Preparation of silica nanoparticles based polymer composites via mussel inspired chemistry and their enhanced adsorption capability towards methylene blue

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1.1 The adsorption of MB by SiO_2@poly(SVS-co-ITA-DA)

The adsorption performance of SiO_2@poly(SVS-co-ITA-DA)nanocompositestowards MB was studied in aqueous solution. The batch adsorption experiments were carried out with 50 mL sample tubes. MBandSiO_2@poly(SVS-co-ITA-DA)nanocomposites were mixed in a sample tubes. The Kinetic experiment were completed by the constant initial concentration (50mgL^{-1}) of MB and 10 mg adsorbents to study the adsorption equilibration time at room temperature and the pH of 7.0. The adsorption thermodynamics batch experiment were studied by 5 °C gradient increase of temperature from room temperature 30 to 60 °C (303,308,313,318,323,328 and 333K) while the other conditions (concentration, pH, contact time) remained unchanged. The study of adsorption isotherm was conducted by adding the same amount of adsorbent into the 40 mL MB aqueous solution with different initial concentrations range from 5 to 500 mgL^{-1} at room temperature and pH 7.0. The influence of pH to the adsorption capacity of SiO_2@poly(SVS-co-ITA-DA) for MB was performed by adding 10 mg adsorbents into 40 mL MB with different pH value (2 to 10). The initial pH value of the adsorption solution was adjusted to a certain value by using 0.1molL^{-1} NaOH and0.1molL^{-1} HCl.

The concentrations of MB remained in the aqueous solution was determined using UV-vis spectrophotometer.

The equilibrium adsorption capacity (Q_e, mg/g) of the adsorbent to the MB aqueous solution was calculated by the following equation:

$$Q_{\mathrm{e}} = \frac{C_0 - C_e}{m} \times V$$

Where Q_e (mg/g) is the amount of adsorbed MB per gram dry weight of the adsorbent atadsorption equilibrium time, C_0 (mg//L) is the initial concentration of MB aqueous solution and C_e (mg/L) is the equilibrium concentration of MB, *m* (g) is the adsorbent's does in the adsorption medium and *V* (mL) is the dye MB aqueous solution's volume.

The adsorption capacity at any time Q_t (mg/g) of the adsorbents to the MB aqueous solution was calculated by the following equation:

$$Q_t = \frac{C_0 - C_t}{m} \times V$$

Where Q_t (mg/g) is the amount of MB adsorbed per gram dry weight of the adsorbent at the time *t* (min), C_0 (mg/L) is the initial concentration of MB aqueous solution and C_t (mg/L) is the concentration of MB at time *t* (min), *m* (g) is the adsorbent's does in the adsorption medium and *V* (L) is the dye MB aqueous solution's volume.

The removal efficiency (R%) of the MB were calculated by the following equation:

$$R = \frac{100(C_0 - C_t)}{C_0}$$

Where R (%) is the removal efficiency of MB. The C_t (mg/L), and C_0 (mg//L) is introduced as the above equation.

2. Results

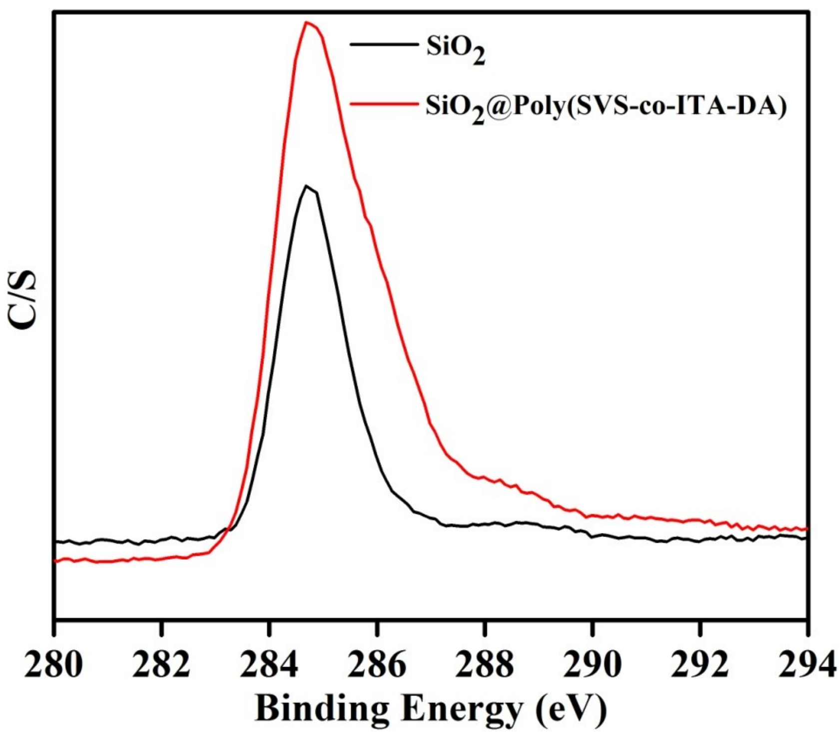

Fig. S1 The detailed XPS Spectra (C1s) of SiO_2 NPs andSiO_2@poly(SVS-co-ITA-DA)nanocomposites.

