Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary material

Fabrication of monodisperse polypyrrole/SBA-15 composite for the selective removal of Cr(Ⅵ) from aqueous solutions

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Text S1 Hexavalent chromium standard curve

The absorption intensity of Cr(VI) solution from 800 to 300 nm wavelength was determined by diphenylcarbazide spectrophotometry[1]. It can be seen from Fig. S1a that the maximum absorption wavelength of Cr(VI) solution was 540 nm. The absorbance of Cr(VI) solution (0.05-1 mg/L) was determined, the relationship between absorbance and concentration was accorded with Lambert-Beer law and showed a linear relationship. The standard curve Fig. S1b of Cr(VI) was drawn.

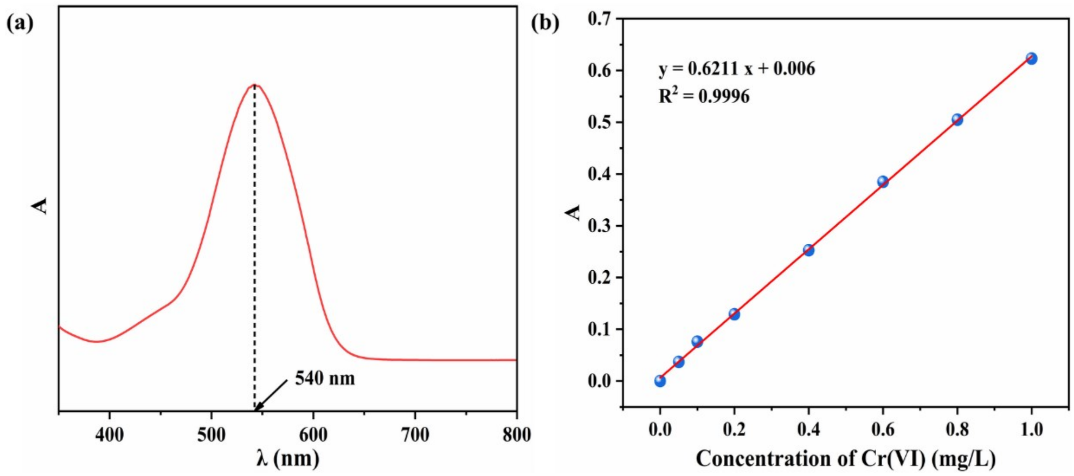

Fig. S1 Absorption intensity of Cr(VI) solution from 800 to 300 nm wavelength (a) and standard curve of Cr(VI) (b)

Test S2 Determination of particle size distribution and dispersion coefficient

SBA-15 and PPy/SBA-15 were dispersed in deionized water with the concentration of 0.1 g/L. After ultrasonic dispersion for 20 minutes, the particle size distribution was tested and analyzed by nano-particle size potentiometer (Zetasizer Nano ZS). Figure S2 showed the particle size distribution of SBA-15 and PPy/SBA-15, in which the dispersion coefficients of SBA-15 and PPy/SBA-15 were 0.241 and 0.342 respectively. It showed that the synthesized SBA-15 and PPy/SBA-15 was monodisperse[2].

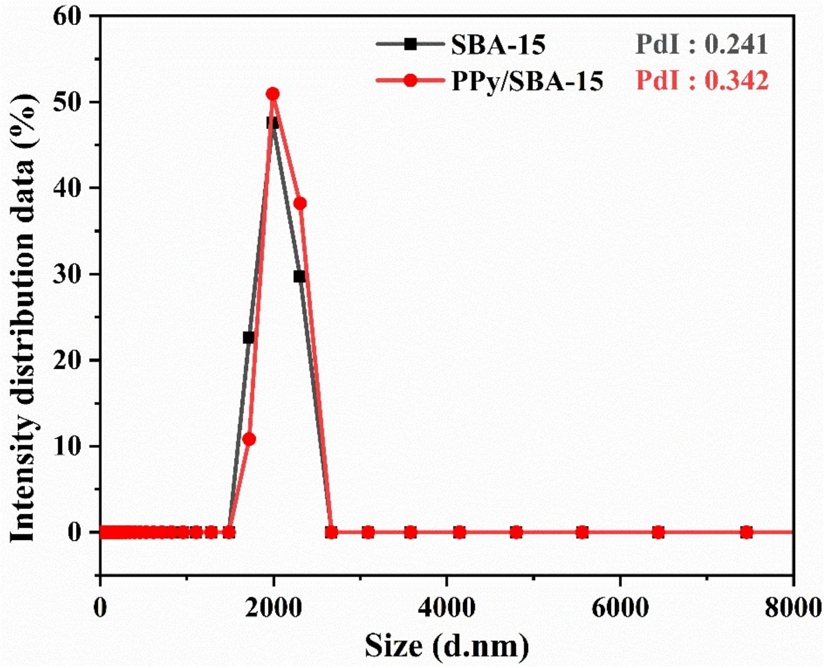

Fig. S2 The particle size distribution of SBA-15 and PPy/SBA-15

Text S3 Effect of Py concentration

PPy/SBA-15 (25 mg, Py concentrations: 10-90 wt%) was added to the Cr(VI) solution (50 mL) with an initial concentration of 200 mg/L at pH 2.0 for 24 h at 298 K. Then, the mixture was filtered to measure the content of Cr(VI). Fig. S3 showed the adsorption properties for Cr(VI) with different Py concentrations.

