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Supplementary Material

Study on adsorption of phosphate from aqueous solution by zirconium modified coal gasification coarse slag

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Text S-1: The removal efficiency (%R) and sorption capacity Qt

The removal efficiency (%R) and sorption capacity Qt (mg/g) were computed according to the following equations: [1]

$$\%R = (C_o - C_t) \times 100/C_o \quad (1)$$

$$Q_t = (C_o - C_t) \times V/m \quad (2)$$

where C_o, C_t are respective phosphate concentrations (mg/L) of the initial and different time, m, V are the mass of sorbent (g) and the solution volume (ml), respectively.

Text S-2: Langmuir and Freundlich isotherm equations

The Langmuir and Freundlich equations can be expressed as follows: [2]

Langmuir isotherm equation:

$$q_e = K_L q_m C_e/(1 + K_L C_e) \quad (3)$$

Freundlich isotherm equation:

$$q_e = K_F C_e^{1/n} \quad (4)$$

Where C_e (mg/L) represents the phosphate concentration at the equilibrium stage of sorption, q_e and q_m represents the sorption amounts of phosphate by CGCS-Zr4 at equilibrium and the theoretical maximum monolayer sorption capacity, respectively, K_L refers to the Langmuir constant, and measures the sorbent affinity to the solute. K_F is the adsorption coefficient. n refers characteristic surface heterogeneity.

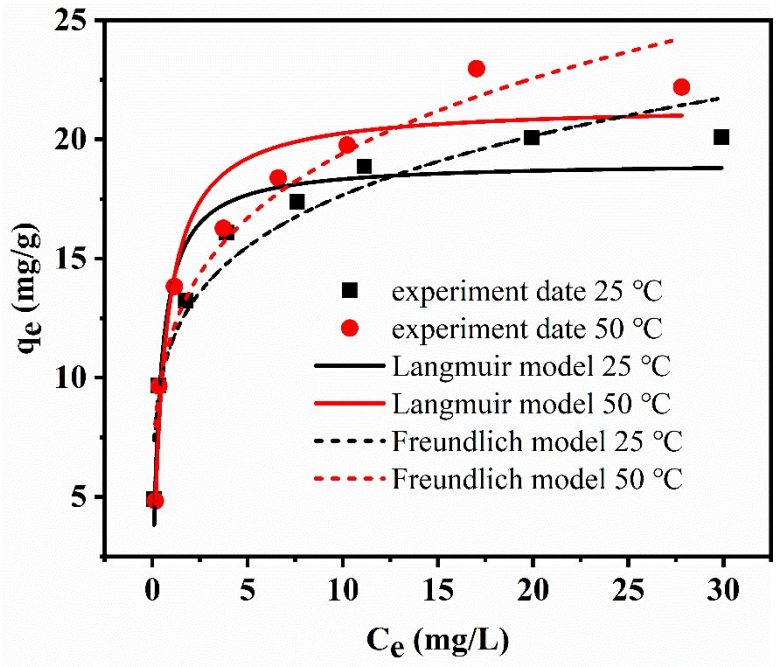


Fig. S-1. Adsorption isotherms of phosphate by CGCS-Zr4 at 25 and 50 ℃. Adsorption conditions: reaction time, 24 h; adsorbent dose, 1 g/L; and shake speed, 160 rpm.

Table S-1

Adsorption isotherm parameters. Experimental conditions: pH value = 6, adsorbent dosage = 1 g/L, reaction time = 24 h.

T (℃)	Langmuir			Freundlich		
	q_m (mg/g)	k_L (L/mg)	R^2	1/n	K_F (mg/g)	R^2
25	19.814	2.582	0.934	0.189	11.437	0.942
50	22.372	1.716	0.941	0.217	11.781	0.931

Table S-2

Comparison of the adsorption capacity of CGCS-Zr4 and adsorbents given in literatures for phosphate.

Adsorbent	Initial concentration (mg P/L)	pH	Temperature (°C)	Sorption capacity (mg/g)	Ref.

