

Biomass-based Cellulose Functionalized by Phosphonic Acid with High Selectivity and Capacity for Capturing U(VI) in Aqueous Solution

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Schematic of the synthetic route of PVKAP

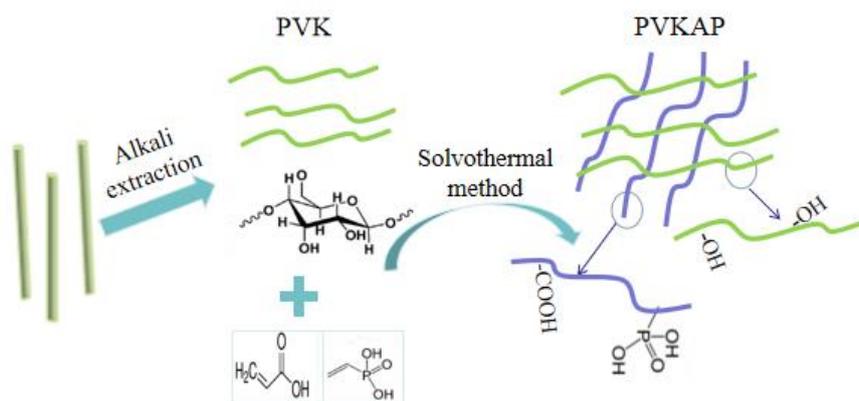


Figure S1. Schematic of the synthetic route of PVKAP.

Details of the Langmuir and Freundlich adsorption models

The Langmuir and Freundlich adsorption models are commonly used to describe adsorption isotherms, which are given as the following equations:

$$\text{Langmuir models } q_e = K_L q_{\max} C_e / (1 + K_L C_e)$$

$$\text{Freundlich models } q_e = K_F C_e^n$$

where q_{\max} (mg g^{-1}) is the maximum monolayer adsorption capacity, C_e (mg L^{-1}) is the equilibrium concentration of the uranyl ion in solution, q_e (mg g^{-1}) is the equilibrium adsorption capacity of the uranyl ion, K_L (L mg^{-1}) is the Langmuir adsorption constant, K_F (mg g^{-1}) and n (ranging between 0 and 1) are the Freundlich adsorption constants.

Details of the calculated equations and method for adsorption thermodynamics

Adsorption thermodynamic parameters (ΔH° , ΔS° and ΔG°) of U(VI) adsorption are calculated from the slope and intercept of the $\ln K_d$ vs $1/T$ curve, which is on the basis of the approach previously reported by Lyubchik et al. [1]. The values of ΔH° and ΔS° are calculated based on the following equations [2]:

$$\ln K_d = \frac{\Delta S^\circ}{R} - \frac{\Delta H^\circ}{RT}$$

$$\Delta G^o = \Delta H^o - T\Delta S^o$$

Where R ($8.314 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$) is the ideal gas constant, and T (K) is the temperature in Kelvin.

Contact time effect and kinetics Study

The pseudo-first-order and the pseudo-second-order models are established to fit the experimental data and describe the control mechanisms of the U(VI) adsorption process, which can be expressed as the following equations [3, 4]:

The pseudo-first-order kinetic model: $\log(q_e - q_t) = \log q_e - k_1 t / 2.303$

The pseudo-second-order model: $t/q_t = 1/k_2 q_e^2 + t/q_e$

Original data for XPS experiments

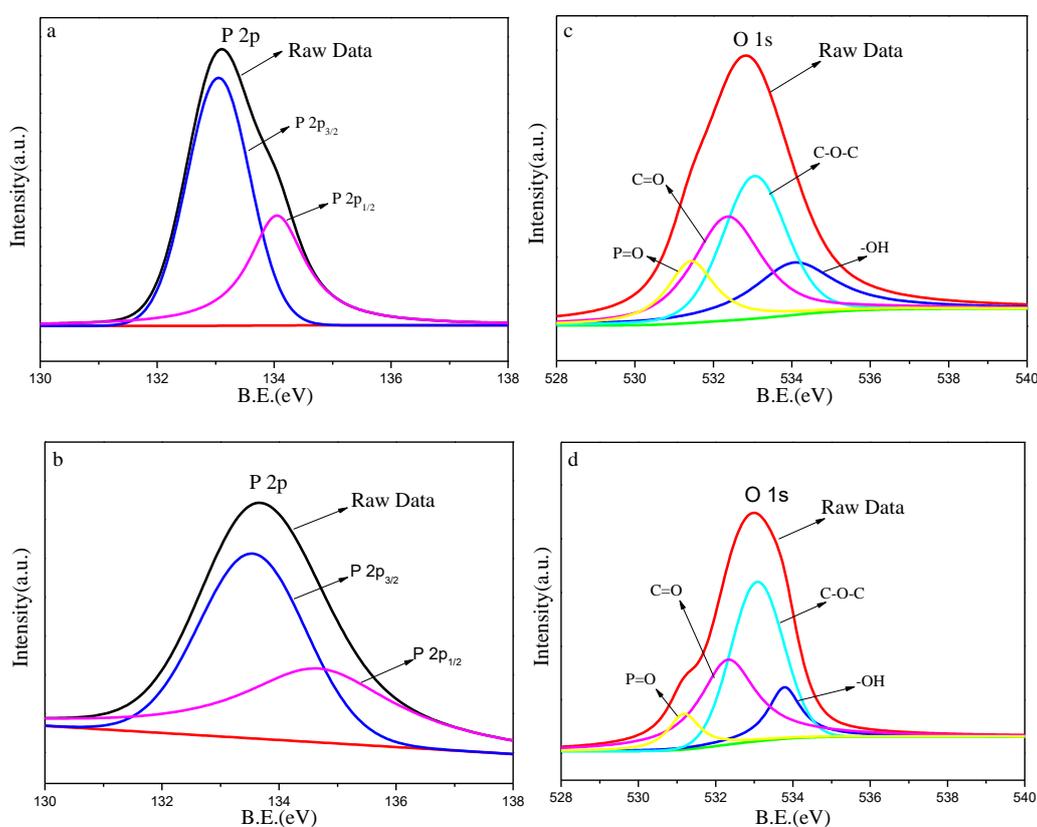


Figure S2. Original data for XPS experiments.

References

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3. Corbett, J. F. Pseudo first-order kinetics. *J. Chem. Educ.* **1972**, *49*, 663-663.
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