Quinoline-Functionalized Graphene Oxide for Enhanced Cadmium Removal: Synthesis, Characterization, and Mechanistic Insights

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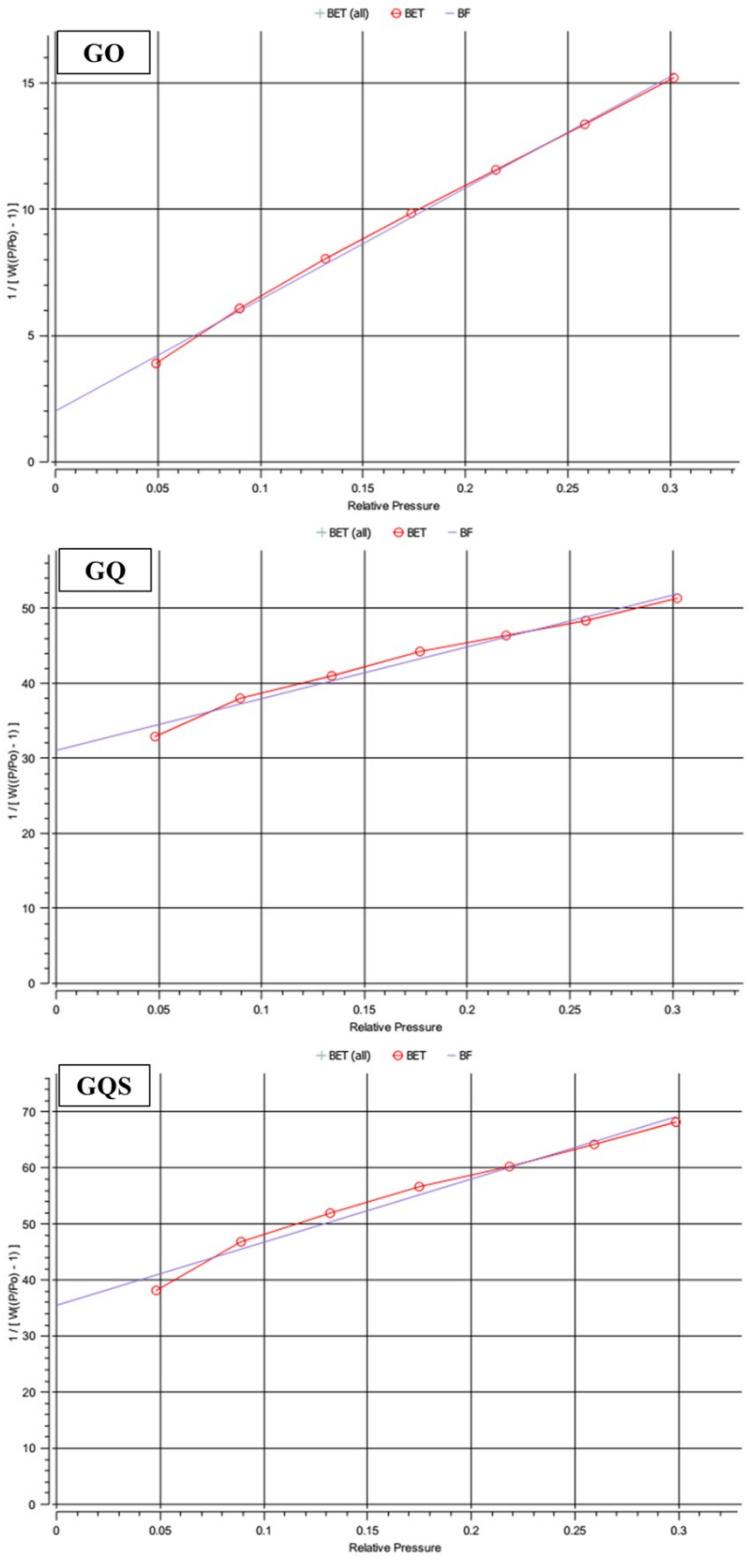

Figure S1: *BET isotherm of graphene oxide (GO), GO functionalized with 8-hydroxyquinoline (GQ), and GO functionalized with 8-hydroxyquinoline-5-sulfonic acid (GQS) sorbents.*