Zr/Al-Mt	20–50	5.0	25	17.2	[3]
BFSs	50-500	7.0	20	18.9	[4]
La-Ves	1.02-5.03	7.1	25	6.7	[5]
Magnetic Fe–Zr binary oxide	0-100	4.0	25	13.65	[6]
Iron oxide tailings	5-150	6.6-6.8	20-21	8.2	[7]
Zr-CNTs	5-50	3	30	10.9	[8]
Lepidocrocite	2–100	7.2	25	3.2	[9]
CGCS-Zr4	5-50	6	30	19.81	This study

Text S-3: kinetic model

The equations of the four kinetic models can be displayed below: [10, 11]

The pseudo first order equation:

$$q_{t=}q_e(1-e^{-k_1t}) \quad (5)$$

The pseudo second order equation:

$$q_t = k_2q_e^2t/(1+k_2q_et) \quad (6)$$

The intraparticle diffusion model:

$$q_t = K_{id}t^{1/2} + C \quad (7)$$

Elovich equation:

$$q_t = \frac{1}{\beta}\ln(1+\alpha\beta t) \quad (8)$$

where q_e and q_t represent the respective adsorbed amount of phosphate at equilibrium and any time t (min). k_1, k_2 and k_{id} are the rate constants of the Eq. (5), Eq. (6) and Eq. (7), respectively. C represents the thickness of the boundary layer. α is the initial adsorption rate; β is the desorption constant.

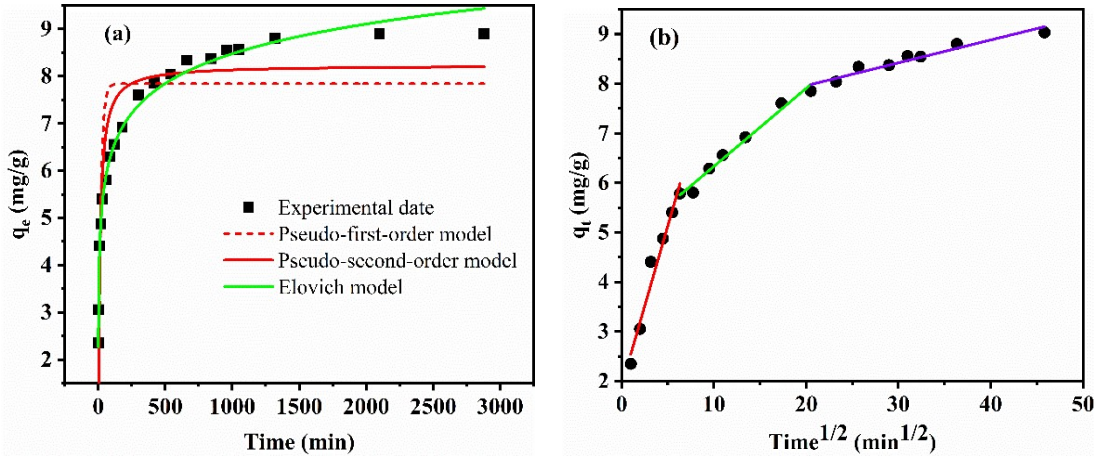


Fig. S-2. Adsorption kinetics of phosphate on CGCS-Zr4: (a) pseudo-first-order, pseudo-second-order and elovich models; (b) intraparticle diffusion model. Adsorption conditions: temperature, 25 ℃; shake speed: 160 rpm, adsorbent dose: 1 g/L, and initial phosphate concentration: 10 mg/L.

Table S-3

Adsorption kinetic parameters of CGCS-Zr4 to phosphate.

