Preparation of Cu-BDC Composite Activated Carbon Materials for

Efficient Removal of Sulfur Compounds

Haitao Wang[a*], Min Xie[a], Yubin Liu[a], Haitao Duan[a], Qinglin Liu[b], Shengwei He[b],

Shuxiang Lyu[b*]

[a] *China tobacco Hebei industrial Co., Ltd, Shijiazhuang 050051, China*

[b] *College of Chemical Engineering and Material Science, Tianjin University of Science*

and Technology, Tianjin 300457, China

*Corresponding author.

Address: College of Chemical Engineering and Material Science, Tianjin University of

Science and Technology, Tianjin 300457, China

Tel: +86-22-60601173

Email address: lshx@tust.edu.cn (Shuxiang Lyu)
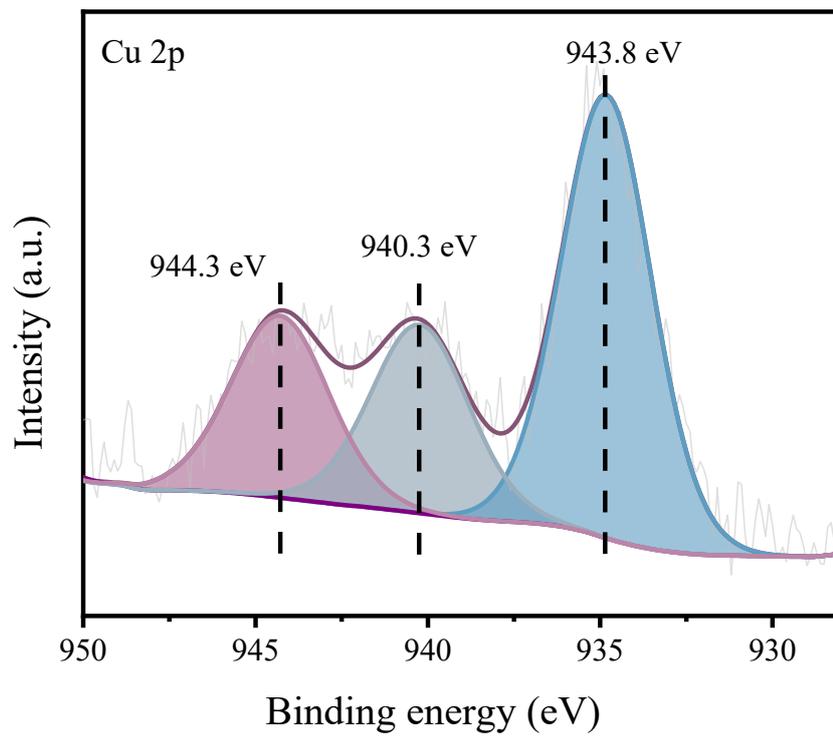
3790834430@qq.com (Haitao Wang)

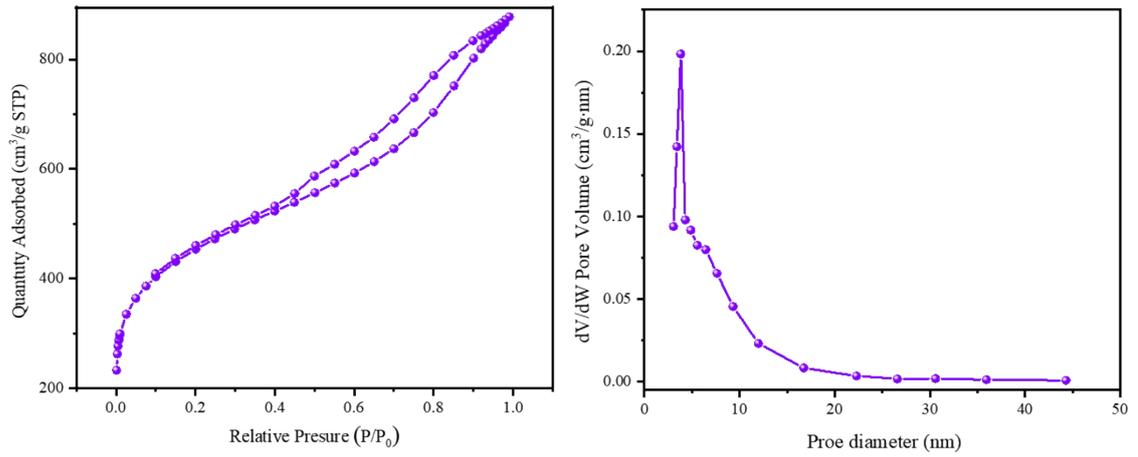Fig. S1 XPS spectra of Cu-BDC@AC1:1 (Cu 2p)

