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Remediation of Cd2+ in aqueous systems by alkali-modified (Ca) biochar and quantitative analysis of its mechanism

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Table S1 The properties of biochar before demineralization.

Sample	SBB	RSB	Ca-SBB	Ca-RSB
Yield (%)	31.38	34.44	34.61	38.03
pH	9.80±0.05b	9.61±0.02c	10.57±0.02a	9.66±0.01c
EC (ms cm^{-1})	1.64±0.01d	8.65±0.06a	6.13±0.05c	6.70±0.12b
DOC (g kg^{-1})	4.24±0.08c	4.06±0.13c	17.83±0.18b	32.99±1.48a
CO_3^{2-} (cmol kg^{-1})	27.41±5.32b	10.81±0.62c	35.05±3.46a	26.85±1.66b
CEC (cmol kg^{-1})	69.46±2.07c	73.49±3.35b	80.82±3.22a	84.32±2.58a
C (%)	61.89±0.49a	56.94±0.77b	55.34±0.39c	53.86±1.16c
H (%)	3.45±0.04b	3.11±0.06c	2.84±0.06d	3.83±0.04a
N (%)	1.33±0.008a	0.96±0.006c	1.16±0.001b	0.44±0.004d
H/C	0.06±0.0002b	0.05±0.001b	0.05±0.0008b	0.07±0.0006a
C/N	46.53±0.33c	59.31±0.43b	47.71±0.34c	122.4±3.41a
K (g kg^{-1})	15.41±0.39c	47.16±0.55a	45.69±0.94a	27.60±1.30b
Ca (g kg^{-1})	32.31±0.86c	24.32±0.54d	75.38±1.37b	82.55±3.44a
Na (g kg^{-1})	0.15±0.03c	6.12±0.12a	0.45±0.02c	1.25±0.27b
Mg (g kg^{-1})	14.41±0.29a	3.67±0.05c	6.38±0.08b	2.54±0.12d
P (g kg^{-1})	0.89±0.02d	2.61±0.08b	4.52±0.04a	2.16±0.09c
S (g kg^{-1})	2.28±0.06c	6.47±0.86a	1.66±0.09c	3.73±0.18b
S_{BET} (m^2 g^{-1})	3.16	5.22	5.51	6.09
Average pore size (nm)	9.21	5.69	8.96	7.33
Total pore volume (cm^3 g^{-1})	0.00728	0.00743	0.0123	0.0112

Note：Subscripts (a, b, c and d) indicate that the differences in the basic properties of biochar in the same treatment is significant ($P<0.05$).

Table S2 Absorption capacity of Cd^{2+} by each mechanism on biochar (mean ± S.D., n=3)

Biochar	Q_{cme} (mg g^{-1})	Q_{cmp} (mg g^{-1})	Q_{co} (mg g^{-1})	$Q_{c\pi}$ (mg g^{-1})
SBB	11.55±0.05d	23.63±0.55b	14.16±0.30a	5.29±0.76a
RSB	19.41±0.20c	14.30±1.79c	8.07±0.15c	3.36±0.10b
Ca-SBB	30.26±0.72b	43.18±0.89a	12.30±0.23b	0.90±0.60c
Ca-RSB	36.66±0.29a	10.94±0.35d	6.80±0.35d	4.81±0.75a

Note: Absorption capacity of Cd^{2+} by ion exchange (Q_{cme}), minerals precipitation (Q_{cmp}), functional groups complexation (Q_{co}) and Cd^{2+}-π coordination ($Q_{c\pi}$) on biochars. Subscripts (a, b, c and d) indicate that the differences in the absorption capacity of Cd^{2+} by each mechanism on biochar in the same treatment is significant ($P < 0.05$)

Table S3 K^+, Ca^{2+}, Na^+ and Mg^{2+} release during Cd^{2+} adsorption on biochar

