Supporting information

Sustainable approach for the sequestration of lead from water involving the synergistic influence of PET waste and L-Cysteine encapsulated in sodium alginate beads

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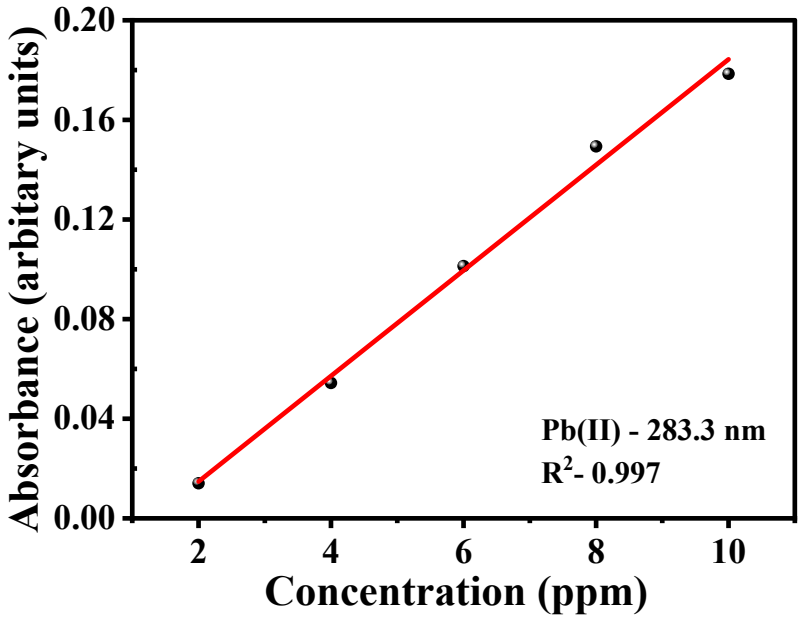