Fig. S2. N_2 adsorption-desorption isotherms (A) and pore size distribution (B) of AC.
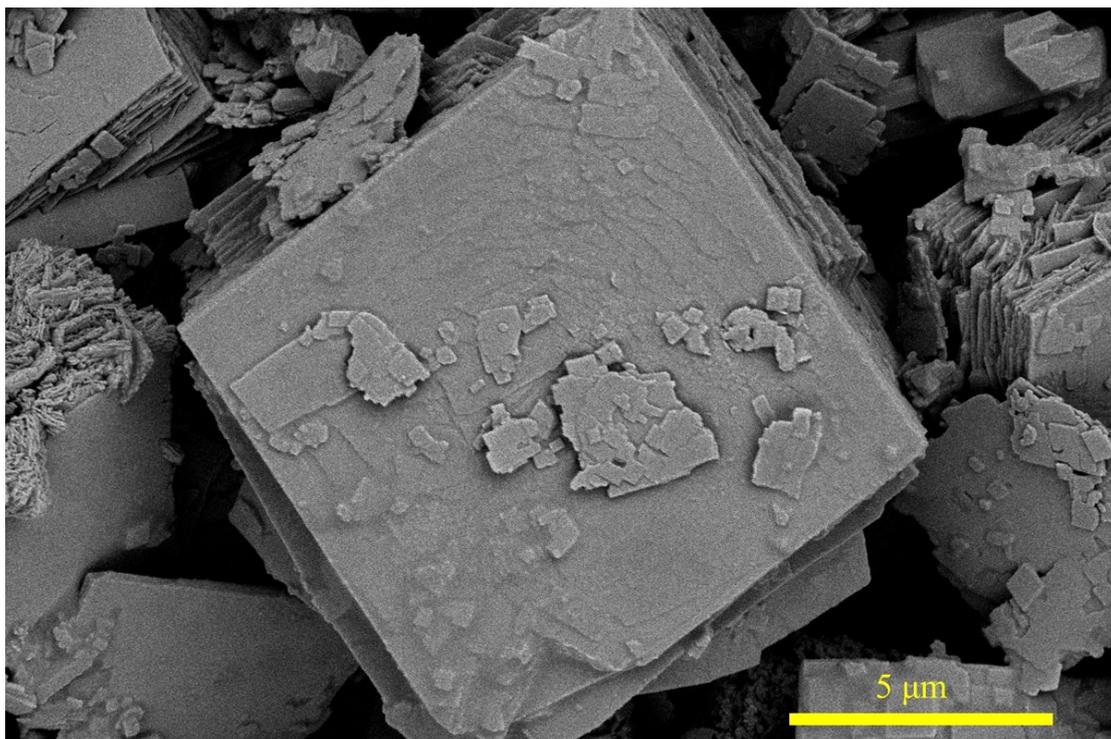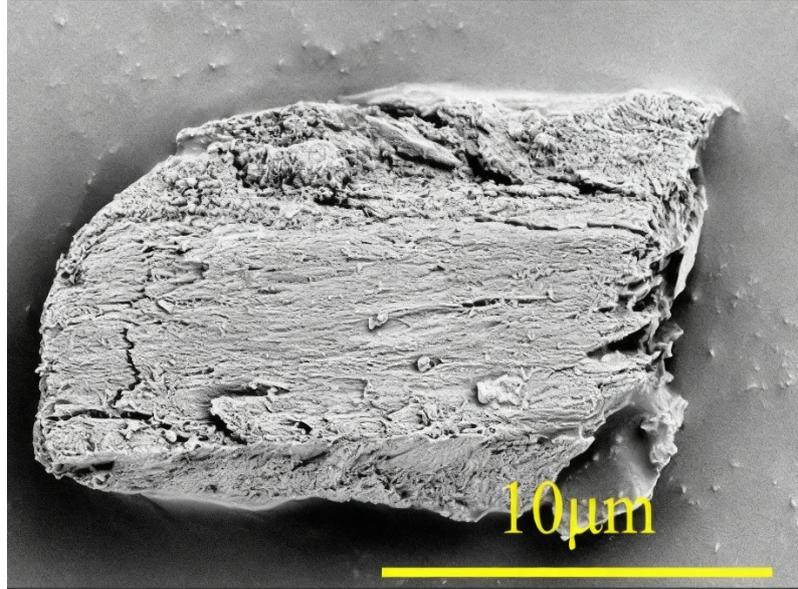
Fig. S3. SEM images of Cu-BDC