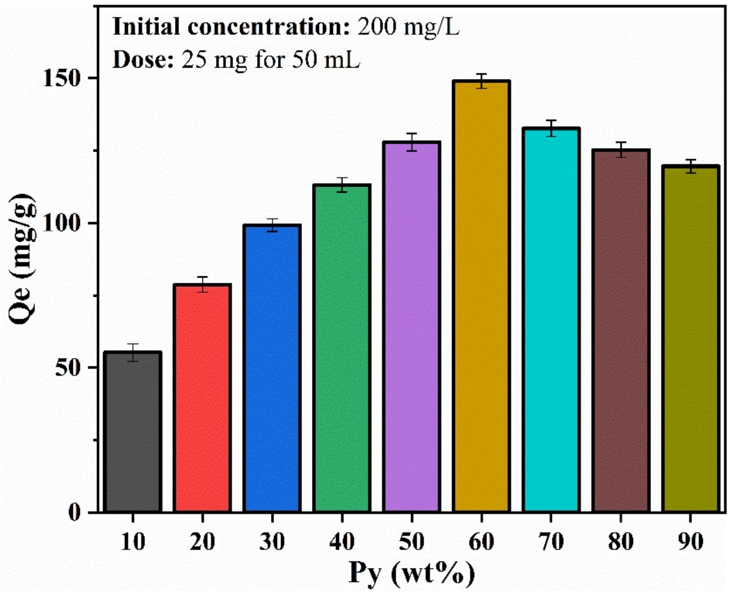

Fig. S3 Adsorption properties for Cr(VI) with different Py concentrations

Text S4 Effect of pH

Influences of solution pH for Cr(Ⅵ) adsorption by PPy, SBA-15 and PPy/SBA-15 were investigated. The adsorbent of 25 mg was added to the initial concentration of solution of 100 mg/L Cr(VI) of 25 mL, the pH (2-8) of the solution was adjusted by HCl (0.2-2 M) or NaOH (0.2-2 M), and adsorbed at 298 K for 24 h. The content of Cr(VI) in the solution was determined after filtration.

Text S5 Effect of adsorbent dose

Effect of the dose of PPy/SBA-15 on the adsorption performance of Cr(VI) was studied. PPy/SBA-15 (10-150 mg) was added to the Cr(VI) solution of 25 mL 100mg/L, and the pH of the solution was adjusted to 2 by was adjusted by HCl (0.2-2 M) or NaOH (0.2-2 M), then adsorbed for 24 hours at 298 K. The content of Cr(VI) in the solution was determined after filtration.

Text S6 Adsorption kinetics

The adsorption process of Cr(VI) was analyzed by adsorption kinetics. In typical kinetic experiments, the PPy/SBA-15 of 30 mg was added to the 200 mL Cr(VI) solution (25, 50 and 75 mg/L) and the pH of the solution was adjusted to 2 by was adjusted by HCl (0.2-2 M) or NaOH (0.2-2 M). It was mixed with the rate of 400 rpm at 298 K and the filtered solution was collected and tested at a predetermined time.

Equations of pseudo-first-order and pseudo-second-order models were expressed as follows[3]:

$$\mathrm{Ln}(Q_e - Q_t) = \mathrm{Ln}Q_e - K_1 t \tag{1}$$

$$\frac{t}{Q_t} = \frac{1}{K_2 Q_e^{\,2}} + \frac{t}{Q_e} \tag{2}$$

Where Q_t (mg/g) was the adsorption capacity of PPy/SBA-15 at t (min) time, K_1 (min^{-1}) was the pseudo-first-order rate constant, and K_2 (mg^{-1} min^{-1}) was the pseudo-second-order rate constant, respectively.

Taking the intraparticle mass transfer diffusion into consideration, the intraparticle diffusion model was also discussed as follows:

$$Q_t = K_i t^{1/2} + C_i \tag{3}$$

Where K_i (mg/g min$^{1/2}$) was the intraparticle diffusion rate constant, and C_i (mg/g) was a constant related to the boundary layer thickness.

Text S7 Adsorption isotherm

Under the condition of pH 2, the Cr(VI) solution (50-500 mg/L) and the adsorbent of 25 mg were adsorbed for 24 hours at 298, 308 and 318 K, respectively. The filtered solution was collected and the adsorption isotherm was determined.

The linear form of Langmuir isotherms was given as follows[3]:

$$\frac{C_e}{Q_e} = \frac{C_e}{Q_m} + \frac{1}{Q_m K_L} \tag{4}$$

Where Q_m (mg/g) was the maximum adsorption capacity, and K_L (L/mg) was the Langmuir adsorption constant.

The Freundlich isotherm model supposed that the surface of the adsorbent was heterogeneous in nature, which could deal with both homogeneous adsorption and heterogeneous adsorption. The linear form of Freundlich was given as follows:

$$\mathrm{LnQ_e = LnK_F + b_F LnC_e} \quad (5)$$

Where K_F (mg/g) (L/mg)$^{1/n}$ was the Freundlich constant and b_F was a constant related to the adsorption intensity.

The Temkin isotherm model indicated that the heat of adsorption decreased linearly with the increase of Cr(Ⅵ) concentration, and was written as follows:

$$\mathrm{Q_e = \frac{RTLna_t}{b_t} + \frac{RTLnC_e}{b_t}} \quad (6)$$

Where a_t (L/mg) was the binding constant corresponding to the maximum binding energy when the adsorption reached equilibrium and b_t (J/mol) was a constant related to the heat of adsorption, R (8.314 J/mol·K) was the ideal gas constant, and T (K) was experimental temperature.

1. L. Du, P. Gao, Y. Meng, Y. Liu, S. Le and C. Yu, *ACS Omega*, 2020, **5**, 6651-6660.
2. A. Sayari, B. H. Han and Y. Yang, *J. Am. Chem. Soc.*, 2004, **126**, 14348-14349.
3. Y. Duan, Y. Song and L. Zhou, *J. Colloid Interface Sci.*, 2019, **546**, 351-360.