Supplementary Material (ESI) for Phys Chem Chem Phys

Experimental and Theoretical Studies on Methylene Blue and Methyl Orange Sorption by Wheat Straw-Derived Biochar with Large Surface Area

Peifang Wang*, Chuangfei Wu, Yong Guo*, Chao Wang

Key Laboratory of Integrated Regulation and Resource Development on Shallow Lakes, Ministry of Education, College of Environment, Hohai University, P.R. China.

E-mail: pfwang2005@hhu.edu.cn;

E-mail: guoyong@hhu.edu.cn;

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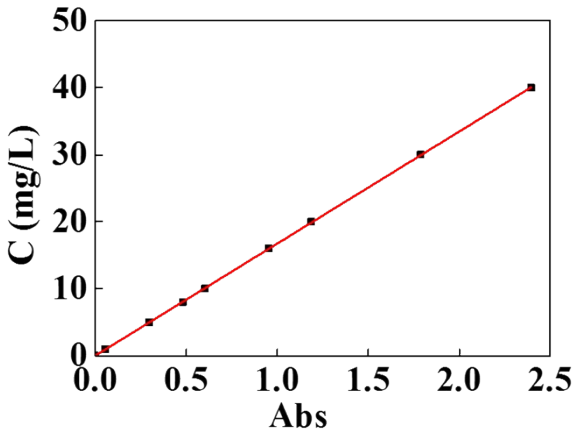


Fig.S1 The standard curve of methyl orange in water.

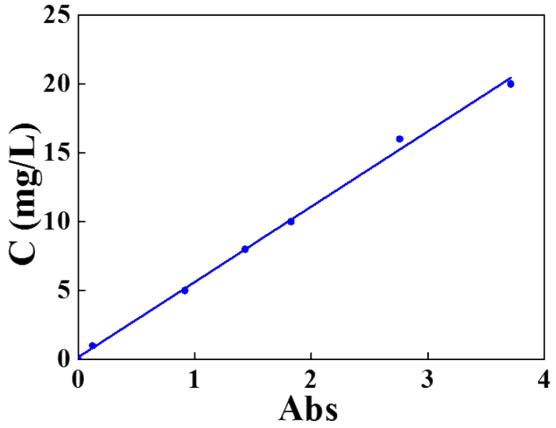


Fig.S2 The standard curve of methylene blue trihydrate in water.

	Concentration (mg/L)	Absorbance before filtration	Absorbance after filtration
MO	50.00	3.526	3.530

Table. S1 The absorbances of MO solution before and after filtration.

	Concentration (mg/L)	Absorbance before filtration	Absorbance after filtration
MB	16.00	2.597	2.557

Table. S2 The absorbances of MB solution before and after filtration.

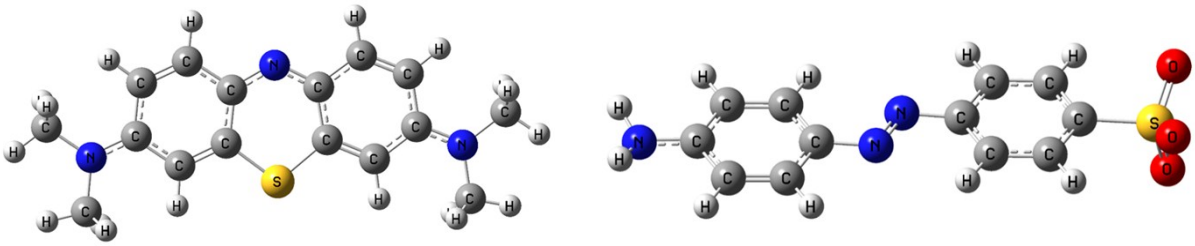


Fig.S3 The optimized structures of MB cation (left) and MO anion (right).

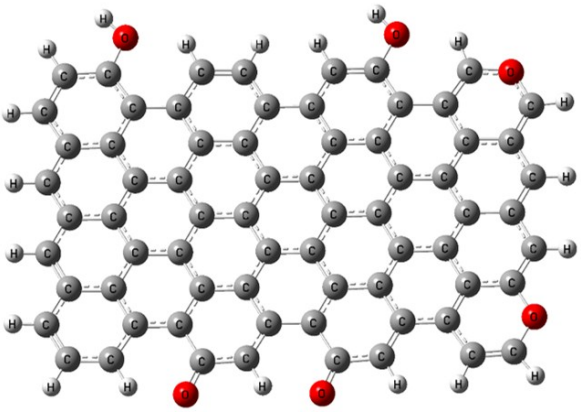


Fig. S4 The optimized structure of BCmodel with negative surface.

