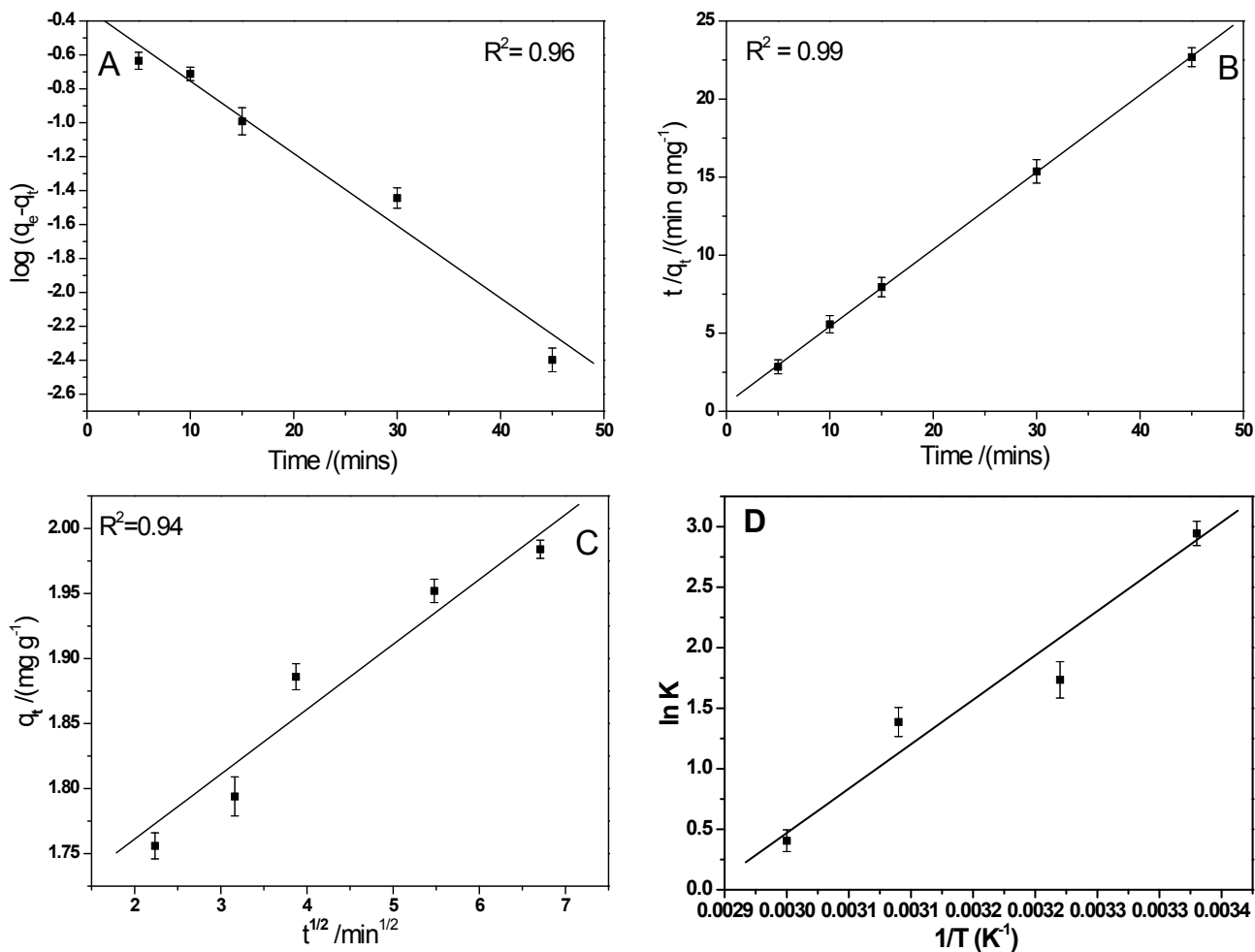


Fig. S4. Effect of (A) Pseudo first order kinetics (B) Pseudo second order kinetics (C) Variation of q_t against $t^{1/2}$ (Weber-Morris) plot (D) Van't Hoff Plot.

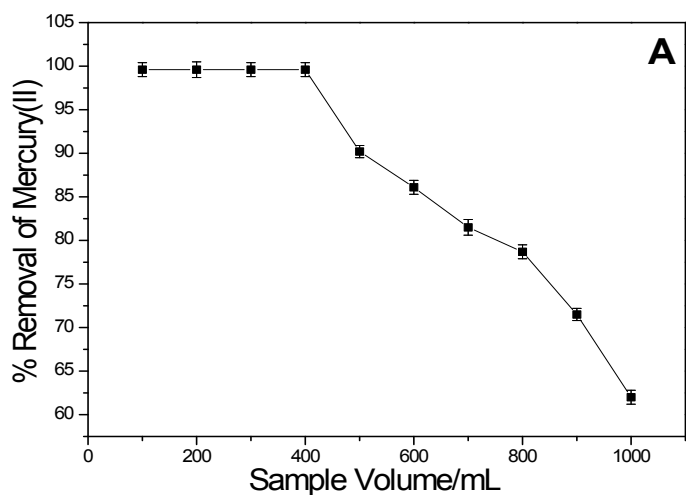
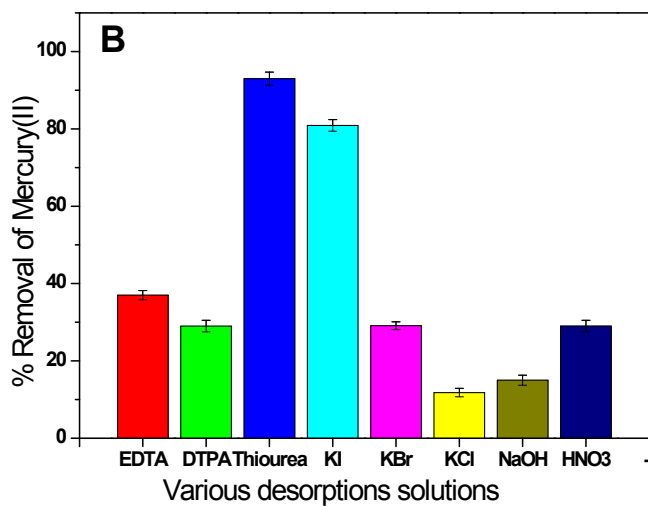