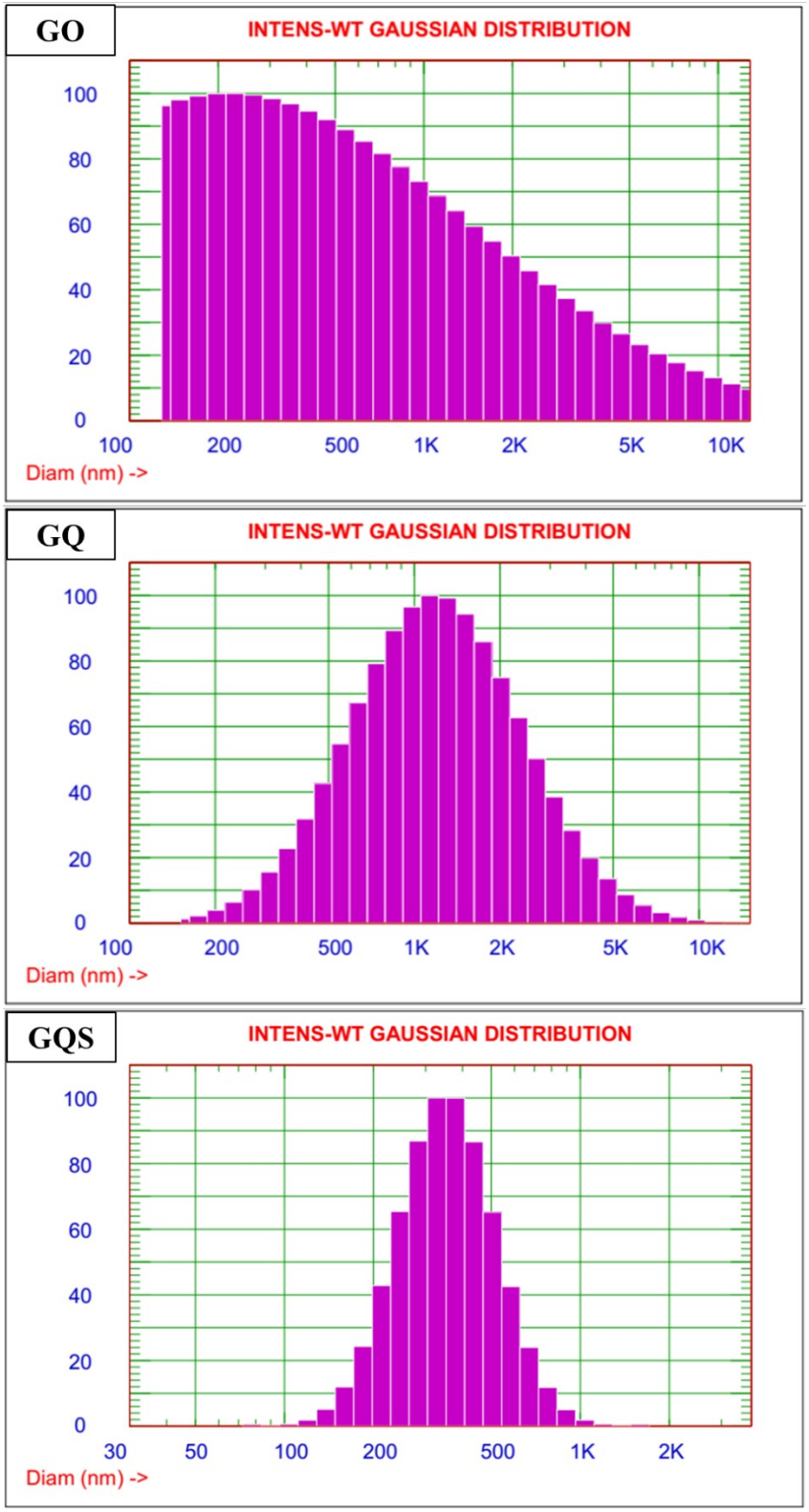

Figure S2: *DLS of graphene oxide (GO), GO functionalized with 8-hydroxyquinoline (GQ), and GO functionalized with 8-hydroxyquinoline-5-sulfonic acid (GQS) sorbents.*

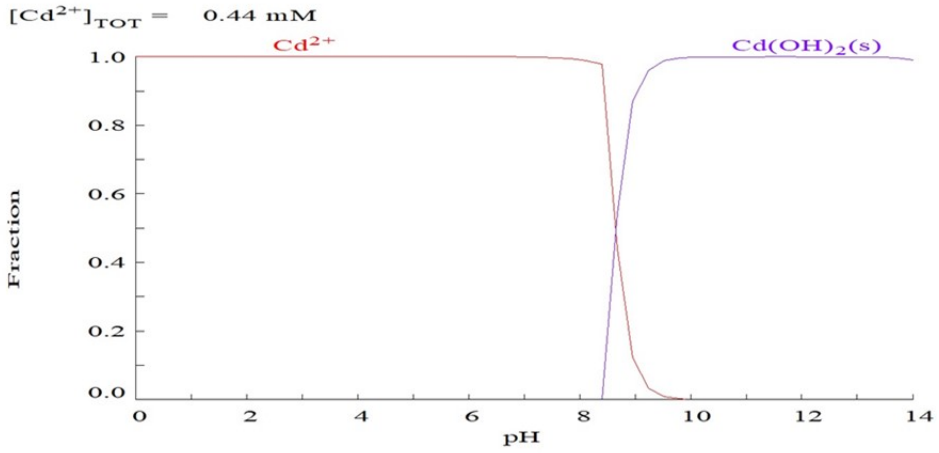

Figure S3: *Expected aqueous speciation of metal ion concentration (50 mg L^{-1}) for cadmium as a function of pH using Medusa/Hydra program.*

