Supporting Information

Synthesis of polyaniline-magnetite nanocomposites using swollen liquid crystals templates for magnetically separable dye adsorbent applications

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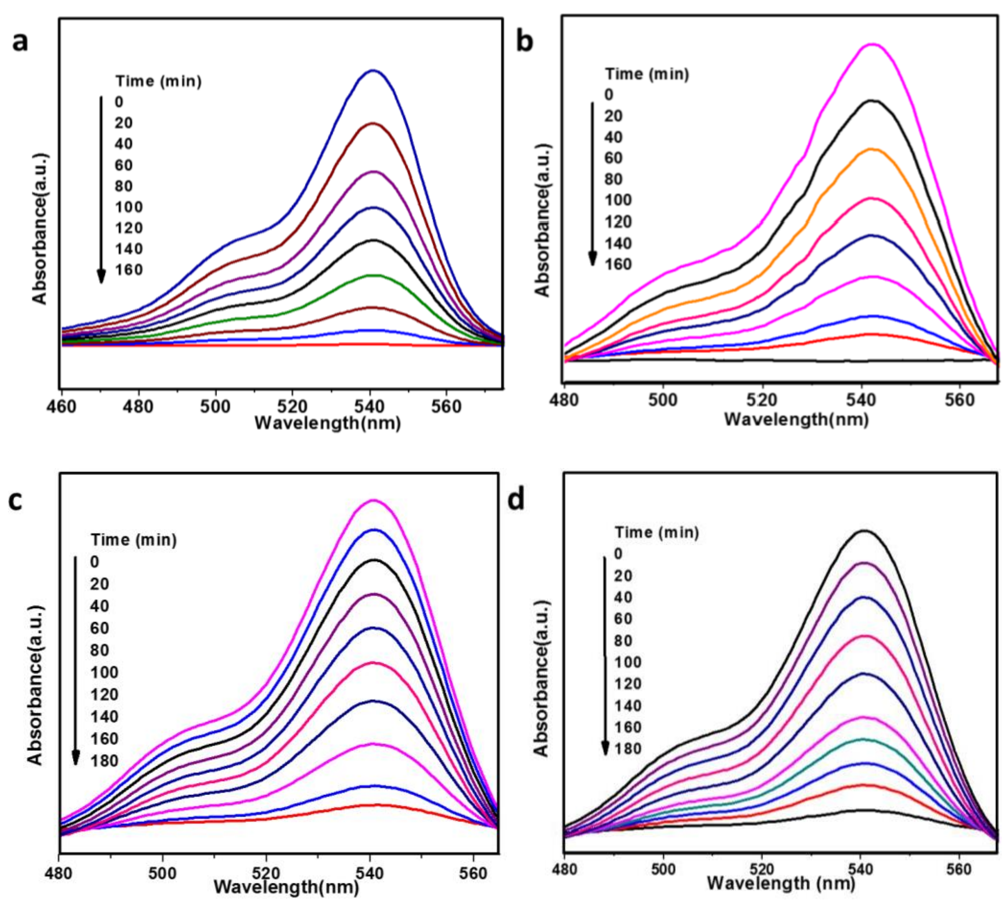

Figure S1. UV-Visible adsorptive plot for the removal of Rose Bengal (RB) dye using (a) PANI.HCl-Fe-M , (b) PANI.HCl-Fe-D, (c) PANI-Fe-M and (d) PANI-Fe-D.