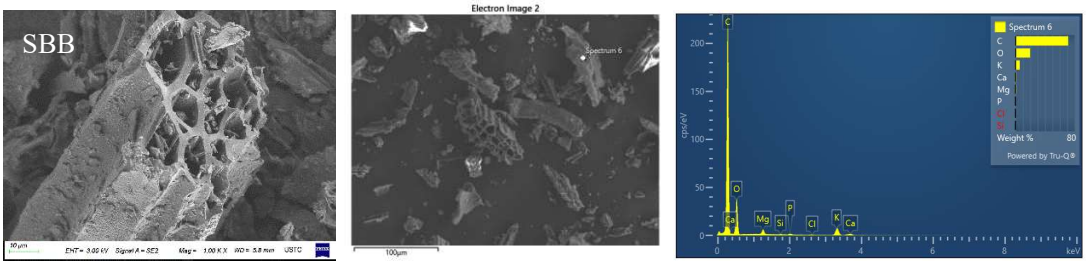
Biochar	Q_K/ (mg g^{-1})	Q_{Ca}/ (mg g^{-1})	Q_{Na}/ (mg g^{-1})	Q_{Mg}/ (mg g^{-1})	Q_{cme} / (mg g^{-1})
SBB	3.35±0.07d	4.55±0.07c	N.D	3.65±0.04a	11.55±0.05d
RSB	16.88±0.19a	1.60±0.10d	0.28±0.03	0.65±0.01d	19.41±0.20c
Ca-SBB	15.74±0.20b	11.49±0.43b	N.D	3.03±0.09b	30.26±0.72b
Ca-RSB	9.38±0.10c	25.92±0.28a	N.D	1.36±0.03c	36.66±0.29a

Note: Q_{cme}, the adsorption capacity resulted from ion exchange mechanism, mg g^{-1}. Subscripts (a, b, c and d) indicate that the differences in the release of K^+, Ca^{2+}, Na^+ and Mg^{2+} during Cd^{2+} adsorption on biochar in the same treatment is significant ($P < 0.05$).

Table S4 Changes in pH of the Cd^{2+} adsorption on demineralized biochar

Biochar	Initial pH	Final pH	Y (%)	Q_{co} (mg g^{-1})
SBB	4.06±0.01	3.38±0.03	78.20	14.16±0.30a
RSB	4.06±0.01	3.57±0.01	66.46	8.07±0.15c
Ca-SBB	4.06±0.01	3.38±0.02	64.47	12.30±0.23b
Ca-RSB	4.06±0.01	3.56±0.03	63.77	6.80±0.35d

Note: Q_{co}, the adsorption capacity resulted from functional group complexation mechanism, mg g^{-1}. Y, the yield of demineralized biochar from original biochar. Subscripts (a, b, c and d) indicate that the differences in the absorption capacity of Cd^{2+} by functional groups complexation (Q_{co}) on biochar in the same treatment is significant ($P < 0.05$).



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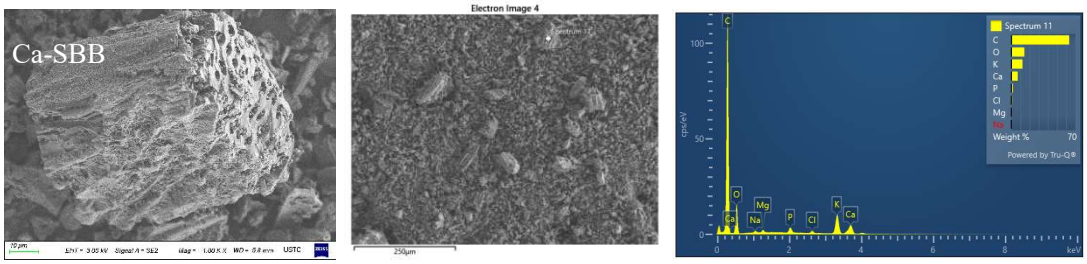

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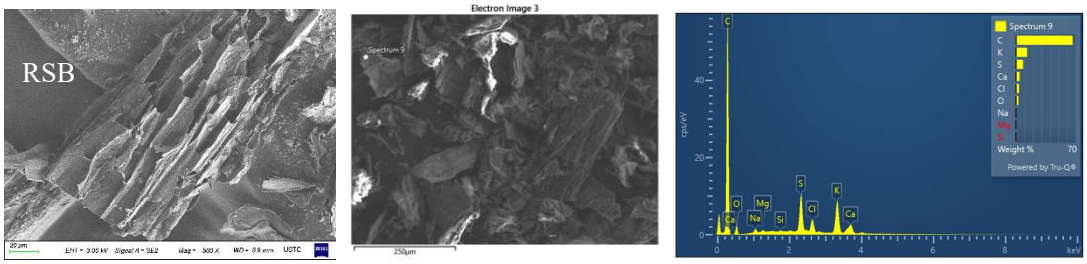