Fig. S4. SEM images of AC

Fig. S5. Evaluation of adsorption for Cu-BDC@AC1:1, Cu-BDC and AC. Reaction conditions: Adsorbent dosage: 200 mg, Temperature: 30 ℃, Initial sulfur concentration: 1500 ppm (nP) 15 mL, Adsorption time: 180 min.
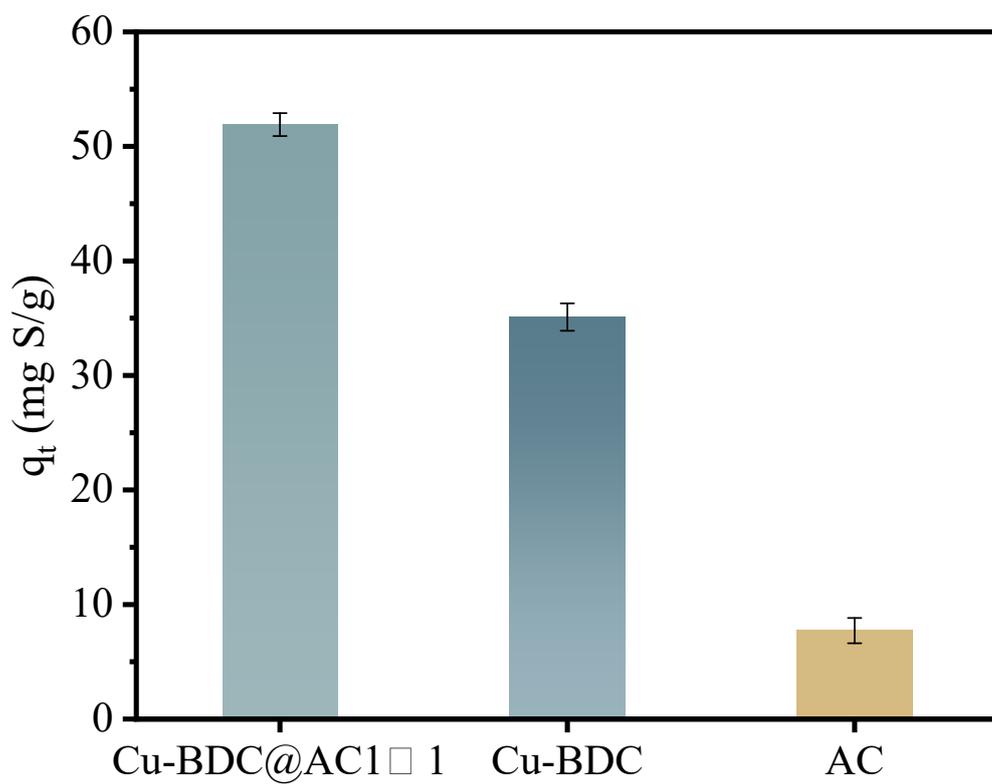
Fig. S6. Evaluation of adsorption for Cu-BDC@AC and Cu-BDC+AC. Reaction conditions: Adsorbent dosage: 200 mg, Temperature: 30 ℃, Initial sulfur concentration: 1500 ppm (nP) 15 mL, Adsorption time: 180 min.

