Zr-Gallic acid based metal organic compound as adsorbent for extraction of Uranium (VI) from Nitrate solution: Adsorption behaviors and mechanisms

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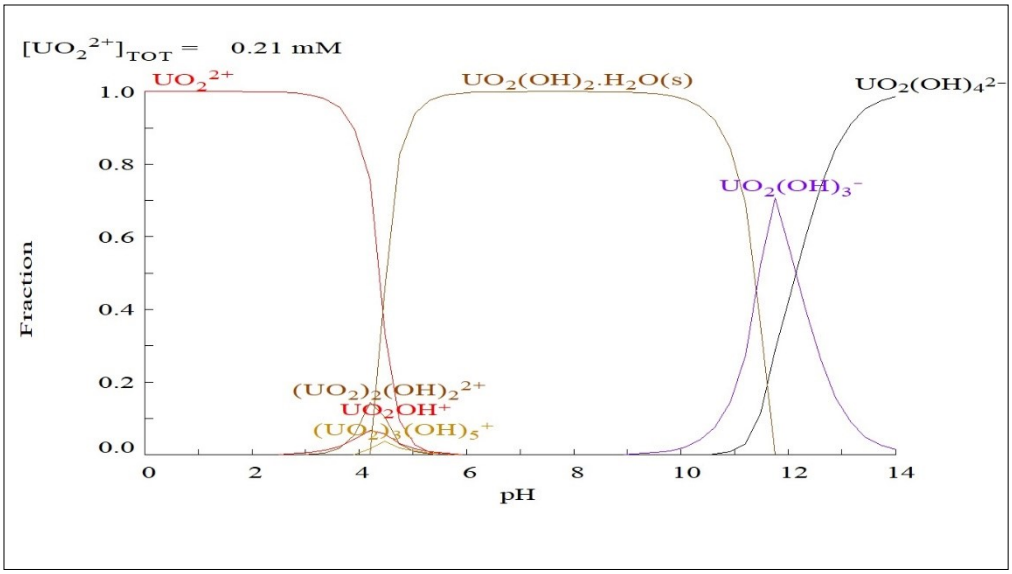

Figure S1: *U(VI) speciation as a function of solution pH, calculated using Hydra-MEDUSA equilibrium calculation program **[1]**.*

1) *Hussein AEM, Taha MH (2013) Uranium removal from nitric acid raffinate solution by solvent immobilized PVC cement. J Radioanal Nucl Chem 295:709–715. https://doi.org/10.1007/S10967-012-2158-3/TABLES/2*

