Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Supporting Information

Preparation of magnetic covalent triazine frameworks by ball milling for efficient removal of PFOS and PFOA substitutes from water

Wei Wang[a,b], Haipei Shao[a], Chang Sun[b], Xiangzhe Jiang[a], Shuangxi Zhou[b], Gang Yu [a], Shubo Deng [a,*]

[a] School of Environment, Beijing Key Laboratory for Emerging Organic Contaminants Control, State Key Joint Laboratory of Environment Simulation and Pollution Control (SKLESPC), Tsinghua University, Beijing 100084, China

[b] State Key Laboratory of Plateau Ecology and Agriculture, Qinghai University, Xi'ning, Qinghai Province 810016, China

[*] Corresponding author, Tel.: +86-10-62792165. Fax: +86-10-62794006.

E-mail: dengshubo@tsinghua.edu.cn (S. Deng)

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Table S1 Primary physiochemical properties of OBS and HFPO-TA

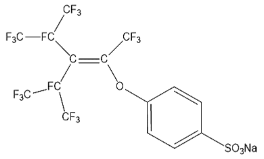
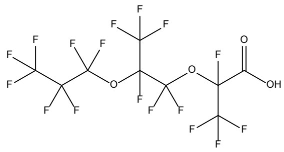
Emerging PFAS	CAS No.	Structural formula	Molecular weight	Log K_{ow}
OBS	87-56-8		626	4.48 (Chen et al., 2020)
HFPO-TA	13252-14-7		496.1	5.55 (Pan et al., 2017)

Table S2 Parameters of the pseudo-first-order and pseudo-second-order equations for fitting OBS and HFPO-TA adsorption kinetics

Emerging PFAS	Pseudo-first-order parameter [a]			Pseudo-second-order parameter [b]		
	q_e (mmol/g)	k_1 (h^{-1})	R^2	q_e (mmol/g)	v_0 (mmol/g/h)	R^2
OBS	0.91	12.48	0.943	0.96	7.61	0.988
HFPO-TA	0.74	49.13	0.991	0.75	44.42	0.998

[a] Pseudo-first-order model: $q_t = q_e\left(1 - e^{\frac{-k_1 t}{2.303}}\right)$

[b] Pseudo-second-order model: $t/q_t = 1/(k_2 q_e^2) + t/q_e = 1/v_0 + t/q_e$

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Table S3 Parameters of the intra-particle diffusion model for fitting OBS and HFPO-TA adsorption

Emerging PFAS	Intra-particle diffusion parameter		
	k_d ($mmol/g/h^{1/2}$)	c (mmol/g)	R^2
OBS	0.786	0.125	0.904
HFPO-TA	1.014	0.153	0.754

Intraparticle diffusion model: $q_t = k_d t^{1/2} + c$, where k_d ($mmol/g/h^{1/2}$) is the diffusion rate constant and c (mmol/g) is the coefficient of boundary layer thickness

Table S4 Parameters of the Langmuir and Freundlich models for fitting OBS and HFPO-TA adsorption isotherms

Emerging PFAS	Langmuir parameters [a]			Freundlich parameters [b]		
	q_m (mmol/g)	b (L/mmol)	R^2	K_f ($mmol^{1-1/n} L^{1/n}/g$)	n	R^2
OBS	1.18	145.68	0.605	1.22	9.66	0.942
HFPO-TA	1.02	16.80	0.779	0.97	5.20	0.967

