Poly(ethyleneimine)-exfoliated g-C$_3$N$_4$ nanosheets implanted in alginate beads

and its application towards adsorptive desulfurization

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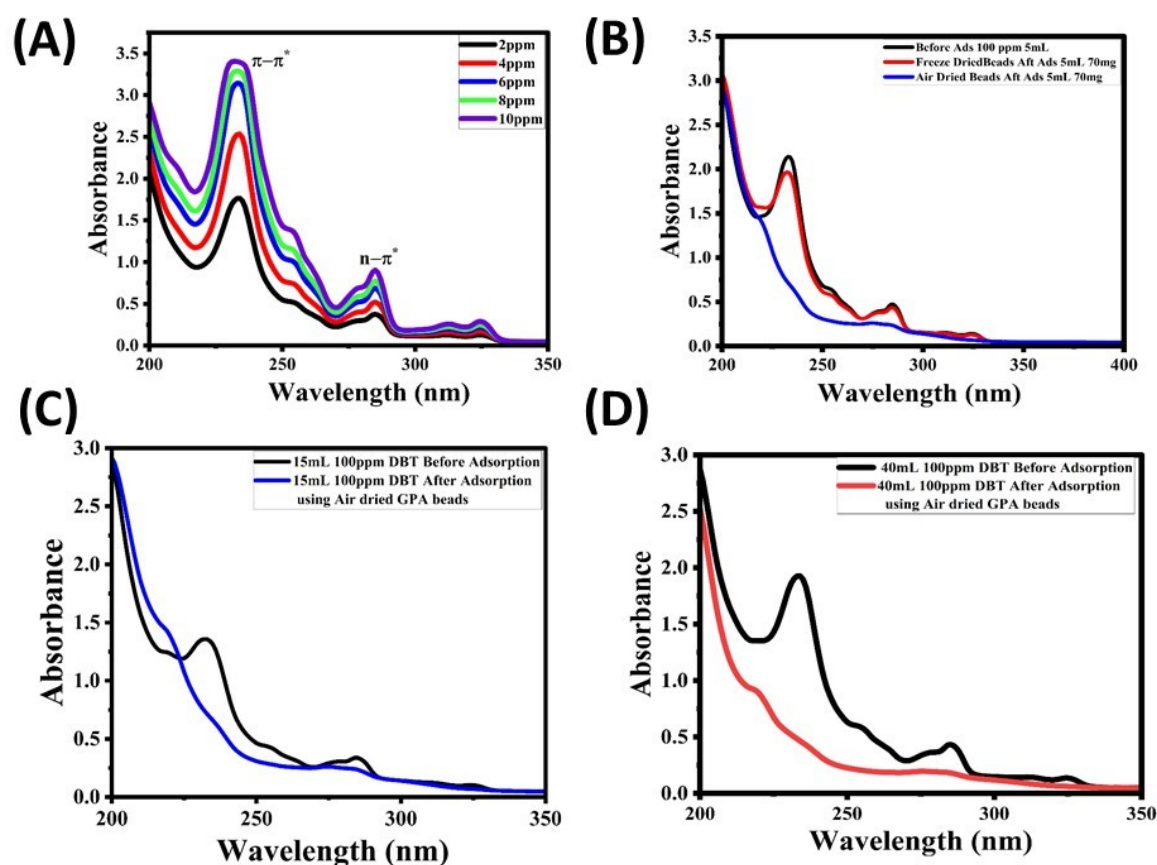
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Figure S1. (A) Absorption spectrum for DBT, **(B, C and D)** Absorbance of DBT before

and after adsorption at varying concentrations conditions in the presence of the as-prepared adsorbent of PEI exfoliated g-C_3N_4NSs@Cal-Alg alginate beads.