Sample	Yield, C(%)	BET (m^2/g)	Micropore Area (m^2/g)	External Surface Area (m^2/g)	Total Volume (cm^3/g)	Micropore Volume (cm^3/g)	mesopore Volume (cm^3/g)	Pore Size (Å)
BC-4-500	16.35	587.57	488.61	98.96	0.32	0.25	0.07	21.66
BC-4-600	14.48	1490.76	1152.52	338.23	0.80	0.59	0.21	21.59
BC-4-700	14.20	2263.10	1170.44	1092.66	1.21	0.63	0.58	21.33
BC-4-800	12.88	2184.50	676.68	1507.82	1.17	0.38	0.80	21.51

Table. S3 The yield, BET surface areas, micropore areas, external surface areas, total volumes, micropore volumes, mesopore volumes and pore sizes of BC-4-500, BC-4-600, BC-4-700 and BC-4-800 samples.

Sample	Yield C(%)	BET (m^2/g)	Micropore Area (m^2/g)	External Surface Area (m^2/g)	Total Volume (cm^3/g)	Micropore Volume (cm^3/g)	mesopore Volume (cm^3/g)	Pore Size (Å)
WS-4-700	4.62	222.17	162.36	59.80	0.16	0.08	0.08	29.55

Table. S4 The yield, BET surface area, micropore area, external surface area, total volume, micropore volume, mesopore volume and pore size of WS-4-700 sample. For the name of WS-4-700, WS represents wheat straw powder, 4 represents that the mass ratio between KOH and WS is 4:1, 700 represents that the activation temperature is 700 °C.

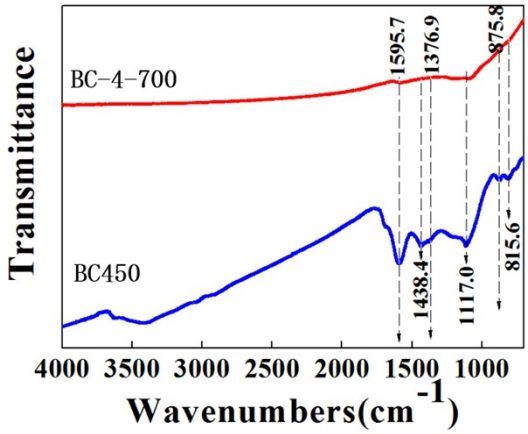


Fig. S5 FTIR spectra of BC-4-700 and BC450 samples.

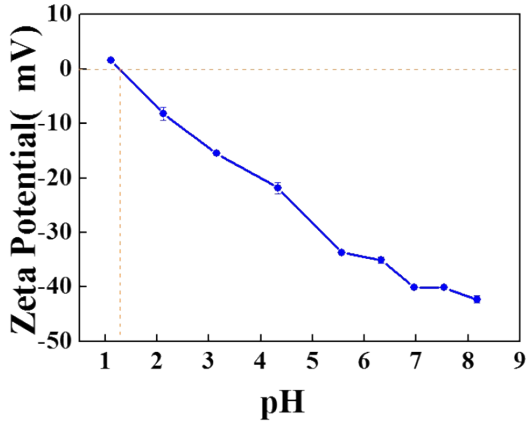
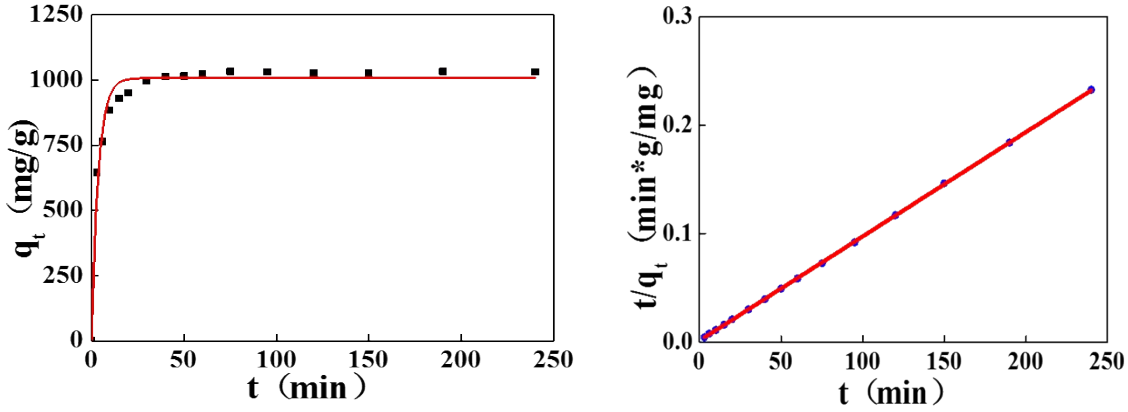


