

Supporting Information

Insight into the mechanism of persulfate activation by hollow MOFs-derived carbon: Electron transfer triggered non-radical oxidization for antibiotic removal

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1. For the effect of inorganic anions, NaCl, NaH₂PO₄, NaHCO₃, Na₂CO₃, Na₂SO₄ with the concentration of 5 mM were added in to TC solution (30 mg/L, 50 mL). After the TC adsorption of 15 min with catalysts (10 mg), 15 mg PDS were added. The concentration of TC at different intervals (5/10/15/30/45 min) were detected by High Performance Liquid Chromatography (HPLC) at 357 nm employing formic acid (0.1%) and acetonitrile as mobile phases.
2. For the effect of pH, the initial pH (2/4/6/8/10/12) was adjusted using 0.1 M HCl or NaOH. After the TC adsorption of 15 min with catalysts (10 mg), 15 mg PDS were added. The concentration of TC at different intervals (5/10/15/30/45 min) were detected by HPLC at 357 nm.
3. For the effect of temperature, the reactive system (30 mg/L, 50 mL TC) was fixed at different temperatures (298/308/318 K). After the TC adsorption of 15 min with catalysts (10 mg), 15 mg PDS were added, and the concentration of TC at different intervals (5/10/15/30/45 min) were detected by HPLC at 357 nm.
4. In the quenching experiment, after the TC adsorption of 15 min with catalysts (10 mg), MeOH (100 mM), TBA (100 mM), FFA (8 mM), BQ (8 mM), and KI (8 mM) were added into TC solution firstly, then adding 15 mg PDS and catalyst. The concentration of TC at different intervals (5/10/15/30/45/60 min) were detected by HPLC at 357 nm.
5. For the regeneration of catalyst, the used catalyst was carbonized at 800 °C for 1 h in N₂ flow with a heating rate of 5 °C/min until it cooled naturally. The carbonized catalysts were collected for reuse.
6. Probe experiments employed nitro-blue tetrazolium (NBT) for O₂^{•-} and 1,3-Diphenylisobenzofuran (DPBF) for ¹O₂. After the TC adsorption of 15 min with catalysts (10 mg), 15 mg PDS were added. The concentration of NBT and DPBF at different intervals (2/5/7/10 min) were detected by UV spectrophotometer at 352 nm and 411 nm, respectively.
7. Galvanic oxidation processes (GOP) were conducted with PDS and TC separately present in two half cells (50 mL) connected by salt bridge (KCl/agar). HZC-800 was coated on graphite electrode in the GOP.

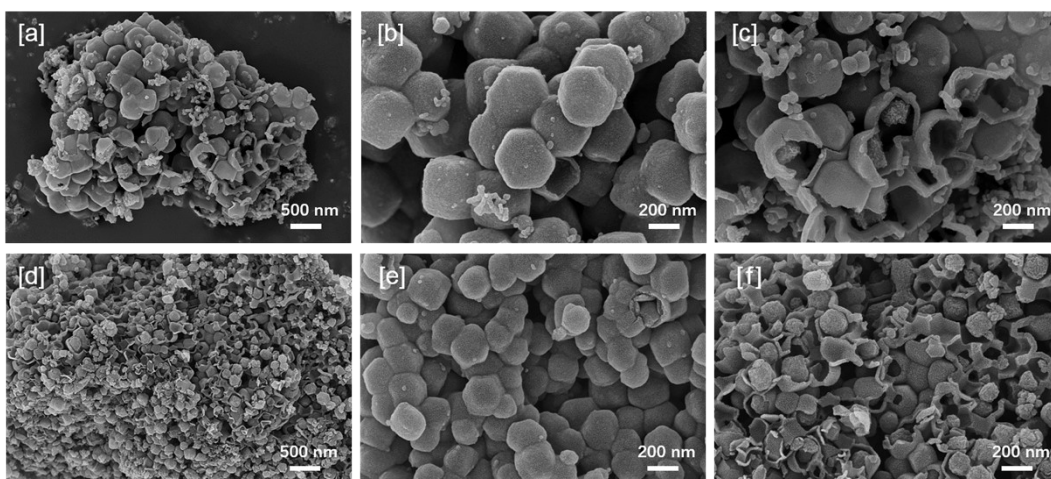


Fig. S1 SEM of HZC-700 (a-c) and HZC-900 (d-f).