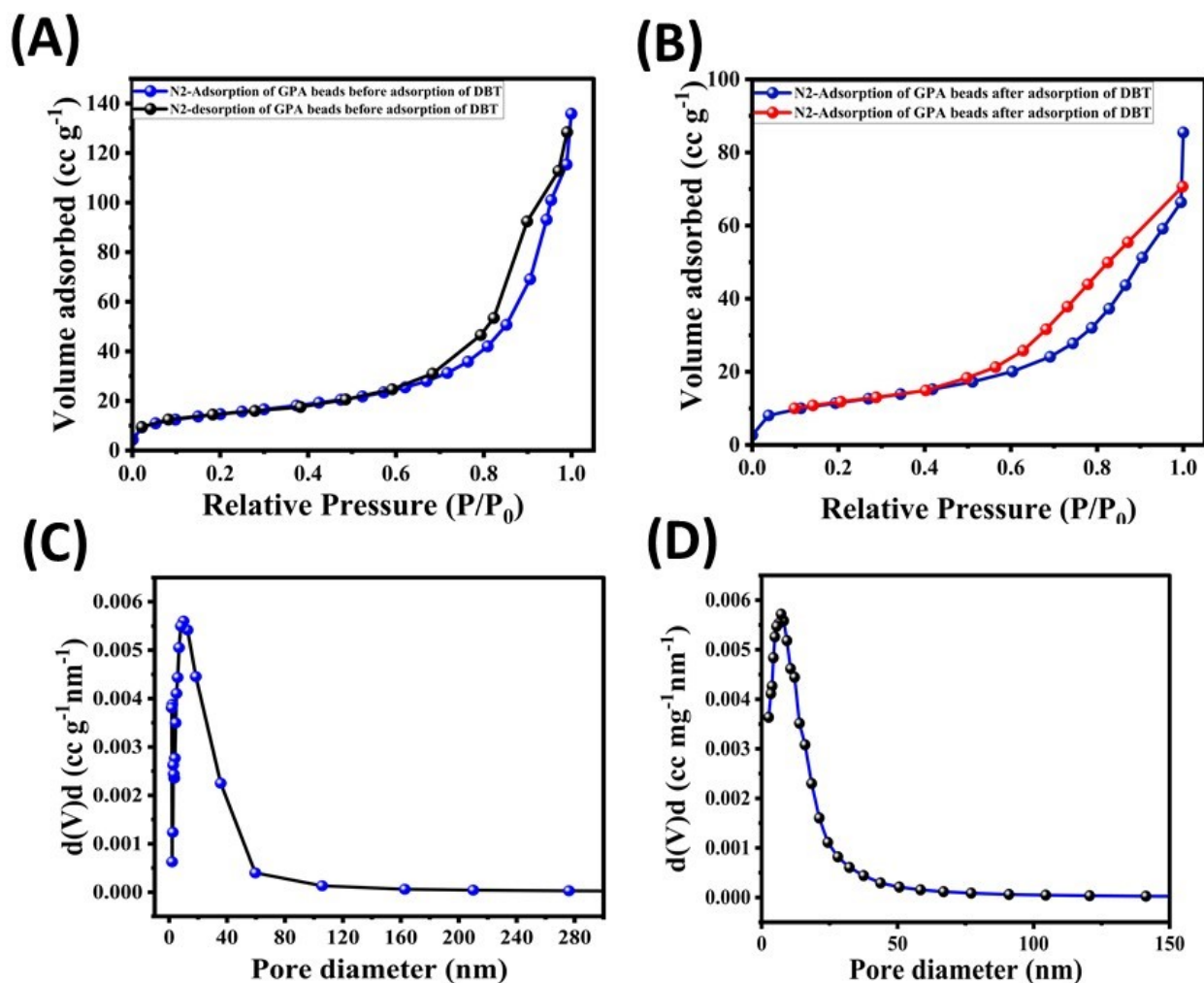**Figure S2.** The as-developed adsorbent of PEI-exfoliated g-C_3N_4NSs@Cal-Alg beads for N_2 adsorption-desorption isotherm **(A and B)** before and after adsorption of DBT; **(C and D)** BJH pore volume plot for before and after adsorption of DBT.

