



## Supplementary Materials

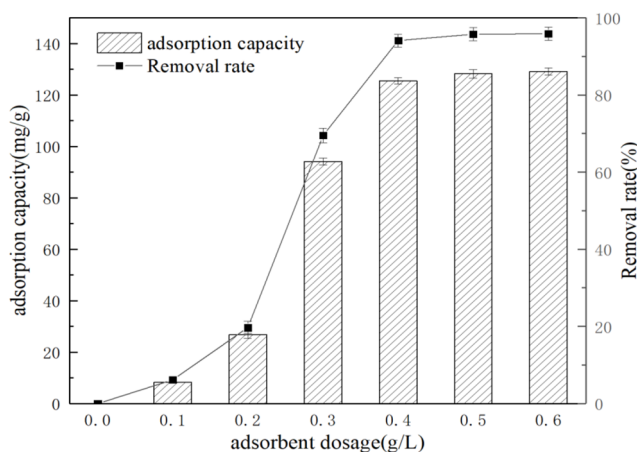
### Text S1. Response Surface Method Model Equation

The experiments were designed and analyzed using BBD of the response surface in the statistical software of Design Expert 8.0, resulting in 17 runs, with the aim of optimizing the best MFDB [1]. Based on the ANOVA, a P-value less than 0.05 indicates that the model terms are significant. In this study, all model terms of the regression quadratic model were determined to be significant [2].

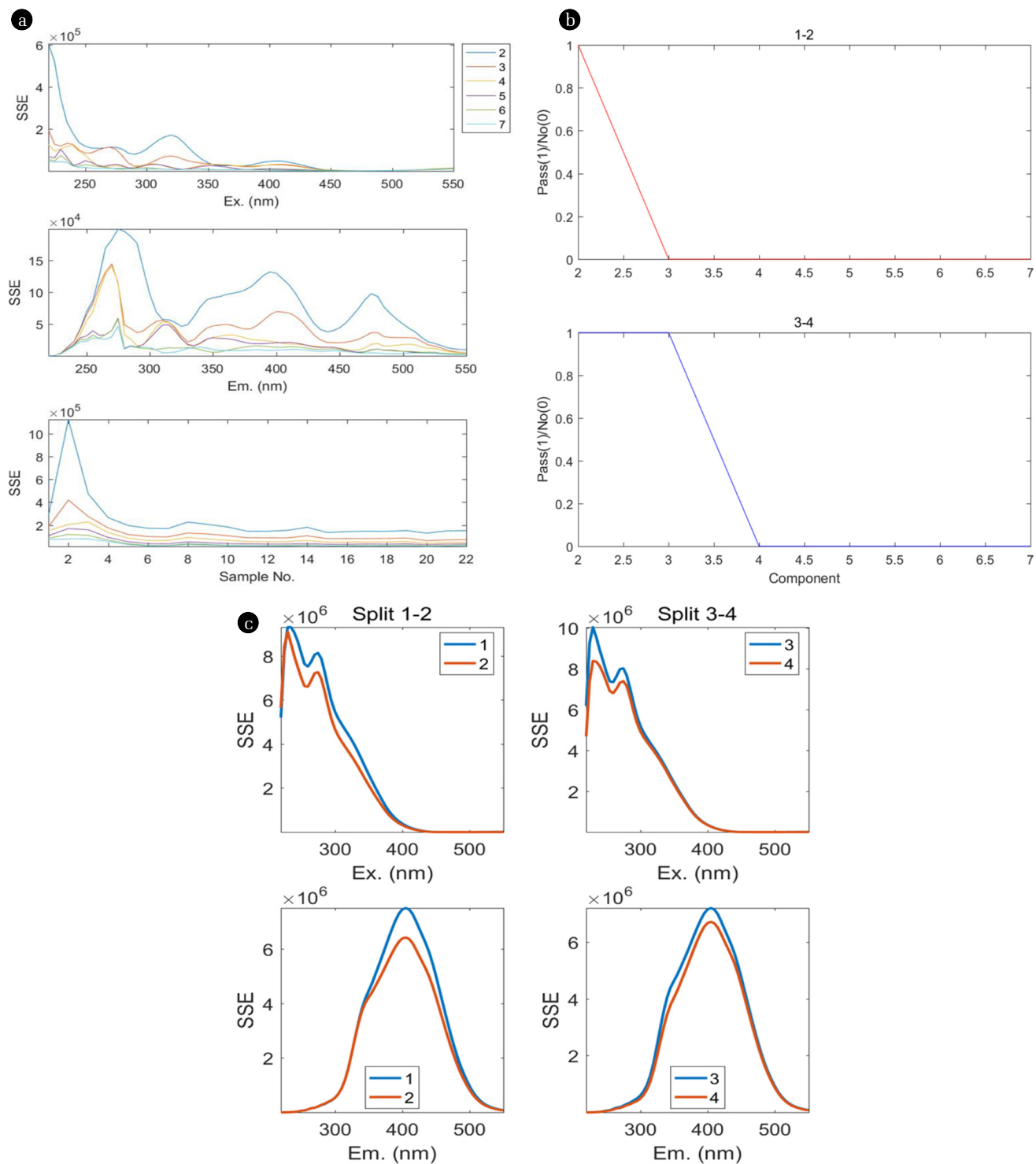
The quadratic model equation is as follows:

