Supplementary Materials for:

Heteroatom-doped highly porous carbons prepared by in-situ activation for efficient adsorptive removal of sulfamethoxazole

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Equations

$$q_e = \frac{(C_0 - C_e)V}{m} \quad \text{(S1)}$$

where C_0 and C_e (mg/L) are the SMX concentrations at initial and equilibrium, respectively. m (g) is the mass of adsorbent and V (L) is the solution volume.

$$q_t = \frac{(C_0 - C_t)V}{m} \quad \text{(S2)}$$

where q_t is the adsorption capacity (mg/g), C_0 is the initial concentration of SMX in solution (mg/L), C_t is the concentration at time t (mg/L), m is the mass of the adsorbent (g), and V is the volume of the solution (L).

$$q_e = q_{max} \cdot K_L \cdot C_e/(1+C_e \cdot K_L) \quad \text{(S3)}$$

where q_{max} is maximum adsorption capacity, and K_L (L/mg) represents Langmuir constant that relates to the affinity of the binding sites which describes the intensity of the adsorption process.

$$q_e = K_F \cdot C_e^{1/n} \quad \text{(S4)}$$

where K_F and n are Freundlich constants indicative of adsorption capacity and adsorption intensity, respectively.

$$q_t = q_e(1 - \exp(-k_1 t)) \quad \text{(S5)}$$

$$q_t = q_e^2 k_2 t/(1 + q_e k_2 t) \quad \text{(S6)}$$

$$h = k_2 \cdot q_e^2 \quad \text{(S7)}$$

where q_t (mg·g^{-1}) and q_e (mg·g^{-1}) are the amount of SMX adsorbed at the contact time of t (min) and equilibrium, respectively; k_1 (min^{-1}) and k_2 (g (mg^{-1} min^{-1})) are the rate constants for the pseudo-first-order and pseudo-second-order models, respectively.