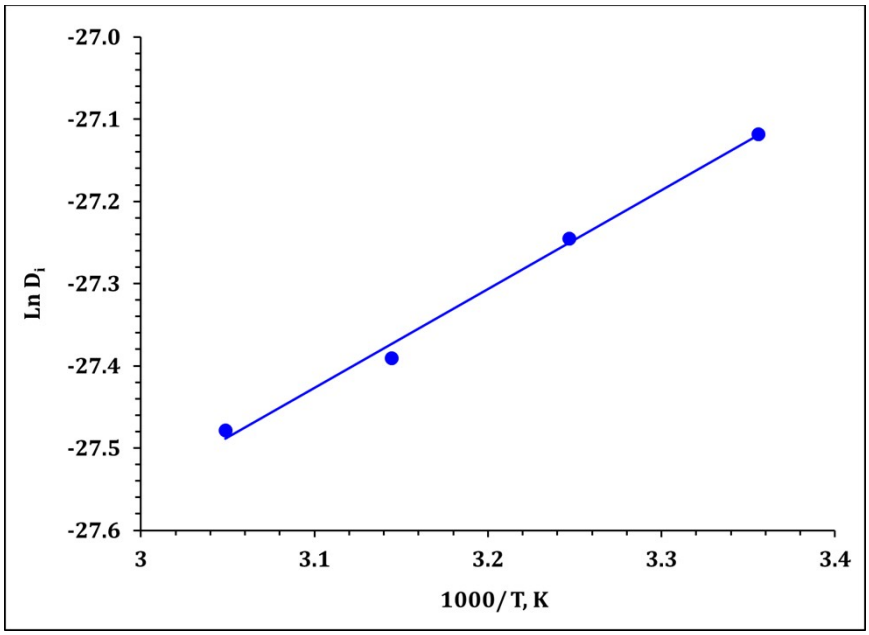

Figure S2: *Arrhenius plot for U(VI) sorption onto prepared composite*

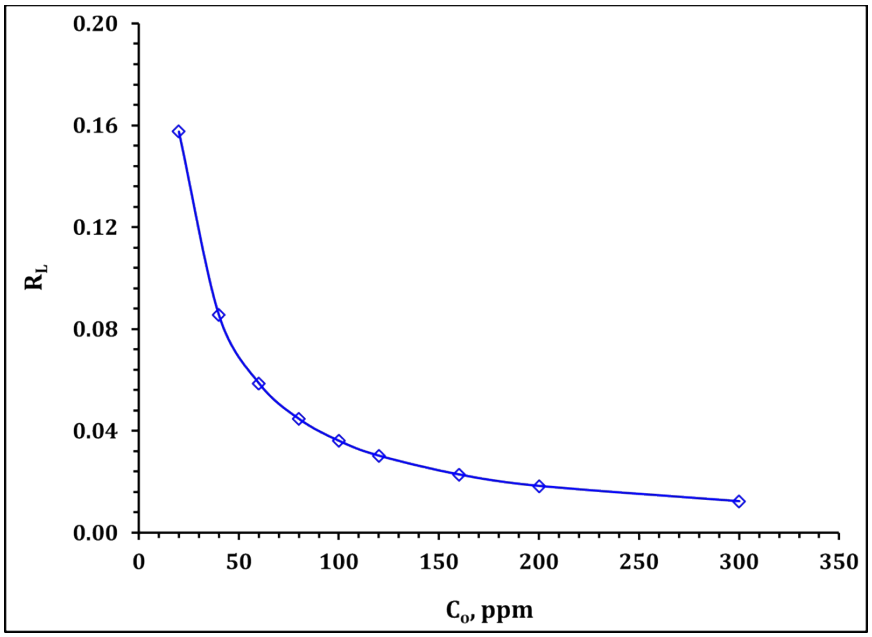

Figure S3: *Separation factor R_L of U(VI) adsorption process.*

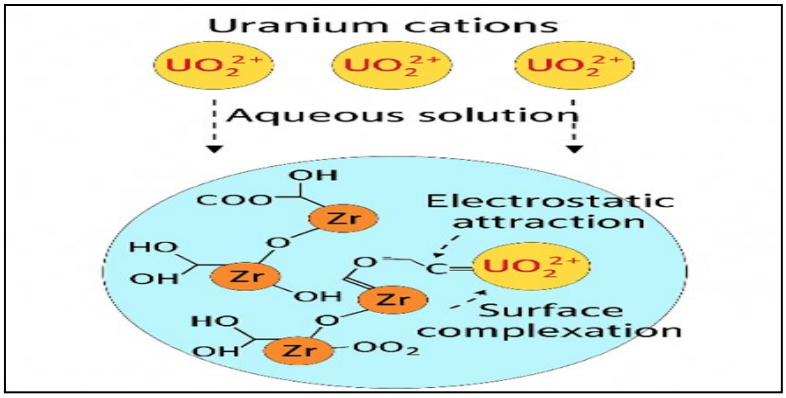

Figure S4. *Schematic representation of the proposed adsorption mechanism of U(VI) onto Zr-GA*

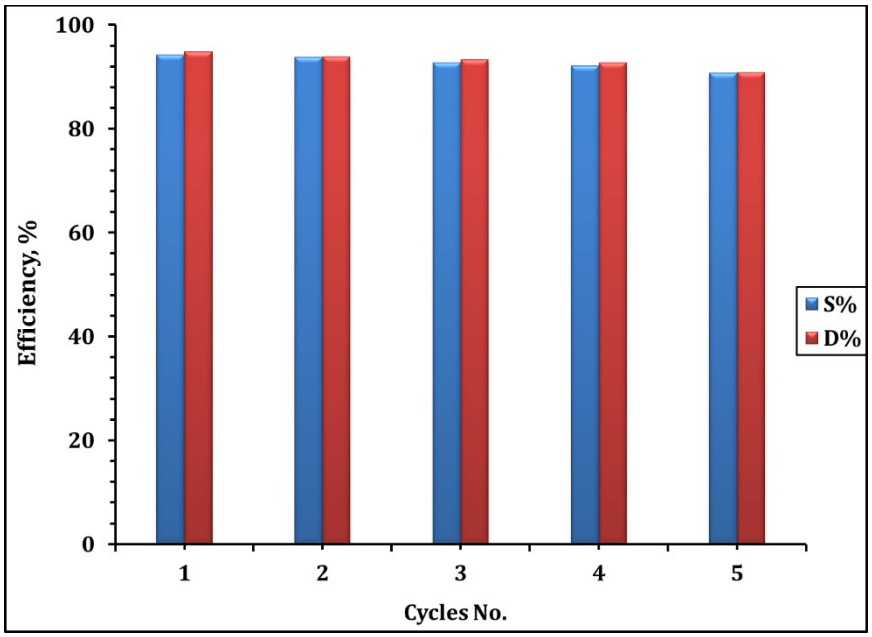

Figure S5: *Sorption/ desorption cycles for uranium capture process.*

Table S1: *Kinetic, isotherm, and thermodynamics equations for U(VI) adsorption process* ***[1-8]***.