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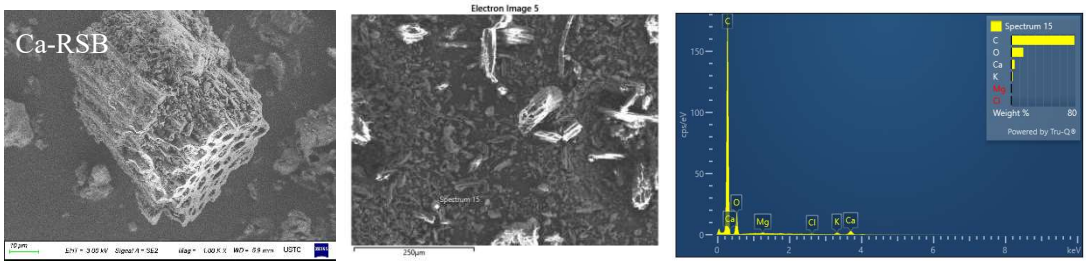

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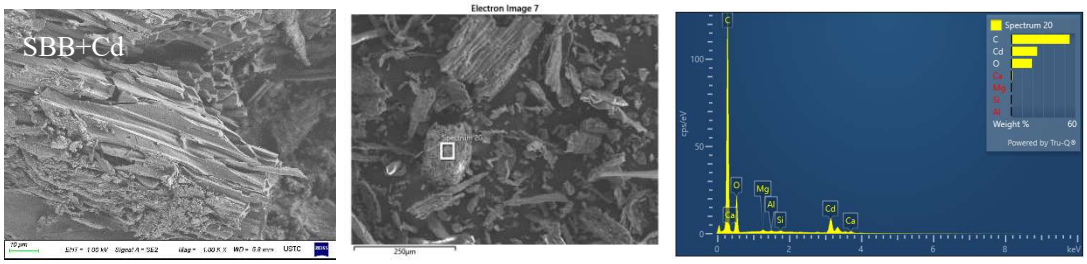

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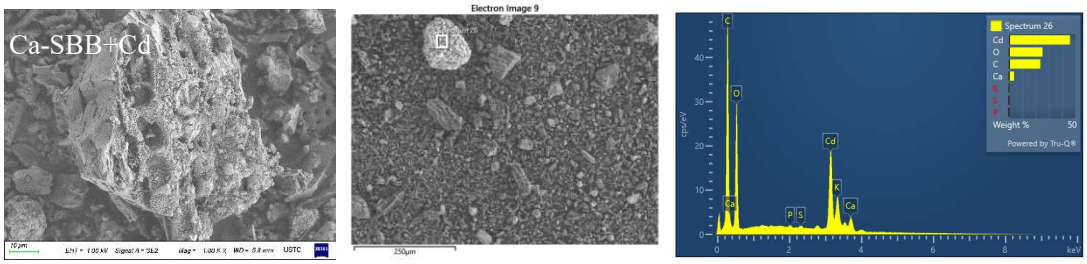

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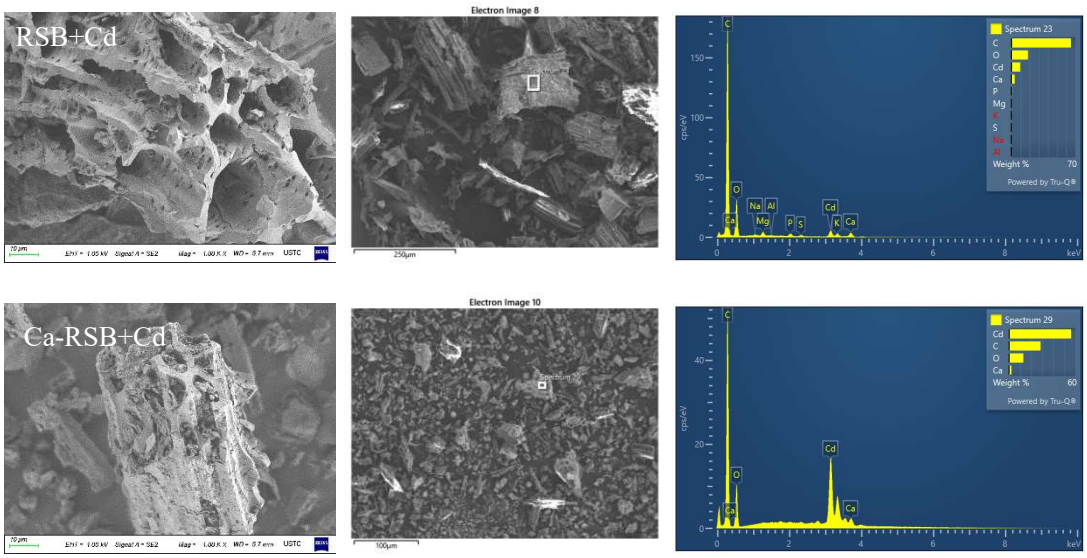

