

## Acid-Base Synergistic Activation of Coal Gasification Fine Slag into Hierarchical Porous

### Carbon for Enhanced Cr(VI) Adsorption and Reduction

Lijuan Bai<sup>1</sup>, Hua Wang<sup>1,2\*</sup>, Kaipeng Guo<sup>1</sup>, Xia Li<sup>1</sup>, , Kaiwen Bai<sup>1</sup>, Zhengyan Shi<sup>1</sup>, Rui Dang<sup>1</sup>

<sup>1</sup> College of Chemistry and Chemical Engineering, Yulin University, Yulin City 719000, China

<sup>2</sup> Shaanxi Provincial Key Laboratory of Clean Utilization of Low-Modified Coal, Yulin University, Yulin City 719000, China

\*Corresponding author at: College of Chemistry and Chemical Engineering, Yulin University, Chongwen Road No.51, Yulin City 719000, Shaanxi Province, China. E-mail address: 99452715@qq.com (H. Wang)

#### Text S1: FHH model

Based on low-temperature nitrogen adsorption data, the fractal dimension (D) of four samples was calculated using the Frenkel-Halsey-Hill (FHH) fractal model. This parameter reflects the degree of pore formation within the material. D was calculated using Equations (1) and (2) [1]:

$$\ln(V) = b + A \ln \left( \ln \frac{P_0}{P} \right) \quad (1)$$

$$D = A + 3 \quad (2)$$

Where V denotes the adsorption volume of N<sub>2</sub> at equilibrium pressure P, and P<sub>0</sub> represents the saturation pressure of N<sub>2</sub>. A is the power-law exponent associated with the fractal dimension (D), and b is a constant. The value of D ranges from 2 to 3.

#### Text S2: Adsorption kinetic models [2]

$$\text{PFO:} \quad q_t = q_e (1 - e^{-k_1 t}) \quad (3)$$

$$\text{PSO:} \quad q_t = \frac{q_e^2 k_2 t}{1 + q_e k_2 t} \quad (4)$$

$$\text{ID:} \quad q_t = k_{id} t^{1/2} + c \quad (5)$$

$q_e$  (mg/g) denotes the equilibrium adsorption capacity;  $k_1$  (1/min) and  $k_2$  (g/(mg·min)) represent the adsorption rate constants for the PFO and PSO models respectively;  $k_{id}$  (mg/(g·min<sup>1/2</sup>)) indicates the particle internal diffusion coefficient;  $c$  (mg/g) reflects the influence of the boundary layer on the adsorption rate, with higher  $c$  values signifying greater impact.

**Text S3: Adsorption isotherm models [3]**

$$\text{Langmuir:} \quad \frac{C_e}{q_e} = \frac{C_e}{q_m} + \frac{1}{K_L q_m} \quad (6)$$

$$\text{Freundlich:} \quad \ln q_e = \ln K_F + \frac{1}{n} \ln C_e \quad (7)$$

Here,  $q_m$  (mg/g) denotes the maximum adsorption capacity. The constant  $K_L$  (L/mg) represents the Langmuir equilibrium constant. The parameter  $K_F$  (mg/g(L/mg)<sup>1/n</sup>) is the Freundlich constant; a higher  $K_F$  value indicates a stronger adsorption reaction. The variable  $n$  is the Freundlich heterogeneity factor; when  $n > 1$ , it signifies high adsorption efficiency, whereas lower values indicate poor adsorption performance.

**Text S4: Adsorption thermodynamics [4]**

$$K_d = \frac{q_e}{C_e} \quad (8)$$

$$\ln K_d = \frac{\Delta S^\theta}{R} - \frac{\Delta H^\theta}{RT} \quad (9)$$

$$\Delta G^\theta = -RT \ln K_d \quad (10)$$

Here,  $K_d$  denotes the thermodynamic equilibrium constant;  $\Delta H^\theta$  and  $\Delta S^\theta$  are derived from the slope and intercept of  $\ln K_d$  versus  $T^{-1}$ .  $R$  (8.314 J/mol·K) represents the molar gas constant.