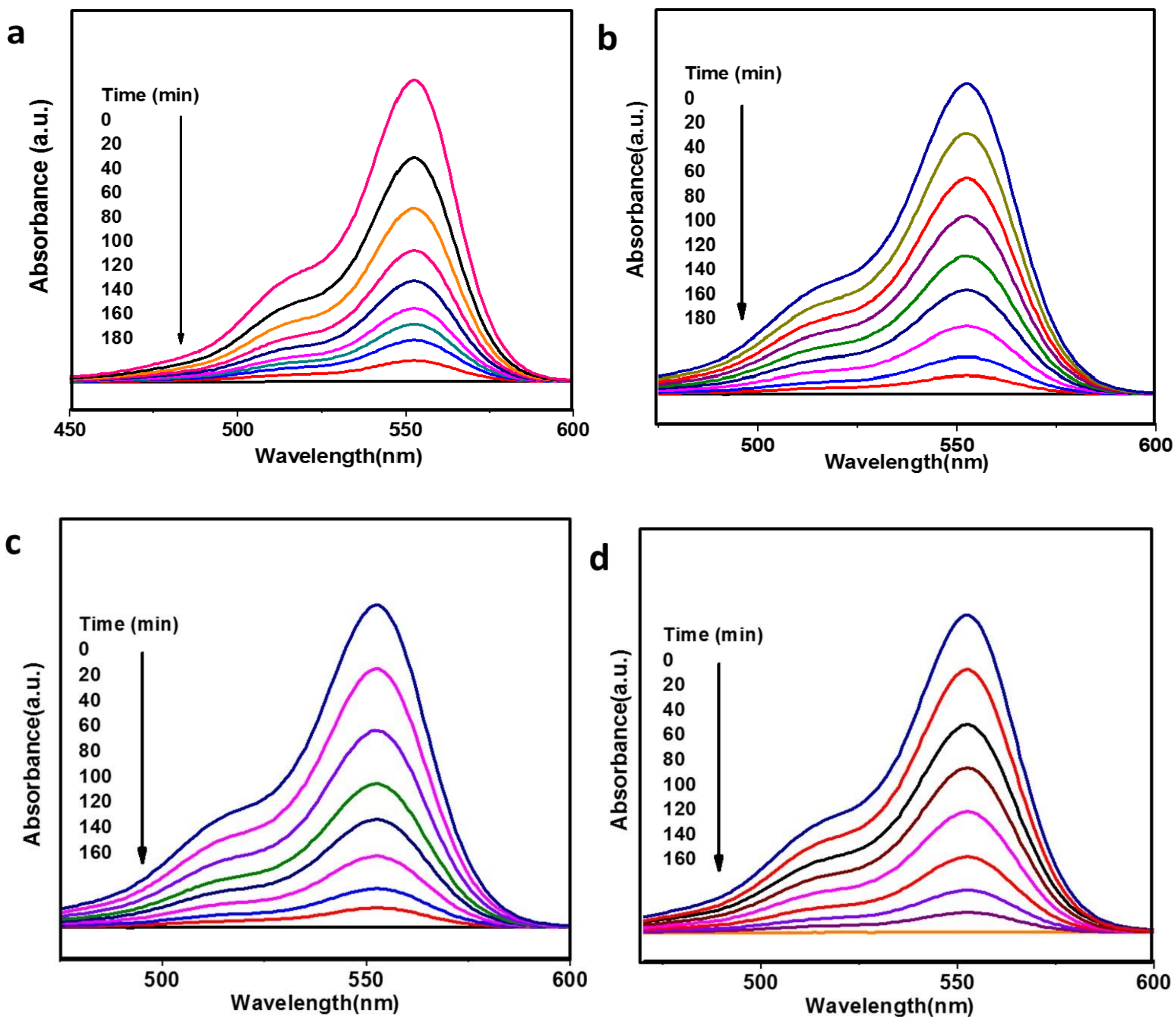

Figure S2. UV-Visible adsorptive plot for the removal of Rhodamine B (RhB) dye using (a) PANI.HCL-Fe-M) (b) PANI.HCL-Fe-D) (c) PANI-Fe-M and (d) PANI-Fe-D.

Kinetics of adsorption:

The adsorption studies of RB and RhB dyes for nanocomposites were studied using UV-visible absorption spectroscopy, as shown figure S1 and S2.

The adsorption of dyes onto PANI-Fe nanocompsoites was the sole act of the electrostatic interaction between PANI and the dye. The mechanism of adsorption reaction and its potential rate controlling steps have been investigated to explore the kinetic model followed by adsorbing polymers. Three expected models: *pseudo-first-order, pseudo-second-order and intraparticle diffusion* have been applied to find out the adsorption behavior of the dye on nanocomposites and the validity of the models were verified by the linear equation analysis: $\ln(Q_e - Q_t)$ vs t, (t/Q_t) vs t and Q_t vs $t^{1/2}$ respectively. Q_e and Q_t (mg/g) denotes to the amount of dye adsorbed at equilibrium and time t (min), respectively. The equations of the three kinetic models are:

