Supplementary Material

Fe$_3$O$_4$-4,4'-Biphenyldicarboxaldehyde superparamagnetic-nanomaterial for high-efficiency removal of 9-Phenanthrol: Experimental combined with DFT investigations

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Detailed description of the formula:

Evaluation on adsorption performance and removal efficiency

The removal efficiency and adsorption capacity of the magnet samples were

determined according to the following formula:

$$R = \frac{(C_0 - C_e)}{C_0} \times 100\% \qquad (1)$$

$$Q = \frac{(C_0 - C_e) \times V}{M} \qquad (2)$$

Where C_0 represented the initial concentration of 9-PROL, the C_e was the

concentration of the suspension at the adsorption reached equilibrium. V (mL) was the

volume of the 9-PROL solution to be treated, M (g) represented the mass of the

adsorbents.

The kinetic models

The Boyd, Weber-Morris-diffusion, Intra-particle diffusion, Elovich, pseudo-first-

order and pseudo-second-order model were applied to fit the experiment data

respectively, and the equations were presented as follows:

Boyd model:

$$B_t = -2.30258 \lg (1 - F) - 0.49770 \qquad (3)$$

$$F = \frac{Q_t}{Q_e} \qquad (4)$$

The intercept (b) of the straight line could obtained by the linear relationship of B_t vs.

time. Where Q_e and Q_t (mg/g) represent the adsorption capacity at equilibrium time

and time t (min).

Weber-Morris-diffusion model:

$$ln\left(1 - \frac{Q_t}{Q_e}\right) = - k_w t$$

$$(5)$$

Whereas k_w (min^{-1}) represent the rate constants of the Weber-Morris adsorption

diffusion models.

Intra-particle diffusion model:

$$Q_t = k_p t^{1/2} + c$$

$$(6)$$

Whereas k_p (mg g^{-1} min$^{0.5}$) represent the rate constants of the Weber-Morris

adsorption diffusion models. Besides, c (mg/g) reperesents the thickness of the

boundary layer.

Elovich model:

$$Q_e = aln\frac{b}{a} + alnt$$

$$(7)$$

Where Q_e (mg/g) represent the adsorption capacity at equilibrium time (min), and a

(mg/g), b (min mg g^{-1}) are the adsorption rate constant of the Elovich model,

respectively.

Pseudo-first-order:

$$Q_t = Q_e(1 - e^{-k_1 t})$$

$$(8)$$

Pseudo-second-order:

$$Q_t = \frac{Q_e^2 k_2 t}{1 + k_2 Q_e t}$$

$$(9)$$

Where Q_e and Q_t (mg/g) represent the adsorption capacity at equilibrium time and

time t (min), and k_1 (min^{-1}), k_2 (g mg^{-1} min^{-1}) are the adsorption rate constant of the

two kinetic models, respectively

The isotherm models:

The Sips, Temkin, Toth, langmuir and Freundlich model were applied to fit the experiment data respectively, and the equations were presented as follows:

Sips model:

$$Q_e = q_{max1}\left(\frac{K_s C_e^{N_s}}{1 + K_s C_e^{N_s}}\right) \quad (10)$$

Where K_s (L mmol^{-1}) is associated with the energy of adsorption and N_s indicates the system heterogeneity, q_{max1} reresent the maximum adsorption capacity (mg/g) caluated by Sips model. Where Q_e (mg/g) was the amount of 9-PROL adsorption at equilibrium

Temkin model:

$$Q_e = \frac{RT}{b_T}lnK_T + \frac{RT}{b_T}lnC_e \quad (11)$$

Where K_T is the equilibrium bond constant related to the maximum energy of bond. R is the universal gas constant and T is the temperature in terms of Kelvin. The b_T constant represents the bond energy.

Toth model:

$$Q_e = \frac{q_{max2}b_T C_e}{\left(1 + (b_T C_e)^{R_T}\right)^{1/R_T}} \quad (12)$$

Where b_T was the Toth constant and R_T was the exponent of heterogeneous adsorption, q_{max2} reresent the maximum adsorption capacity (mg/g) caluated by Toth model.

Langmuir model:

$$Q_e = \frac{q_m k C_e}{1 + k C_e}$$

(13)

Where Q_e (mg/g) and C_e (mg/L) were the amount of 9-PROL adsorption and residual

9-PROL concentration at equilibrium; q_m (mg/g) represented the maximum adsorption

capacity of 9-PROL, and k is the Langmuir adsorption equilibrium constant (L mg^{-1}).

Freundlich model:

$$Q_e = K_F C_e^n$$

(14)

Where K_F is the Freundlich constant (mg $^{(1-n)}$ L^n g^{-1}) and n (dimensionless) is the

Freundlich intensity parameter.