Fig. S6 The surface charge of BC-4-700 at different pH values

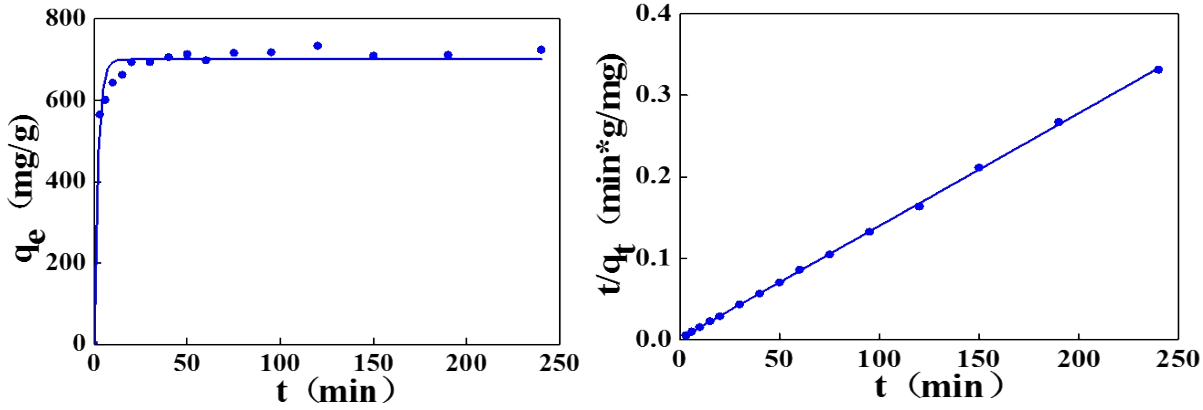


(a) (b)

Fig. S7 The kinetic sorption of MO by BC-4-700, which was fitted by (a) pseudo-first-order model and (b) pseudo-second-order model, respectively.

Table S5 Kinetic parameters for MO sorption by BC-4-700.

Model	Parameters	Values
Pseudo-first-order	k_1 (1/min)	0.2719
	q_e (mg/g)	1007
	R^2	0.9772
Pseudo-second-order	k_2 (g/ (mg*min)	0.0006
	q_e (mg/g)	1040
	R^2	0.9999

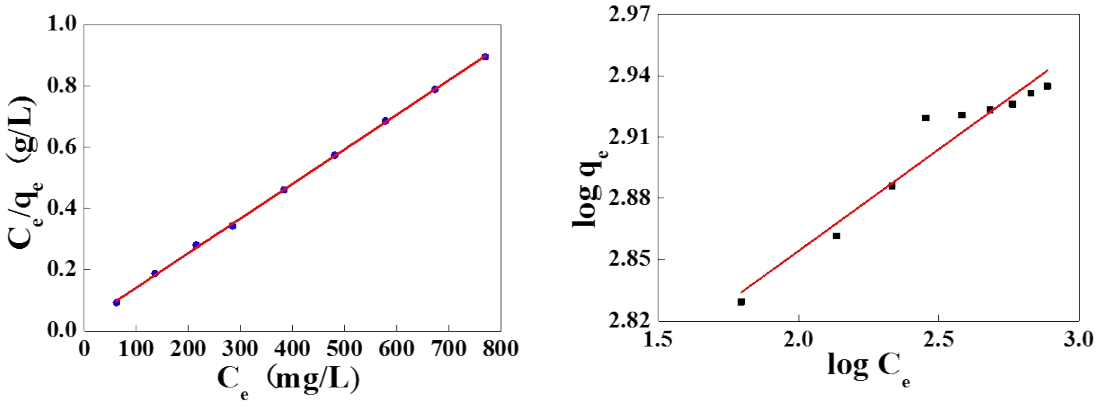


(a) (b)

Fig. S8 The kinetic sorption of MB by BC-4-700, which were fitted by (a) pseudo-first-order model and (b) pseudo-second-order model, respectively.