Fig. S1 SEM images and corresponding EDS spectra of biochar before and after Cd^{2+} adsorption.

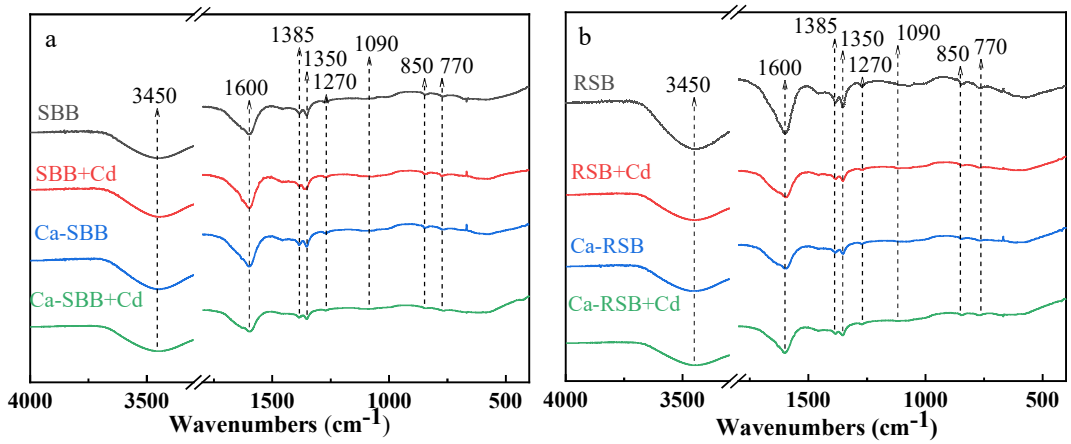

Fig. S2 FTIR spectra of SBB, Ca-SBB (**a**) and RSB, Ca-RSB (**b**) before and after Cd^{2+} adsorption, respectively

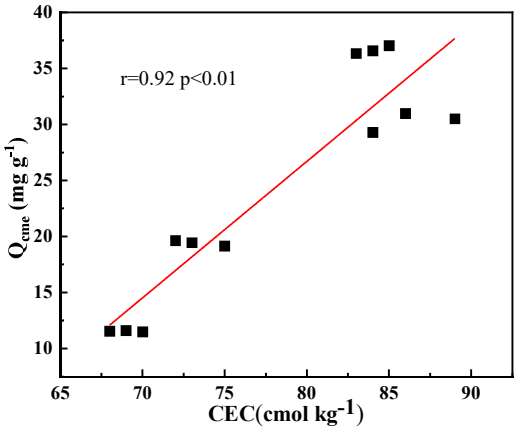

Fig. S3 Correlation between CEC and Q_{cme} in biochar. Q_{cme}, the adsorption capacity resulted from metal ion exchange mechanism, mg g^{-1}

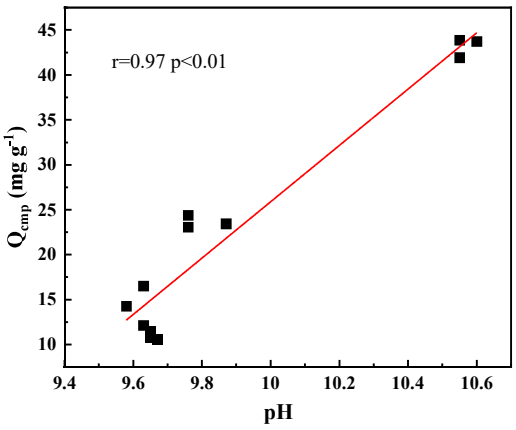

Fig. S4 Correlation between pH and Q_{cmp} in biochar. Q_{cmp} the adsorption capacity resulted from precipitation with minerals mechanism, mg g^{-1}