[a] Langmuir model: $q_e = q_m C_e / (1/b + C_e)$

[b] Freundlich model: $q_e = K_f C_e^{1/n}$

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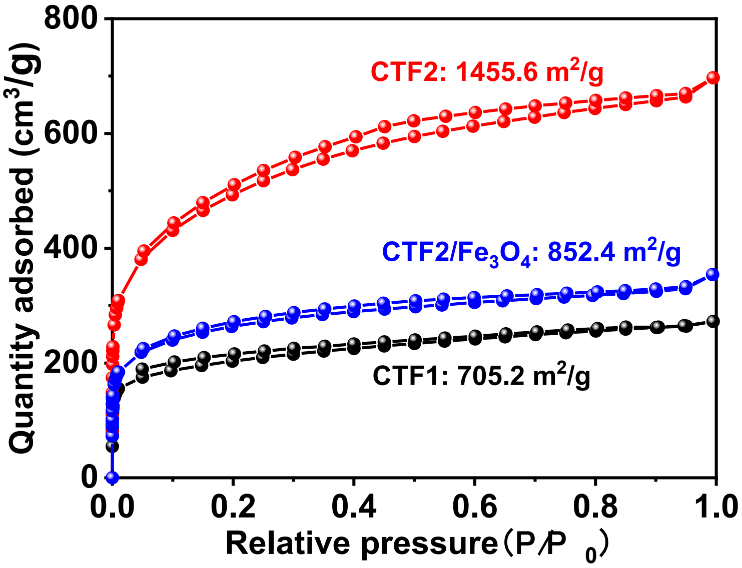

Fig. S1 Nitrogen adsorption isotherm curves on CTF1, CTF2, and CTF2/Fe_3O_4 at CTF/Fe_3O_4 ratio of 6:1.

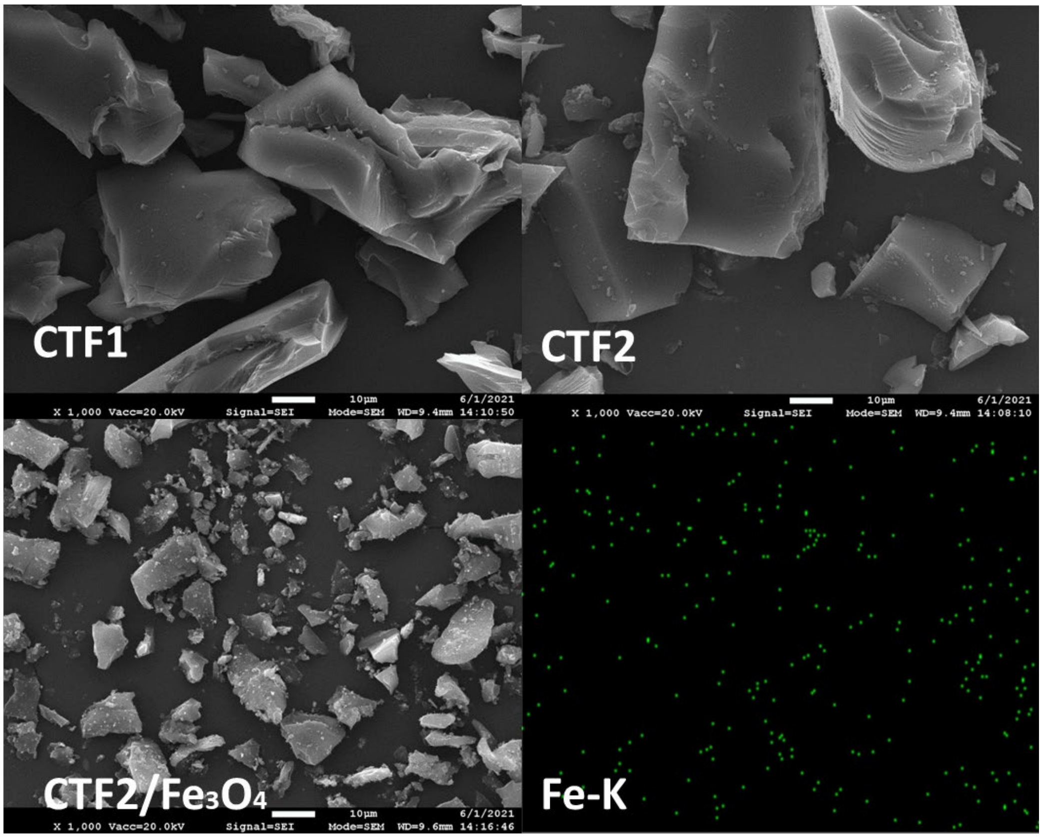

Fig. S2 SEM images of CTF1, CTF2 and CTF2/Fe_3O_4 as well as the SEM-EDS analysis on Fe element (bright green color) of CTF2/Fe_3O_4.