Model	Parameters	Values
Pseudo-first-order	k_1（1/min）	0.4704
	q_e（mg/g）	700.2
	R^2	0.9704
Pseudo-second-order	k_2（g/（mg*min）	0.0013
	q_e（mg/g）	724.6
	R^2	0.9997

Table S6 Kinetic parameters for MB sorption by BC-4-700.



(a) (b)

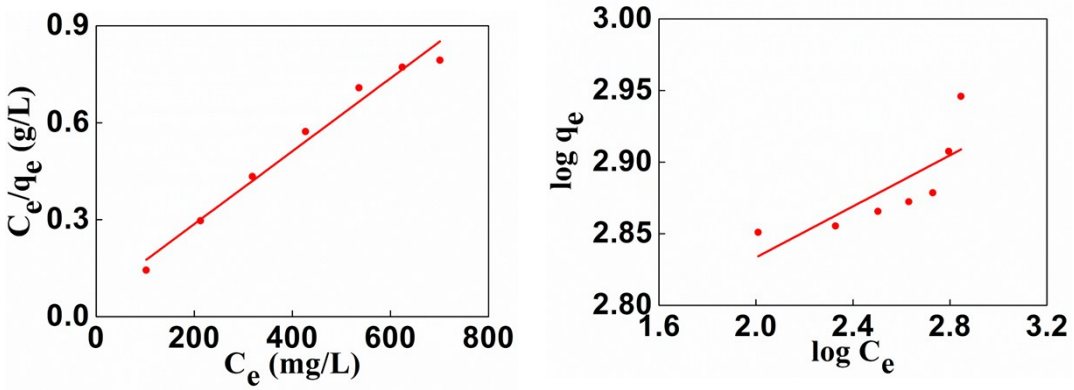
Fig. S9 The isotherm sorption of MO by BC-4-700, which were fitted by (a) Langmuir model and (b) Freundlich model, respectively.

Model	Parameters	Values
Langmuir	Q_0(mg/g)	1109
	K_L（L/mg）	0.0381
	R^2	0.9996
Freundlich	K_F（mg/g）（L/mg）$^{1/n}$	452.2
	n	10.05
	R^2	0.9339

Table. S7 Isotherm parameters for MO sorption by BC-4-700.

The concentrations of the prepared MB solution（mg/L）	The detected concentrations of MB solution four hours later（mg/L）
456.9 (1.22 mmol/L)	456.4 (1.22 mmol/L)
571.1 (1.53 mmol/L)	538.5 (1.44 mmol/L)
685.4 (1.83 mmol/L)	667.3 (1.78 mmol/L)
799.6 (2.14 mmol/L)	799.1 (2.14 mmol/L)
913.8 (2.44 mmol/L)	913.4 (2.44 mmol/L)
1028 (2.75 mmol/L)	1029 (2.75 mmol/L)
1142 (3.06 mmol/L)	1121 (3.00 mmol/L)
1256 (3.36 mmol/L)	1217 (3.25 mmol/L)
1370 (3.67 mmol/L)	1311 (3.51 mmol/L)

Table.S8 The concentrations of the prepared MB solutions and the detected concentrations of MB solutions four hours later.

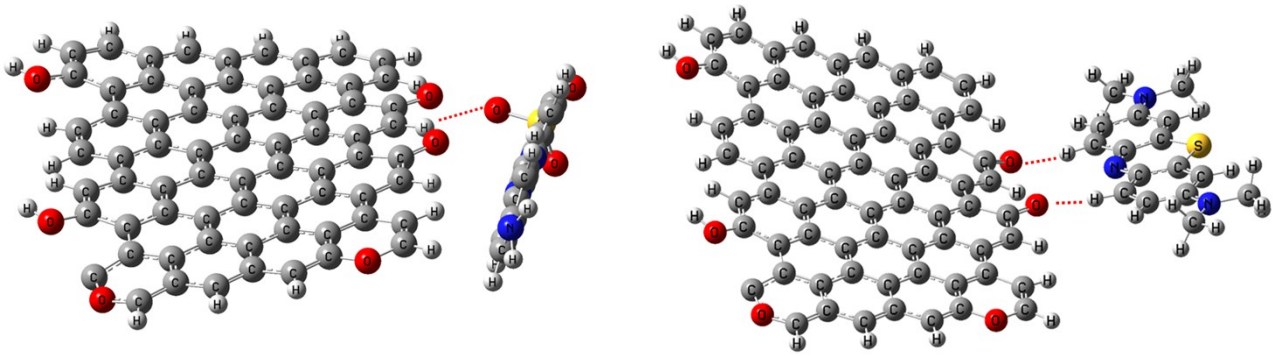


(a) (b)

Fig. S10 The isotherm sorption of MB by BC-4-700 with the concentrations ranging from 1.22 mmol/L to 3.06 mmol/L, which was fitted by (a) Langmuir method and (b) Freundlich method, respectively.

