

Supplementary Information:

Adsorption of Cd²⁺ ions onto zeolites synthesized from mixture of coal fly ash and oil shale ash in aqueous media

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Supplementary Tables

Tab. S1. Chemical composition of CFA and OSA

Component content (mass%)	SiO ₂	Al ₂ O ₃	CaO	Fe ₂ O ₃	Na ₂ O	MgO	SO ₃	TiO ₂	K ₂ O	others	SiO ₂ /Al ₂ O ₃
CFA	45.78	39.05	4.56	2.50	0.15	1.46	2.45	2.62	1.01	0.42	1.17
OSA	52.67	14.67	12.57	6.48	3.47	2.18	4.34	1.26	0.91	1.45	3.59

Tab. S2. Kinetics parameters for Cd²⁺ adsorption onto zeolites

Models	Samples	OSA100	OSA75	OSA50	OSA25	CFA100
Experiment	$q_{e,exp}$ (mg·g ⁻¹)	97.92	99.66	94.73	89.88	88.52
Pseudo-first-order	k_1 (min ⁻¹)	0.034	0.069	0.034	0.036	0.030
	$q_{e,cal}$ (mg·g ⁻¹)	24.19	43.99	27.66	23.25	31.89
	R^2	0.8879	0.9251	0.9684	0.9769	0.9708
Pseudo-second-order	k_2 (g·mg ⁻¹ ·min ⁻¹)	0.0036	0.0047	0.0036	0.0041	0.0025
	$q_{e,cal}$ (mg·g ⁻¹)	99.70	101.52	96.15	92.94	91.58
	R^2	0.9997	0.9999	0.9998	0.9998	0.9999
Intraparticle diffusion (stage 1)	k_p (mg·g ⁻¹ ·min ^{-1/2})	4.58	3.77	4.88	3.50	7.04
	C (mg·g ⁻¹)	62.25	70.96	59.24	61.72	39.53
	R^2	0.9474	0.7819	0.8508	0.7530	0.9559
Intraparticle diffusion (stage 2)	k_p (mg·g ⁻¹ ·min ^{-1/2})	0.32	0.36	0.97	0.61	1.07
	C (mg·g ⁻¹)	93.91	95.56	83.40	82.86	76.42
	R^2	0.7181	0.9721	0.7466	0.8631	0.8602

The adsorption capacity (q_e) at equilibrium was calculated using Eq. (S1):

$$q_e = \frac{(C_0 - C_e)V}{m} \quad \text{Eq. (S1)}$$

where C_0 (mg·L⁻¹) represents the initial Cd²⁺ concentration, C_e (mg·L⁻¹) is the Cd²⁺ concentration at equilibrium, V (L) is the volume of the solution, and m (g) is the mass of the adsorbent.

The uptake efficiency (E%) was calculated using Eq. (S2):

$$E\% = \frac{(C_0 - C_e) \times 100\%}{C_0} \quad \text{Eq. (S2)}$$

where C_0 and C_e (mg·L⁻¹) are the initial and equilibrium Cd²⁺ concentrations, respectively.

The linear expressions for the pseudo-first-order, pseudo-second-order, and intraparticle diffusion models are given as follows:

$$\ln(q_e - q_t) = \ln q_e - k_1 t \quad \text{Eq. (S3)}$$

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{1}{q_e} t \quad \text{Eq. (S4)}$$

$$q_t = k_p t^{1/2} + C \quad \text{Eq. (S5)}$$

In these equations, q_e and q_t ($\text{mg}\cdot\text{g}^{-1}$) denote the adsorption capacities at equilibrium and at any given time t , respectively. The rate constants k_1 (min^{-1}), k_2 ($\text{g}\cdot\text{mg}^{-1}\cdot\text{min}^{-1}$) and k_p ($\text{mg}\cdot\text{g}^{-1}\cdot\text{min}^{-1/2}$) correspond to the pseudo-first-order, pseudo-second-order, and intraparticle diffusion models, respectively. C ($\text{mg}\cdot\text{g}^{-1}$) represents the intercept of the plot of q_t as a function of $t^{1/2}$.