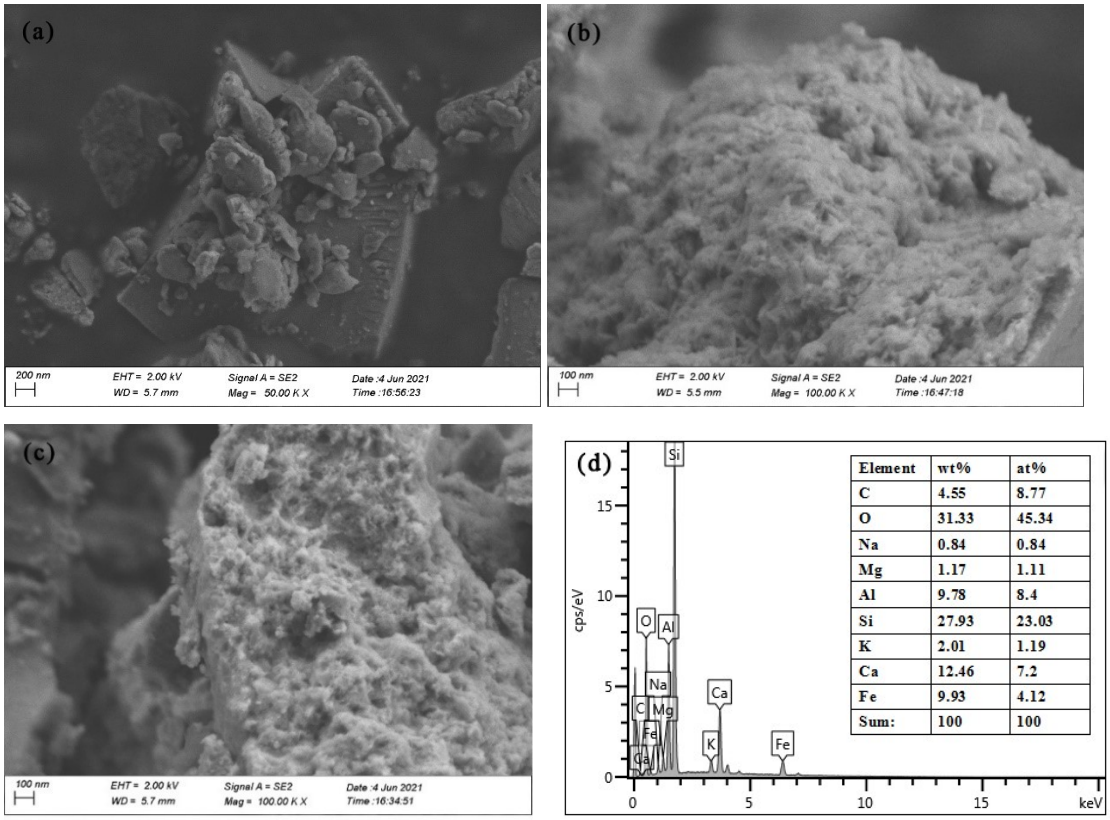
Kinetic models and Experimental results	Plot parameters	Values
Experimental adsorption capacity	$q_{e,exp}$ (mg/g)	9.14
Pseudo-first-order	$q_{e,cal}$ (mg/g)	7.84
	k_1 (min^{-1})	0.055
	R^2	0.718
Pseudo-second-order	$q_{e,cal}$ (mg/g)	8.233
	K_2 (g/(mg min))	0.010
	R^2	0.861
Elovich	α (mg/ (g min))	10.181
	β (g/mg)	1.100
	R^2	0.990
Intraparticle diffusion	K_{id1} (mg/g min$^{1/2}$)	0.646
	C	1.899
	R^2	0.965
	K_{id2} (mg/g min$^{1/2}$)	0.158

	C	4.758
	R^2	0.982
	K_{id3} (mg/g $min^{1/2}$)	0.046
	C	7.039
	R^2	0.936

Table S-4

Main chemical constituents of ditch water before and after adsorption.