Reactions

$$K_2CO_3 \rightarrow K_2O + CO_2 \quad \text{(S1)}$$

$$K_2CO_3 + 2C \rightarrow 2K + 3CO \quad \text{(S2)}$$

$$K_2O + C \rightarrow 2K + CO \quad \text{(S3)}$$

$$CO_2 + C \rightarrow 2CO \quad \text{(S4)}$$

$$C + H_2O \rightarrow CO + H_2 \quad \text{(S5)}$$

$$CO + H_2O \rightarrow CO_2 + H_2 \quad \text{(S6)}$$

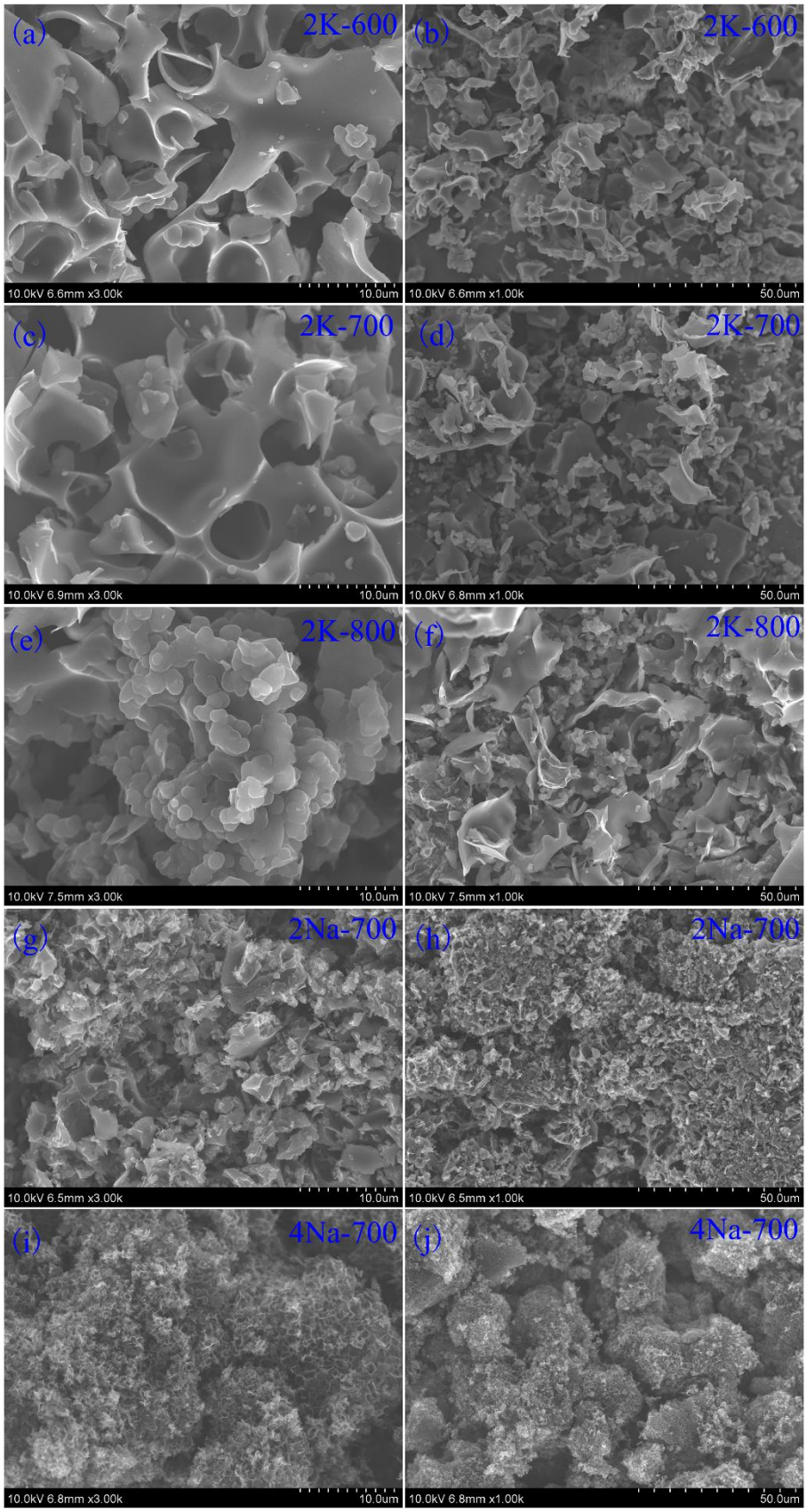

Figure S1. High resolution (a, c, e, g, i) and low resolution (b, d, f, h, j) SEM image of porous carbons.