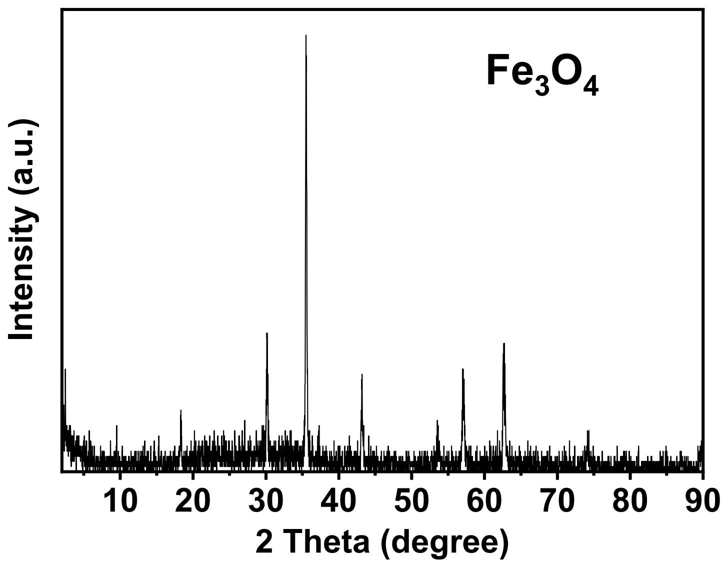

Fig. S3 XRD pattern of Fe_3O_4.

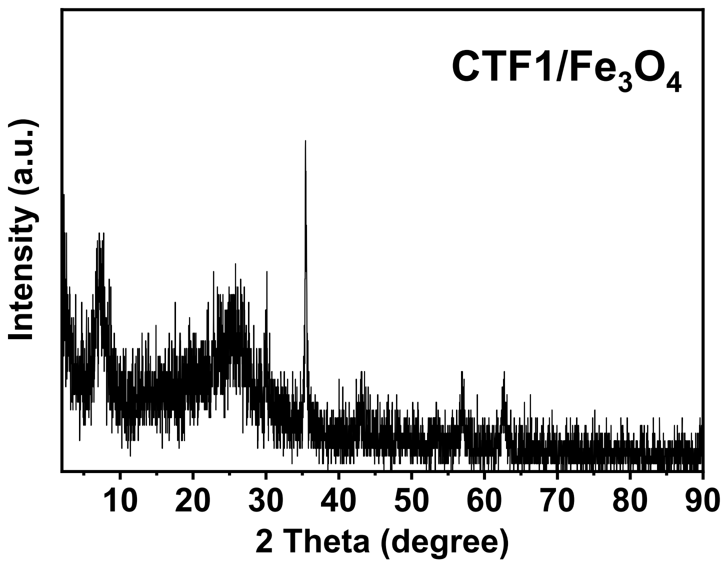

Fig. S4 XRD pattern of CTF1/Fe_3O_4 at ratio of 6:1.