Fig. S5A Effect of sample volume



B) Effect of desorption studies.

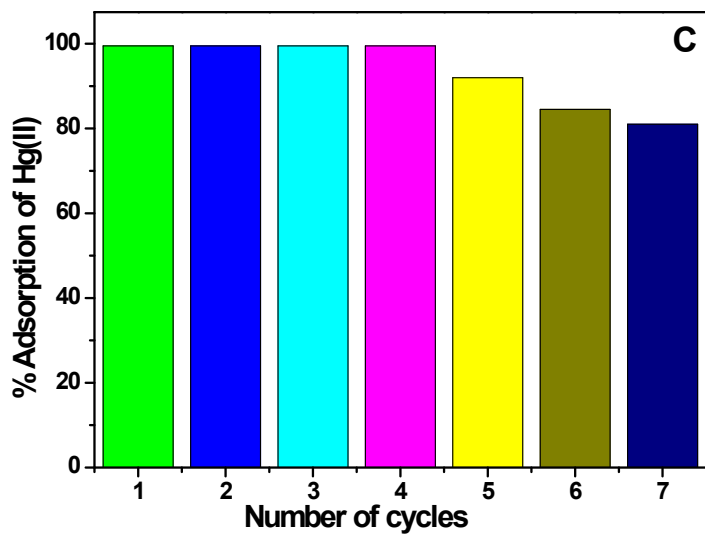


Fig. S5C Adsorbent regeneration cycles

Table T1 Operating conditions of ICP-MS analysis

Sl.No	ICP-MS plasma	Parameters
1	RF power	1300 W
2	Plasma gas (Ar) flow rate	15 L min ⁻¹
3	Auxiliary gas (Ar) flow rate	1.325 L min ⁻¹
4	Carrier gas (Ar) flow rate	0.97 L min ⁻¹
5	Sampler/skimmer diameter orifice	Nickel 1.0 mm/0.4 mm
6	Data acquisition scanning mode	Peak-hopping
7	Dwell time	50 ms
8	Points per spectral peak	1
9	Isotopes	²⁰² Hg
10	Integration mode	Peak area

Table T2. R_L values and type of equilibrium isotherms

Sl.No	R_L value	Nature of equilibrium isotherm
1	$R_L > 1$	Unfavorable
2	$R_L = 1$	Linear
3	$0 < R_L < 1$	Favorable
4	$R_L > 0$	Irreversible

Table T3 Isotherm parameters acquired from various models

Sl. No	Isotherm	Characteristic values	
1	Langmuir	q_0 (mg g ⁻¹)	79.36
		b (L mg ⁻¹)	0.27
		R_L	0.034
		r^2	0.99
2	Freundlich	K_F (mg ^{1-1/n} g ⁻¹ L ^{1/n})	19.1
		n	2.42
		r^2	0.95

Table T4 Adsorption kinetics

Rate constant k_2 /(g mg ⁻¹ min ⁻¹)	Regression coefficient	Rate constant k_1 / (min ⁻¹)	Regression coefficient	Intraparticle rate constant k_{int} /(mg g ⁻¹ min ^{-1/2})
0.50	0.99	0.067	0.96	0.049

Table T5. Thermodynamic parameters

Temperature/ (Kelvin)	q_e (mg g ⁻¹)	ΔG^0 / (kJ mol ⁻¹)	ΔS^0 / (J mol ⁻¹ K ⁻¹)	ΔH^0 / (kJ mol ⁻¹)
300	1.9	-7.34	-179.08	-60.99
310	1.7	-4.47		
323	1.6	-3.72		
333	1.2	-1.12		

Table T6 Effect of co-existing ions

Sample name	Co-existing ions	Concentration in mg L ⁻¹	(%) Removal of Hg(II)
Synthetic mixture - A	Ag, Al, As, Ba, Bi, Ca, Cd, Co, Cr, Cs, Cu, Ga, In, K, Li, Mg, Mn, Na, Ni, Pb, Rb, Se, Sr, Ti, U, V, Zn	10	80.0
Synthetic mixture - B	As, Cd, Co, Cu, Ni, Pb, Se, Zn, Au	100	91.0
Synthetic mixture -C	SO ₄ ²⁻ , NO ₃ ⁻ , PO ₄ ³⁻ , Cl ⁻	100	90.0