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Supplementary Material

Carboxylated carbon nanotubes – graphene oxide aerogels as ultralight and renewable high performance adsorbents for efficient adsorption of glyphosate

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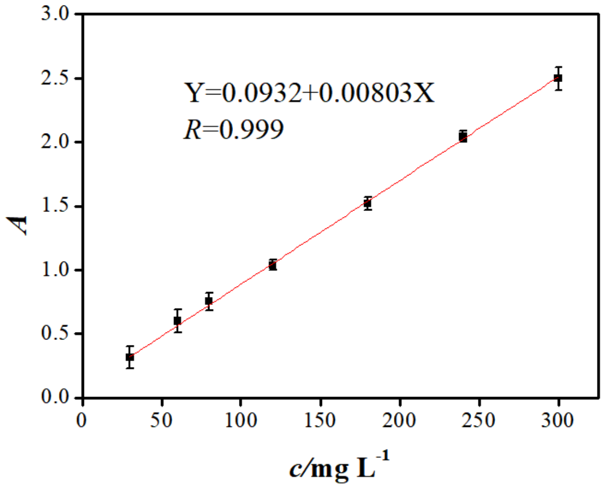

Fig.S1 The standard curve of glyphosate concentration

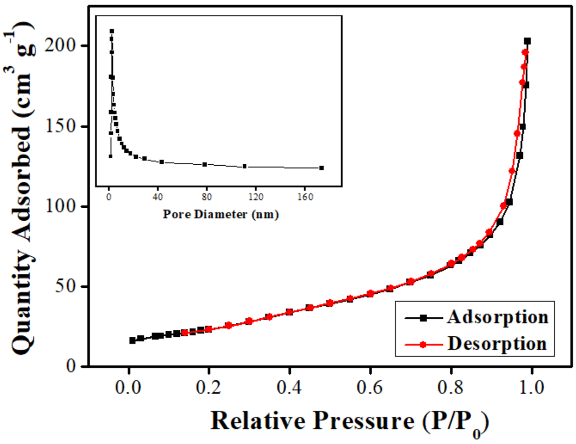

Fig.S2 Typical nitrogen adsorption-desorption isotherms for cCNTs with an inset of the pore size distribution curves.

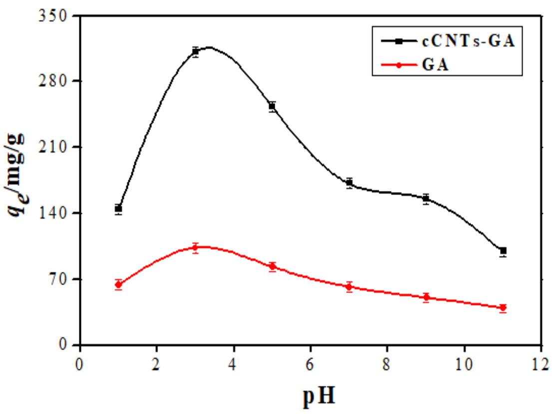

Fig.S3 Effects of pH value on the adsorption capacities of glyphosate on the cCNTs-GA and GA (T = 298 K)

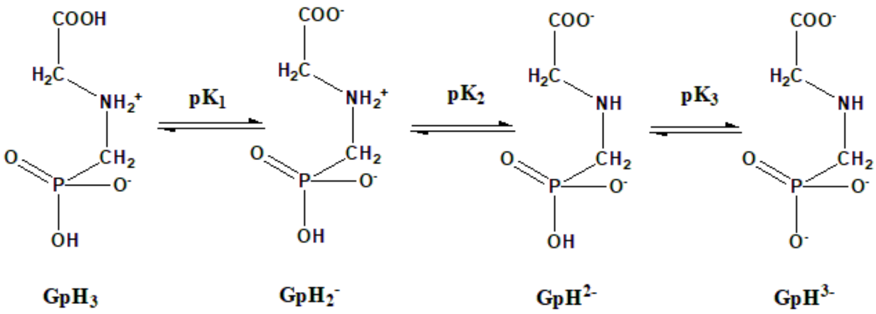

Fig.S4 Species of glyphosate depending on the pH value and protonation constants

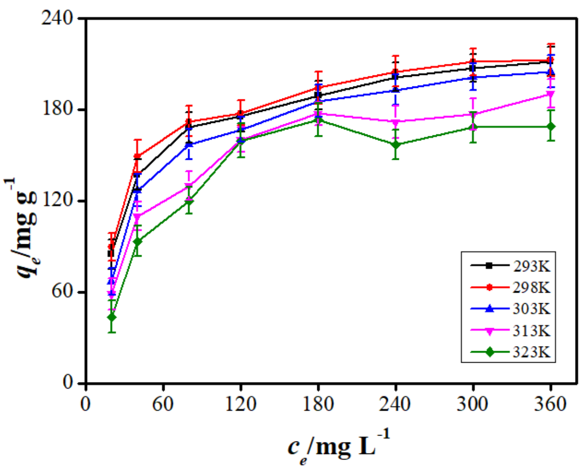

Fig.S5 Adsorption isotherm for glyphosate onto GA ($c_{adsorbent}$ = 0.14 g L^{-1}, pH = 3)