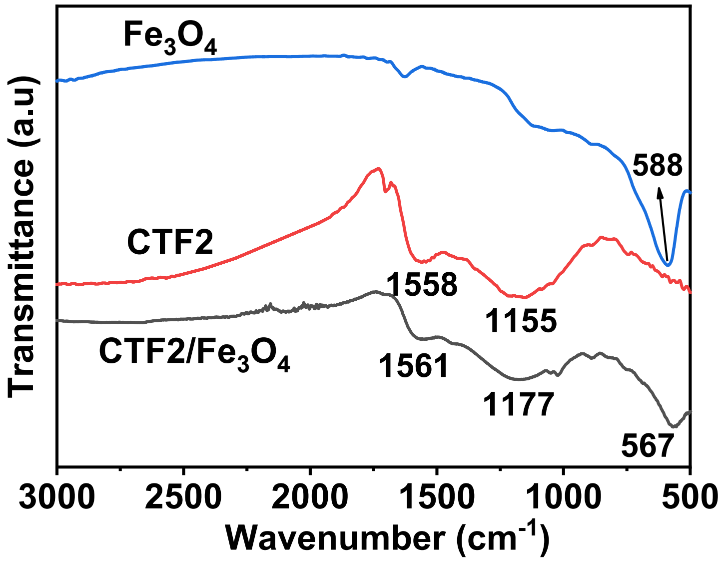

Fig. S5 FTIR spectra of Fe_3O_4, CTF2 and CTF2/Fe_3O_4.

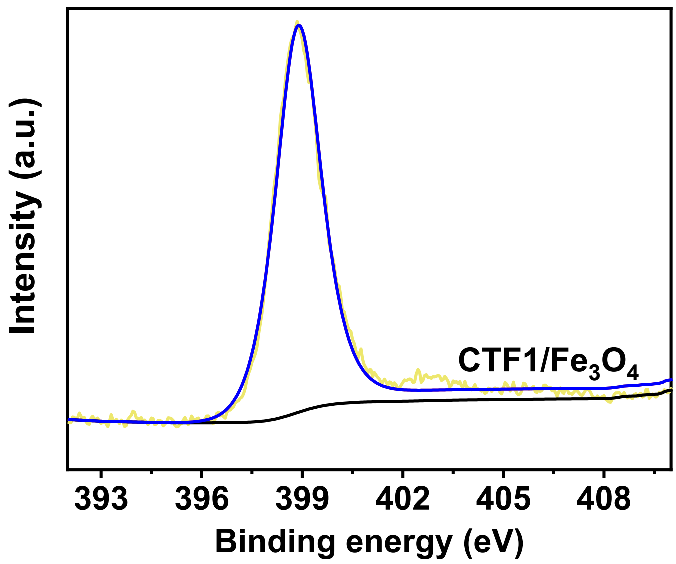

Fig. S6 N1s spectrum of CTF1/Fe_3O_4 at CTF/Fe_3O_4 ratio of 6:1.

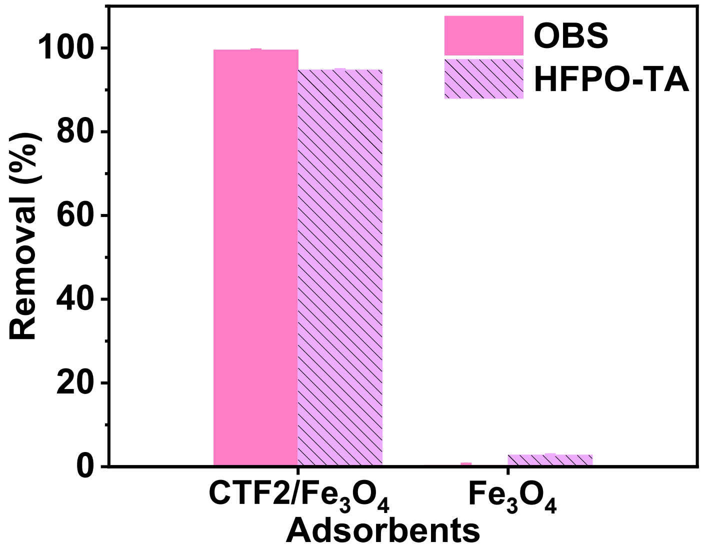

Fig. S7 OBS and HFPO-TA removal byFe_3O_4 and CTF2/ Fe_3O_4.