Fig S1. Linear Calibration plot of Lead from 2 ppm to 10 ppm

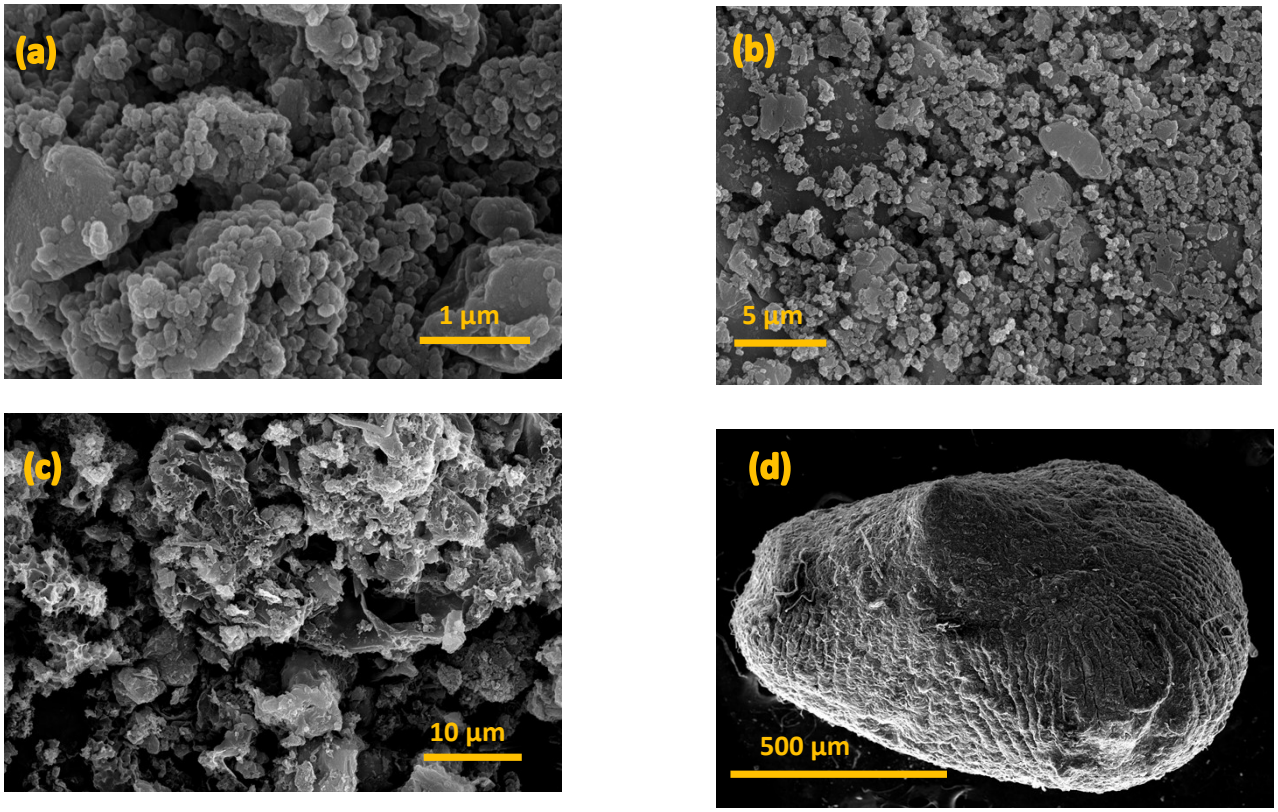

Fig S2. SEM images of NaOH-activated carbon (a-c), (d) Ox-carbon@cysteine-Na-Alg beads

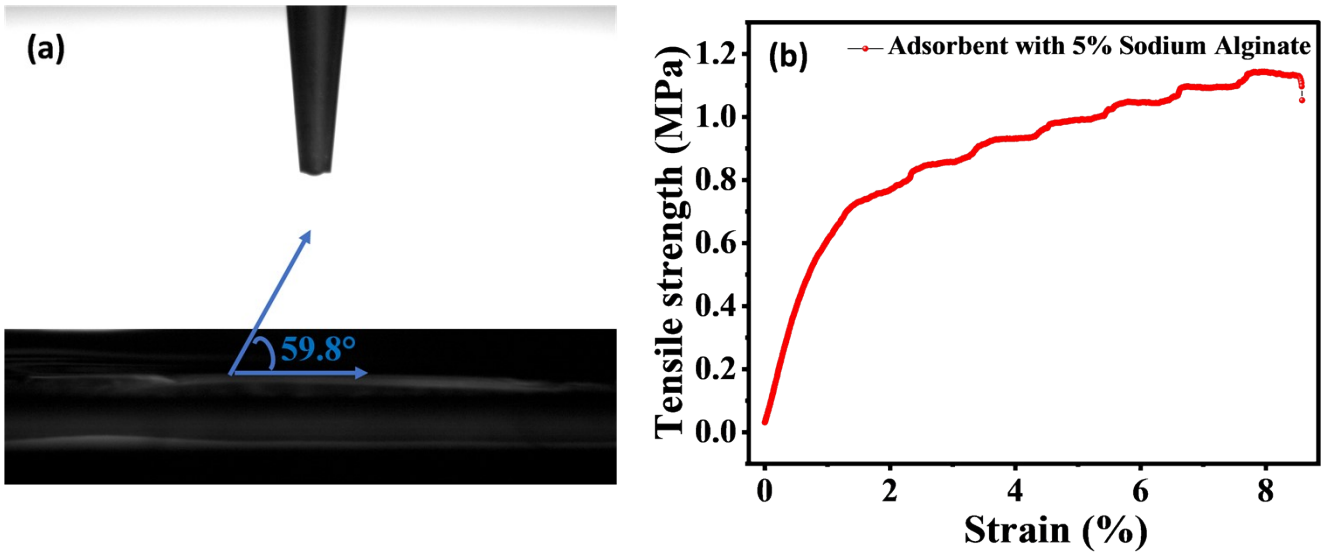

Fig S3. (a) Contact angle measurement of the adsorbent (b) Stress-Strain curve of the adsorbent.