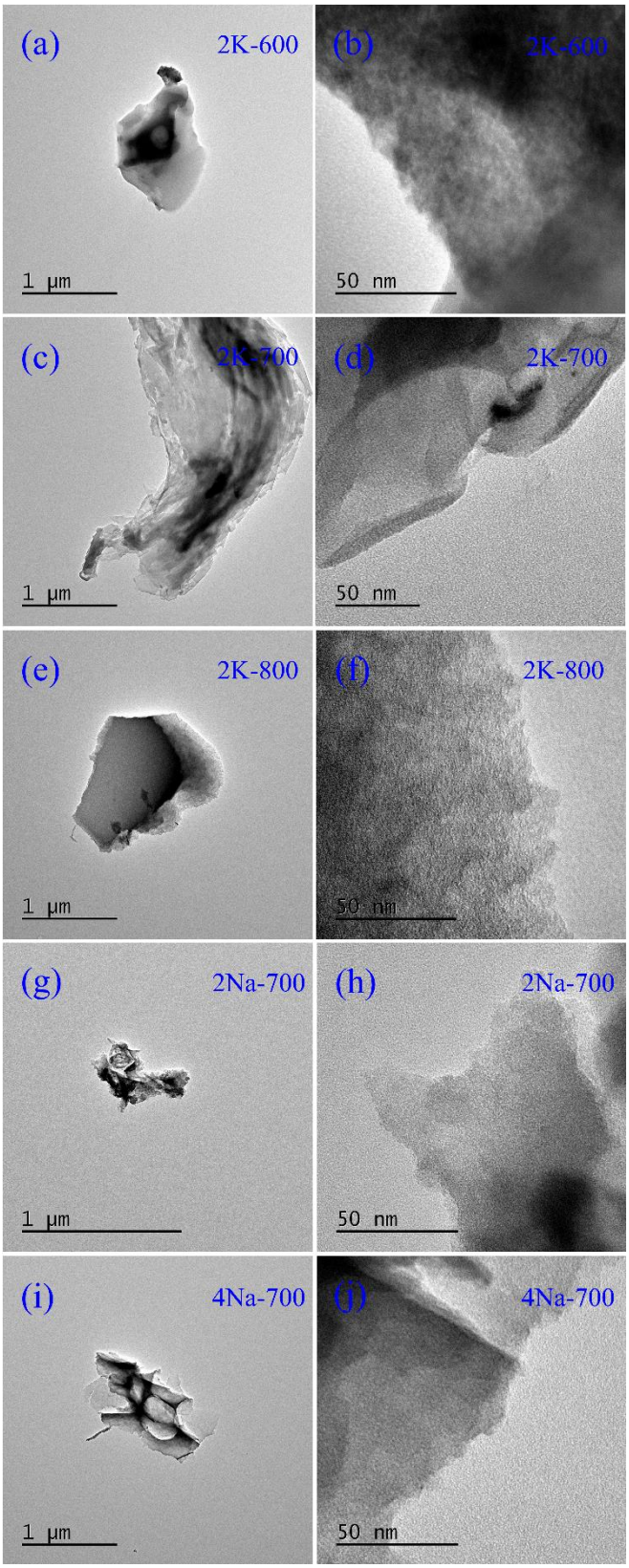

Figure S2. Low resolution (a, c, e, g, i) and high resolution (b, d, f, h, j) TEM image of porous carbons.