$$Y = \beta_0 + \sum_{i=1}^n \beta_i X_i + \sum_{i=1}^n \beta_{ii} X_i^2 + \sum_{i=1}^n \sum_{j=1}^n \beta_{ij} X_i X_j + e$$

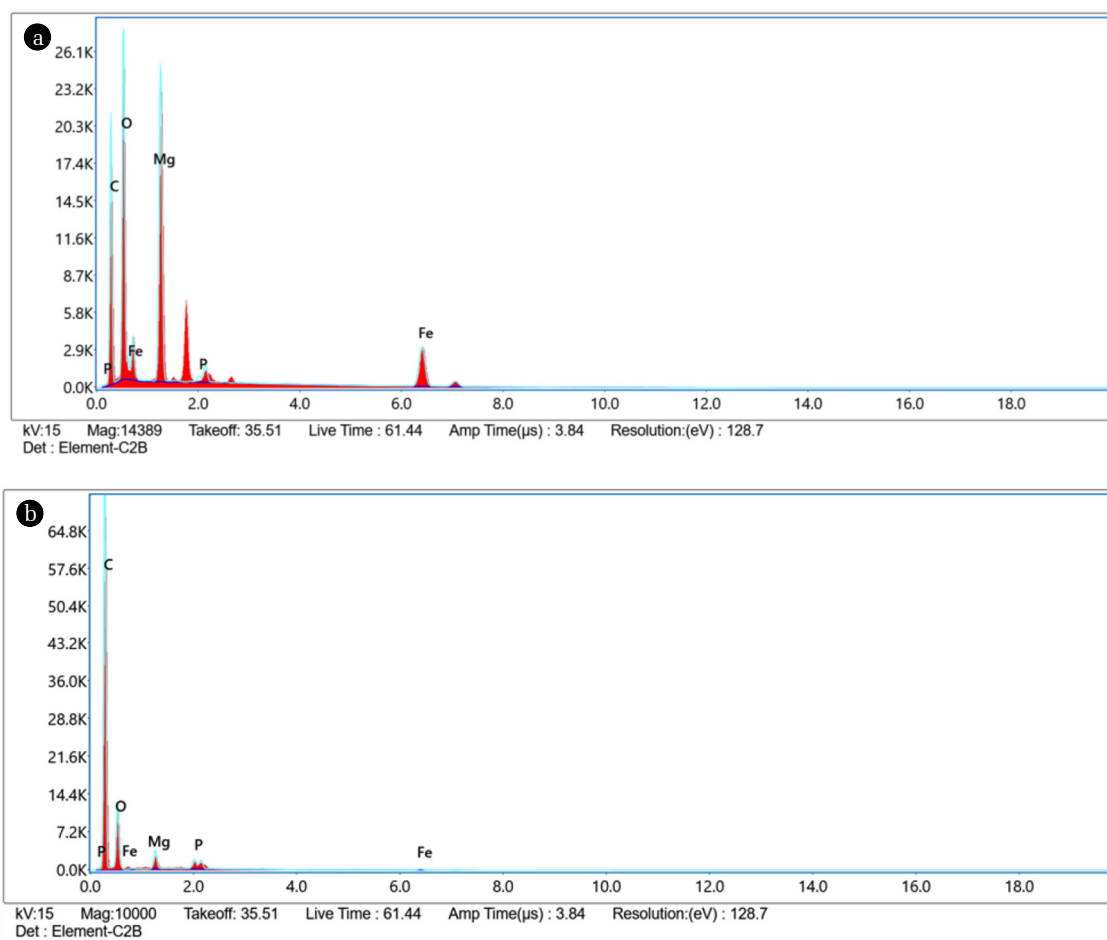
where  $Y$  is the response factor (Phosphorus adsorption),  $\beta_0$  is the constant coefficient,  $\beta_i$  is the constant coefficient of first order,  $\beta_{ii}$  is the constant coefficient of quadratic term,  $\beta_{ij}$  is the constant coefficient of interaction term,  $X_i, X_j$  are the coded values of the independent process variables and  $e$  is the residual error [2].