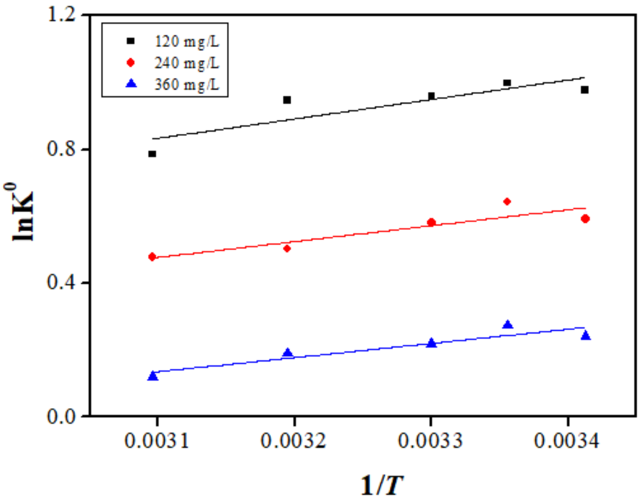

Fig.S6 Plots of $\ln K^0$ vs. 1/*T* for estimation of thermodynamic parameters of the adsorption of glyphosate at different equilibrium glyphosate concentrations

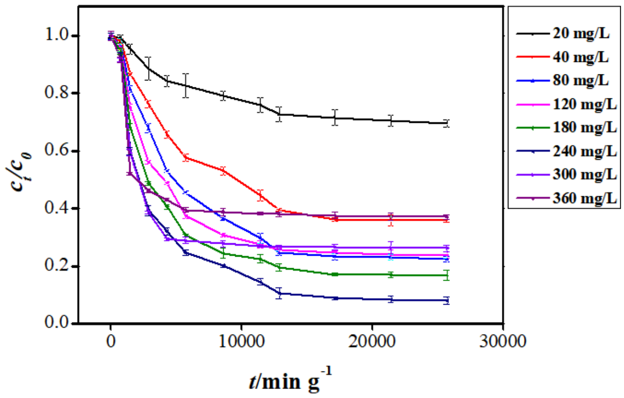

Fig.S7 The breakthrough curve of cCNTs-GA adsorbing different initial concentrations of glyphosate solution

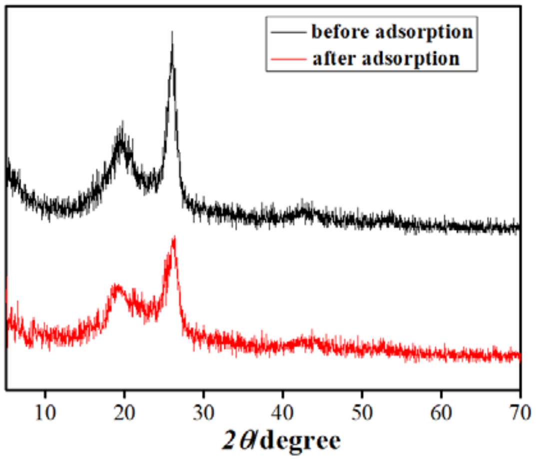

Fig.S8 XRD spectra before and after adsorption of cCNTs-GA

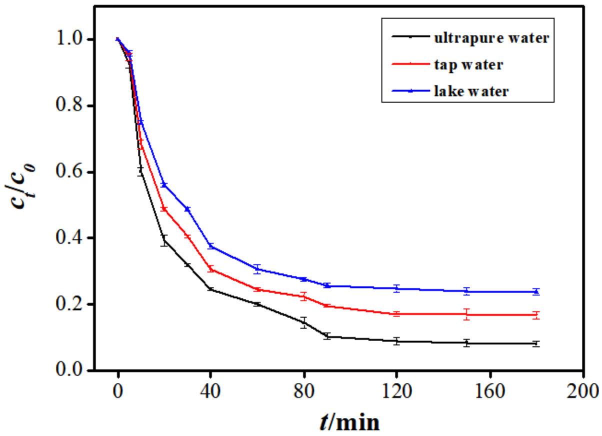

Fig.S9 Adsorption of glyphosate via cCNTs-GA in different water matrices

Table S1 Evaluate the Adsorption capacity of cCNTs-GA and GA in glyphosate solutions with different pH values (*T* = 298 K)

pH	1	3	5	7	9	11
			PC (mg g^{-1} uM^{-1})			
cCNTs-GA	0.656	1.59	1.24	0.795	0.711	0.439
GA	0.277	0.458	0.365	0.267	0.216	0.168

Table S2 Evaluate the Adsorption capacity of cCNTs-GA and GA in glyphosate solutions with different contact time (*T* = 298 K)

t (min)	5	10	20	30	40	60	80	90	120
PC (mg g^{-1} uM^{-1})									
cCNTs-GA	0.904	1.56	3.05	4.65	5.85	7.93	10.5	11.8	12.6
GA	0.493	0.828	1.25	1.91	2.14	2.48	3.05	3.30	3.31

