

Novel thiol-grafted composite of chitosan and rice straw biochar (TH@CT-BC): A two-step fabrication for highly selective adsorption of cadmium from contaminated water

Yasir Hamid^{1*}, Lei Liu¹, Muhammad Haris², Muhammad Usman³, Qiang Lin¹, Yonglong Chen¹, Muhammad Saqib Rashid⁴, Zaid Ulhassan⁵, M. Iftikhar Hussain⁶, Xiaoe Yang^{1*}

¹Ministry of Education (MOE) Key Lab of Environ. Remediation and Ecol. Health, College of Environmental and Resources Science, Zhejiang University, Hangzhou 310058, China

²School of Environmental Science and Engineering, Shaanxi University of Science & Technology, Xi'an 710021, PR China

³Université de Rennes, Ecole Nationale Supérieure de Chimie de Rennes, CNRS, ISCR-UMR 6226, F-35000, Rennes, France

⁴CAS-Key Laboratory of Crust-Mantle Materials and the Environments, School of Earth and Space Sciences, University of Science and Technology of China, Hefei 230026, P.R. China

⁵Institute of Crop Science, Ministry of Agriculture and Rural Affairs Laboratory of Spectroscopy Sensing, Zhejiang University, Hangzhou 310058, China

⁶Department of Plant Biology & Soil Science, Universidade de Vigo, Campus Lagoas Marcosende, 36310-Vigo, Spain

* For correspondence:

xeyang@zju.edu.cn (X. E Yang), yasirs2007@gmail.com (Y. Hamid)

Table S1: Kinetic parameters for Cd adsorption on BC, CT-BC, and TH@CT-BC.

	Pseudo first order			Pseudo second order		
	Q _e (mg g ⁻¹)	k ₁ (min ⁻¹)	R ²	Q _e (mg g ⁻¹)	K ₂ (g mg ⁻¹ min ⁻¹)	R ²
BC	11.07	17.26	0.908	8.13	0.0014	0.992
CT-BC	17.48	19.31	0.678	18.72	0.0620	0.990
TH@CT-BC	55.37	33.42	0.977	51.65	0.0090	0.997

Here, BC: rice straw biochar, CT-BC: chitosan-modified rice straw biochar, and TH@CT-BC: thiol grafted chitosan-modified biochar

Table S2: Intraparticle diffusion parameters for Cd adsorption on BC, CT-BC, and TH@CT-BC

	K_{p1} (mg g ⁻¹ min ⁻¹)	C (mg g ⁻¹)	R ²	K_{p2} (mg g ⁻¹ min ⁻¹)	C (mg g ⁻¹)	R ²	K_{p3} (mg g ⁻¹ min ⁻¹)	C (mg g ⁻¹)	R ²
BC	1.550	0.280	0.820	0.120	8.946	0.958	0.045	10.093	0.997
CT-BC	2.652	4.890	0.686	0.144	17.310	0.972	0.051	18.870	0.924
TH@CT-BC	5.578	27.485	0.998	0.130	52.169	0.975	0.036	53.950	0.967

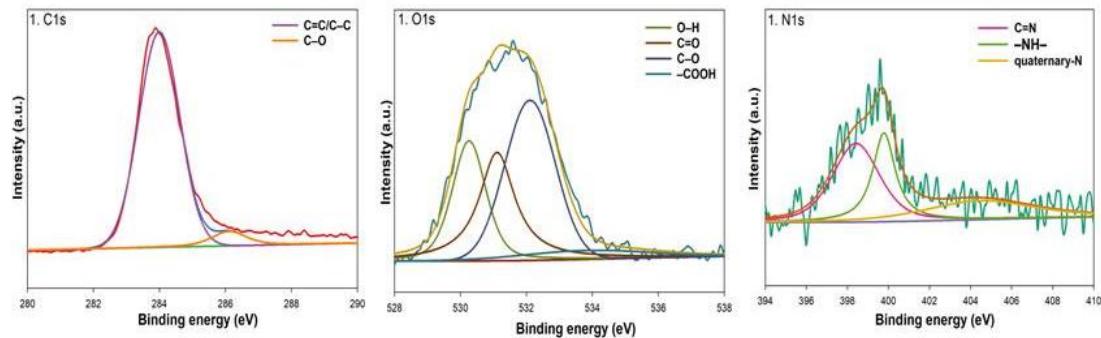
Here, BC: rice straw biochar, CT-BC: chitosan-modified rice straw biochar, and TH@CT-BC: thiol grafted chitosan-modified biochar