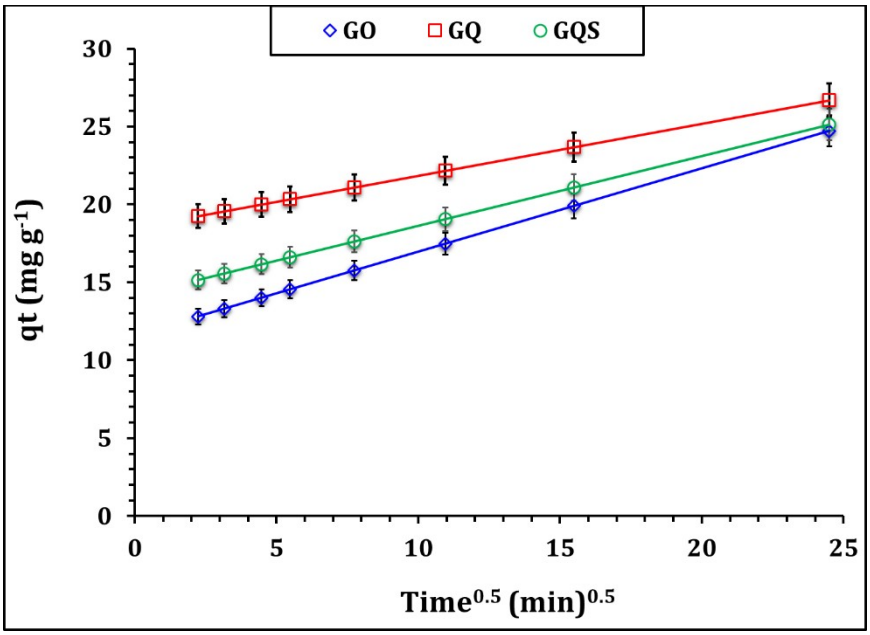

Figure S4: *Intraparticle diffusion (IPD) model plots for Cd(II) adsorption. Experimental conditions: initial ion concentration = 50 mg L^{-1}, pH = 5.01, dose = 0.5 g L^{-1}, temperature = 25°C.*

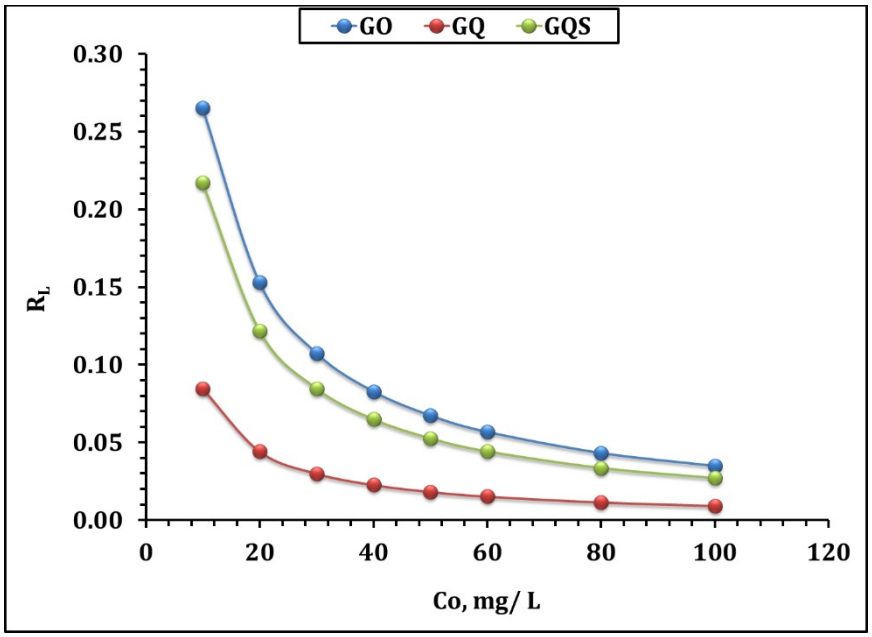

Figure S5: *Separation factor (R_l) for Cd(II) adsorption process using* GO, GQ, GQS sorbents.

Table S1: *Kinetic, isotherm, and thermodynamics equations for and Cd(II) sorption process* ***[1-7]***.