Kinetics	Equations
Pseudo-first-order	$q_t = q_1\left(1 - e^{-k1t}\right)$
Pseudo-second-order	$q_t = \frac{1}{\left(1 \middle\vert k_2 q_2^2\right) + \left(t \middle\vert q_2\right)}$
Intra-particle diffusion model (IPD)	$q_t = K_{id}\, t^{0.5} + C_i$
Boyd model	$Bt = -0.4977 - Ln(1 - F)$
Isotherms	**Equations**
Langmuir model	$q_e = \frac{q_m k_L C_e}{1 + k_L C_e}$
Freundlich model	$q_e = K_F C_e^{1/n_F}$
Sips model	$q_e = \frac{q_S \left(k_S C_e\right)^{mS}}{1 + \left(k_S C_e\right)^{mS}}$
Thermodynamics	**Equations**
	$\log K_C = -\frac{\Delta H^o}{2.303\, R} X \frac{1}{T} + C$
	$-\Delta G^o = 2.303\, RT \log K_C$
	$\Delta G^o = \Delta H^o - T\, \Delta S^o$
Fitting	**Equations**
Coordination coefficient (R^2)	$R^2 = 1 - \frac{\sum_1^n \left(q_{exp} - q_{pred}\right)^2}{\sum_1^n \left(q_{exp} - \bar{q}_{exp}\right)^2}$

qe (mg g^{-1}) is the equilibrium concentration of U(VI) species, and qt (mg g^{-1}) is the adsorbed amount of U(VI) species ions after time t (min), Ce (mg L^{-1}) is equilibrium concentration of U(VI) species. k_1 (min^{-1}) and k_2 (min^{-1}) are the rate constants for the pseudo first and second order, respectively. K_{id} (mg/g. $min^{0.5}$) is a rate constant, and C is the thickness of the boundary layer. F is

the ratio of the sorbed quantity at time t and that sorbed at equilibrium; B is the time constant and it equals $\pi^2 D_i / r_o^2$ **[4]**; Di is the effective diffusion coefficient of metal ions; ro is the radius of the solid particles; and n is an integer. q_m and q_S are the maximum sorption capacity (mg. g^{-1}) of Langmuir and Sips models. k_L (L. mg^{-1}), K_F (L/ mg), and K_S (L/ mg) are represent the constants of Langmuir, Freundlich, and Sips models. n refer to the sorption intensity, $\boldsymbol{q_s}$ is the theoretical isotherm saturation capacity (mg/g). K_C is a non-dimensional equilibrium constant and it equals K_d X 1000 X ρ **[5]**; T is the temperature (K), $\boldsymbol{R}$ is the universal gas constant (8.314 J mol^{-1}. K^{-1}), ρ is solution density g/ L, and C is a constant. R^2 is the coordination coefficient, the number of test points is n, the experimental equilibrium capacity is q_{exp} (mg g^{-1}), while the predicted capacity is q_{pred} (mg g^{-1}).

Table S2: *Surface charges and mean particle sizes of Zr-GA before and after adsorption process*

Analysis	***Before***	***After***
DLS analysis, nm	*549.5*	*1116.1*
Zeta potential, mV	*-46.69*	*-26.49*

Table S3: *The values of Morris-Weber model parameters.*

		25 °C	**35 °C**	**45 °C**	**55 °C**
Weber and Morris model	**k_i (mg/g $min^{1/2}$)**	1.06	0.88	0.67	0.44
	C	20.5	13.5	10.4	5.3
	R^2	0.98	0.97	0.98	0.96

References:

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3) Tho, P.T., Van, H.T., Nguyen, L.H., Hoang, T.K., Tran, T.N.H., Nguyen, T.T., Nguyen, T.B.H., Le Sy, H., Tran, Q.B., Sadeghzadeh, S.M. and Asadpour, R., 2021. Enhanced simultaneous adsorption of As (iii), Cd (ii), Pb (ii) and Cr (vi) ions from aqueous solution using cassava root husk-derived biochar loaded with ZnO nanoparticles. *RSC advances*, *11*(31), pp.18881-18897.
4) Hassan, H.S., El-Kamash, A.M. and Ibrahim, H.A.S., 2019. Evaluation of hydroxyapatite/poly (acrylamide-acrylic acid) for sorptive removal of strontium ions from aqueous solution. *Environmental Science and Pollution Research*, *26*, pp.25641-25655.
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