

Supporting Information

Activation of biomass with volatilized KOH

Chao Li^a, Yuannian Li^a, Yuewen Shao^a, Lijun Zhang^a, Shu Zhang^b, Shuang Wang^c, Bin Li^c, Zhenhua Cui^d, Yonggui Tang^d, Xun Hu^{a,}*

^aSchool of Material Science and Engineering, University of Jinan, Jinan, 250022, P. R. China

^bJoint International Research Laboratory of Biomass Energy and Materials, College of Materials Science and Engineering, Nanjing Forestry University, Nanjing, 210037, P. R. China

^cSchool of Energy and Power Engineering, Jiangsu University, Zhenjiang, 212013, P. R. China

^dShandong Basan Graphite New Material, Zibo, 255000, P. R. China

Corresponding authors: Xun.Hu@outlook.com (X. Hu);

Table S1 Peak height and particle size of the biochar or activated carbon from the activation with KOH as activators with different activation methods

Entry	Samples	Peak height		FWHM		
		C (0 0 2)	C (1 0 0)	C (0 0 2)	C (1 0 0)	
1	Biochar	Sawdust	1.3×10^4	1.2×10^3	0.5	0.3
2	Biochar	Cellulose	1.3×10^4	1.6×10^3	0.7	0.7
3	Biochar	Lignin	1.6×10^4	4.1×10^3	0.6	0.7
4	AC	DA-Sawdust	9.7×10^4	7.7×10^3	0.4	0.2
5	AC	DA-Cellulose	1.6×10^5	1.4×10^4	0.3	0.2
6	AC	DA-Lignin	1.1×10^5	7.8×10^3	0.3	0.1
7	AC	AVK-Sawdust	1.1×10^5	4.5×10^3	0.5	0.2
8	AC	AVK -Cellulose	8.7×10^4	8.6×10^3	0.6	0.2
9	AC	AVK -Lignin	3.8×10^4	7.6×10^3	0.3	0.2

DA: Direct activation of the mixture of biomass and KOH with a mass ratio of 1:1;

AVK: Activation with volatilized KOH of biomass in the upper bed while KOH in the lower bed with a mass ratio of 1:1.

Table S2 Abundance of the functional groups of the AC from the activation with KOH as activators with different activation methods

Entry	Samples	Abundance (a.u.)				
		-OH	=C-H	C-H	-CH ₃	C-O-C
1	DA-Sawdust	0.04	0.01	0.02	0.01	0.05
2	DA-Cellulose	0.05	0.01	0.04	0.01	0.10
3	DA-Lignin	0.05	0.01	0.02	0.01	0.09
4	AVK-Sawdust	0.07	0.02	0.04	0.02	0.11
5	AVK-Cellulose	0.06	0.01	0.03	0.02	0.07
6	AVK-Lignin	0.05	0.01	0.03	0.01	0.11

DA: Direct activation of the mixture of biomass and KOH with a mass ratio of 1:1;

AVK: Activation with volatilized KOH of biomass in the upper bed while KOH in the lower bed with a mass ratio of 1:1.

Table S3 Environmental impacts, energy consumption, and resource depletion for production of the AC

Feedstock	DA-	DA-	DA-	AVK-	AVK-	AVK-
	Sawdust	Cellulose	Lignin	Sawdust	Cellulose	Lignin
Acidification (kg SO₂ eq)	3.22E+05	2.46E+05	2.57E+05	2.22E+05	2.48E+05	1.91E+05
Carcinogenics (CTUh)	2.15E+02	1.64E+02	1.71E+02	1.48E+02	1.66E+02	1.28E+02
Ecotoxicity (CTUe)	3.14E+09	2.40E+09	2.50E+09	2.17E+09	2.42E+09	1.87E+09
Eutrophication (kg N eq)	2.45E+05	1.87E+05	1.95E+05	1.69E+05	1.89E+05	1.46E+05
Fossil fuel depletion (MJ surplus)	5.63E+07	4.31E+07	4.49E+07	3.89E+07	4.35E+07	3.35E+07
Global warming (kg CO₂ eq)	7.74E+07	5.93E+07	6.17E+07	5.35E+07	5.97E+07	4.60E+07
Non carcinogenics (CTUh)	7.77E+01	5.95E+01	6.20E+01	5.37E+01	5.99E+01	4.62E+01
Ozone depletion (kg CFC-11 eq)	4.69E+00	3.59E+00	3.74E+00	3.24E+00	3.62E+00	2.79E+00
Respiratory effects (kg PM2.5 eq)	1.12E+05	8.57E+04	8.93E+04	7.74E+04	8.64E+04	6.66E+04
Smog (kg O₃ eq)	4.56E+06	3.49E+06	3.63E+06	3.15E+06	3.52E+06	2.71E+06

DA: Direct activation of the mixture of biomass and KOH with a mass ratio of 1:1;

AVK: Activation with volatilized KOH of biomass in the upper bed while KOH in the lower bed with a mass ratio of 1:1.