Table S1. Structural information of the original magnetic oxides and the derived magnetic

nanocomposite.

Samples	S_{BET} (m^2/g)	V_{pores} (cm^3/g)	Pore size (nm)
Fe_3O_4	35.55	0.178	20.03
Fe_3O_4-AMINO	4.73	0.0215	18.22
Fe_3O_4-0.75BIPHENY	3.47	0.0174	19.98

Table S2. Adsorption kinetics parameters for adsorption of 9-PROL on magnetic samples.

Models	Parameters	Fe_3O_4	Fe_3O_4-AMINO	Fe_3O_4-0.75BIPHENY
	k (min^{-1})	0.00514	0.00597	0.00615
Boyd	b	-0.62009	-0.80516	-0.78911
	R^2	0.92481	0.87196	0.83599
Weber-Morris	k_w (min^{-1})	0.00514	0.00597	0.00615
adsorption diffusion	R^2	0.92481	0.87196	0.83599
	k_{p1} (mg g^{-1} min$^{1/2}$)	1.69537	1.65071	2.39518
	R^2	0.98657	0.99102	0.99415
Intra-particle diffusion	k_{p2} (mg g^{-1} min$^{1/2}$)	0.98083	0.90868	1.15802
	R^2	0.98633	0.99672	0.99509
	k_{p3} (mg g^{-1} min$^{1/2}$)	0.50105	0.36029	0.55674
	R^2	0.7895	0.6844	0.63482
	a	8.0238	7.4962	10.4461
Elovich	b	0.41705	0.34768	0.56118
	R^2	0.99815	0.99813	0.99833
	Q_e (mg g^{-1})	29.7397	27.2781	38.3679
Pseudo-first order	k_1 (min^{-1})	0.00482	0.00439	0.00514
	R^2	0.9905	0.99239	0.98666
	Q_e (mg g^{-1})	37.5381	35.1829	48.0475
Pseudo-second order	k_2 (g mg^{-1} min^{-1})	0.000128	0.000119	0.000109
	R^2	0.99576	0.99544	0.99607

Table S3. Isotherm fitting results of 9-PROL adsorption on magnetic samples.

Models	Parameters	Fe_3O_4	Fe_3O_4-AMINO	Fe_3O_4-0.75BIPHENY
Sips	q_{max1} (mg g^{-1})	49.1033	43.1546	89.2646
	K_s (L mmol^{-1})	0.66527	0.53262	4.023
	N_s	1.17793	1.16132	1.15139
	R^2	0.99648	0.99873	0.99903
Temkin	b_T	202.5135	234.6849	124.0314
	K_T (L mg^{-1})	4.8367	4.1268	28.2025
	R^2	0.99963	0.99749	0.98369
Toth	q_{max2} (mg g^{-1})	48.1364	41.2109	80.8035
	B_t (L mg^{-1})	0.53054	0.44465	2.6675
	N_T	1.32843	1.37678	1.47748
	R^2	0.99529	0.99851	0.99863
Langmuir	q_m (mg g^{-1})	56.5999	48.8424	109.7346
	k (L mg^{-1})	0.5242	0.4476	2.2472
	R^2	0.99498	0.99683	0.99772
Freundlich	K_F (mg$^{(1-n)}$ L^n g^{-1})	18.9036	15.2187	94.5572
	n	0.53043	0.51384	0.66163
□	R^2	0.96282	0.95988	0.98153

Table S4. The distance between the Fe$_3$O$_4$-0.75BIPHENY and 9-PROL molecular under different bonding modes.

	Bond lengths between specific atoms (Number 1 Atom *A*-Number 2 Atom *B*)					
A	Atoms	9*C*-43*C*	10*C*-46*C*	11*C*-45*C*	12*C*-44*C*	13*C*-40*C*	14*C*-39*C*
	Bond lengths (Å)	3.56258	3.79979	3.73294	3.47785	3.29166	3.33104
B	Atoms	9*C*-43*C*	10*C*-46*C*	11*C*-45*C*	12*C*-44*C*	13*C*-40*C*	14*C*-39*C*
	Bond lengths (Å)	3.50008	3.40317	3.3937	3.41339	3.46194	3.54937
C	Atoms	3*C*-43*C*	4*C*-39*C*	5*C*-40*C*	6*C*-44*C*	7*C*-45*C*	8*C*-46*C*
	Bond lengths (Å)	3.87865	3.48128	3.43846	3.78523	4.15081	4.24026
D	Atoms	3*C*-43*C*	4*C*-39*C*	5*C*-40*C*	6*C*-44*C*	7*C*-45*C*	8*C*-46*C*
	Bond lengths (Å)	3.29317	3.8702	4.22789	4.12006	3.56431	3.09543