Table S3: Ionic characteristics of various cations

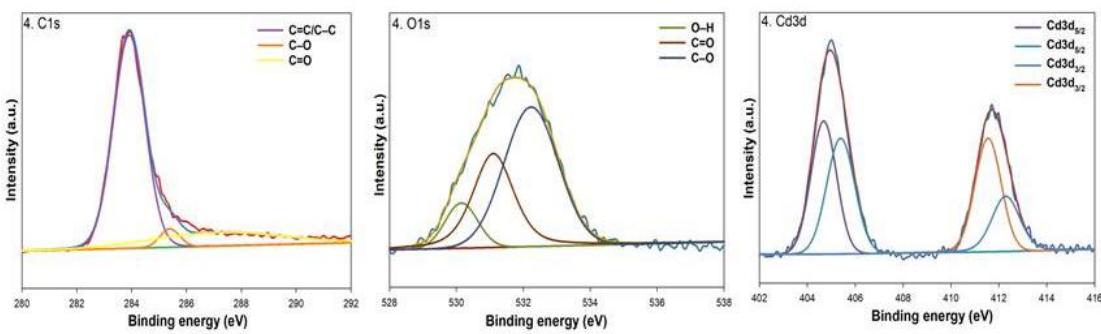
Cation	Atomic number	Electronegativity	Ionic radius (nm)	Hydrated ionic radius (Å)
Cd	48	1.7	0.097	4.26
Pb	82	1.8	0.132	4.01
Zn	30	1.65	0.880	4.30
Mg	12	1.31	0.065	4.30
Cu	29	1.9	0.096	4.19
Ni	28	1.91	0.069	4.04

Figure S1: C1s, O1s, N1s, and Cd3d, XPS spectra of BC and CT-BC before and after Cd adsorption

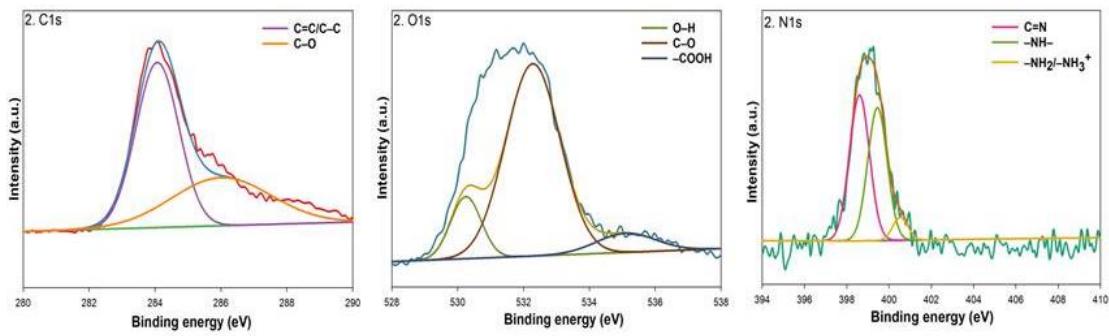
BC (Before Cd adsorption)



BC (After Cd adsorption)



CT-BC (Before Cd adsorption)



CT-BC (After Cd adsorption)