Figure S3. Field Emission Scanning Electron Microscopic (FE-SEM) images of the as-developed Ca-alginate beads functionalized with PEI-g-C_3N_4 NSs (PEI exfoliated g-C_3N_4NSs@alginate beads), **(A and B)** air dried Ca-Alg alginate beads, **(C and D)** Freeze dried Ca-alginate beads, **(E and F)** air dried alginate beads after adsorption of DBT, **(G)** EDX spectra and elemental composition of the as-developed Ca-alginate beads functionalized with PEI-g-C_3N_4 NSs (PEI exfoliated g-C_3N_4NSs@alginate beads) after adsorption of DBT.
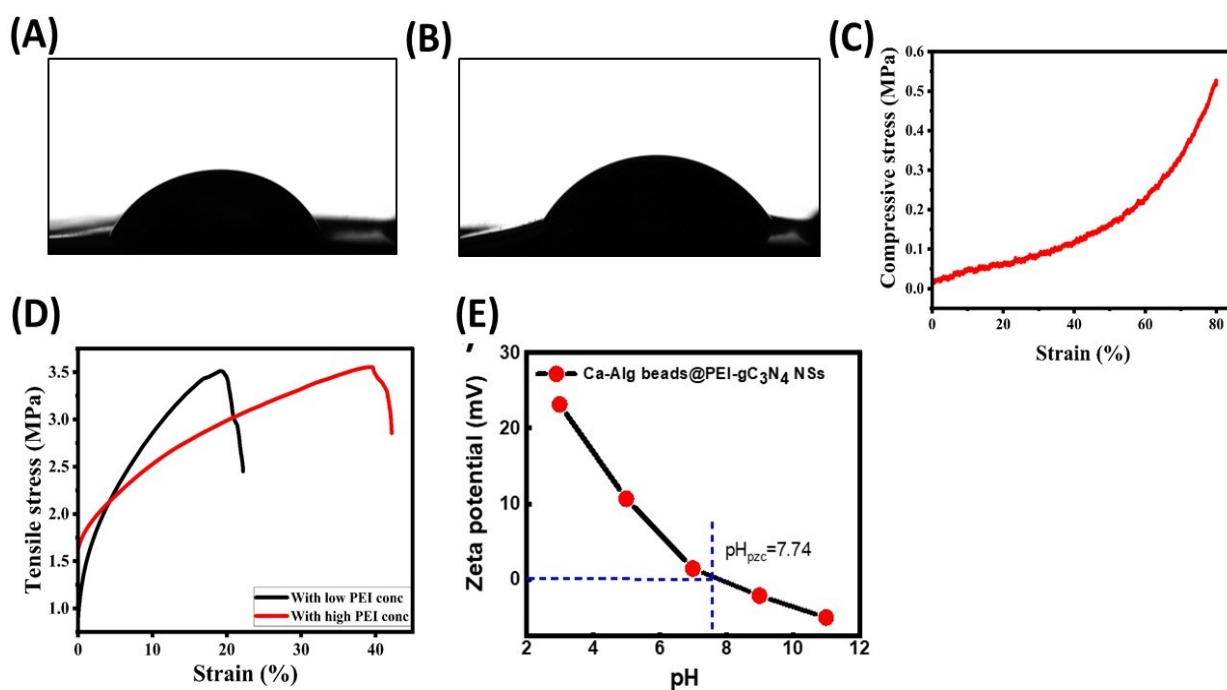

Figure S4. Contact angle images for calcium alginate beads (Ca-Alg beads) functionalized with PEI- g-C_3N_4 NSs for (A)before and (B) after adsorption of DBT; **(C)** compressive stress-strain curves for PEI-g-C_3N_4 NSs; **(D)** Tensile stress-strain curves for calcium alginate beads (Ca-Alg beads) functionalized with PEI- g-C_3N_4 NSs **(D)** with less concentration of PEI 5% (**D, black line**); a high concentration of PEI 15% concentration (**D, red line**); **(E)** Point of Zero Charge (pH$_{pzc}$) measurements of calcium alginate beads (Ca-Alg beads) functionalized with PEI- g-C_3N_4 NSs.
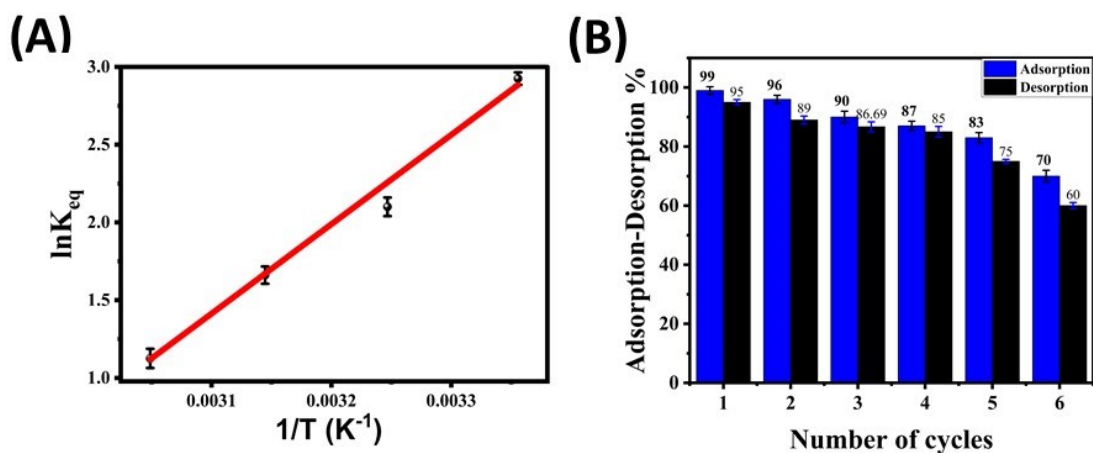
Figure S5. (A and B) The as-developed adsorbent of calcium alginate beads (Ca-Alg beads) functionalized with PEI-g-C_3N_4 NSs for thermodynamic adsorption using Van't Hoff plot for adsorption of DBT **(A);** Regeneration cycles for adsorption-desorption of DBT **(B).**