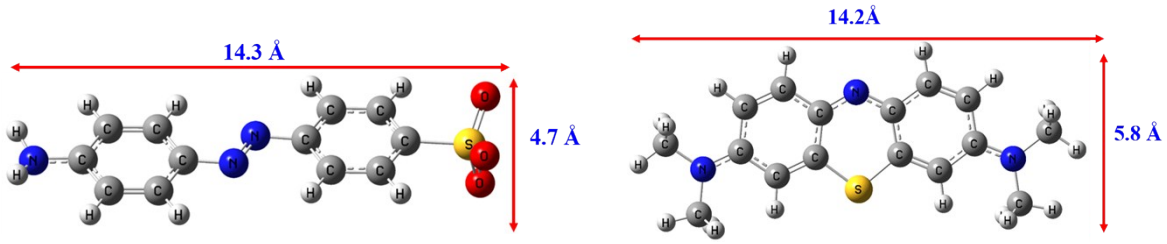
Model	Parameters	Values
Langmuir	Q_0(mg/g)	885.0
	K_L（L/mg）	0.0186
	R^2	0.9763
	R_L	0.0450
Freundlich	K_F（（mg/g）*（L/mg）$^{1/n}$）	451.9
	n	11.21
	R^2	0.5458

Table S9 Isotherm parameters for MB sorption by BC-4-700 with the concentrations ranging from 1.22 mmol/L to 3.06 mmol/L.



(a) (b)

Fig. S11 The optimized structures of (a) BCmodel-MO^- complex formed via hydrogen bonding interaction; (b) BCmodel-MB^+ complex formed via hydrogen bonding interaction.



(a) (b)

Fig. S12 The calculated sizes of (a) MO anion and (b) MB cation.

MO			MB		
concentration (mg/L)	pH before sorption	pH after sorption	concentration (mg/L)	pH before sorption	pH after sorption
400.0 (1.22 mmol/L)	6.80	6.61	456.9 (1.22 mmol/L)	6.08	3.56
500.0 (1.53 mmol/L)	6.78	6.78	571.1 (1.53 mmol/L)	5.15	3.54
600.0 (1.83 mmol/L)	6.74	6.70	685.3 (1.83 mmol/L)	4.96	3.53
700.0 (2.14 mmol/L)	6.82	6.75	799.6 (2.14 mmol/L)	4.81	3.53
800.0 (2.44 mmol/L)	6.86	6.87	913.8 (2.44 mmol/L)	4.88	3.54
900.0 (2.75 mmol/L)	6.91	6.95	1028 (2.75 mmol/L)	4.80	3.53
1000 (3.06 mmol/L)	7.73	6.93	1142 (3.06 mmol/L)	4.65	3.52
1100 (3.36 mmol/L)	7.34	6.96	1257 (3.36 mmol/L)	4.71	3.53
1200 (3.67 mmol/L)	7.20	6.99	1371 (3.67 mmol/L)	4.64	3.53

Table.S10 the pH values of MO and MB solutions with different concentrations before and after isotherm sorption.

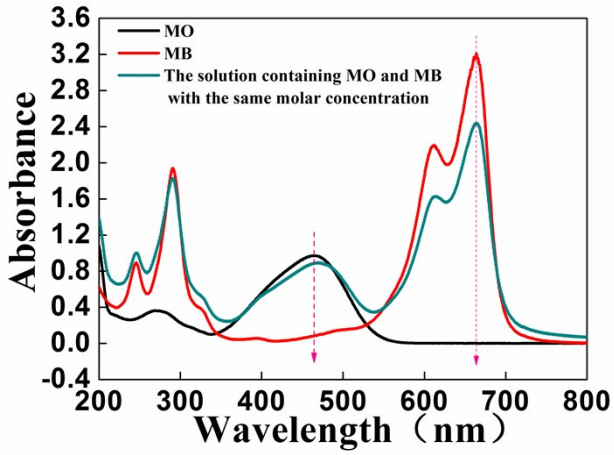


Fig. S13 The Uv absorption peaks of MO, MB and the solution containing MO and MB with the same molar concentration. The concentrations of MO and MB are 800.0 mg/L (2.44 mmol/L) and 913.8mg/L (2.44 mmol/L).