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Electronic Supplementary Information for

Efficient removal of uranium (VI) from simulated seawater with hyperbranched polyethylenimine (HPEI) – functionalized polyacrylonitrile fiber

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Fig. S1 shows the FT-IR spectra of raw PANF, PAN-HPEI$_{0.07}$, PAN-HPEI$_{0.17}$, PAN-HPEI$_{0.33}$ and PAN-HPEI$_{0.66}$.

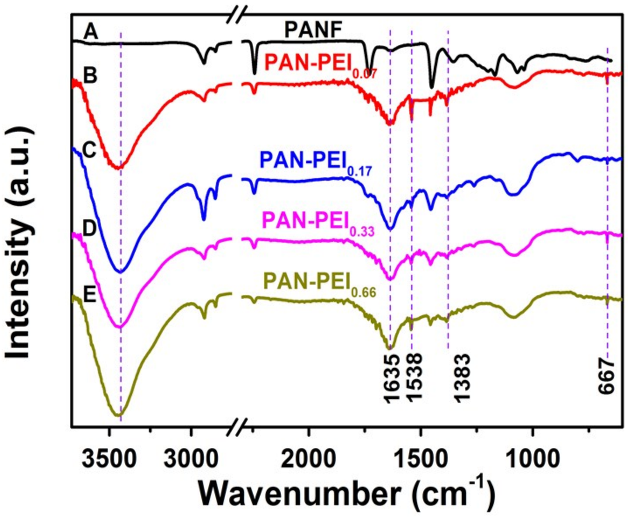

Fig. S2 shows the SEM morphology of raw PANF, PAN-HPEI$_{0.07}$, PAN-HPEI$_{0.17}$, PAN-HPEI$_{0.33}$ and PAN-HPEI$_{0.66}$.

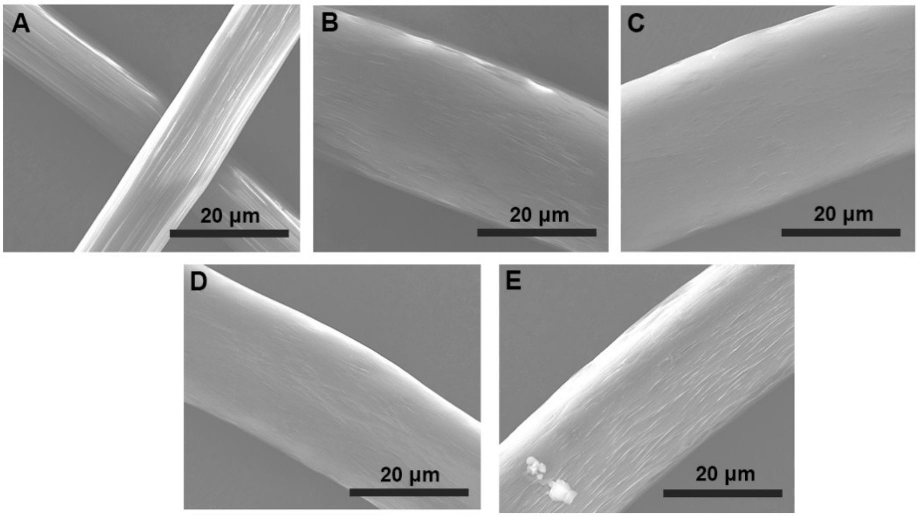

Fig. S3 shows the effect of concentrations on the adsorption of U(VI) with different grafting degrees of PAN-HPEI. (V= 50 mL, T= 298 K, m= 0.02 g)

