Supporting Information

Phosphonate-Functionalized Polystyrene Microspheres with Controlled Zeta Potential for Efficient Uranium Sorption

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1. Characterization methods

¹H nuclear magnetic resonance (¹H NMR) spectrum of DEVBP was obtained on a Varian INVOA-400 instrument. The critical micelle concentration (CMC) was determined using pyrene as a fluorescence probe, and the fluorescence spectra were recorded using FLS920 fluorescence spectrometer at the emission wavelength of 382 and 371 nm ($\lambda_{excitation} = 334$ nm). Field-emitting scanning electron microscopy (FE-SEM) images were performed on a HITACHI S-570 microscope with an accelerating voltage of 15 kV, and energy-dispersive X-ray (EDX) analysis was carried out with an EDAX-PV 9100 energy dispersion X-ray fluorescence analyzer. Malvern Zetasizer (632.8 nm, He-Ne laser) was used to determine zeta potential and Z-average size distribution of the nanoparticles. Transmission electron microscopy (TEM) images of particles were obtained by a FEI Tecnai G20 electron microscope (120 kV). The concentration of uranyl ions was measured by thermo inductively coupled plasma mass spectrometer (ICP-MS, Element II).

2. Sorption kinetics

The pseudo-first-order equation is generally expressed as Equation $(1)^{1}$:

$$\log(q_{\rm e} - q_{\rm t}) = \log q_{\rm e} - (\frac{k_{\rm l}}{2.303}) \times t \qquad (1)$$

where q_t and q_e (mg/g) are the concentrations of uranium at time *t* and equilibrium time (min), respectively. k_1 (h⁻¹) is the pseudo first order kinetic constant. k_1 and q_e can be obtained from the slope and intercept of the plot of log (q_e - q_t) versus *t*, respectively (Figure S2A).

And the pseudo-second-order equation is given as Equation (2) 2,3 :

$$\frac{t}{q_{t}} = \frac{1}{k_{2} \times q_{e}^{2}} + \frac{t}{q_{e}}$$
(2)

where k_2 (g/mg/h) is the rate constant of the pseudo-second order, which can be obtained from the plot of t/q_t against t (Figure S2B).

3. Sorption isotherm

The equilibrium data were applied to Langmuir and Freundlich isotherm models. Langmuir model is represented by Equation (3), which describes monolayer sorption based on the assumption that all the sorption sites have equal affinity, and that desorption at one site doesn't affect an adjacent site ⁴.

$$\frac{C_e}{q_e} = \frac{1}{q_{\max}b} + \frac{C_e}{q_{\max}}$$
(3)

where q_{max} (mg/g) is the maximum sorption amount (i.e. sorption capacity), C_{e} (mg/L) is equilibrium concentration of uranium solution, b (L/mg) is the Langmuir adsorption equilibrium constant. And q_{max} and the Langmuir constant b can be calculated from the linear plot of $C_{\text{e}}/q_{\text{e}}$ against C_{e} , respectively (Figure S3A).

The Freundlich model can be applied for multilayer sorption and the sorption on heterogeneous surfaces, which can be expressed as Equation $(4)^{5}$:

$$\log q_{\rm e} = \log K_{\rm F} + \frac{1}{n_{\rm F}} \log C_{\rm e} \tag{4}$$

Where $n_{\rm F}$ and $K_{\rm F}$ (mol¹⁻ⁿLⁿ/g) are Freundlich constants related to sorption capacity and sorption intensity, respectively, which can be obtained from the linear plot of log $q_{\rm e}$ versus log $C_{\rm e}$, respectively (Figure S3B).



Figure S1. (A) SEM image, (B) particle size distribution of polystyrene microspheres and (C) EDX of sorbent after uranium sorption. (Experimental conditions: 0.14 g/L sorbent (47.2 mV), 1.36 mg/L uranyl ions, 298.15 K, pH 8.0, 298.15 K.)



Figure S2. (A) Pseudo-first order and (B) Pseudo-second order kinetics of uranium (VI) by sorbents with different zeta potentials (i.e. 47.2, -2.83 and -23.8 mV). (Experiment condition: 28.0 mg sorbent, 200 mL solution, 1.36 mg/L uranium (VI), pH 8.0, and 298.15K.)



Figure S3. (A) Langmuir and (B) Freundlich sorption isotherm plots for the sorption of uranium (VI) onto sorbents with different zeta potentials (i.e. 47.2, -2.83 and -23.8 mV). (Experiment condition: 28.0 mg sorbent, 200 mL solution, pH 8.0, and 298.15K.)

References

(1) Lagergren, S., zur theorie der sogenannten adsorption gelöster stoffe. K. Sven. Vetenskapsakad., Handl., Band 24 1898, 4, 1-39.

(2) Ho, Y. S., Review of second-order models for adsorption systems. *J. Hazard. Mater.*2006, *136* (3), 681-689.

(3) Ho, Y. S.; McKay, G., Sorption of dye from aqueous solution by peat. *Chem. Eng. J.***1998,** *70* (2), 115-124.

(4) Sadeghi, S.; Aboobakri, E., Magnetic nanoparticles with an imprinted polymer coating for the selective extraction of uranyl ions. *Microchim. Acta* **2012**, *178* (1-2), 89-97.

(5) Freundlich, H., Concerning adsorption in solutions. *Zeitschrift Fur Physikalische Chemie--Stochiometrie Und Verwandtschaftslehre* **1906**, *57* (4), 385-470.