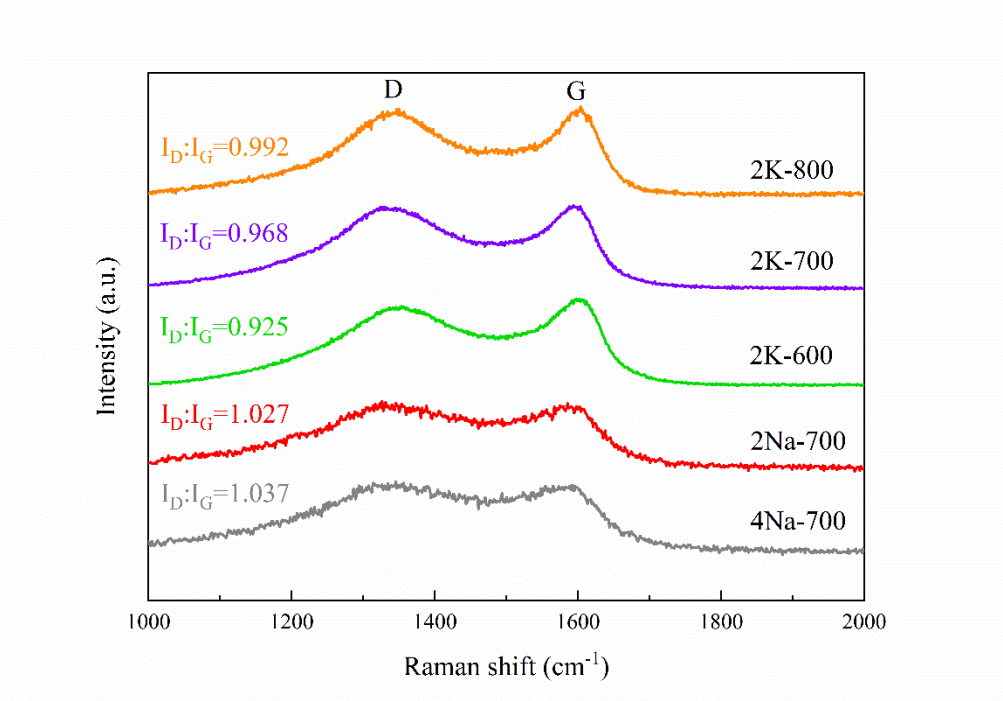

Figure S3. Raman spectra of porous carbons

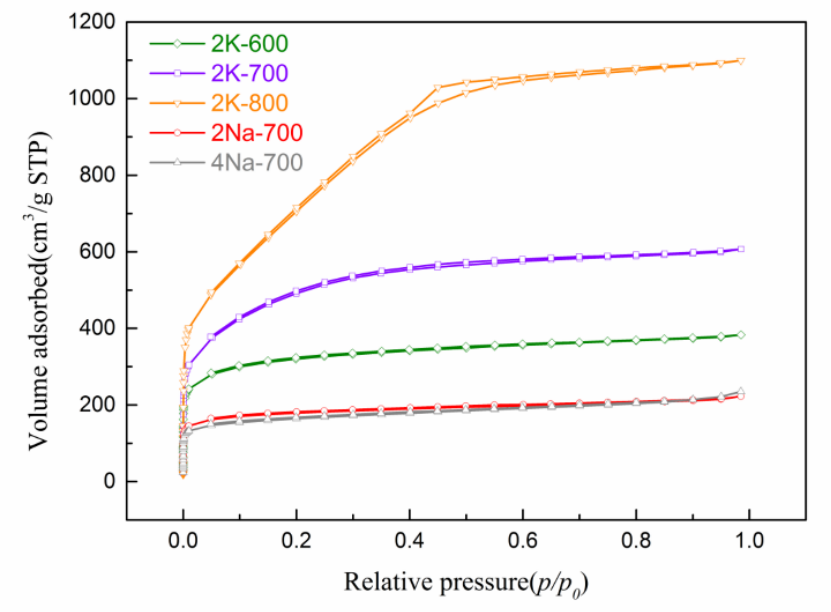

Figure S4. Nitrogen sorption isotherms of the porous carbons.