The first model is the pseudo-first order rate equation [1]:

$$\ln(Q_e - Q_t) = \ln Q_e - k_1 t$$

the rate constant for pseudo-first order reaction referred by k_1. The amount of dye adsorbed per unit weight of polymer adsorbent, Q_e (mg g^{-1}), was calculated from the mass balance equation given by [2]:

$$Q_e = (C_o - C_e)\, Vm^{-1}$$

Where C_o is the initial dye concentration in liquid phase (mgL^{-1}), C_e is the dye concentration at equilibrium (mgL^{-1}), V is the volume of dye solution used (L), and m is the mass of adsorbent in the system (g). Plotting a graph between $\ln(Q_e - Q_t)$ and time (t) of the pseudo-first order equation would give the value for the parameters, k_1. The fitting plot is shown below in figures S3 & S4.

The second model tried was pseudo-second-order. In this model, reaction is dependent on the amount of solute adsorbed on the surface of adsorbent and the amount adsorbed at equilibrium.

The pseudo-second order model was displayed in the following form [3]:

$$t/Q_t = 1 / k_2 Q_e^2 + t / Q_e$$

k_2 is rate constant (g $mg^{-1}min^{-1}$). The plot of t/Q_t for different nanocomposites are shown in Figure 8 and 9 .

Also, the third kinetic model (intraparticle diffusion model) was also analyzed. In this model the uptake of adsorbate varies with the square root of time, the root time dependence equation is given below [4]:

$$Q_t = k_i t^{1/2} + C$$

Where, k_i is the intraparticle diffusion rate parameter in Q_t versus $t^{1/2}$ plot (shown in Figure S3 & S4).

So, based on the values of correlation coefficients, we observed that the pseudo second-order kinetic model gave the best fit over the other models for our dye adsorption experimental data.

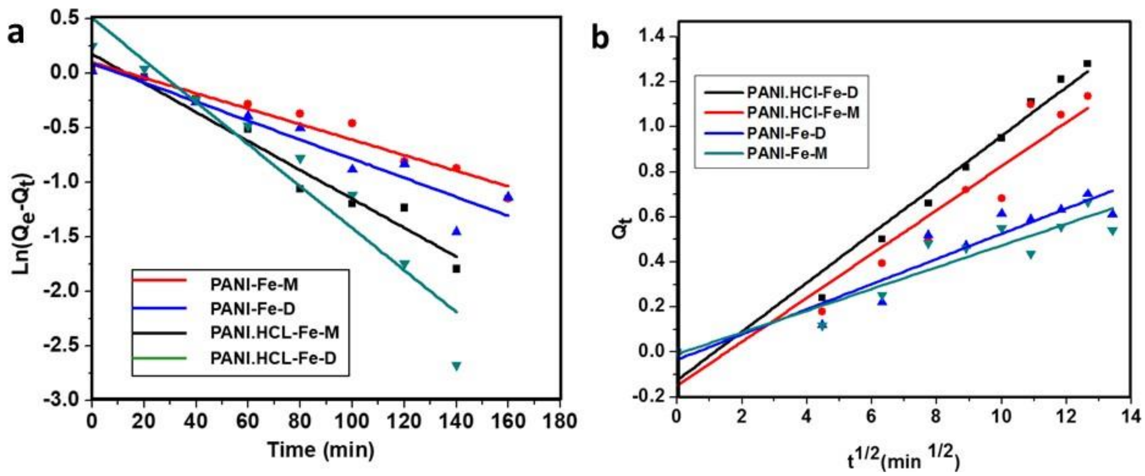

Figure S3. Kinetic model plots for PANI nanocomposites for the adsorption of RB dye (a) pseudo-first order plots (b) intraparticle diffusion plots.