**Table S1 Fractal dimensions of FHH model for CGFS, FC and CGFS-H.**

samples	P/P <sub>0</sub> =0~0.4			P/P <sub>0</sub> =0.4~1		
	A <sub>1</sub>	D <sub>1</sub>	R <sub>1</sub> <sup>2</sup>	A <sub>2</sub>	D <sub>2</sub>	R <sub>2</sub> <sup>2</sup>
CGFS	-0.1887	2.8113	0.9652	-0.4705	2.5295	0.9992
CGFS-H	-0.1723	2.8277	0.9415	-0.4456	2.5544	0.9995
FC	-0.1332	2.8668	0.9796	-0.3190	2.6810	0.9904

**Table S2 Carbon microstructure parameters of CGFS and FC.**

samples	$I_D/I_G$	$A_{D1}/A_{all}$	$A_G/A_{all}$	$A_{(D3+D4)}/A_{all}$
CGFS	0.6997	0.2463	0.3520	0.4016
FC	0.9827	0.3223	0.3279	0.3497

**Table S3 pH value changes of various anions before and after adsorption.**

pH	Cl <sup>-</sup>	SO <sub>4</sub> <sup>2-</sup>	NO <sub>3</sub> <sup>-</sup>	HPO <sub>4</sub> <sup>2-</sup>	CO <sub>3</sub> <sup>2-</sup>	Without Ion
Initial	5.19	4.85	4.91	4.43	10.86	5.28
Final	5.76	5.56	5.57	4.63	10.66	5.92

**Table S4 Adsorption kinetic parameters fitted based on PFO, PSO and ID models.**

models	Parameters	C <sub>0</sub> ,Cr(VI)
		100 mg/L
PFO	q <sub>e,exp</sub> (mg/g)	135.6739
	q <sub>e,cal</sub> (mg/g)	130.1276
	k <sub>1</sub> (1/min)	0.0278
	R <sup>2</sup>	0.4114
PSO	q <sub>e,cal</sub> (mg/g)	136.3703
	k <sub>2</sub> (g/mg/min)	0.0073
	R <sup>2</sup>	0.9944
	k <sub>id,1</sub> (mg/(g · min <sup>1/2</sup> ))	1.5375
ID	c <sub>1</sub>	94.7002
	R <sup>2</sup>	0.9772
	k <sub>id,2</sub> (mg/(g · min <sup>1/2</sup> ))	0.3564
	c <sub>2</sub>	120.2107
	R <sup>2</sup>	0.9029

**Table S5 Adsorption isotherm parameter of Cr(VI) by FC.**

models	Parameters	Temperature		
		298 K	308 K	318 K
Langmuir	$q_m$ (mg/g)	172.7115	173.9130	179.8561
	$K_L$	0.1170	0.1339	0.1513
	$R^2$	0.9871	0.9859	0.9902
Freundlich	$K_F(\text{mg/g}(\text{L/mg})^{1/n})$	69.0361	75.6290	80.4310
	$n$	5.3444	5.8685	5.9684
	$R^2$	0.9164	0.9065	0.9483

**Table S6 Comparison of the adsorption capacity of FC and other adsorbents for Cr(VI).**

Adsorbent	Temperature (K)	$q_{\max}$ (mg/g)	Reference
NiCo-LDHM	298 K	132.00	[5]
PACFs	298 K	93.20	[6]
Al/BC	298 K	176.23	[7]
Fe <sub>3</sub> O <sub>4</sub> @SiO <sub>2</sub> -UiO-66-EDTA	298 K	75.11	[8]
FC	298 K	172.71	This study

**Table S7 Adsorption thermodynamic parameter.**

T (K)	$\Delta G^\theta$ (KJ/mol)	$\Delta H^\theta$ (KJ/mol)	$\Delta S^\theta$ ((J/(mol·K))
298	-7.674		
308	-8.476	17.663	84.974
318	-9.376		