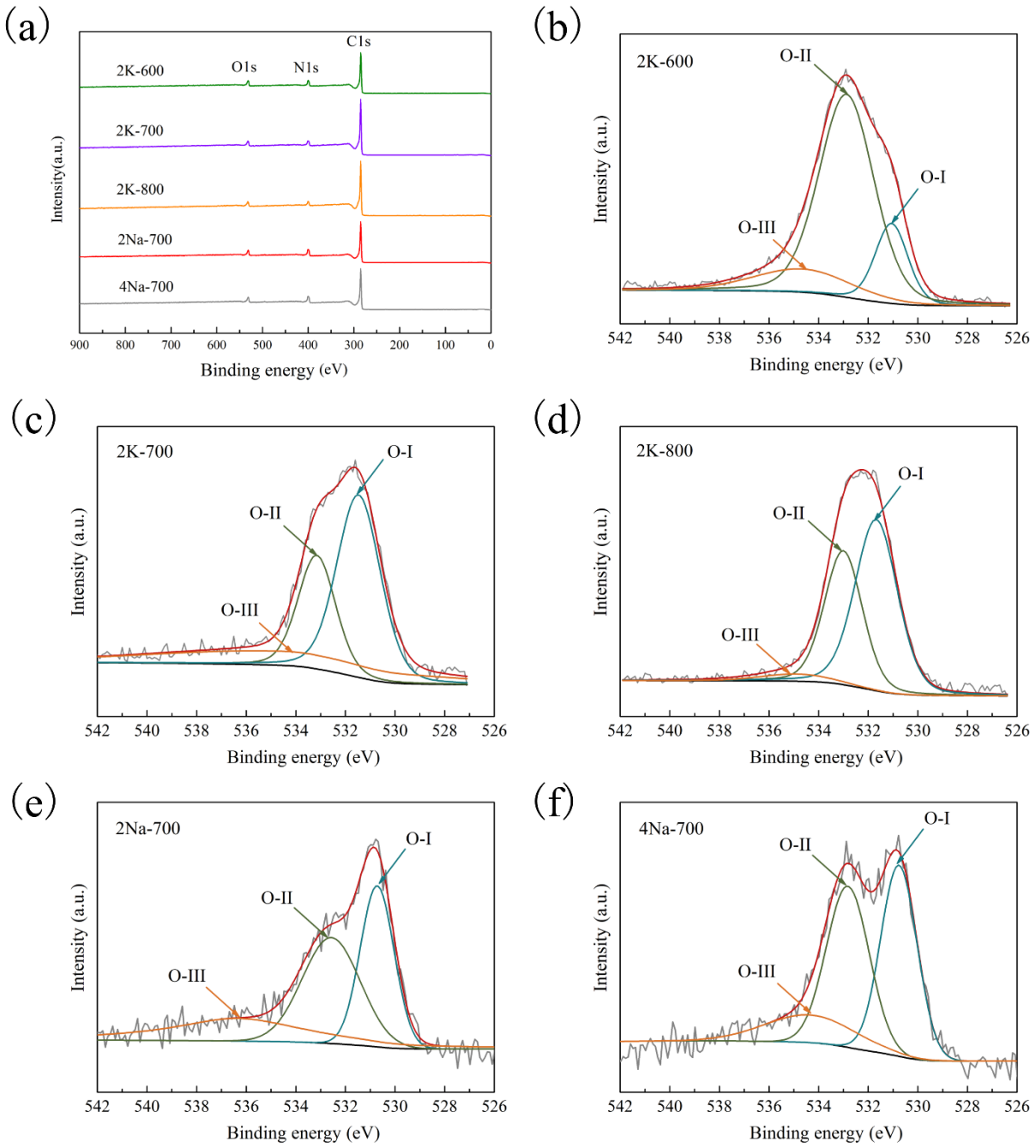

Figure S5 XPS spectra (a) and deconvolution of the high-resolution O1s spectra(b–f) of the porous carbons