Table S1 BET-N_2 isotherm data for g-C_3N_4-PEI NSs@Cal-Alginate beads

No.	Type of material	Surface area m²g⁻¹	Pore diameter (nm)	Pore volume cm³g⁻¹	Volume of N₂ uptake in BET ccg⁻¹
1	g-C_3N_4-PEI NSs@Cal-Alginate beads **Before Adsorption**	142.06	13.80	0.182	135
2	g-C_3N_4-PEI NSs@Cal-Alginate beads **After Adsorption**	35.19	11.08	0.097	83

Table S2 Isotherm Parameters

Model of Isotherm	Non-linear equation	Type of adsorbent	Parameters	Values
Langmuir	$q_e = \dfrac{q_m b C_e}{1 + b C_e}$	PEI-g-C$_3$N$_4$-NSs	q_{max} (mg g^{-1})	**107.17**
			K$_L$ (L mg^{-1})	0.05
			R$_L$	0.166
			R^2	0.98
		PEI-g-C$_3$N$_4$ NSs@Ca-Alg beads	q_{max}	**183.03**
			K$_L$ (L mg^{-1})	0.011
			R$_L$	0.476
			R^2	0.98
Freundlich	$q_e = K_F C_e^{1/n}$	PEI-g-C$_3$N$_4$-NSs	K$_F$ (mg$^{1-1/n}$g^{-1} L$^{1/n}$)	6.62
			n	1.66
			R^2	0.89
		PEI-g-C$_3$N$_4$ NSs@Ca-Alg beads	K$_F$ (mg$^{1-1/n}$g^{-1} L$^{1/n}$)	2.19
			n	1.34
			R^2	0.95
Temkin	$q_e = \dfrac{RT}{b} \ln A C_e$	PEI-g-C$_3$N$_4$-NSs	b_T (J mol^{-1})	25.53
			K_T (L g^{-1})	5.44x10^{-2}
			R^2	0.96
		PEI-g-C$_3$N$_4$ NSs@Ca-Alg beads	b_T (J mol^{-1})	28.51
			K_T (L g^{-1})	4.35x10^{-2}
			R^2	0.91

Table S3 Kinetic and rate parameters

Kinetic models	Parameters	Values
Pseudo-first order	q_e (mg g^{-1})	42.02
	k_1 (min^{-1})	0.01
	R^2	0.981
Pseudo-second order	q_e (mg g^{-1})	58.16
	k_2 (min^{-1})	0.001
	R^2	0.987
Intra-particle diffusion	C_1 (mg g^{-1})	-0.49
	K_{i1} (mg g^{-1} min$^{1/2}$)	3.68
	R^2	0.99
	C_2 (mg g^{-1})	1.21
	K_{i2} (mg g^{-1} min$^{1/2}$)	2.74
	R^2	0.98
	C_3 (mg g^{-1})	10.39
	K_{i3} (mg g^{-1} min$^{1/2}$)	2.14
	R^2	0.99

Temperature (Kelvin)	ΔG^o (kJ mol^{-1})	ΔH^o (kJ mol^{-1})	ΔS^o (kJ mol^{-1} K^{-1})	R^2

			)		
298	-7.562	-47.797	-0.1364	0.991	**Table**
308	-5.561				**S4**
318	-4.392				**Therm**
328	-3.070				**odyna**

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Table S5 Fixed based column adsorptive desulfurization data

Models	**Parameters**	**Values**
Thomas model	q_o (mg g^{-1})	132.8
	K_{Th} (mL min^{-1} mg^{-1})	0.054
	R^2	0.947
Yoon-Nelson model	K_{yn} (min^{-1})	0.0534
	τ (min)	135
	R^2	0.932