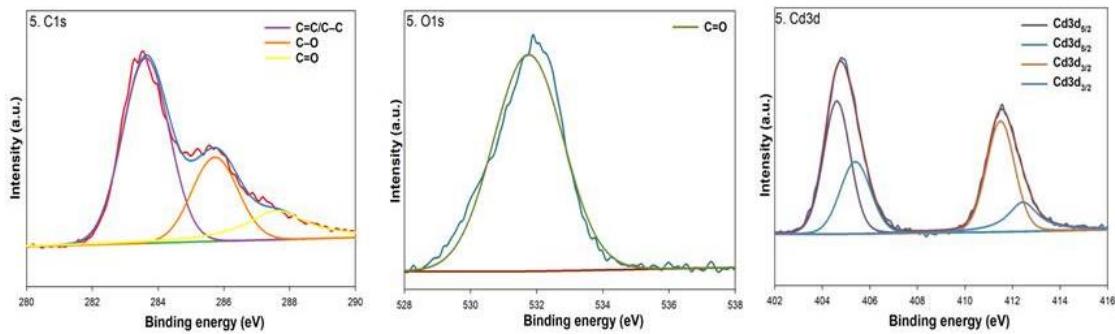


Figure S2: Effect of solution pH on Cd adsorption onto BC, CT-BC, and TH@CT-BC. Reaction settings: Adsorbent dosage 0.05 g, metal solution 30 mg L⁻¹ Cd, temperature 26±2 °C, pH 1-10, and 200 rpm for 24 h.

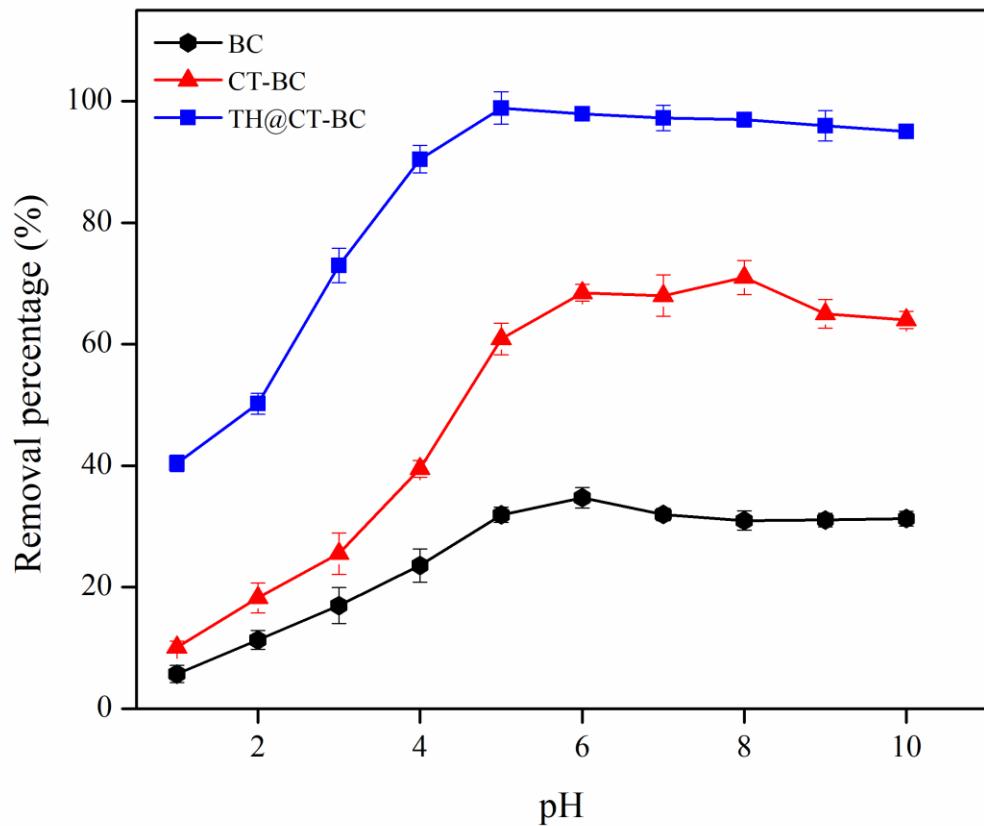


Figure S3: Effect of competing cations on Cd adsorption onto BC, CT-BC, and TH@CT-BC. Reaction settings: Adsorbent dosage 0.05 g, temperature 26 ± 2 °C, pH 5.5 ± 0.5 , and 200 rpm for 24 h.