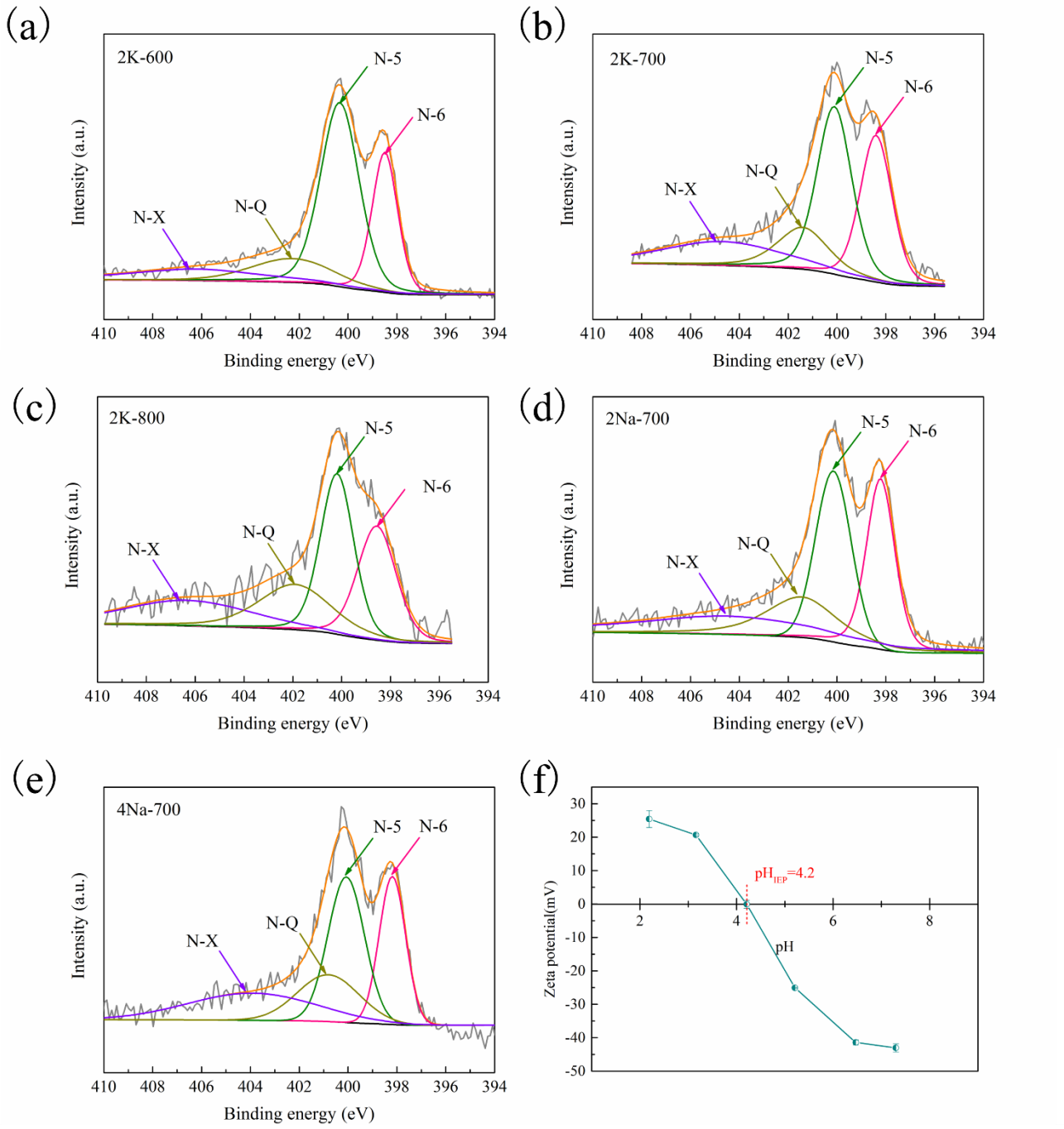

Figure S6 Deconvolution of the high-resolution N1s spectra(a-e) and Effect of pH on zeta-potential of 2K-700 (f)

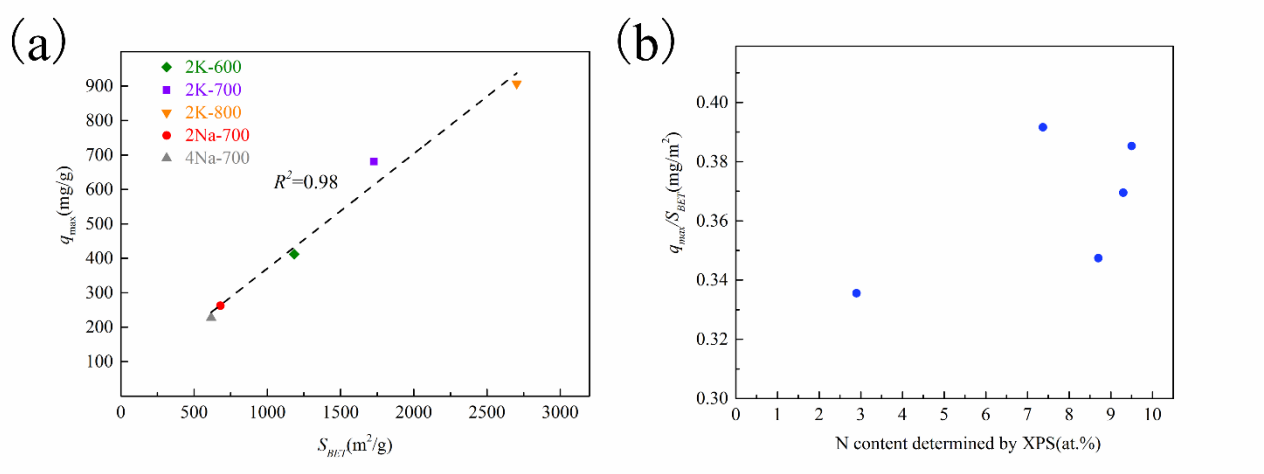

Figure S7 Effects of S_{BET} on the adsorption of SMX (a) Effect of nitrogen content on relative adsorption amount (b)