Table S4 Input and output on the basis of production of 1 ton of AC

Feedstock	DA-Sawdust	DA-Cellulose	DA-Lignin				
Input/Output	Quantity			Unit			
Step 1: Transportation							
Input							
Feedstock	11570.9	8306.1	8925.9	kg			
transportation	11.5	8.3	8.9	tkm			
Output							
Feedstock, after transportation	10992.3	7890.8	8479.0	kg			
Step 2: Pretreatment							
Input							
Feedstock, after transportation	10992.3	-	8479.0	kg			
Electricity	27700.8	-	21367.0	MJ			
Deionized water	32977.1	-	25436.9	kg			
Hydrochloric acid	3790.2	-	-	kg			
Sulfuric acid	-	-	423.9	kg			
Output							
Feedstock, after pretreatment	9893.1	-	7631.1	kg			
Wastewater	32977.1	-	25436.9	kg			
Step 3: Grinding							
Input							
Feedstock,	32977.1	-	25436.9	kg			

after pretreatment				
Electricity	783.5	625.0	604.4	MJ
Output				
Feedstock, after grinding	9398.4	7496.3	7249.5	kg
Step 4: Activation				
Input				
Feedstock, after grinding	9398.4	7496.3	7249.5	kg
Natural gas	6286.7	5014.3	4849.3	m ³
Electricity	84.5	67.5	65.2	MJ
KOH	9398.5	7496.3	7249.5	kg
Output				
Mixture	1785.7	1724.1	1754.4	kg
Waste gas	7612.8	5772.1	5495.1	kg
Step 5: Post-treatment				
Input				
Mixture	1785.7	1724.1	1754.4	kg
Hydrochloric acid	615.7	594.5	587.4	kg
Deionized water	5357.1	5172.4	5263.2	kg
Outputs				
AC	1000	1000	1000	kg
wastewater	5357.1	5172.4	5263.2	kg

DA: Direct activation of the mixture of biomass and KOH with a mass ratio of 1:1.

Table S5 Input and output on the basis of production of 1 ton of AC

Feedstock	AVK-Sawdust	AVK-Cellulose	AVK-Lignin				
Input/Output	Quantity			Unit			
Step 1: Transportation							
Input							
Feedstock	8414.3	6835.3	6534.0	kg			
transportation	8.4	6.8	6.5	tkm			
Output							
Feedstock, after transportation	7993.6	6493.5	6207.3	kg			
Step 2: Pretreatment							
Input							
Feedstock, after transportation	7993.6	-	6207.3	kg			
Electricity	20143.9	-	15642.5	MJ			
Deionized water	23980.8	-	18621.9	kg			
Hydrochloric acid	2756.2	-	-	kg			
Sulfuric acid	-	-	310.4	kg			
Output							
Feedstock, after pretreatment	7194.2	-	5586.6	kg			
Wastewater	23980.8	-	18621.9	kg			
Step 3: Activation							
Input							
Feedstock,	7194.2	6493.5	5586.6	kg			

after pretreatment

Natural gas	4812.3	4343.6	3736.9	m ³
Electricity	64.7	58.4	50.3	MJ
KOH	7194.2	6493.5	5586.6	kg
Output				
AC	1000	1000	1000	kg
Waste gas	6194.2	5493.5	4586.6	kg
Waste KOH	2474.8	2194.8	1877.1	kg

AVK: Activation with volatilized KOH of biomass in the upper bed while KOH in the lower bed with a mass ratio of 1:1.