Ion	TOC	Ca^{2+}	K^+	Mg^{2+}	Na^+	PO_4^{3-}	F^-	Cl^-	NO_3^-	SO_4^{2-}	pH
Unit	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	
Content before adsorption	14.03	66.6	7.75	120	533	0.063	1.06	508	3.24	709	7.98
Content after adsorption	11.41	58.4	7.50	111	495	0.000	0.036	512	3.16	715	8.19



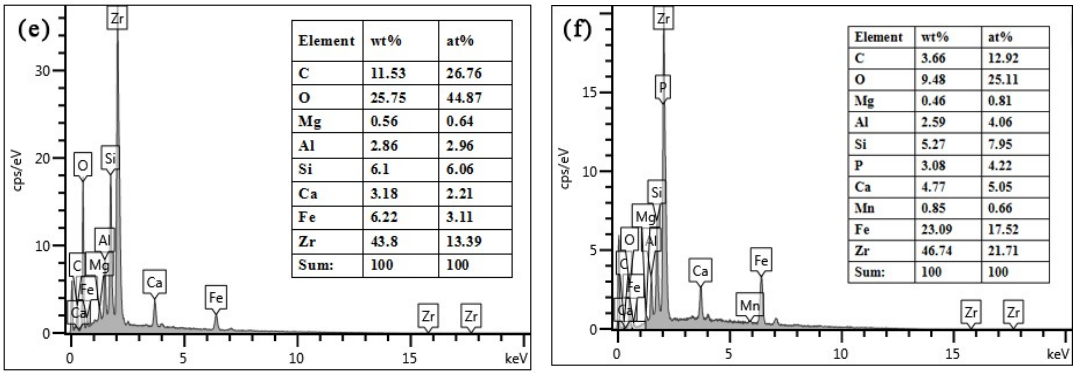


Fig. S-3. SEM images of (a) CGCS, (b) CGCS-Zr, (c) CGCS-Zr after phosphate adsorption, (d) EDS spectrum of CGCS, (e) CGCS-Zr, and (f) P-loaded CGCS-Zr .

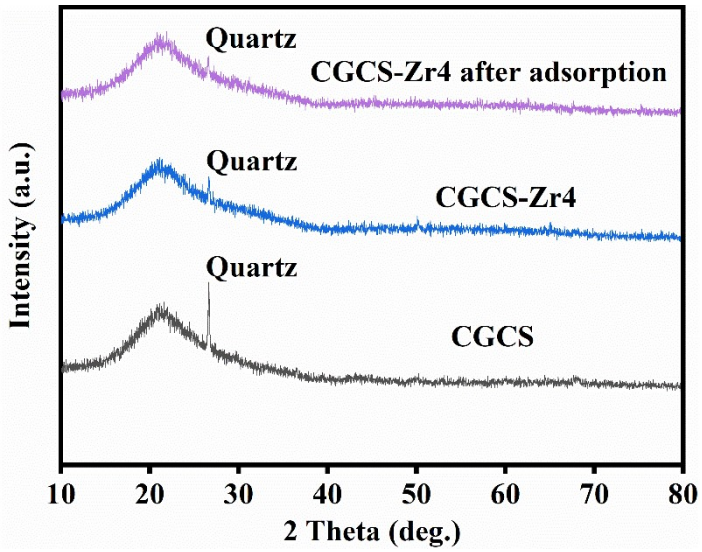


Fig. S-4. XRD spectrum of samples.

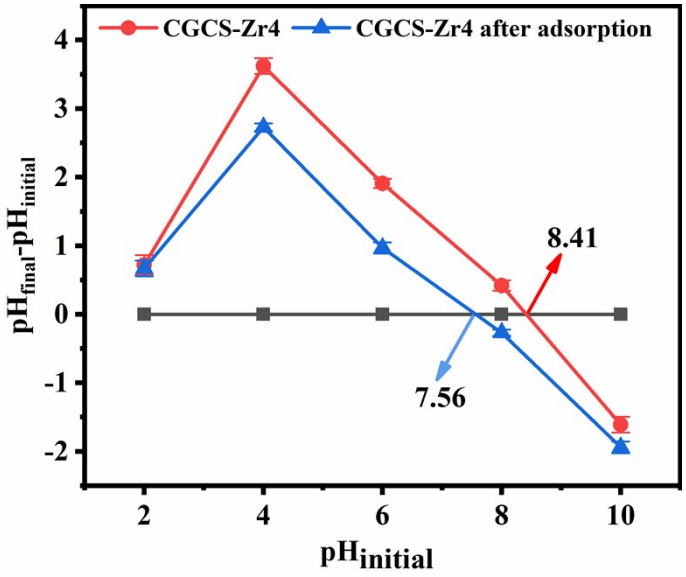


Fig. S-5. the changes of pH_{PZC} of CGCS-Zr4 and CGCS-Zr4 after phosphate adsorption.