Kinetics	Equations
Pseudo-first-order	$q_t = q_1\left(1 - e^{-k1t}\right)$
Pseudo-second-order	$q_t = \frac{1}{\left(1 \middle\vert k_2 q_2^2\right) + \left(t \middle\vert q_2\right)}$
Intra-particle diffusion model (IPD)	$q_t = K_{id}\, t^{0.5} + C_i$
Isotherms	**Equations**
Langmuir model	$q_e = \frac{q_m k_L C_e}{1 + k_L C_e}$
Freundlich model	$q_e = K_F C_e^{1/n_F}$
Temkin model	$q_e = \frac{RT}{b_T} \ln K_T C_e$
Sips model	$q_e = \frac{q_S \left(k_S C_e\right)^{mS}}{1 + \left(k_S C_e\right)^{mS}}$
Thermodynamics	**Equations**
	$\log K_C = -\frac{\Delta H^o}{2.303\, R} X \frac{1}{T} + C$
	$-\Delta G^o = 2.303\, RT \log K_C$
	$\Delta G^o = \Delta H^o - T\, \Delta S^o$
Fitting	**Equations**
Coordination coefficient (R^2)	$R^2 = 1 - \frac{\sum_1^n \left(q_{exp} - q_{pred}\right)^2}{\sum_1^n \left(q_{exp} - \bar{q_{exp}}\right)^2}$
Average relative error (ARE)	$ARE = \frac{100}{n} \sum_1^n \frac{\left\vert q_{exp} - q_{pred} \right\vert}{q_{exp}}$

qe (mg g^{-1}) is the equilibrium concentration of metal ions species, and qt (mg g^{-1}) is the adsorbed amount of metal ions species ions after time t (min), Ce (mg L^{-1}) is equilibrium concentration of metal ions species. k_1 (min^{-1}) and k_2 (min^{-1}) are the rate constants for the pseudo first and second order, respectively. K_{id} (mg/g. $min^{0.5}$) is a rate constant, and C is the thickness of the boundary layer. q_m and q_S are the maximum sorption capacity (mg. g^{-1}) of Langmuir and Sips models. k_L (L. mg^{-1}), K_F (L/ mg), K_T (L min^{-1}), and K_S (L/ mg) are represent the constants of Langmuir, Freundlich, Temkin, and Sips models. n refer to the sorption intensity, b_T is Temkin constant that refers to the adsorption heat, mS is Sips constant. $\boldsymbol{q_s}$ is the theoretical isotherm saturation capacity (mg/g). K_C is a non-dimensional equilibrium constant and it equals K_d X 1000 X ρ **[4-5]**; T is the temperature (K), $\boldsymbol{R}$ is the universal gas constant (8.314 J mol^{-1}. K^{-1}), ρ is solution density g/ L, and C is a constant. R^2 and x^2 are the coordination and Chi-square coefficients respectively, the number of test points is n, the experimental equilibrium capacity is q_{exp} (mg g^{-1}), while the predicted capacity is q_{pred} (mg g^{-1}).

References:

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Table S2: *The relationship between Cd(II) adsorption capacity and* sorbent *dose under the following conditions: room temperature, a pH of 6.0, a starting concentration of 50 mg* L^{-1}*, reaction time of 240 min.*

Sorbent dose, g/ L	**Sorption capacity, mg/ g**		
	GO	**GQ**	**GQS**
0.3	39.3	78.8	65.5
0.5	36.2	58.2	48.2
1.0	30.9	36.4	33.5
2.0	20.0	24.3	21.2
3.0	14.3	16.5	15.5

Table S3: *The values of Morris-Weber model parameters.*

		GO	GQ	GQS
Weber and Morris model	**k_i (mg/g $min^{1/2}$)**	0.54	0.33	0.45
	C	11.6	18.5	14.1
	R^2	0.98	0.98	0.98

Table S4: *Cd(II) desorption from loaded sorbent using different solutions (2.0 g/L, room temperature; 120 min).*

Eluent type	Sorption efficiency, %
1.0 M Hydrochloric acid	98.1
1.0 M Sulfuric acid	76.7
1.0 M Nitric	64.3

Table S5: *Initial concentrations of constituents in raffinate wastewater, along with calculated removal efficiency (%), and distribution coefficient (kd) after treatment with* GQ sorbent.

Parameter	Initial concentration, mg/ L	Removal efficiency, %	distribution coefficient, Kd
Cd(II)	120.0	94.2	8.07
V(V)	60.0	20.0	0.13
Cr(III)	80.0	11.3	0.06
Si(IV)	300.0	23.3	0.15
Ca(II)	504.0	19.8	0.12
Na(I)	320.0	15.0	0.09
Cl-	800.0	8.8	0.05