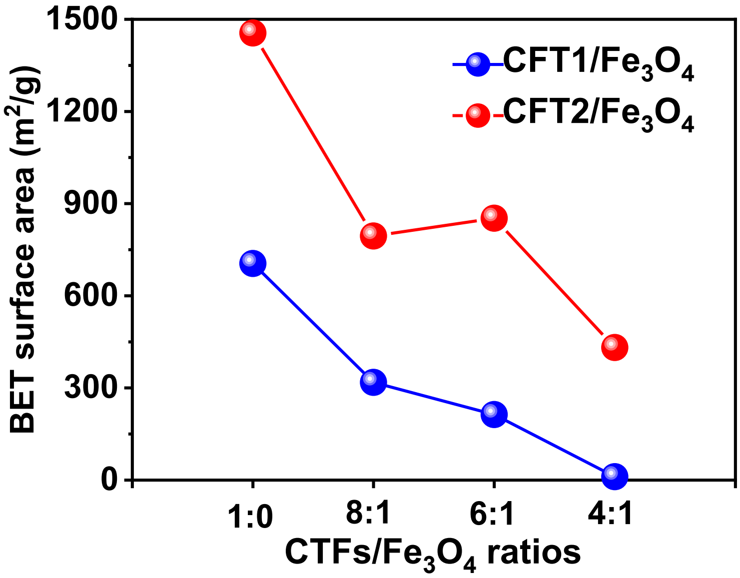

Fig. S8 BET surface area of CTFs and CTFs/ Fe_3O_4 composites with different mass ratios.

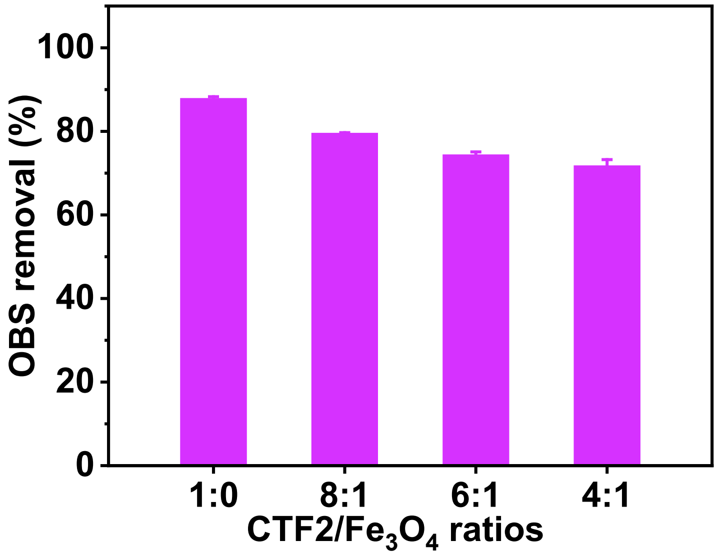

Fig. S9 Effects of CTF/Fe_3O_4 ratios on OBS adsorption at adsorbent dosage of 0.125g/L.

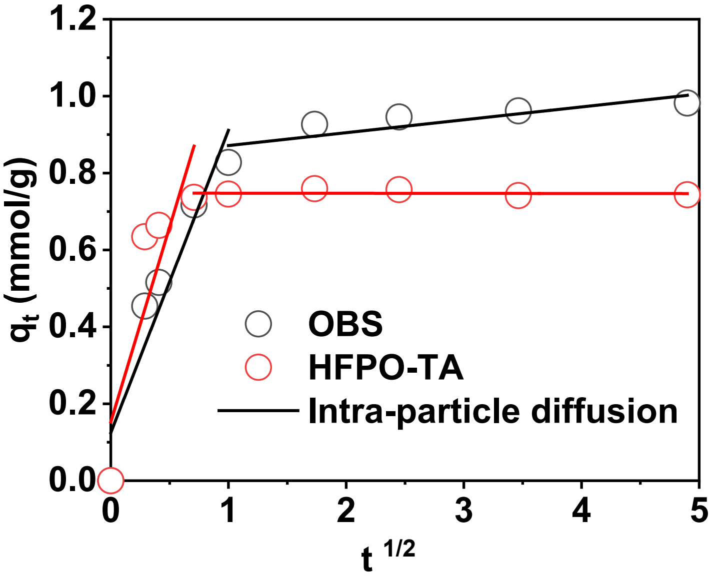

Fig. S10 Intra-particle diffusion model for fitting OBS and HFPO-TA sorption kinetics.

