nanomaterials

Supplementary Materials

Exfoliated Clay Decorated with Magnetic Iron Nanoparticles for Crystal Violet Adsorption: Modeling and Physicochemical Interpretation

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Table S1. Kinetic and isotherm linear models for CV uptake by MNP/CTAB-EC composite.

Kinetic Model	Linear	Parameters	Refs.
Pseudo first-order	$ln(q_e - q_t) = ln\, q_e - k_1 t$	q_t (mg g^{-1}) is the removed amount of CV at time t. q_e is the equilibrium adsorption uptake (mg g^{-1}). k_1 is the rate constant of the first-order adsorption $(min)^{-1}$.	[16]
Pseudo Second-order	$\frac{t}{q_t} = \frac{1}{k_2\, q_e^2} + \frac{t}{q_e}$	k_2 is the rate constant of the second-order adsorption (g(mg min)$^{-1}$).	[17]
Isotherm Model			
Langmuir	$\frac{C_e}{q_e} = \frac{1}{q_{max}\, b} + \frac{C_e}{q_{max}}$	C_e (mg L^{-1}): equilibrium concentration of the CV in the solution q_e (mg g^{-1}): removed amount of CV at equilibrium. q_{max} (mg g^{-1}): maximum adsorption capacity K_L (L mg^{-1}): Langmuir constant	[19]
Freundlich	$log\, q_e = log\, K_F + \frac{1}{n} log\, C_e$	K_F (mg g^{-1} (mg $L^{-1})^{-1/n}$) CV adsorption capacity. n: heterogeneity factor.	[20]
D–R	$ln\, q_e = ln\, q_m - \beta\varepsilon^2$	β(mol^2/kJ^2): D–R constant ε (kJ^2/mol^2): Polanyil potential, equal to $RT\, ln\left(1 + \frac{1}{C_e}\right)$. R: universal gas constant (8.31 J/mol K). T (K): absolute temperature. q_m (mg g^{-1}): theoretical adsorption capacity.	[21]

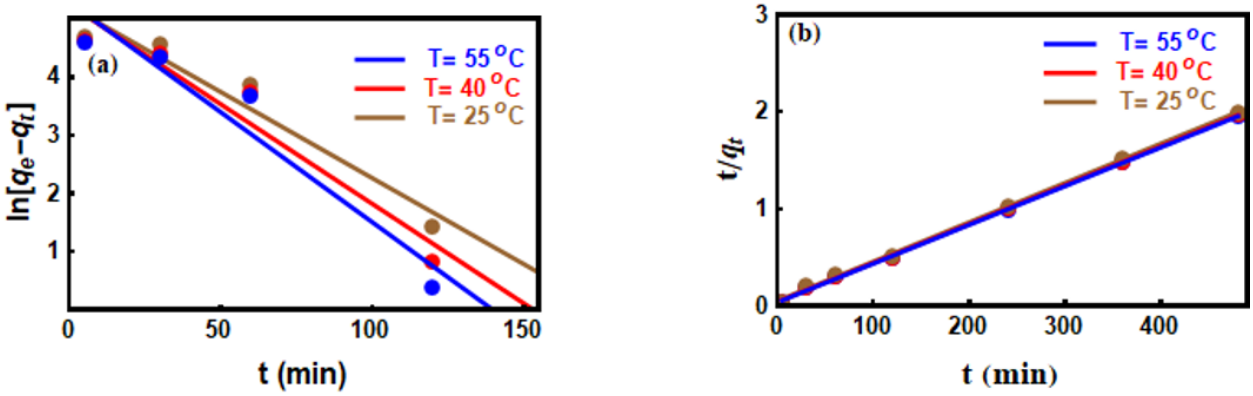

Figure S1. Linear forms of the Pseudo-first order model (**a**) and the Pseudo-second order model (**b**) for CV uptake by MNP/CTAB-EC composite at different temperatures.