Table S6 E-factor and material efficiency data for production of the AC^a

Entry	Samples^b	E-factor	Material efficiency
1	DA-Sawdust	45.9	2.1×10^{-2}
2	DA-Cellulose	10.9	8.3×10^{-2}
3	DA-Lignin	36.2	2.7×10^{-2}
4	AVK-Sawdust	30.1	3.2×10^{-2}
5	AVK -Cellulose	2.2	3.1×10^{-1}
6	AVK -Lignin	20.5	4.7×10^{-2}

^aE (environmental) – factor = $\frac{\text{Mass of wastes}}{\text{Mass of products}}$;

Material efficiency = $\frac{\text{Mass of products}}{\text{Mass of products} + \text{Mass of wastes}}$;

calculated considering output of wastewater and waste gas as waste, and activated carbon as product; The data could refer to the Table S4 and S5;

^bDA: Direct activation of the mixture of biomass and KOH with a mass ratio of 1:1;

AVK: Activation with volatilized KOH of biomass in the upper bed while KOH in the lower bed with a mass ratio of 1:1.

Table S7 Pore characteristics of the biochar and activated carbon (AC) from the activation of various feedstocks in the absence/presence of activator

Entry	Samples*		S _{BET}	V _b ^a	D _a ^c	S _{micro} ^b	V _{micro} ^d
			(m ² /g)	(cm ³ /g)	(nm)	(m ² /g)	(cm ³ /g)
AVA-							
1	AC	Sawdust (ZnCl ₂)	704.1	0.32	0.92	103.3 (14.7)	0.08
2	Biochar	Ceiba	110.4	0.06	1.1	34.7 (31.4)	0.02
AVK-							
3	AC	Ceiba (KOH)	118.6	0.09	1.6	92.1 (77.7)	0.04
4	Biochar	Walnut shell	107.1	0.06	1.2	0 (0)	0
AVK-							
5	AC	Walnut shell (KOH)	152.0	0.08	1.1	62.3 (41.0)	0.03
6	Biochar	Pine needle	88.4	0.05	1.2	46.9 (53.1)	0.02
AVK-							
7	AC	Pine needle (KOH)	119.6	0.1	1.7	92.2 (77.1)	0.04

^aTotal pore volume at P/P₀ = 0.99; ^bMicropore surface area, the percentage of

S_{micro}/S_{BET} is given in parentheses; ^cAverage pore diameter; ^dMicropore volume;

* DA: Direct activation of the mixture of biomass and KOH with a mass ratio of 1:1;

AVA: Activation with volatilized activator of biomass in the upper bed while KOH in the lower bed with a mass ratio of 1:1;

AVK: Activation with volatilized KOH of biomass in the upper bed while KOH in the lower bed with a mass ratio of 1:1.