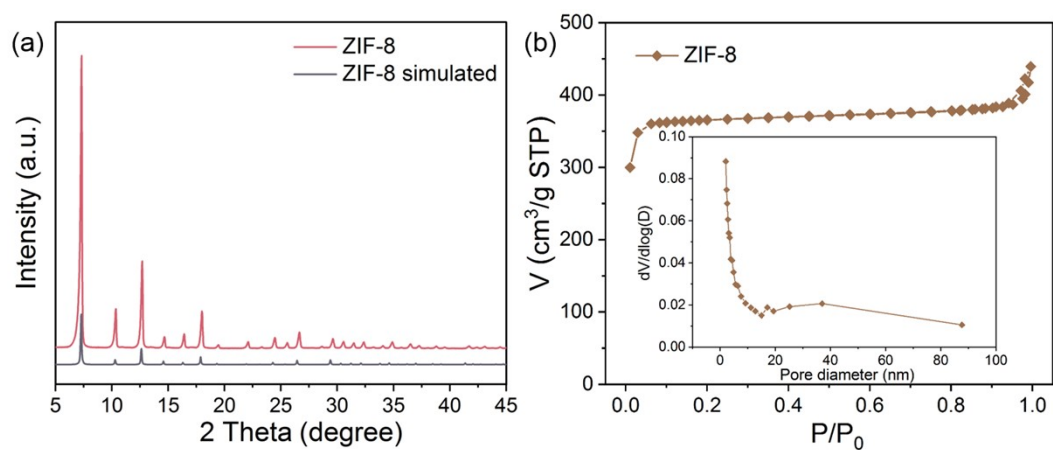


Fig. S2 XRD of ZIF-8 and simulated ZIF-8 (a), and N_2 adsorption-desorption curves and pore diameter distribution of ZIF-8 (b).

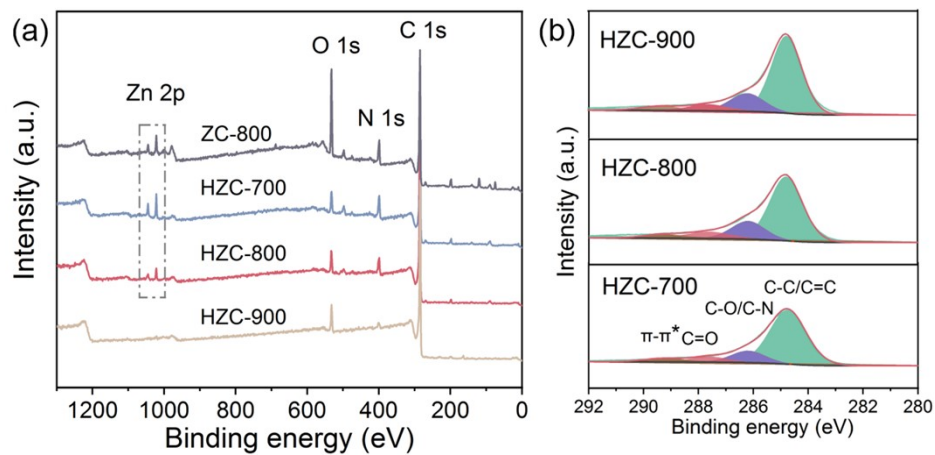


Fig. S3 XPS survey of HZC and ZC-800 (a), and C 1s of HZC (b).

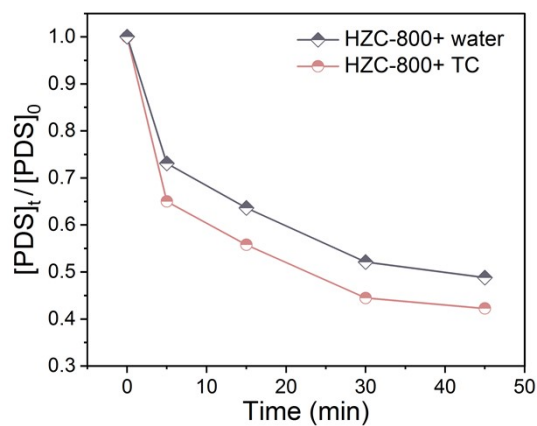


Fig. S4 PDS consumption in HZC-800/PDS/TC and HZC-800/PDS/water systems.

Condition: $C_0 = 30$ mg/L, $V = 50$ mL, catalyst = 0.2 g/L, PDS = 0.3 g/L, pH = 4.3, T =