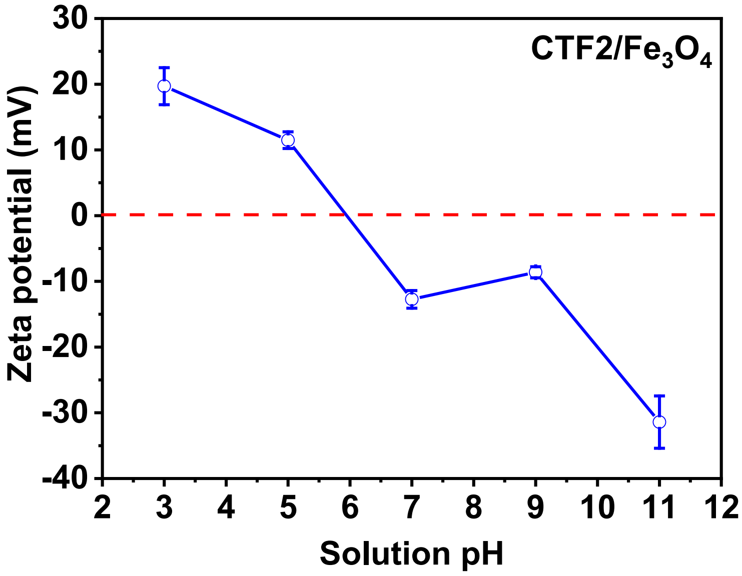

Fig. S11 zeta potentials of $CTF2/Fe_3O_4$ at different solution pH.

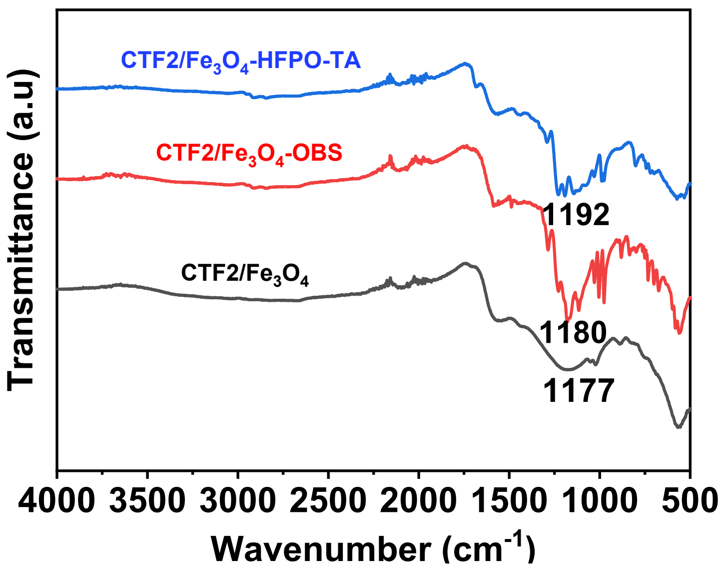

Fig. S12 FTIR spectra of $CTF2/Fe_3O_4$ before and after OBS and HFPO-TA adsorption.