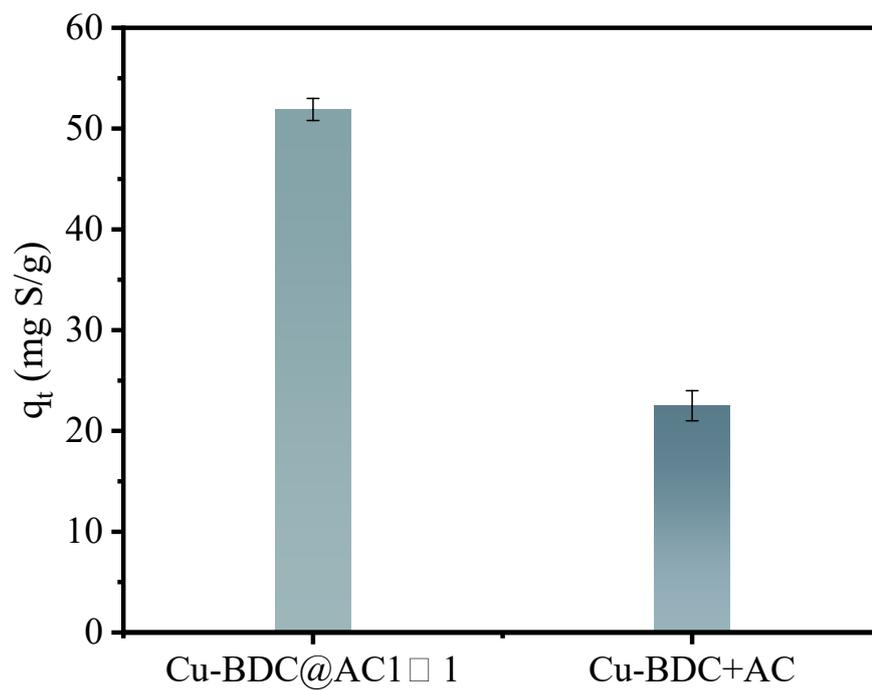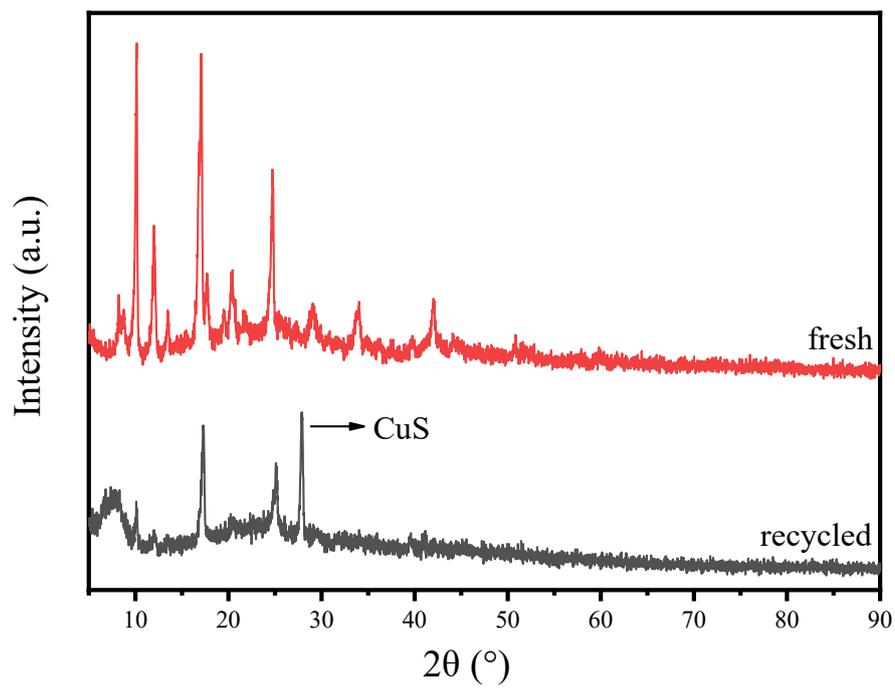Fig. S7 XRD of Fresh and recycled after 4 cycles for Cu-BDC@AC1:1.