**Table S8 Specific surface area and pore distribution of FC and FC-Cr(VI)**

samples	Specific surface area (m <sup>2</sup> /g)	Micropore surface area (m <sup>2</sup> /g)	Mesopore Surface area (m <sup>2</sup> /g)	Total pore volume (cm <sup>3</sup> /g)
FC	630.308	63.794	250.078	0.728
FC-Cr(VI)	151.577	0.000	73.918	0.205

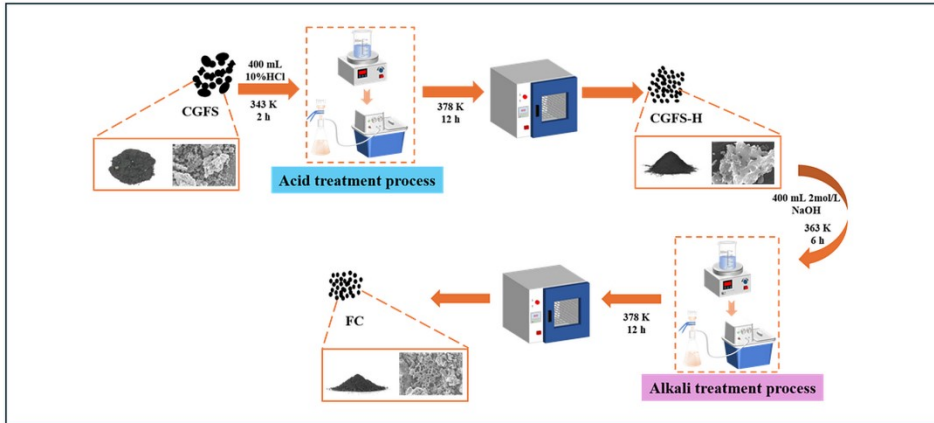
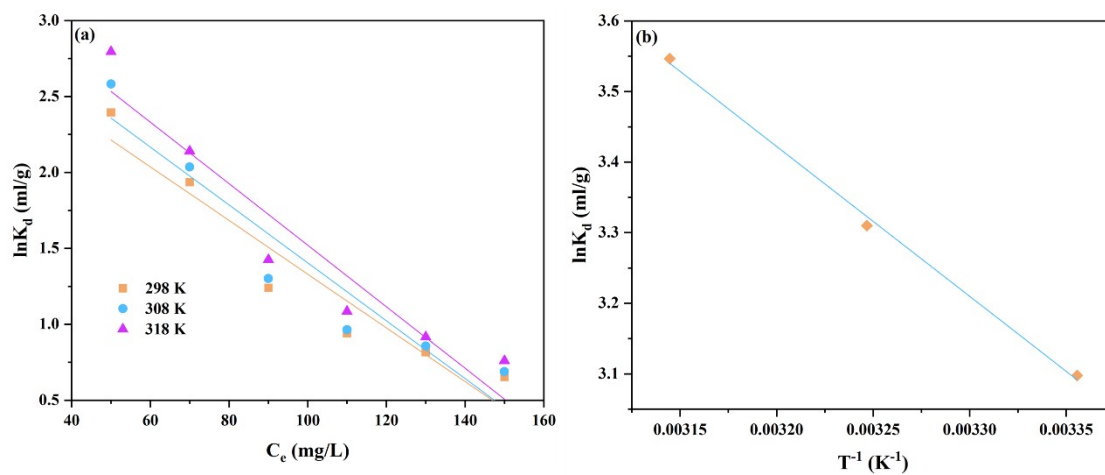


Figure S1. Schematic diagrams of the preparation processes for FC and CGFS-H



**Figure S2 (a)**The relationship curve between  $\ln K_d$  and  $C_e$ ; **(b)**The relationship curve between  $\ln K_d$  and  $T^{-1}$

**Figure S3 (a) N<sub>2</sub> adsorption-desorption isotherms of FC and FC-Cr(VI); (b) pore size distribution**

## References

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