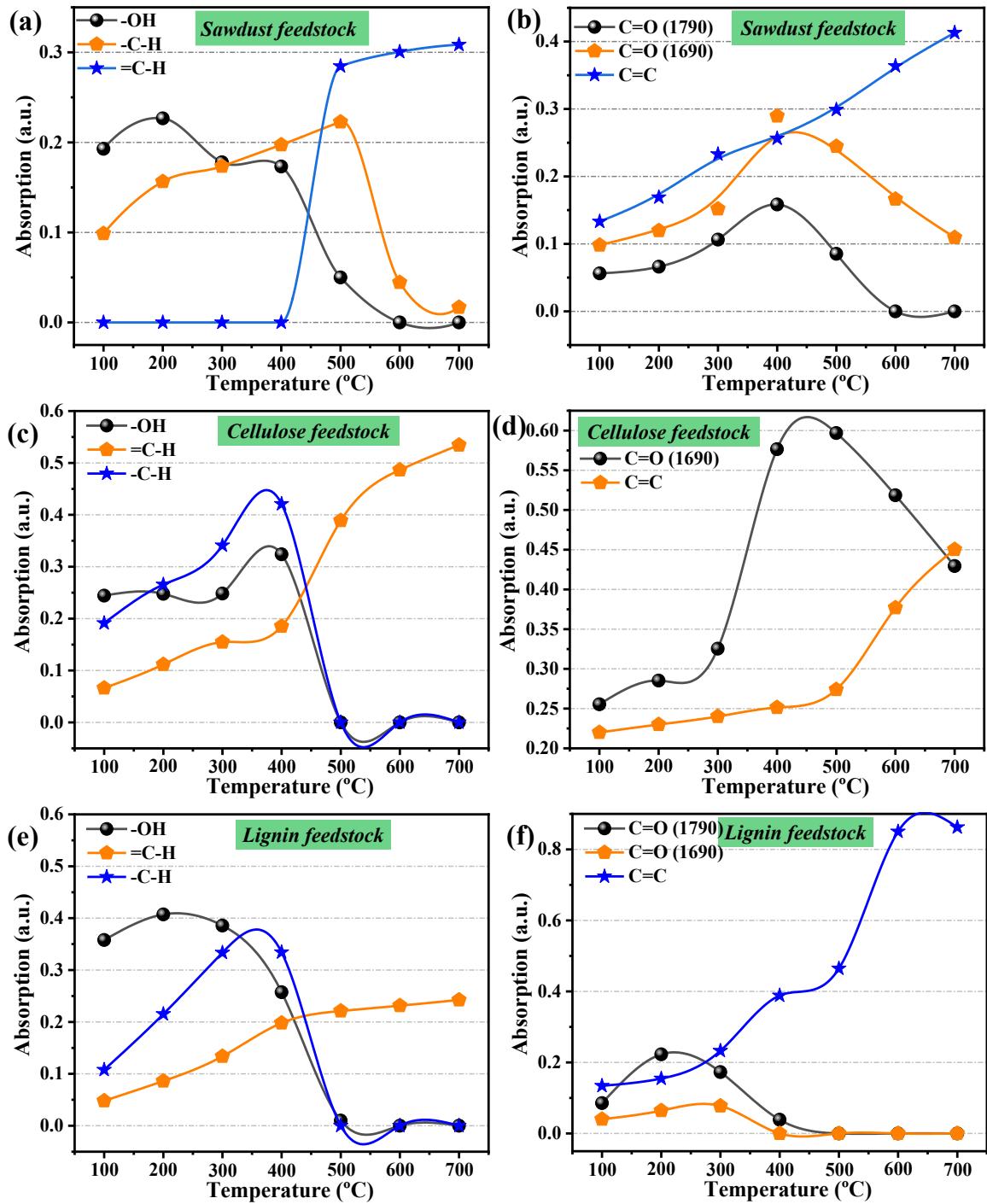


Fig. S1 Abundance of various functional groups derived from the in-situ DRIFTS spectra of different feedstocks; (a): Sawdust feedstock; (b): Cellulose feedstock; (c): Lignin feedstock.