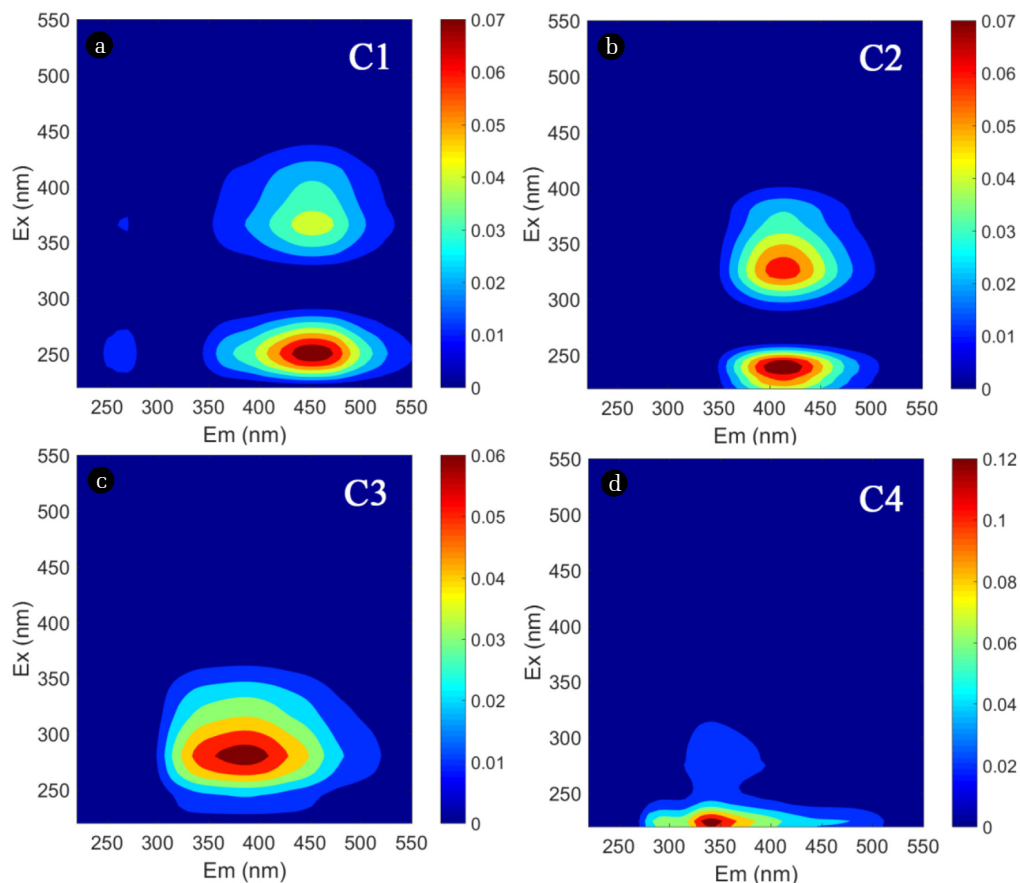
**Fig. S1.** Effect of MFDB dosage on phosphate- removal rate.



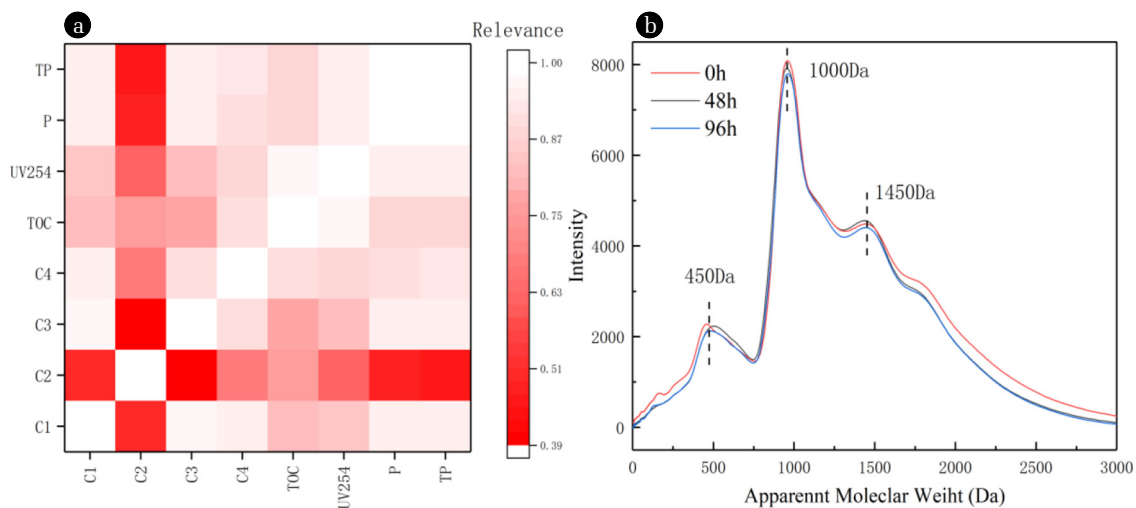
**Fig. S2.** PARAFAC model validation. (a) Sum of squares error diagram; (b) core consistency; (c) half-score tests.