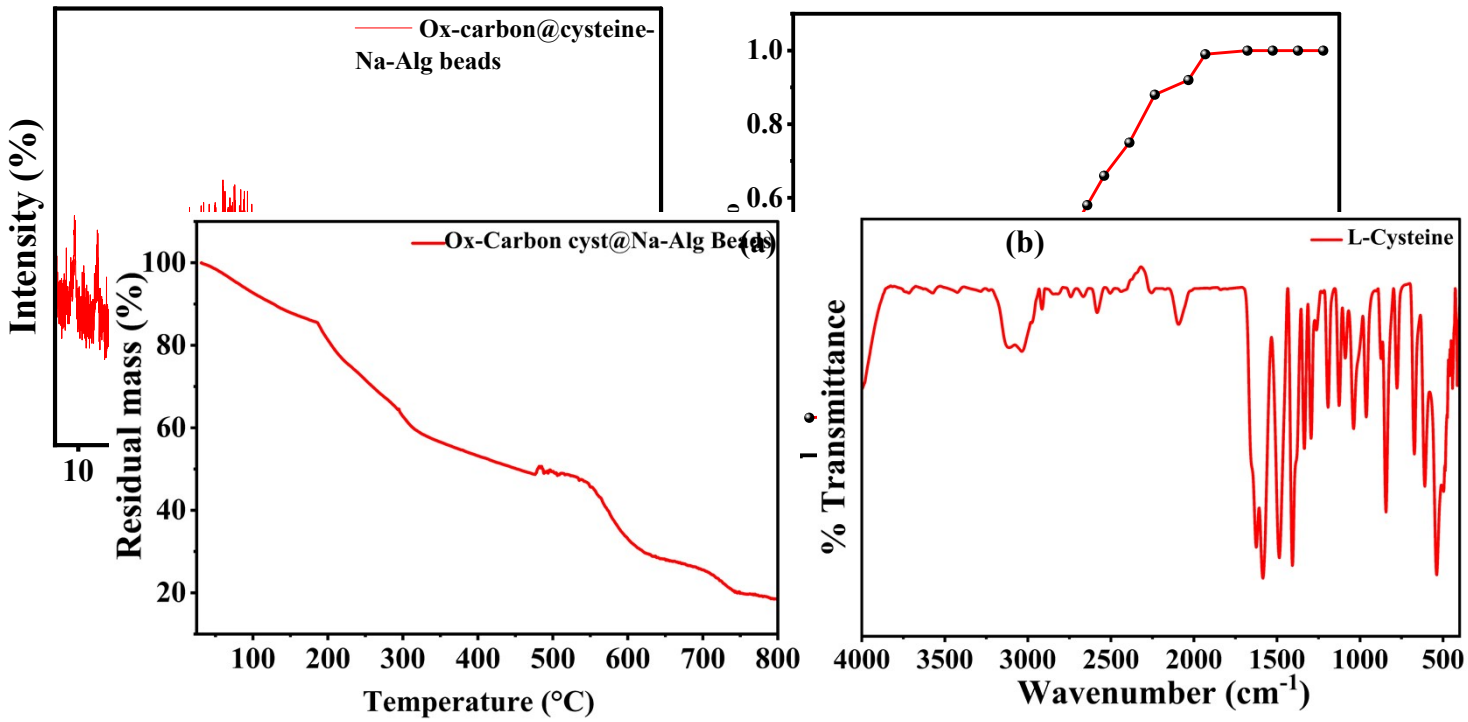

Fig S4. PXRD pattern of Ox-carbon@cysteine-Na-Alg beads and Breakthrough graph for fixed bed adsorption study.

Fig S5. (a) TGA curve of Ox-Carbon cyst@Na-Alg Beads (b) FTIR-Spectra of L-Cysteine.

S1. Molecular dynamics methodology

Molecular dynamics (MD) simulations were conducted to investigate the interaction of Pb^{2+} ions with the surface of the adsorbent featuring various chemical functionalities. The molecule model was constructed using Avogadro 2.[1] The carbonised PET was considered to have a structure similar to that of a disordered graphite, which was oxidized and functionalized with L-cysteine (Fig. S6). The disordered graphite sheet was constructed based on representative structural motifs that contain hydroxyl and carboxyl groups. Functionalization was modelled by grafting epichlorohydrin to the disordered graphite oxide surface and subsequently coupling L-cysteine.

The structure was parameterised using the CHARMM General Force Field (CGenFF).[2] Initial topologies were generated using CGenFF, reviewed for penalty scores, and converted to GROMACS-compatible formats via the standard cgenff-to-gromacs workflow. The resulting parameters were incorporated into the CHARMM36 force field framework.[3] The l-cysteine functionalised PET carbon model was placed at the centre of a cubic simulation box with a minimum of 1.0 nm between the sheet and the box boundaries, solvated with the SPC water model[4], represented water molecules, and added Pb^{2+} and neutralised by adding chloride ions using gmx genion.