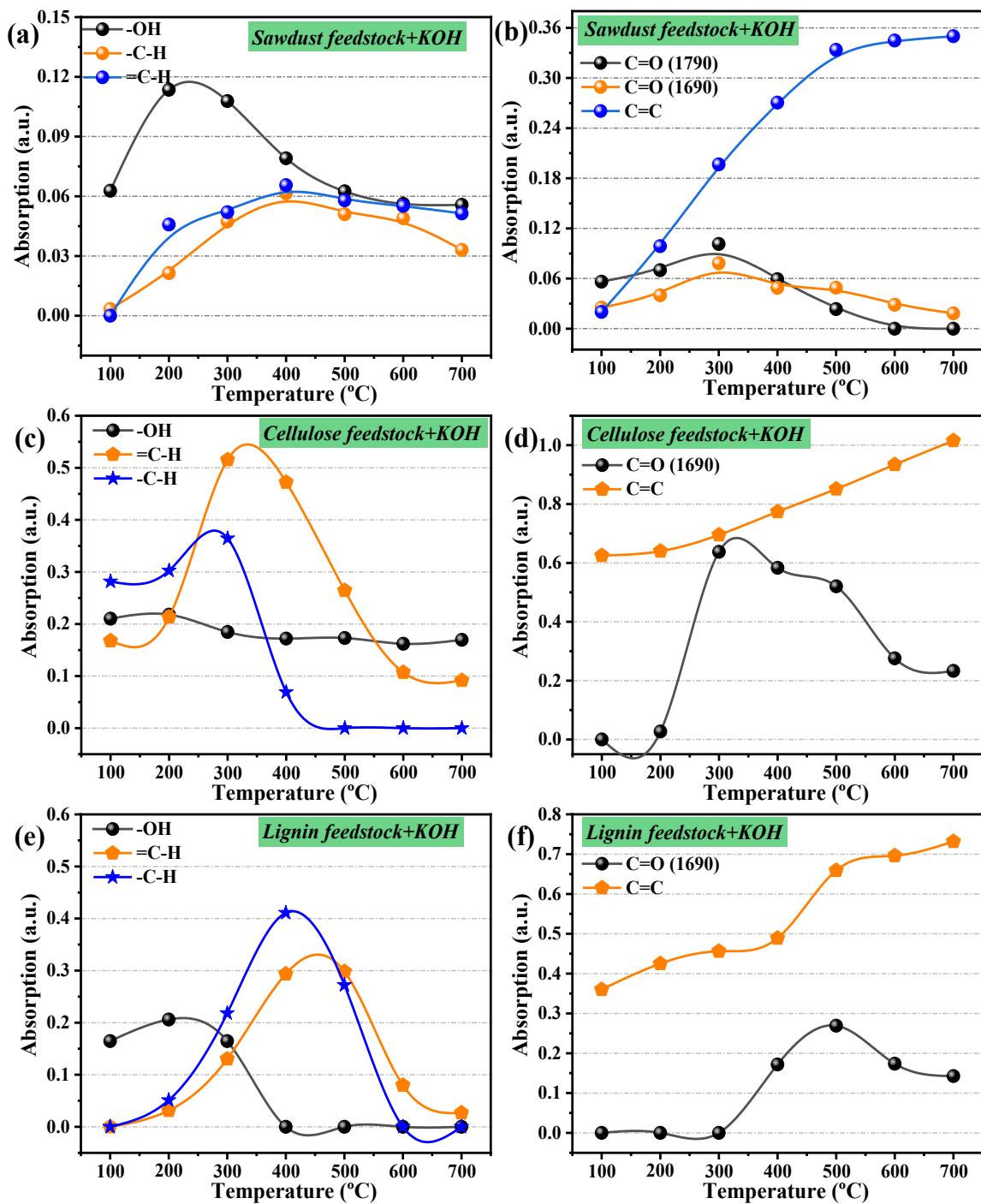


Fig. S2 Abundance of various functional groups derived from the in-situ DRIFTS spectra of different feedstocks; (a): Mixture of sawdust feedstock and KOH; (b): Mixture of cellulose feedstock and KOH; (c): Mixture of lignin feedstock and KOH.