Table S3 Kinetic parameters of pseudo-first-order and pseudo-second-order models for glyphosate onto cCNTs-GA and GA (T = 298 K, $c_{adsorbent}$ = 0.14 g L^{-1}, $c_{glyphosate}$ = 240 mg L^{-1}, pH = 3)

	pseudo-first-order model			pseudo-second-order model		
Adsorbent	k_1 (min^{-1})	q_e (mg g^{-1})	R^2	k_2 (g (mg min)$^{-1}$)	q_e (mg g^{-1})	R^2
cCNTs-GA	-0.0434±0.0038	260.59±1.27	0.887	$9.87\times10^{-5}\pm5.5\times10^{-6}$	431.03±2.08	0.997
GA	-0.01679±0.0017	79.02±1.08	0.859	$9.24\times10^{-4}\pm2.13\times10^{-5}$	172.71±6.13	0.995

Table S4 Kinetic parameters of intraparticle diffusion models for glyphosate onto cCNTs-GA and GA (T = 298 K, $c_{adsorbent}$ = 0.14 g L^{-1}, $c_{glyphosate}$ = 240 mg L^{-1}, pH = 3)

	intraparticle diffusion model					
adsorbent	k_1(mg (g $min^{1/2})^{-1}$)	k_2(mg (g $min^{1/2})^{-1}$)	C_1(mg g^{-1})	C_2 (mg g^{-1})	R_1^2	R_2^2
cCNTs-GA	58.0±1.6	20.2±4.3	-47.9	243.7	0.993	0.764
GA	28.2±1.8	8.7±3.4	-14.7	133.5	0.960	0.424

Table S5 Thermodynamic parameters for glyphosate adsorption onto cCNTs-GA

T/K	ΔG^0(kJ mol^{-1})	ΔH^0(kJ mol^{-1})	ΔS^0(J mol^{-1} k^{-1})
293	-2.29	-5.25	-10.1
298	-2.24		
303	-2.19		
313	-2.09		
323	-1.99		

Table S6 Evaluate the Adsorption capacity of cCNTs-GA at 5%, 10%, 50% and 100% breakthrough points in glyphosate solutions with different initial concentrations (*T* = 298 K, pH = 3)

c_0 (mg L^{-1}) / BT (%)	20	40	80	120	180	240	300	360
	Adsorption capacity (mg g^{-1})							
5%	0.476	1.83	7.38	12.6	24.1	45.2	62.7	75.8
10%	2.31	13.2	37.1	75.2	142	240	305	430
50%	10.3	46.9	126	207	339	479	541	551
100%	14.2	63.7	153	225	373	546	550	561

Table S7 Evaluate the partition coefficient (PC) of cCNTs-GA at 5%, 10%, 50% and 100% breakthrough points in glyphosate solutions with different initial concentrations (T = 298 K, pH = 3)

c_0 (mg L^{-1}) / BT (%)	20	40	80	120	180	240	300	360
	PC (mg g^{-1} uM^{-1})							
5	0.024	0.046	0.095	0.110	0.141	0.204	0.228	0.229
10	0.121	0.383	0.569	0.836	1.15	1.66	1.71	2.29
50	0.656	2.21	4.34	5.64	7.69	9.92	6.49	3.94
100	0.993	4.40	8.26	7.57	12.1	25.5	6.89	4.14

Table S8 The PC values of cCNTs-GA and GA at different breakthrough points (T = 298 K, $c_{glyphosate}$ = 240 mg L^{-1}, pH = 3)

BT (%)	5	10	50	100
		PC (mg g^{-1} uM^{-1})		
cCNTs-GA	0.204	1.66	9.92	25.5
GA	0.121	0.454	1.29	2.50

Table S9 The PC values after repeated use of cCNTs-GA and GA (T = 298 K, $c_{glyphosate}$ = 240 mg L^{-1}, pH = 3)

Cycle number	5	10	15	20	25	30	35	40
				PC (mg g^{-1} uM^{-1})				
cCNTs-GA	26.6	24.6	22.0	18.3	15.0	11.4	7.91	5.61
GA	3.03	2.33	1.95	1.80	1.60	1.17	0.691	0.642

Table S10 Adsorption of glyphosate via cCNTs-GA in different water matrices (T = 298 K, $c_{glyphosate}$ = 240 mg L^{-1}, pH = 3)

t (min)	5	10	20	30	40	60	80	90	120	150	180
					PC (mg g^{-1} uM^{-1})						
Ultrapure water	1.17	2.06	4.27	6.94	9.19	13.7	20.8	25.2	26.1	26.5	26.9
Tap water	1.17	2.01	3.75	5.59	7.25	11.0	17.1	16.3	15.0	15.6	16.1
Lake water	1.17	1.99	3.41	4.86	6.03	8.98	13.6	13.2	12.9	13.2	13.5