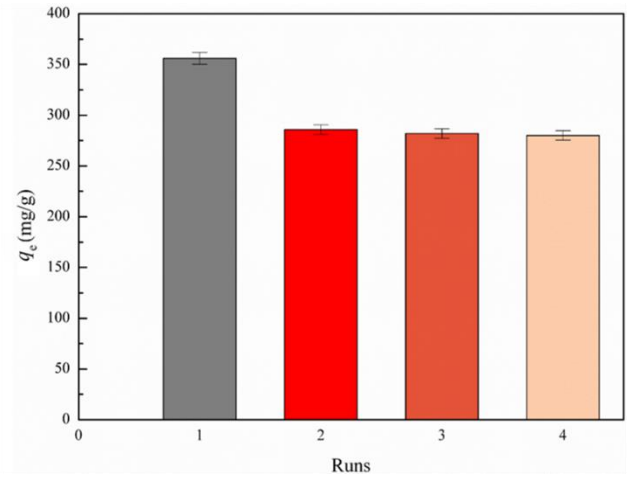

Figure S8 Recyclability of 2K-700 for adsorption of SMX from water.

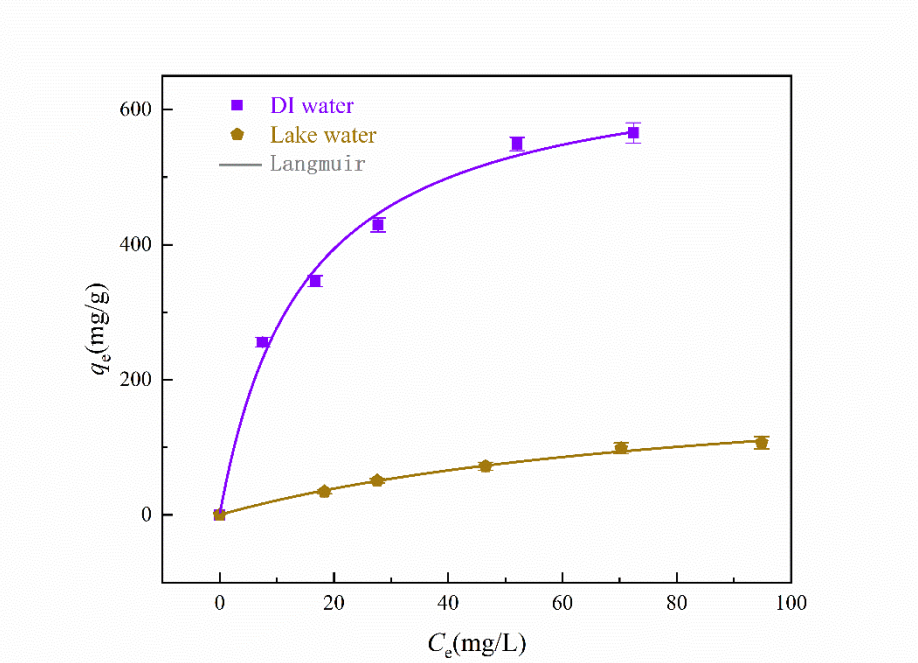

Figure S9. Effect of properties of the water matrices on adsorption of SMX by 2K-700.

Table S1 Pseudo-first-order and Pseudo-second-order models for SMX adsorption on 2K-700

Solution concentration (mg/L)	Exp.q_e (mg/g)	Pseudo-first-order model			Pseudo-second-order model			
		Cal. q_e (mg/g)	k_1 (10^{-1}min^{-1})	R^2	Cal. q_e (mg/g)	k_2 (10^{-3}g/(mg·min))	R^2	h (mg/(g·min))
20	281.7	270.9	2.668	0.786	285.0	1.500	0.930	121.88
50	439.3	423.1	2.927	0.778	442.2	1.130	0.922	221.00
100	594.3	577.3	3.283	0.862	603.8	0.901	0.971	328.29

Table S2 the Intra-particle diffusion constants for SMX adsorption on 2K-700

Solution concentration (mg/L)	Intra-particle-diffusion model					
	k_1 (mg·g^{-1}min$^{-0.5}$)	C_1 (mg/g)	R_1^2	k_2 (mg·g^{-1}min$^{-0.5}$)	C_2 (mg/g)	R_2^2
20	29.827	105.3	0.961	3.386	247.6	0.578
50	50.708	164.6	0.977	0.651	433.3	0.210
100	68.585	234.5	0.917	1.316	584.7	0.878