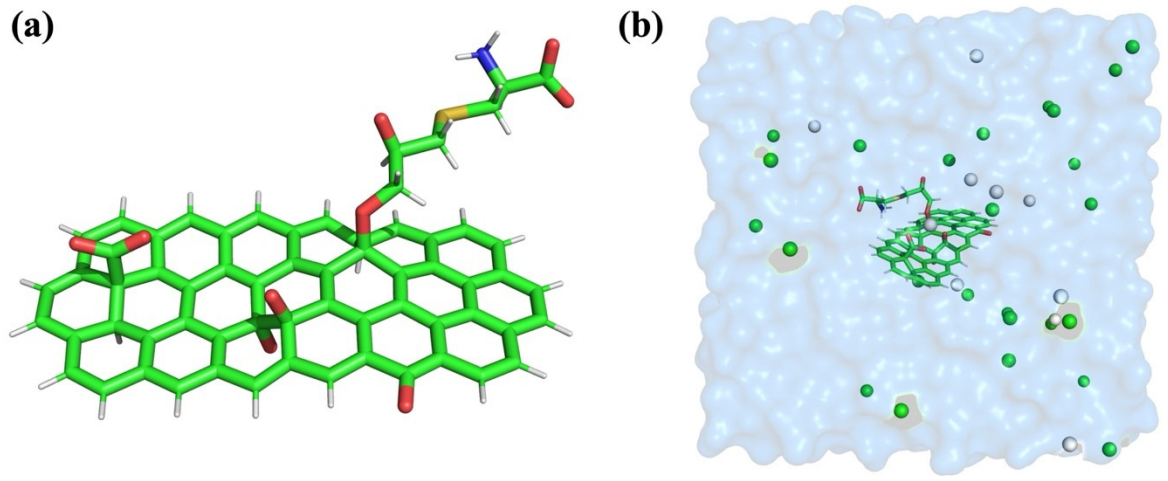

Fig. S6. (a) L-cysteine functionalised PET carbon (b) Simulation box consist of L-cysteine functionalised PET carbon along with lead ion, chloride and water.

All simulations were carried out using GROMACS 2024.4.[5] With GPU support, the PyMol software was utilised to visualise and analyse all trajectories. Energy minimisation was performed using the steepest descent algorithm until a maximum force of below 1000 kJ mol^{-1} nm^{-1} was reached. The minimised system was equilibrated in two stages: a 1 ns NVT equilibration at 300 K using the V-rescale thermostat, followed by a 1-2 ns NPT equilibration at 1 bar pressure using the Parrinello-Rahman barostat.[6] During the equilibration, heavy atoms of the disordered GO structures were position-restrained to allow solvent and ion relaxation. Production MD simulations were then run for 200 ns under NPT conditions (300 K, 1 bar). Long-range electrostatics were computed using the Particle Mesh Ewald (PME)

method,[7] while van der Waals interactions employed a 1.2 nm cutoff. All bonds involving hydrogen atoms were constrained using the LINCS algorithm, allowing for a 2 fs timestep.[8]

Table S1. Isotherm parameters for Lead adsorption

Isotherm models	**Isotherm parameters**	**Values**
Langmuir	q_{max} (mg g^{-1})	370.84
	K_L (L mg^{-1})	0.3371
	R^2	0.9778
Freundlich	K_F ($mg^{1-1/n}$ g^{-1} $L^{1/n}$)	24.322
	n	2.520
	R^2	0.978
Temkin	b_T (J mol^{-1})	40.110
	K_T (L g^{-1})	4.81 ×10^3
	R^2	0.9410
Sips	q_m (mg g^{-1})	646.2
	n	0.564
	K (L $mg^{-1})^n$	7.8039 E^{-4}
	R^2	0.9655

Table S2. Kinetic parameters for the adsorption of Lead.

Kinetics models	**Parameters**	**Values**
pseudo–first order	k_1 (min^{-1})	0.001
	q_{e1} (mg g^{-1})	102.329

	R^2	0.9469
pseudo-second order	k_2 (g mg^{-1} min^{-1}) q_{e2} (mg g^{-1}) R^2	0.002 159.6 0.978
Intra–particle diffusion	C_1 (mg g^{-1}) K_{i1} (mg g^{-1} min$^{1/2}$) R^2 C_2 (mg g^{-1}) K_{i2} (mg g^{-1} min$^{1/2}$) R^2	66.19 0.718 0.978 49.31 1.859 0.970

Table S3. Thermodynamic parameters (enthalpy, entropy, and free energy changes) for the adsorption of Lead.

Temperature (Kelvin)	ΔG° (kJ mol^{-1})	ΔH° (kJ mol^{-1})	ΔS° (kJ mol^{-1} K^{-1})	R^2
298.15 to 328.15	-31.442	-34.046	-0.017	0.997

Table S4. Comparision of Ox-carbon@cysteine, Ox-carbon@cysteine-Na-Alg beads, Ox-carbon-Na-Alg beads

Sl.No	**Material**	**Adsorption (%)**
1.	Ox-carbon@cysteine (50 mg, 10 ppm, 100 mL)	74.32
3.	Ox-carbon-Na-Alg beads (50 mg, 10 ppm, 100 mL)	82.60
2.	Ox-carbon@cysteine-Na-Alg beads (50 mg, 10 ppm, 100 mL)	92.40

Table S5. Fixed-bed column adsorption data

Model	Parameters	Values
Thomas	K_{Th} (mL $min^{-1}mg^{-1}$)	0.03
	q_o (mg g^{-1})	245.33
	R^2	0.932
Yoon-Nelson	K_{yn} (min^{-1})	0.03
	τ (min)	245.3
	R^2	0.935

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