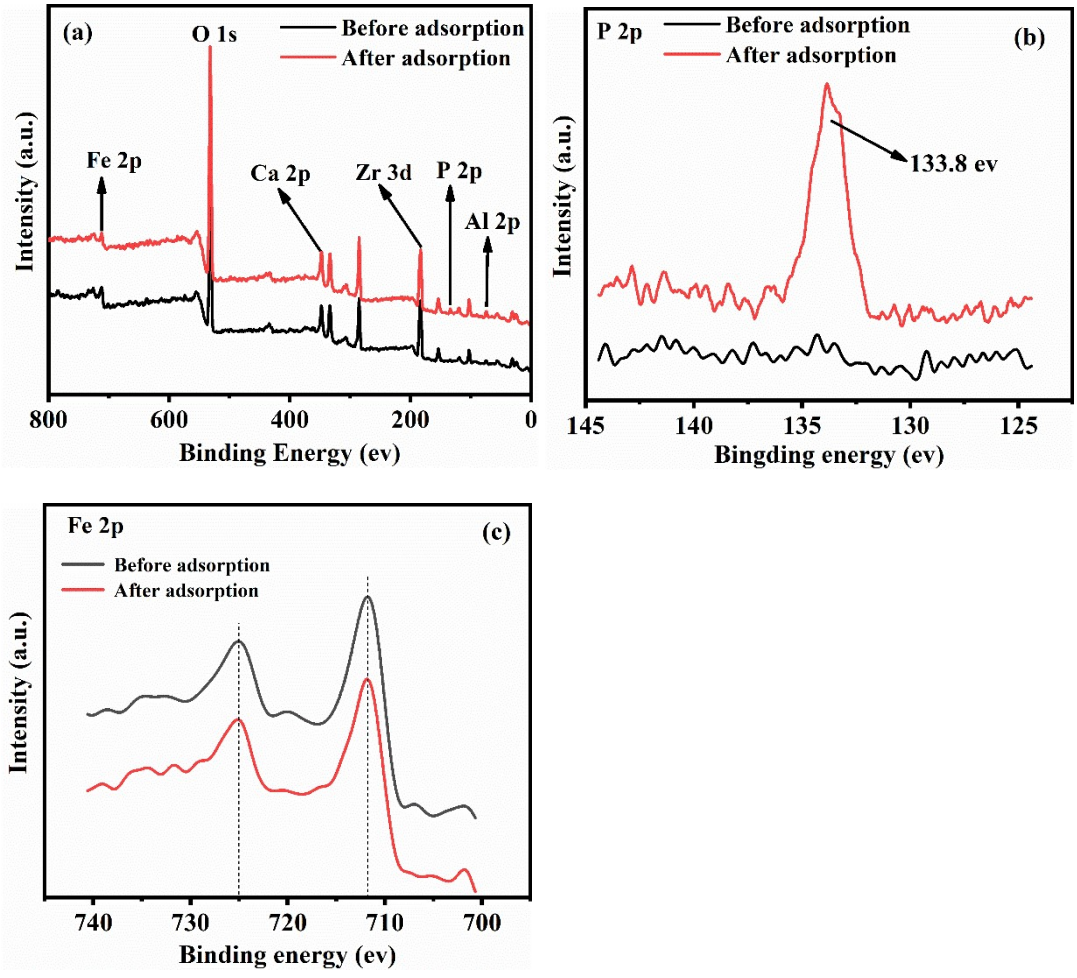


Fig. S-6. XPS analysis of CGCS-Zr4 before and after phosphate adsorption: (a) wide-scan spectra; (b) P 2p; (c) Fe 2 p.

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