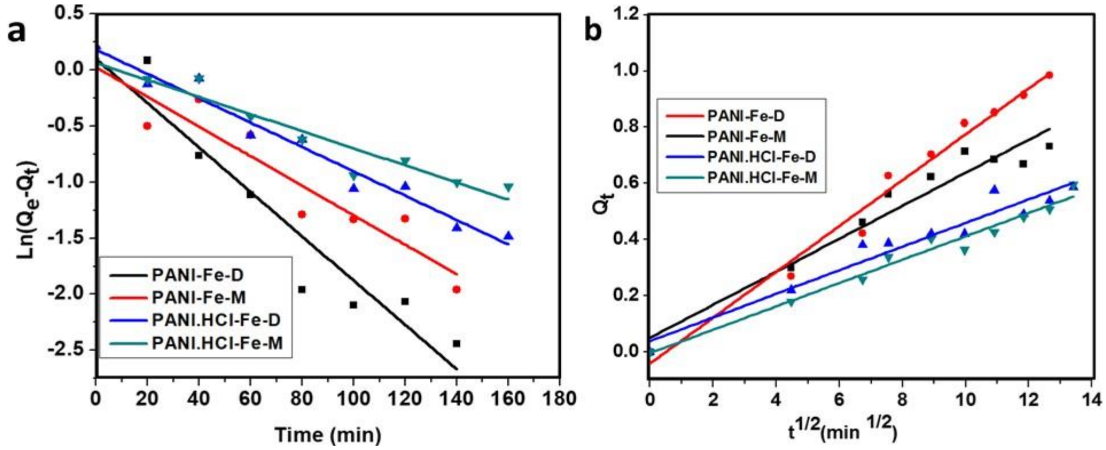

Figure S4. Kinetic model plots for PANI nanocomposites for the adsorption of RhB dye (a) pseudo first order plots (b) intraparticle diffusion plots.

Catalyst	Pseudo first order R^2	Pseudo second order R^2	k_2 ($gmg^{-1}min^{-1}$)	Intraparticle diffusion R^2
PANI-Fe-M	0.95	0.98	0.1672	0.86
PANI-Fe-D	0.94	0.973	0.1972	0.88
PANI.HCl-Fe-M	0.89	0.99	0.2639	0.90
PANI.HCl-Fe-D	0.91	0.983	0.3022	0.96

Table ST1. Table contains correlation coefficients (R^2) of pseudo-first-order, pseudo-second-order, intraparticle diffusion models and rate constant (k) values of pseudo-second-order for RB dye.

Catalyst	Pseudo first order R^2	Pseudo second order R^2	k_2($g\ mg^{-1}\ min^{-1}$)	Intraparticle diffusion R^2
PANI-Fe-M	0.95	0.99	0.2521	0.93
PANI-Fe-D	0.93	0.983	0.2972	0.95
PANI.HCl-Fe-M	0.89	0.999	0.1818	0.91
PANI.HCl-Fe-D	0.91	0.993	0.2072	0.92

Table ST2. Table contains correlation coefficients (R^2) of pseudo-first-order, pseudo-second-order, intraparticle diffusion models and rate constant (k) values of pseudo-second-order for RhB dye.

Sr. No.	Concentration of Dye (mg/L)	Amount of adsorbent (g)	Q_e(mg/g) PANI.HCl-Fe-D	Q_e(mg/g) PANI-Fe-D
1.	70	0.05	104.2	100.3
2.	60	0.05	100.2	96.0
3.	50	0.05	94.2	91.7
4.	40	0.05	81.7	78.1
5.	30	0.05	57.6	52.1
6.	20	0.05	31.9	27.3
7.	10	0.05	18.8	16.1

Table ST3. Summary of the model parameters for the adsorption of RB on PANI.HCl-Fe-D and PANI-Fe-D nanocomposites (at room temperature under suitable pH condition).

Sr. No.	Concentration of Dye (mg/L)	Amount of adsorbent (g)	Q_e (mg/g) PANI.HCl-Fe-D	Q_e (mg/g) PANI-Fe-D
1.	70	0.05	95.4	100.2
2.	60	0.05	88.1	98.0
3.	50	0.05	83.2	91.8
4.	40	0.05	78.7	86.1
5.	30	0.05	52.1	57.0
6.	20	0.05	30.1	39.1
7.	10	0.05	15.2	17.1

Table ST4. Summary of the model parameters for the adsorption of RhB on PANI.HCl-Fe-M and PANI.HCl-Fe-D nanocomposites (at room temperature under suitable ph condition).