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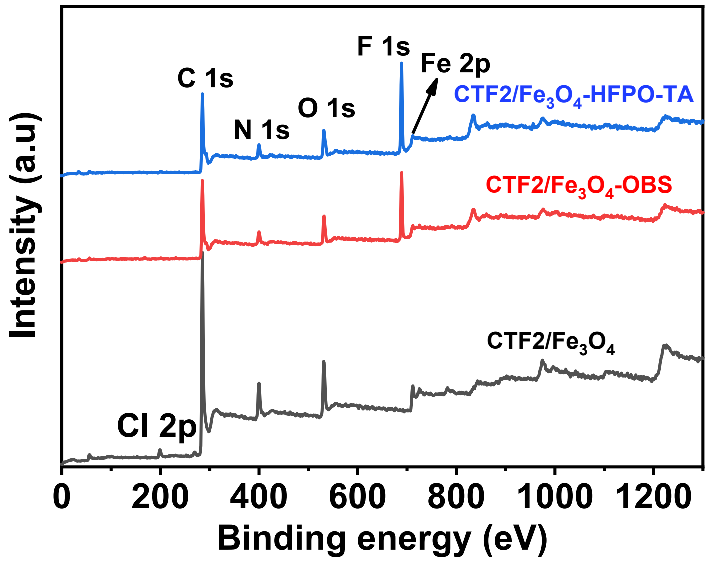

Fig. S13 XPS wide scan spectra of CTF2/Fe_3O_4 before and after OBS and HFPO-TA adsorption.

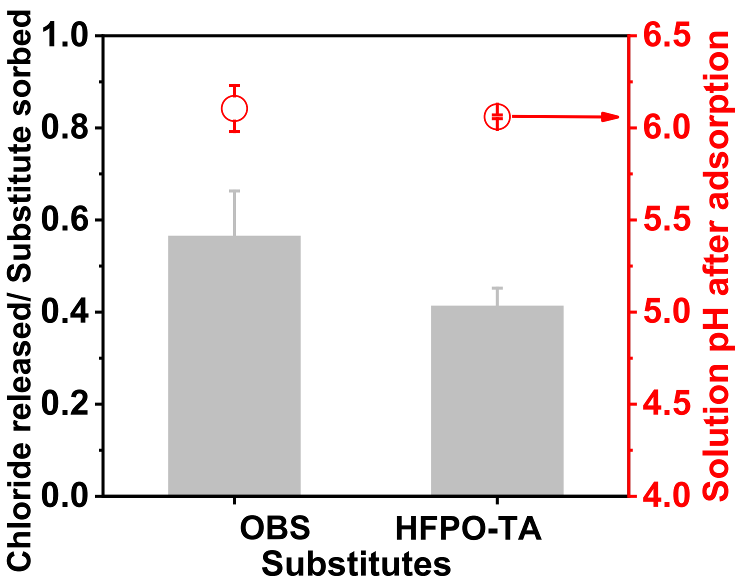

Fig. S14 Ratios of chloride desorbed to substitutes adsorbed as well as solution pH after adsorption with 0.015 g of CTF2/Fe_3O_4 in 40 mL of 1.2 mmol/L PFAS solution at pH 5.

(The contribution of OH^- was calculated according to the formula

$CB_{OH^-} = C_{OH^-}/(C_{OH^-} + C_{Cl^-}) \times 100\%$, where CB_{OH^-} is contribution of OH^- in the ion exchange process, C_{OH^-} and C_{Cl^-} is the released amount after PFAS adsorption.)

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References

Chen, H., Munoz, G., Duy, S. V., Zhang, L., Yao, Y., Zhao, Z., Yi, L., Liu, M., Sun, H., Liu, J., Sauvé, S., 2020. Occurrence and distribution of per- and polyfluoroalkyl substances in Tianjin, China: The contribution of emerging and unknown analogues. Environ. Sci. Technol. 54 (22), 14254-14264.

Pan, Y., Zhang, H., Cui, Q., Sheng, N., Yeung, L. W. Y., Guo, Y., Sun, Y., Dai, J., 2017. First report on the occurrence and bioaccumulation of hexafluoropropylene oxide trimer acid: An emerging concern. Environ. Sci. Technol. 51(17), 9553-9560.