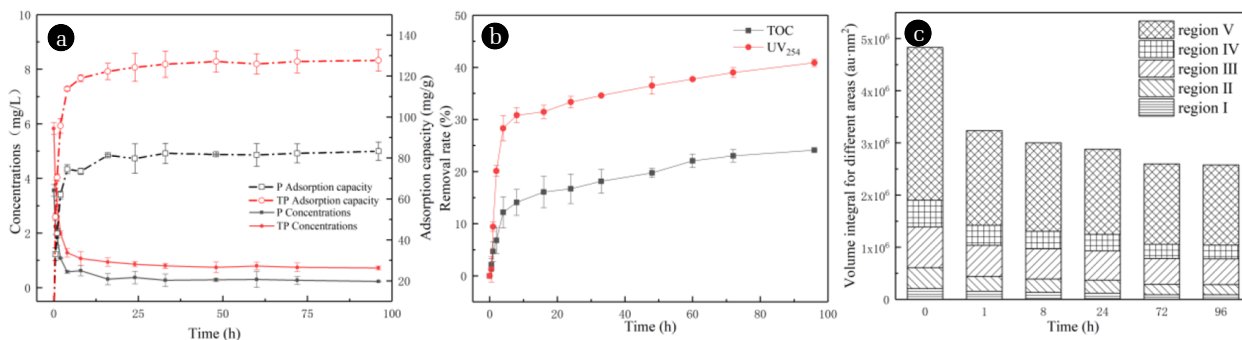
**Fig. S3.** (a) EDS spectrum of MFDB before adsorption; (b) EDS spectrum of MFDB after adsorption.



**Fig. S4.** Analysis of four PARAFAC components by EEM fluorescence spectroscopy of actual water adsorbed by MFDB.



**Fig. S5.** (a) Correlation analysis of different components; (b) Apparent molecular weight (AMW) distribution of actual water at different adsorption times.



**Fig. S6.** (a) Removal of phosphorus and total phosphorus by MFDB in real wastewater. (b) Removal of TOC and UV<sub>254</sub> by MFDB. (c) Area integral volume of EEM fluorescence spectrum by MFDB.

**Table S1.** MFDB's Experimental Design Table

Run	Coded level			Actual level of variables			Response Adsorption capacity (mg/g)
	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	Factor 1 A:Mg	Factor 2 B:Fe	Factor 3 C:T	
1	1	0	-1	4	1.5	450	74.23
2	-1	0	-1	0	1.5	450	19.06
3	-1	1	0	0	3	550	2.80
4	0	0	0	2	1.5	550	67.77
5	-1	0	1	0	1.5	650	23.91
6	0	0	0	2	1.5	550	69.42
7	1	1	0	4	3	550	27.36
8	0	-1	-1	2	0	450	42.35
9	1	0	1	4	1.5	650	56.35
10	0	1	1	2	3	650	29.63
11	0	0	0	2	1.5	550	68.61
12	0	-1	1	2	0	650	30.53
13	0	1	-1	2	3	450	28.66
14	0	0	0	2	1.5	550	67.18
15	1	-1	0	4	0	550	43.70
16	-1	-1	0	0	0	550	0.23
17	0	0	0	2	1.5	550	72.64