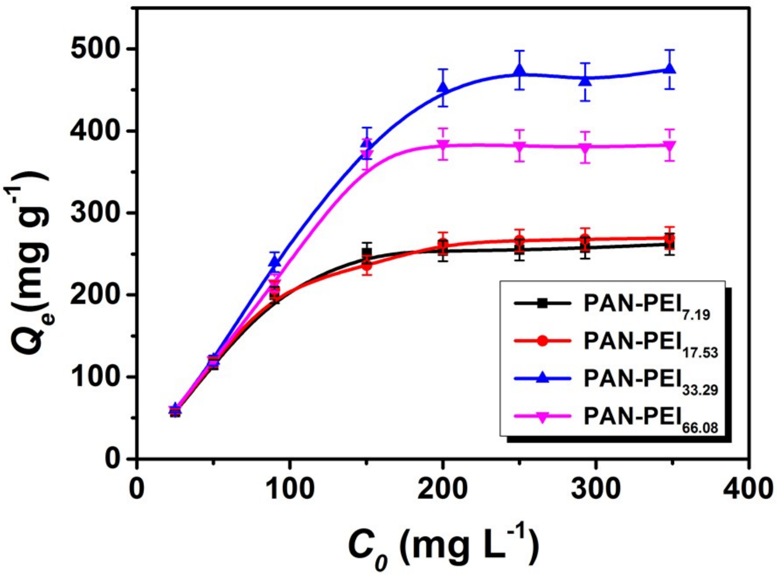

Fig. S4 shows the experimental data of desorption with HCl of different concentration.

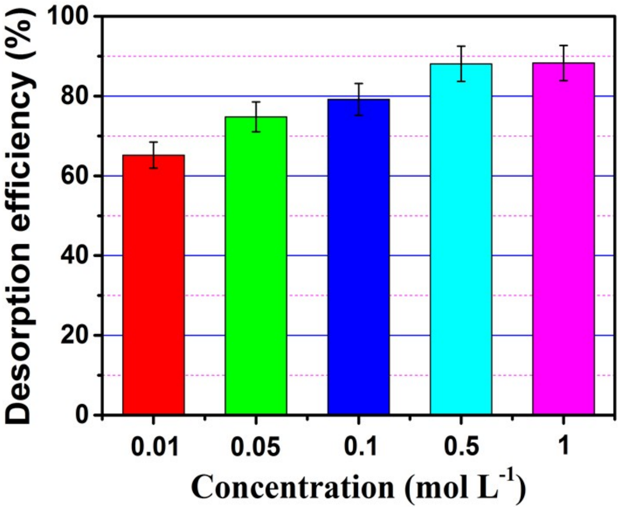

Fig. S5 shows the contact angles of the PAN and PAN-HPEI with different grafting degrees.

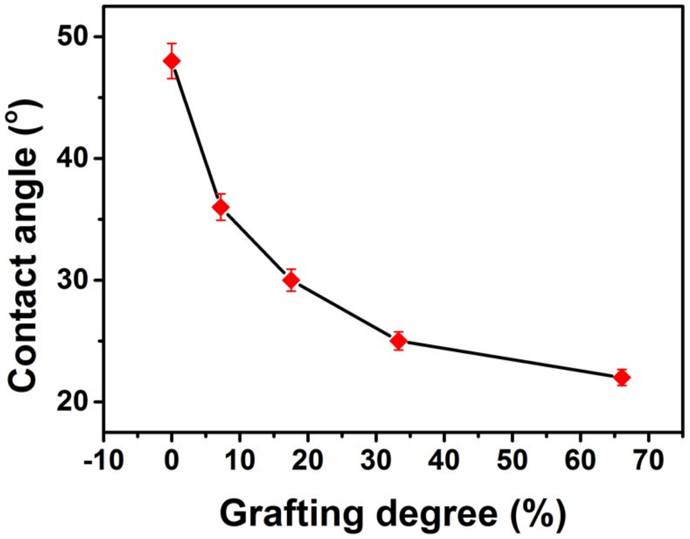

Fig. S6 shows the machanical properties (A) Elongation and (B) Tensile strength of the PAN-HPEI with different grafting degrees.