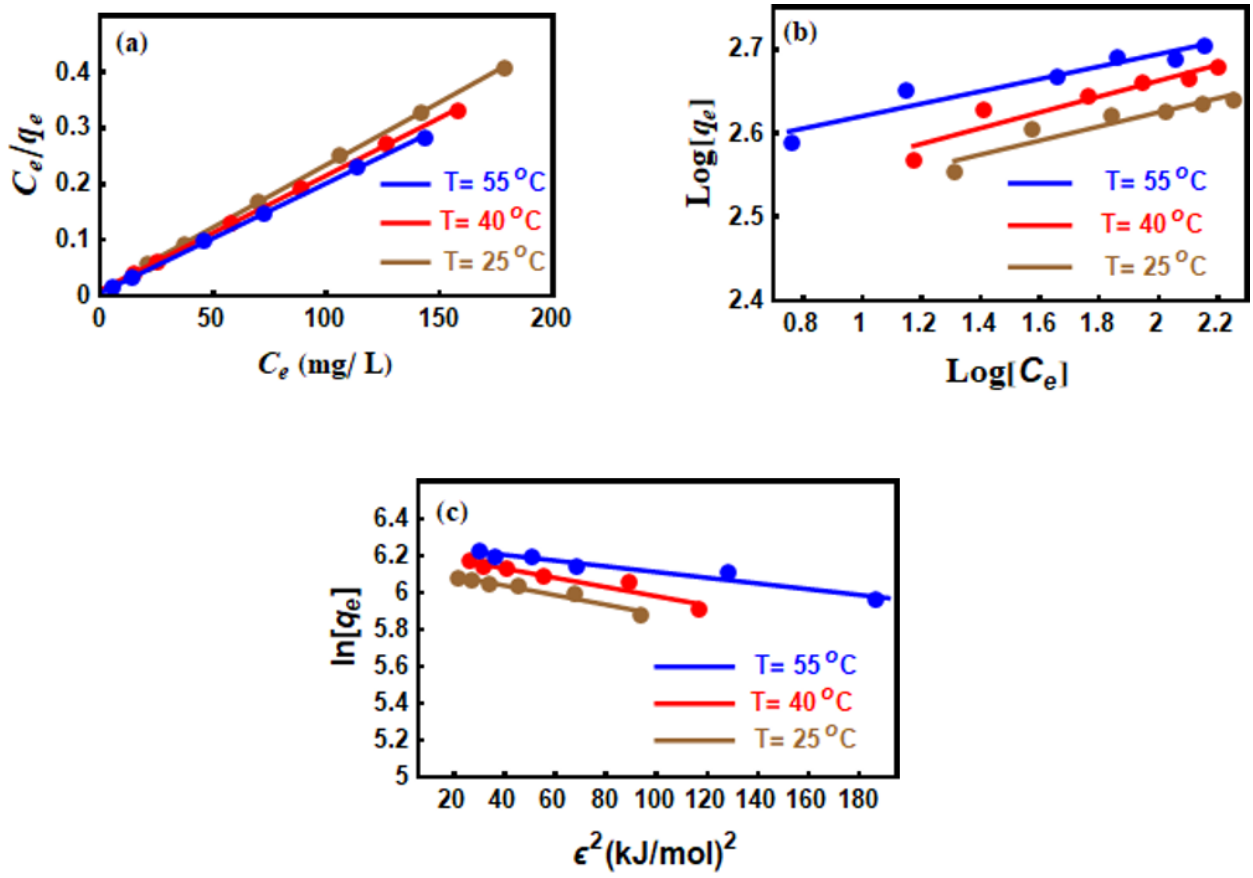

Figure S2. Linear Langmuir, Freundlich, and D–R isotherms models for CV uptake by MNP/CTAB-EC composite at different temperatures.

Table S2. Parameters of linear of kinetic and isotherm models for the adsorption of CV onto MNP/CTAB-EC composite.

Kinetic Model	T = 25 °C	T = 40 °C	T = 55 °C
Pseudo-first-order			
$q_{e(exp)}$ (mg g^{-1})	239.72	243.8	244.9
$q_{e(cal)}$ (mg g^{-1})	185.82	189.94	198.28
k_1 (min^{-1})	0.03	0.034	0.038
R^2	0.9401	0.9315	0.9247
Pseudo-second-order			
$q_{e(cal)}$ (mg g^{-1})	246.37	249.22	250.1
k_2 (g (mg $min)^{-1}$)	0.00032	0.00038	0.00044
R^2	0.9989	0.9993	0.9994

Isotherm Model			
Langmuir			
q_{max} (mg g^{-1})	447.41	486.76	509.11
k_L (L mg^{-1})	0.2	0.21	0.37
R^2	0.9998	0.9992	0.9996
Freundlich			
k_F (mg g^{-1})	286.5	297.98	351.96
$1/n$	0.08	0.09	0.07
R^2	0.8925	0.8881	0.913
D−R			
q_m(mg g^{-1})	465.01	507.77	526.36
E(kJ mol^{-1})	13.89	14.16	17.99
R^2	0.9414	0.9252	0.9458