Table S3 Properties of the water matrices employed in this work [a]

	pH	TOC (mg/L)	UV254 (AU/cm)	Conductivity(mS/cm)
Lake water	8.60	8.25	0.1716	2.32

[a] Data reported in a just accepted work of the authors' research group (Chem. Eng. J, 2020, DOI: 10.1016/j.cej.2019.124009)

Table S4 The fitting parameters of Langmuir isotherm models

Sample	q_{max}(mg·g^{-1})	K_L (L·mg^{-1})	R^2
DI	681.24	6.84×10^{-2}	0.992
Lake water	213.58	1.11×10^{-2}	0.995

Table S5 SMX adsorption capacity in comparison to previous reports

Adsorbents	S_{BET}(m^2/g)	q_{max}(mg/g)	References
MOF-5-derived carbon calcined at 1000 ℃	1731	625	[1]
Sulfonic acid functionalized biochar	-	425	[2]
Sulfonated coffee waste	-	406	[3]
Single-layer graphene oxide	>2000	240	[4]
ZIF-8-derived carbon calcined at 1000 ℃	1855	435	[5]
Fe_2O_3/CeO_2 loaded activated carbon	1536	60	[6]
Wood-based activated carbon	1541	329	[7]
Activated carbon with a membrane bioreactor	>1000	282	[8]
Organo-Vermiculites	7.6	74	[9]
Organo-montmorillonites	23.9	243	[10]
MIL-101(Cr)@GO	3352	101	[11]
MIL-101(Cr)	2338	182	[12]
Ag-FMWCNTs	-	119	[13]
Peanut shells	2	27	[14]
2K-700	1728	681	This work
2K-800	2703	907	This work

References

[1] X. Li, H. Yuan, X. Quan, S. Chen and S. You, J. Environ. Sci. (China), 2018, 63, 250-259.

[2] M. A. Ahsan, M. T. Islam, C. Hernandez, H. Kim, Y. Lin, M. L. Curry, J. Gardea-Torresdey and J. C. Noveron, J. Environ. Chem. Eng., 2018, 6, 4215-4225.

[3] M. A. Ahsan, M. T. Islam, M. A. Imam, A. H. M. G. Hyder, V. Jabbari, N. Dominguez and J. C. Noveron, J. Environ. Chem. Eng., 2018, 6, 6602-6611.

[4] H. Chen, B. Gao and H. Li, J. Hazard. Mater., 2015, 282, 201-207.

[5] I. Ahmed, B. N. Bhadra, H. J. Lee and S. H. Jhung, Cataly. Today, 2018, 301, 90-97.

[6] J. Akhtar, N. S. Amin and A. Aris, Chem. Eng. J., 2011, 170, 136-144.

[7] C. B. Vidal, M. Seredych, E. Rodriguez-Castellon, R. F. Nascimento and T. J. Bandosz, J. Colloid. Inter. Sci., 2015, 449, 180-191.

[8] X. Li, F. I. Hai and L. D. Nghiem, Bioresource. Technol., 2011, 102, 5319-5324.

[9] S. Guo, M. Gao, T. Shen, Y. Xiang and G. Cao, Micropor. Mesoporous Mat., 2019, 286, 36-44.

[10] L. Lu, M. Gao, Z. Gu, S. Yang and Y. Liu, J. Environ. Sci., 2014, 26, 2535-2545.

[11] X. Jia, S. Li, Y. Wang, T. Wang and X. Hou, J. Chem. Eng. Data, 2019, 64, 1265-1274.

[12] X. Huang, Q. Hu, L. Gao, Q. Hao, P. Wang and D. Qin, RSC Adv., 2018, 8, 27623-27630.

[13] Q. Song, H. Wang, B. Yang, F. Wang and X. Sun, RSC Adv., 2016, 6, 75855-75861.

[14] R. Li, Y. Zhang, W. Chu, Z. Chen and J. Wang, RSC Adv., 2018, 8, 13546-13555.