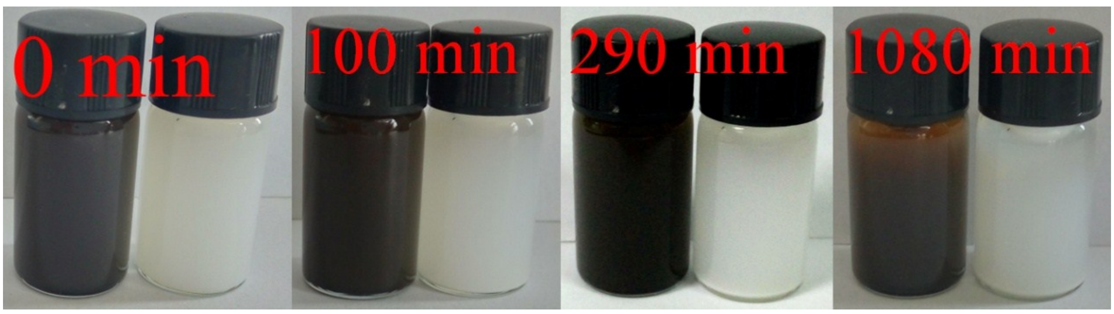

Fig. S2 The water dispersibility of modified (Left bottle) and unmodified silica nanoparticles (right bottle) at different deposition time points.

Table S1 Element contents (%) of silica nanoparticles based on XPS analysis.

Sample	**Atom percentage (%)**				
	C1s	**N1s**	**O1s**	**Si2p**	**S2p**
SiO_2 NPs	17.65	0	56.2	26.15	0
SiO_2@poly(SVS-co-ITA-DA)	37.07	3.37	42.84	15.98	0.73

TableS2 Data of Pseudo-first-order, Pseudo-second-order and Intraparticle diffusion models parameters at 303K

Models	Parameters	Initial concentration (mg/L)
		50
Pseudo-first-order equation	$Q_{e\,(cal)}$ (mg/g)	61.586
	k_1 (min^{-1})	0.0681
	R^2	0.991
Pseudo-second-order equation	$Q_{e\,(cal)}$ (mgg^{-1})	69.1
	k_2 (g mg^{-1} min^{-1})	0.00128
	h (mg g^{-1} min^{-1})	6.099
	R^2	0.988
Intraparticle diffusion	k_p(mg g^{-1} min$^{-0.5}$)	17651.16
	C	7.076
	R^2	0.895

Table S3 Data of the thermodynamic parameters for the adsorption of MB by SiO_2@poly(SVS-co-ITA-DA)

T **(K)**	***ΔG^0*** **(kJ/mol)**	***ΔH^0*** **(kJ/mol)**	***ΔS^0*** **(kJ/mol K)**
308.15	-2.244	13.37	0.05066
313.15	-2.497		
318.15	-2.750		
323.15	-3.003		
328.15	-3.257		
333.15	-3.510		

120 min.

Table S4 Data of adsorption isotherm of Langmuir and Freundlich models for the adsorption on SiO_2@poly(SVS-co-ITA-DA) for MB at 303 K.

Isotherms	Parameters	Temperatures(K)
		303
Langmuir	Q_m(mg/g)	75.76
	K_L(L/mg)	0.2326
	R_L	0.02327-0.8269
	R^2	0.9906
Freundlich	K_F [(mg/g)(L/mg)$^{1/n}$]	26.21
	n	4.456
	R^2	0.8896

Table S5 Comparison of adsorption capacity qm(mg•g-1) of MB on various materials.

Materials	Maximum adsorption capacity qm (mg • g-1)	References
Persian Kaolin	20.40	[1]
Naturalmontmorillonite	78.20	[2]
Natural zeolite	14.40	[3]
Zeolite MCM-22	57.60	[3]
chitosan/graphene oxide	130.10	[4]
mesoporous SBA-15	49.28	[5]
SiO_2@poly(SVS-co-ITA-DA)	62.20	This work

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