Tab. S3. Isotherm parameters for Cd²⁺ adsorption onto zeolites

Models	Samples	OSA100	OSA75	OSA50	OSA25	CFA100
Experiment	$q_{e,exp}$ (mg·g ⁻¹)	187.18	227.24	205.87	179.54	156.21
Langmuir	q_{max} (mg·g ⁻¹)	192.31	236.41	211.86	182.84	159.24
	K_L (L·mg ⁻¹)	0.13	0.09	0.10	0.07	0.10
	R^2	0.9908	0.9954	0.9961	0.9914	0.9928
Freundlich	K_F (mg·g ⁻¹)	60.59	60.66	57.10	50.78	52.05
	n_F	4.76	4.20	4.26	4.20	5.18
	R^2	0.7307	0.7908	0.7553	0.8469	0.7951
Dubinin-Radushkevich	q_{max} (mg·g ⁻¹)	129.14	153.30	143.54	126.23	116.51
	K_{DR} (mol ² ·J ⁻²)	$5.67 \cdot 10^{-8}$	$1.03 \cdot 10^{-7}$	$1.17 \cdot 10^{-7}$	$5.14 \cdot 10^{-8}$	$6.48 \cdot 10^{-8}$
	R^2	0.4934	0.8385	0.7051	0.5701	0.8777
	E_{DR} (kJ·mol ⁻¹)	2.97	2.21	2.07	3.12	2.78

The Langmuir isotherm model, which assumes monolayer adsorption onto a homogeneous surface with a finite number of identical adsorption sites, is widely employed for modeling equilibrium data in solid-liquid systems. The linearized form of the Langmuir equation is expressed as:

$$\frac{C_e}{q_e} = \frac{1}{q_{max}K_L} + \frac{C_e}{q_{max}} \quad \text{Eq. (S6)}$$

where K_L (L·mg⁻¹) is the Langmuir adsorption constant, which is related to the energy of adsorption, C_e (mg·L⁻¹) is the equilibrium concentration of Cd²⁺ ions in the solution, q_e (mg·g⁻¹) is the amount of Cd²⁺ ions adsorbed by the adsorbent at equilibrium, and q_{max} (mg·g⁻¹) represents the maximum monolayer adsorption capacity of the adsorbent.

The Freundlich isotherm, an empirical model, is typically used to describe adsorption on heterogeneous surfaces. The equation for the Freundlich isotherm is expressed as:

$$\ln q_e = \ln K_F + \frac{1}{n_F} \ln C_e \quad \text{Eq. (S7)}$$

where K_F ($\text{mg}\cdot\text{g}^{-1}$) is the Freundlich constant, and n_F is the characteristic constant of the adsorption system.

The Dubinin-Radushkevich (D-R) isotherm is similar to the Langmuir isotherm but is more general as it does not assume a homogeneous surface or constant adsorption potential. The linear form of the D-R equation is expressed as:

$$\ln q_e = \ln q_{\max} - K_{\text{DR}} \varepsilon^2 \quad \text{Eq. (S8)}$$

where q_{\max} ($\text{mg}\cdot\text{g}^{-1}$) is the maximum adsorption capacity, and K_{DR} ($\text{mol}^2\cdot\text{J}^{-2}$) is the affinity coefficient related to the adsorption energy $E = 1/(2K_{\text{DR}})^{1/2}$ ($\text{kJ}\cdot\text{mol}^{-1}$). The Polanyi potential ε is given by:

$$\varepsilon = RT \ln(1 + 1/C_e) \quad \text{Eq. (S9)}$$

where R ($\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$) is the ideal gas constant, T (K) is the absolute temperature, and C_e ($\text{mg}\cdot\text{L}^{-1}$) is the equilibrium concentration of the adsorbate in the solution.