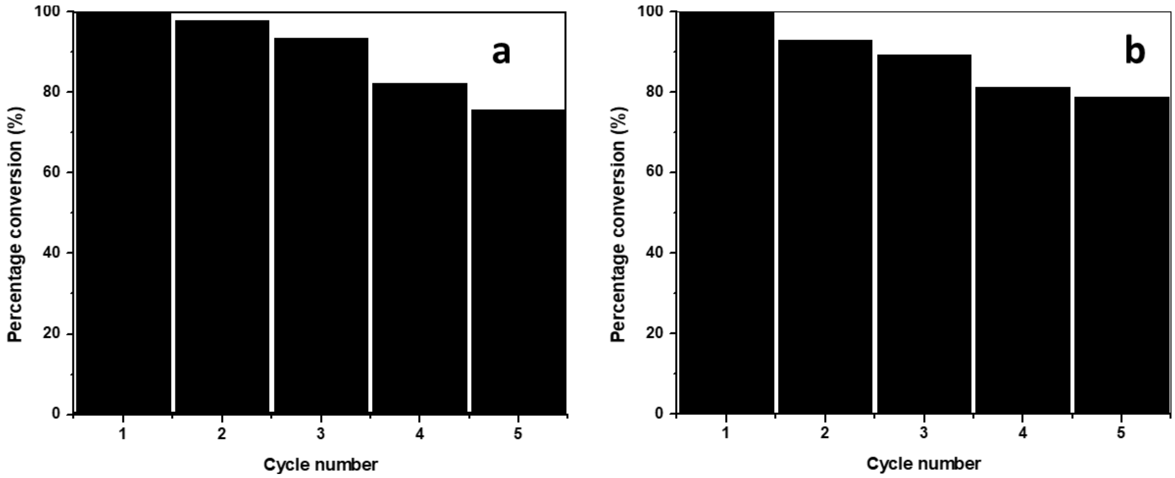

Figure S5. Plot of percentage adsorption with number of cycles for PANI-Fe-D nanocomposite for the adsorption of (a) RB and (b) RhB dyes.

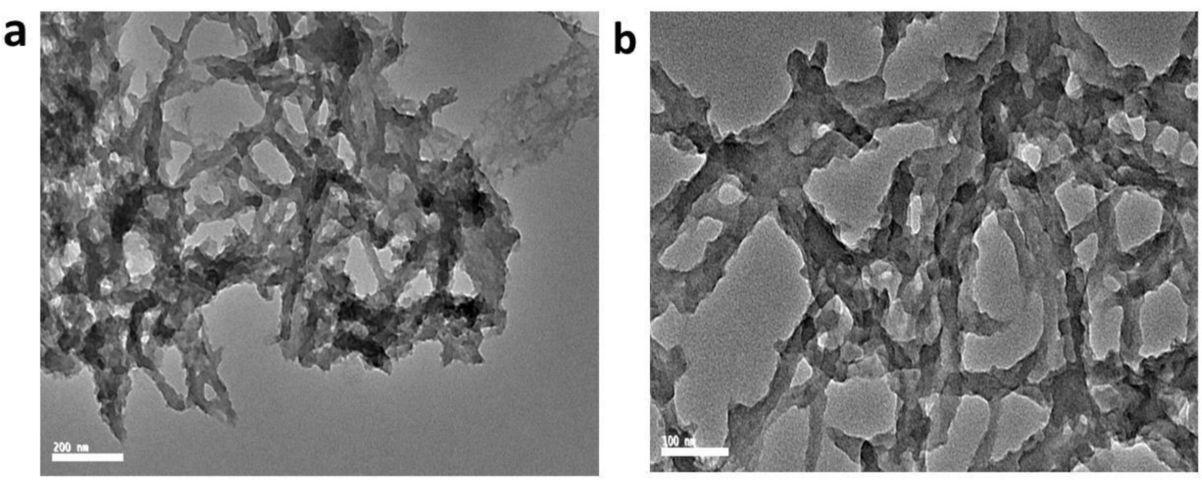

Figure S6. TEM images of PANI.HCl-Fe-D nanocomposites (a) before the 1st cycle and (b) after the 5th cycle RB dyes adsorption.

References:

[1]. D. Mahanta, G. Madras, S. Radhakrishnan and S. Patil, *The Journal of Physical Chemistry B*, 2009, 113, 2293-2299.

[2]. A. N. Chowdhury, S. Jesmeen and M. Hossain, *Polymers for Advanced Technologies*, 2004, 15, 633-638.

[3]. D. Mahanta, G. Madras, S. Radhakrishnan and S. Patil, *The Journal of Physical Chemistry B*, 2008, 112, 10153-10157.

[4]. D. Li, J. Huang and R. B. Kaner, *Accounts of Chemical Research*, 2009, 42, 135-145.