Table. S1 Physical properties of AC

Adsorbent	$S_{BET}(m^2/g)$	V (cm^3/g)	D (nm)
AC	1619	1.36	3.54

Table S2. ANOVA for the quadratic response surface model developed for Cu-BDC@AC1:1. Temp, temperature (°C); Conc, initial sulfur concentration (ppm); Time, adsorption time (min). Significant terms were identified at $p < 0.05$.

Source	df	Sum of Squares	Mean Square	F-value	p-value
Temp	1	668.712	668.712	362.75	0.000316
Conc	1	837.837	837.837	454.49	0.000226
Time	1	6.444	6.444	3.50	0.1583
Temp^2	1	4.521	4.521	2.45	0.2153
Conc^2	1	28.160	28.160	15.28	0.0298
Time^2	1	~0	~0	~0	0.9994
Temp×Conc	1	0.648	0.648	0.35	0.5950
Temp×Time	1	0.168	0.168	0.09	0.7824
Conc×Time	1	0.203	0.203	0.11	0.7621
Residual	3	5.530	1.843	—	—

Table. S3 Fitting parameters for the adsorption kinetics of the four adsorbents.

Adsorbent	Pseudo-first-order kinetic			Pseudo-second-order kinetic		
	q_e (mg S/g）	K_1 (min^{-1})	R^2	q_e(mg S/g)	K_2 (g/ (mg S·min))	R^2
Cu-BDC@AC1：0.5	21.9	1.06×10^{-3}	0.975	41.7	1.34×10^{-3}	0.998
Cu-BDC@AC1：1	25.7	1.42×10^{-3}	0.993	55.56	1.55×10^{-3}	0.998
Cu-BDC@AC1：2	13.24	1.22×10^{-3}	0.994	42.21	3.16×10^{-3}	0.999
Cu-BDC@AC1：5	11	1.17×10^{-3}	0.991	28.9	3.23×10^{-3}	0.997

Table. S4 Fitting parameters for the four adsorbent internal diffusion models

Adsorbent	First stage (exter)			Second stage (intra)		
	K_{3i}(mg S/(g min$^{1/2}$))	C (mg S/g)	R^2	K_{3ii}(mg S/(g·min$^{1/2}$))	C (mg S/g)	R^2
Cu-BDC@AC1：0.5	2.11	13.66	0.987	0.41	32.1	0.871
Cu-BDC@AC1：1	2.23	26.33	0.967	0.47	44.5	0.983
Cu-BDC@AC1：2	1.17	26.91	0.994	0.28	36.6	0.891
Cu-BDC@AC1：5	1.04	15.30	0.981	0.26	23.7	0.891

Table. S5 Adsorption thermodynamic fitting data of the four adsorbents

Adsorbent	ΔG (KJ/mol)			ΔH (KJ/mol)	ΔS (J/(mol·K))
	303.15K	313.15K	323.15K		
Cu-BDC@AC1:0.5	-8.93	-8.66	-8.46	-15.55	-21.95
Cu-BDC@AC1:1	-10.23	-9.66	-9.36	-22.78	-41.57
Cu-BDC@AC1:2	-9.20	-8.86	-8.65	-17.04	-26.02
Cu-BDC@AC1:5	-7.79	-7.40	-7.15	-16.96	-30.51