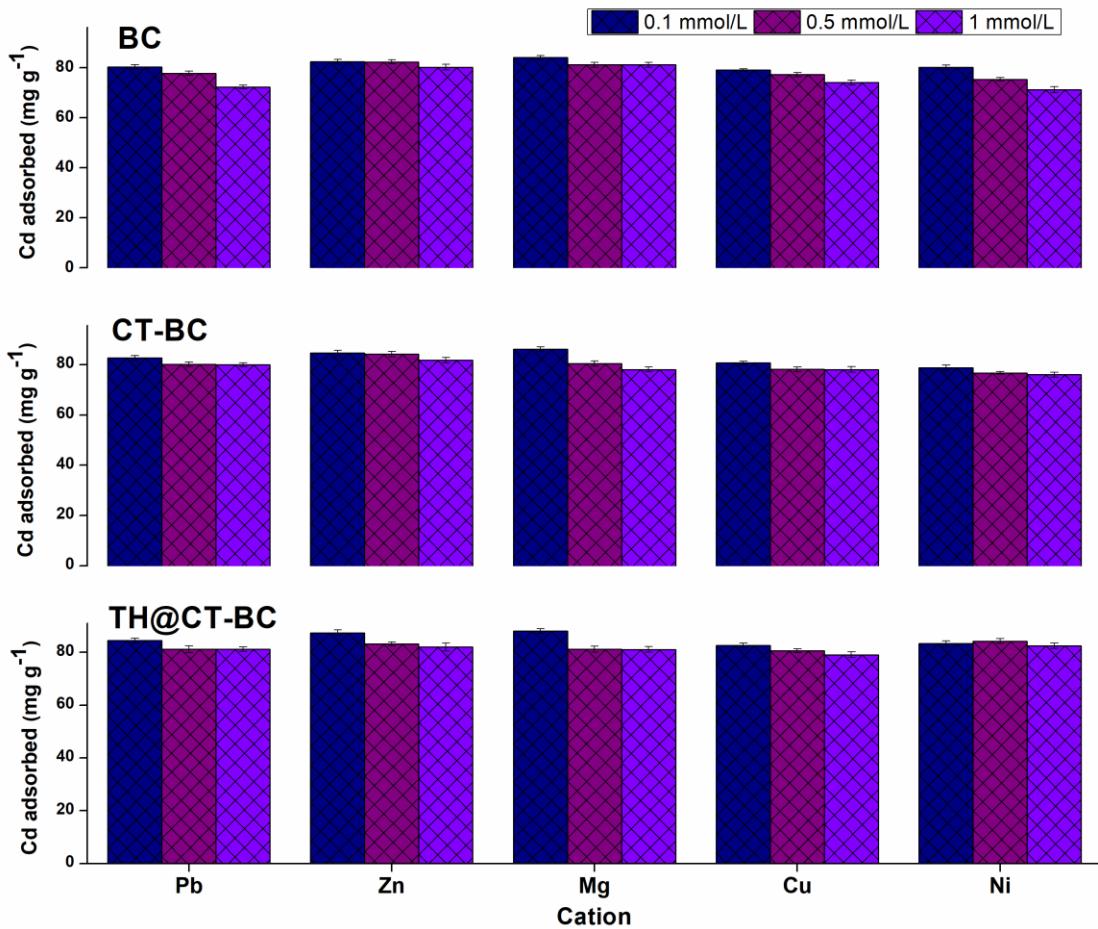


Figure S4: Regeneration efficiency of BC, CT-BC, and TH@CT-BC for Cd removal (A) and effect on Cd removal using Cd spiked river water (B). Reaction settings: Adsorbent dosage 0.05 g, temperature 26 ± 2 °C, pH 5.5 ± 0.5 .