**Table S2.** Analyses of Variance (ANOVA) Table for the Model

Source	Sum of Squares	df	Mean Square	F Value	p-value	prob > F
Model	9,682.74	9	1,075.86	112.46	< 0.0001	significant
X <sub>1</sub> -Mg:BM	3,027.92	1	3,027.92	316.52	< 0.0001	
X <sub>2</sub> -Fe:BM	100.5	1	100.5	10.51	0.0142	
X <sub>3</sub> -T	71.26	1	71.26	7.45	0.0294	
X <sub>1</sub> X <sub>2</sub>	89.44	1	89.44	9.35	0.0184	
X <sub>1</sub> X <sub>3</sub>	129.2	1	129.2	13.51	0.0079	
X <sub>2</sub> X <sub>3</sub>	40.9	1	40.9	4.28	0.0775	
X <sub>1</sub> <sup>2</sup>	1,684.73	1	1,684.73	176.11	< 0.0001	
X <sub>2</sub> <sup>2</sup>	3,941.87	1	3,941.87	412.06	< 0.0001	
X <sub>3</sub> <sup>2</sup>	138.45	1	1,38.45	14.47	0.0067	
Residual	66.96	7	9.57	-	-	
Lack of fit	48.64	3	16.21	3.54	0.1269	not significant
Pure error	18.33	4	4.58	-	-	
Cor total	9,749.7	16	-	-	-	

R<sup>2</sup> = 0.993, Coefficient of variance = 7.21%.

**Table S3.** Kinetic Parameters of Phosphorus Adsorption by MFDB (25°C)

phosphate concentration mg/L	q <sub>e,exp</sub> mg/g	Pseudo-first-order			Pseudo-second-order			intraparticle diffusion model	
		k <sub>1</sub> 1/h	q <sub>e,cal</sub> mg/g	R <sup>2</sup>	k <sub>2</sub> g/(mg·h)	q <sub>e,cal</sub> mg/g	R <sup>2</sup>	k <sub>3</sub> mg/(g·h <sup>0.5</sup> )	R <sup>2</sup>
5	11.21	0.098	10.03	0.803	0.0126	11.14	0.916	0.839	0.948
10	21.87	0.064	21.3	0.974	0.0023	26.39	0.982	2.573	0.989
25	56.67	0.022	67.4	0.998	0.0001	101.05	0.997	7.396	0.993
50	103.24	0.037	109.6	0.998	0.0002	144.19	0.997	13.274	0.983

**Table S4.** The Isotherm of Phosphorus Adsorption by MFDB

Temperature K	q <sub>e,exp</sub> mg/g	Langmuir model			Freundlich model			Tempkin		
		q <sub>m</sub> mg/g	b L/mg	R <sup>2</sup>	K <sub>F</sub>	1/n	R <sup>2</sup>	A	B	R <sup>2</sup>
283	128.71	211.73	0.0136	0.938	2.778	0.894	0.99	0.194	33.11	0.769
298	158.21	228.53	0.0063	0.934	3.769	0.843	0.993	0.279	41.88	0.860
313	179.21	246.25	0.0099	0.957	2.183	0.822	0.972	0.431	15.19	0.892

**Table S5.** Thermodynamic Parameters of Phosphorus Adsorption by MFDB

Temperature	qe	Ce	Kd	$\Delta G_0$	$\Delta H_0$	$\Delta S_0$
K	mg/g	mg/L		KJ/mol	KJ/mol	J/(mol·K)
283	108.37	62.245	1741.02	-17.558		
298	119.17	64.062	1860.22	-18.652	15.91	71.168
313	131.72	62.851	2095.76	-19.901		

**Table S6.** Physical and chemical properties of materials (SBC is wheat straw biochar; MFDB is Mg/Fe-doped biochar;  $S_{BET}$  is the BET surface area; TPV is total pore volume; APR is average pore radius)

Adsorbents	C (%)	H (%)	O (%)	H/C	O/C	Fe (%)	Mg (%)	P (%)	$S_{BET}$ (m <sup>2</sup> /g)	TPV (cm <sup>3</sup> /g)	APR (nm)
SBC	53.3	2.26	10.5	0.042	0.197	0.551	0.535	0.304	10.5	0.015	1.483
MFDB	6.47	5.17	43.6	0.799	6.738	13.6	29.1	0.079	112.8	0.14	1.092

## References

1. Karimifard S, Moghaddam MRA. Application of response surface methodology in physicochemical removal of dyes from wastewater: A critical review. *Sci. Total Environ.* 2018;640:772-797. <https://doi.org/10.1016/j.scitotenv.2018.05.355>.
2. Singh KP, Gupta S, Singh AK. Optimizing adsorption of crystal violet dye from water by magnetic nanocomposite using response surface modeling approach. *J. Hazard. Mater.* 2011;186:1462-1473. <https://doi.org/10.1016/j.jhazmat.2010.12.032>.