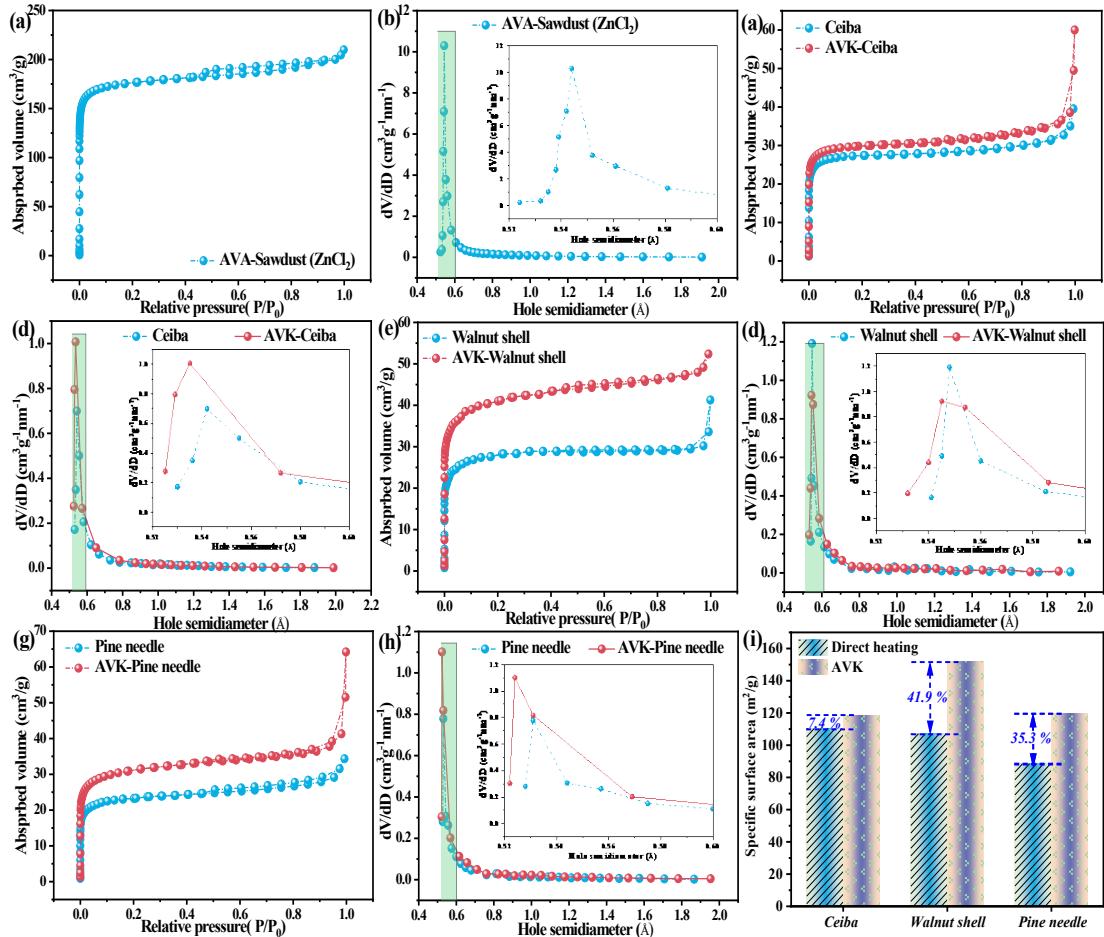


Fig. S3 Pore structure analysis of the biochar or AC from the activation of various feedstocks in the absence/presence of activator; (a and b): AC from activation with volatilized ZnCl_2 as activator; (c and d): Activation of ceiba; (e and f): Activation of walnut shell; (g and h): Activation of pine needle; (i): Specific surface area of the biochar or AC; AVA: Activation with volatilized activator of biomass in the upper bed while KOH in the lower bed with a mass ratio of 1:1; AVK: Activation with volatilized KOH of biomass in the upper bed while KOH in the lower bed with a mass ratio of 1:1.

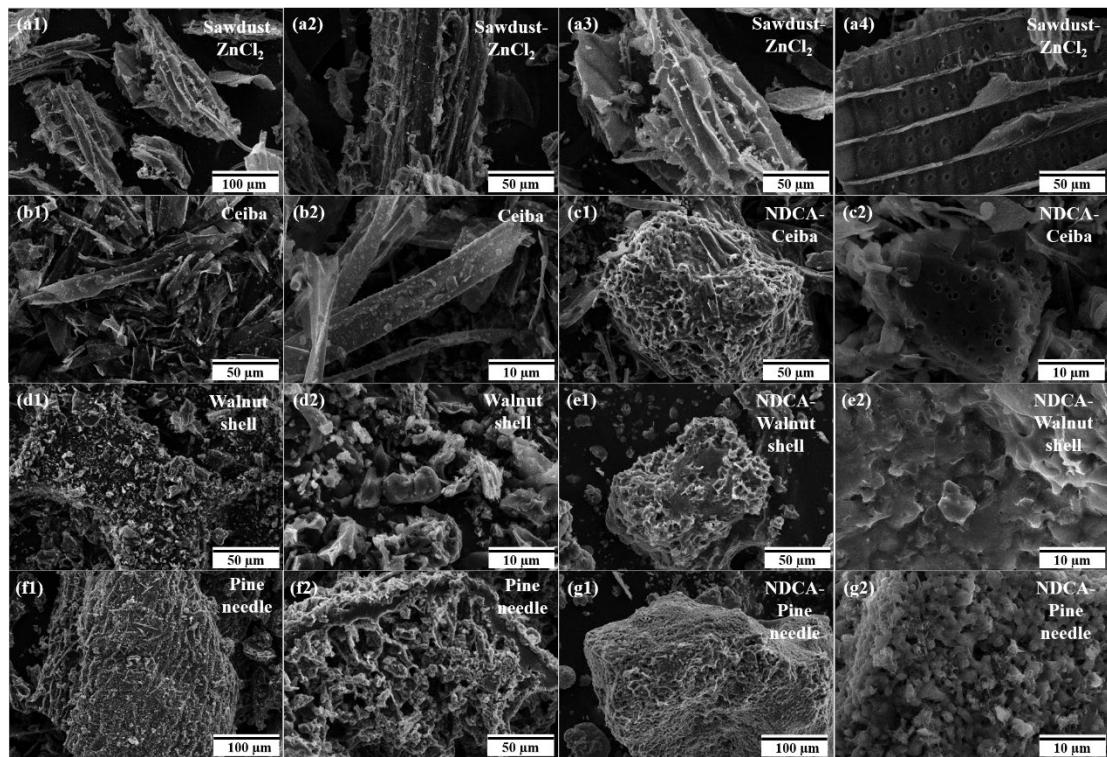


Fig. S4 SEM analysis of the biochar or AC from the activation of various feedstocks in the absence/presence of activator; (a): AC from activation with volatilized ZnCl_2 as activator; (b): Biochar from direct heating of ceiba; (c): AC from activation with volatilized KOH of ceiba; (d): Biochar from direct heating of walnut shell; (e): AC from activation with volatilized KOH of walnut shell; (f): Biochar from direct heating of pine needle; (g): AC from activation with volatilized KOH of pine needle; AVK: Activation with volatilized KOH of biomass in the upper bed while KOH in the lower bed with a mass ratio of 1:1.