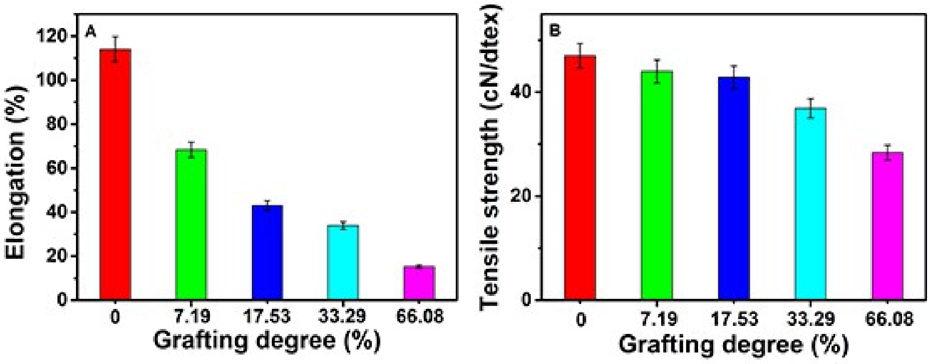

Fig. S7 shows the porosity of the PAN and PAN-HPEI with different grafting degrees.

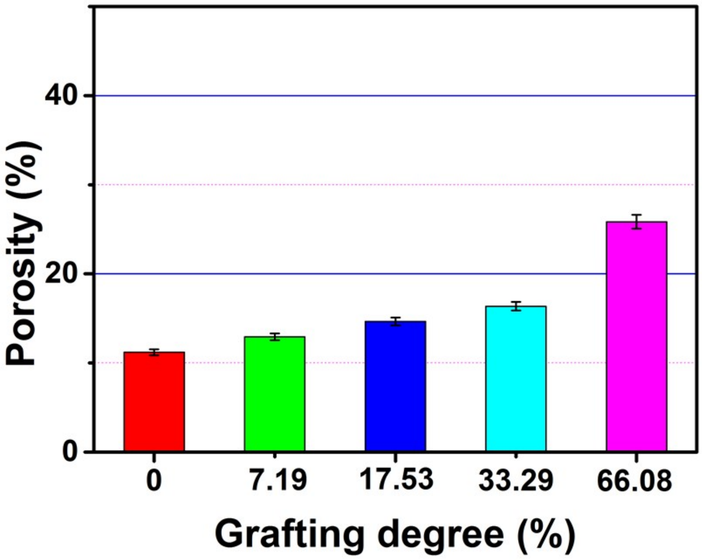

Table S1. The concentrations of the competing ions and the "V", "T", "m" and "t".

V (mL)	T (K)	M (g)	t (h)	C_0 (mg L^{-1})							
				Sr	Ba	Ca	U	V	Na	Mg	Zn
50	298	0.02	12	73	115	23.4	200	42.68	19.2	20.3	54.9

Adsorption Kinetics:

Assuming that the adsorption is controlled by diffusion step, the pseudo-first order equation is written as:

$$\ln\left(Q_e - Q_t\right) = \ln Q_e - k_1 t \qquad (1)$$

Where k_1 is the rate constant of pseudo-first order adsorption, Q_e and Q_t (mg g^{-1}) are the amount of U(VI) adsorbed at equilibrium and at time (t), respectively.

And assuming that the adsorption process is controlled by the chemical adsorption, the pseudo-second order equation is given as:[1]

$$t / Q_t = 1 / (k_2 \cdot Q_e^{\,2}) + t / Q_e \qquad (2)$$

Where k_2 is the rate constant of pseudo-second order equation.

To further catch on the rate controlling steps, intra-particular diffusion model in view of the assumption that liquid film diffusion resistance is negligibly small was applied to study the adsorption process, and the equation based upon Weber-Morris equation was described as follows:

$$Q_t = k_3 t^{0.5} + C \qquad (3)$$

Where k_3 (mg g^{-1} $\mathrm{min}^{-0.5}$) is the intra-particular diffusion rate constant and C (mg g^{-1}) is a constant proportional to the boundary layer, respectively. The higher value of C is, the greater contribution of the boundary layer makes.

[1] S.W. Zhang, M.Y. Zeng, J.X. Li, J. Li, J.Z. Xu, X.K. Wang, Porous magnetic carbon sheets from biomass as an adsorbent for the fast removal of organic pollutants from aqueous solution, J. Mater. Chem. A 2 (2014) 4391–4397.

[2] Y.-S. Ho, G. McKay, The kinetics of sorption of divalent metal ions onto sphagnum moss peat, Water Res. 34 (2000) 735–742.

[3] T. Wen, Q. Fan, X. Tan, Y. Chen, C. Chen, A. Xu, X. Wang, A core–shell structure of polyaniline coated protonic titanate nanobelt composites for both Cr(VI) and humic acid removal, Polym. Chem. 7 (2016) 785–794.

Adsorption isotherms:

The Langmuir isotherm, as one of the most famous well-adopted models used to describe the adsorption systems from solutions, has been utilized extensively for dilute solutions in the following equation:[2]

$$Q_e = b \cdot q_m \cdot C_e / (1 + bC_e) \qquad (4)$$

Where Q_m (mg g^{-1}) is the maximum adsorption capacity, *b* is the Langmuir adsorption equilibrium constant.

The separation factor constant (R_L) is a factor revealing the applicability of the fiber towards a targeted metal ion and may be calculated from the equation:

$$R_L = \frac{1}{1 + \mathrm{b}C_0} \qquad (5)$$

The value of R_L provides guidance for the possibility of the adsorption process to proceed. R_L> 1.0, unsuitable; R_L= 1.0, linear; 0< R_L = 1.0, suitable; R_L= 0, irreversible. The values of R_L, as displayed in **Fig. 6B**, were found to range from 0.00587 to 0.19333, indicating the suitability of PAN-HPEI as adsorbents for the recovery of U(VI) ions from aqueous solutions.

Another factor can help understanding the behavior of the adsorption of U(VI) ions on PAN-HPEI, is the Langmuir surface coverage rate (θ), which relates the surface coverage of the fiber to the initial concentration of U(VI) ions and can be calculated using the following equation:[3]

$$\theta = \frac{bC_0}{1 + \mathrm{b}C_0} \qquad (6)$$

The relationship of θ and initial concentration of U(VI) ions was depicted in **Fig. 6B**. Evidently, the adsorption of U(VI) ions on PAN-HPEI in the early age was very fast (low coverage of fiber surface and plenty of free active sites are available for binding with the metal ions) then tends to be a plateau at higher surface coverage where most of the active sites are occupied. This implies the applicability of Langmuir model to describe the adsorption of U(VI) ions on PAN-HPEI.

The Freundlich model is based on a reversible heterogeneous adsorption since it is not restricted to monolayer adsorption capacity [1]. The Freundlich isotherm equation is given as:

$$Q_e = K_f \cdot C_e^{1/n} \qquad (7)$$

Where *k* and *n* are the Freundlich constants related to the adsorption capacity and adsorption intensity, respectively.

The Sips model is according to the combination of Langmuir and Freundlich model, and the mathematical formula is as follows:

$$Q_e = \frac{Q_s K_s C_e^m}{1 + K_s C_e^m} \tag{8}$$

Where Q_s is the saturated adsorption capacity, K_s is the Sips constant related to the adsorption energy and m is the Sips constant. When the 1/m equals to zero the adsorption is heterogeneous adsorption, while the homogeneous adsorption happens when 1/m is 1.

The D-R model, which is applied to get further information of the nature of the adsorption process [2], is on the basis of assumption that a Gaussian energy distribution onto a heterogeneous surface with an expression of the following equations:

$$Q_e = Q_{DR} e^{(-\beta \varepsilon^2)} \tag{9}$$

$$\varepsilon = RT \ln(1 + \frac{1}{C_e}) \tag{10}$$

$$E = 1/\sqrt{2\beta} \tag{11}$$

Where Q_{DR} (mg g^{-1}) is the monolayer saturated adsorption capacity, β (mol^2 kJ^{-2}) is related to the free energy of adsorption and E (kJ mol^{-1}) stands for the mean free energy which can be used as the indicator whether the process is manipulated by physical adsorption.

1. I. Langmuir, *J. Am. Chem. Soc.*, 1918, **40**, 1361-1403.
2. K. Y. Foo and B. H. Hameed, *Chemical Engineering Journal*, 2010, **156**, 2-10.