298 K.

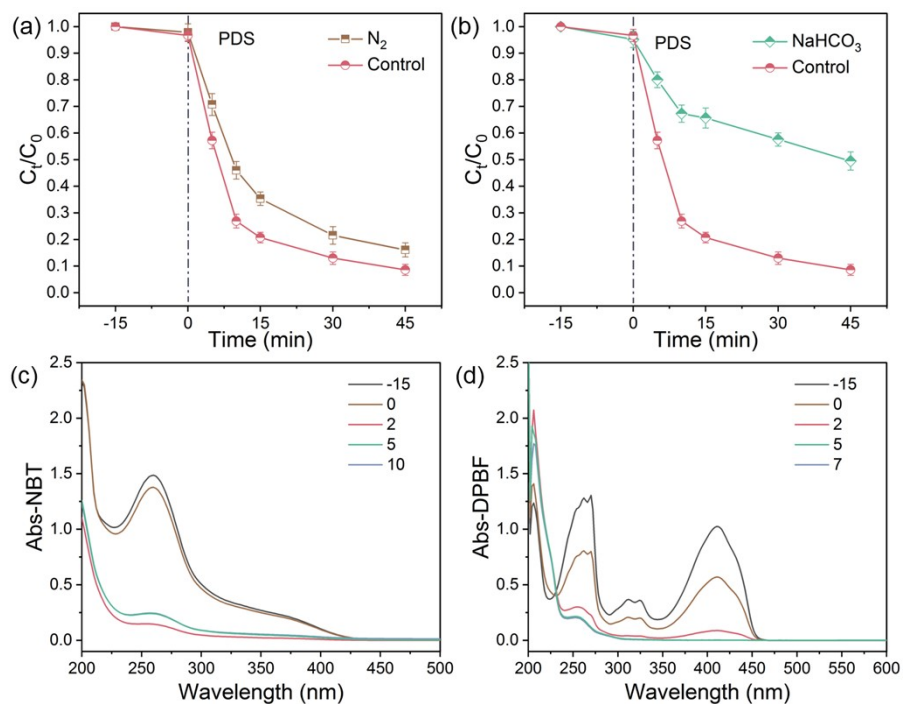


Fig. S5 Oxygen-limited experiment in N_2 (a) and the effect of $NaHCO_3$ on TC removal (b) in the ZC-800/PDS system; Condition: Catalyst= 0.2 g/L, C_{TC} = 30 mg/L, V =50 mL, PDS= 0.3 g/L, pH= 4.3, T =298 K; Probe experiments employing nitro-blue tetrazolium (NBT) for $O_2^{\cdot-}$ (c) and 1,3-Diphenylisobenzofuran (DPBF) for 1O_2 (d) in the ZC-800/PDS system. Condition: Catalyst= 0.2 g/L, C_{NBT} = 25 μ M, C_{DPBF} = 50 μ M, V =50 mL, PDS= 0.3 g/L, T =298 K.

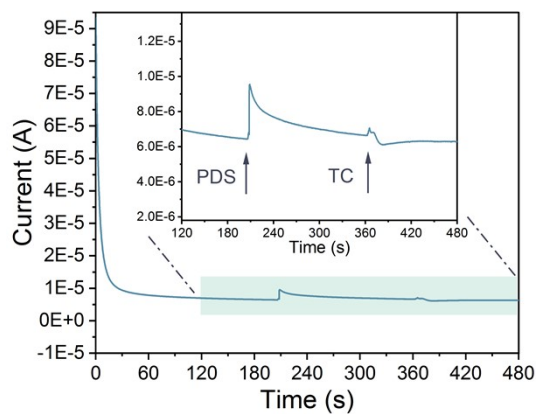


Fig. S6 Chronoamperometry of ZC-800 system.

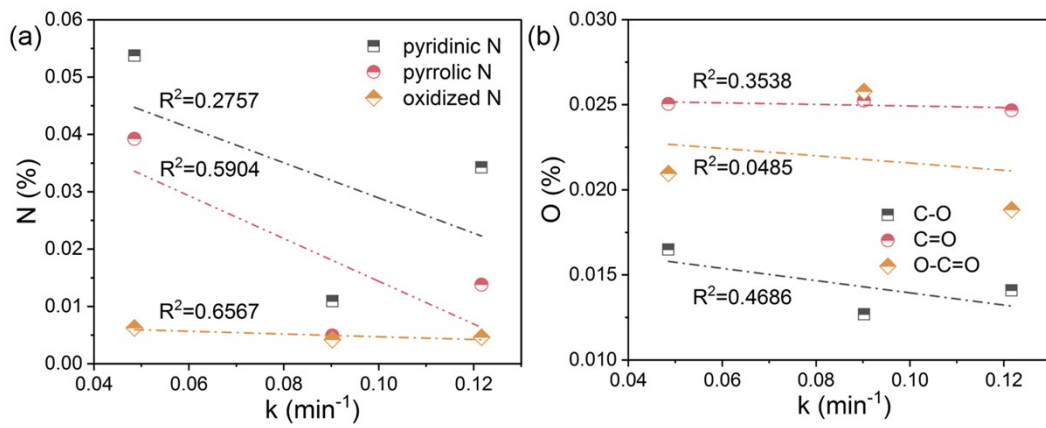


Fig. S7 The correlation analysis of N configuration (a) and O configuration (b) with kinetic constants.

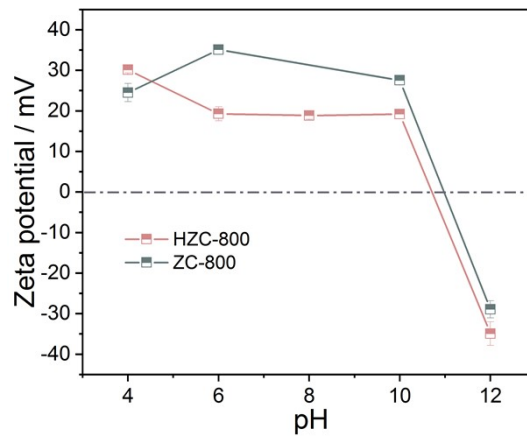


Fig. S8 Zeta potential of HZC-800 and ZC-800.

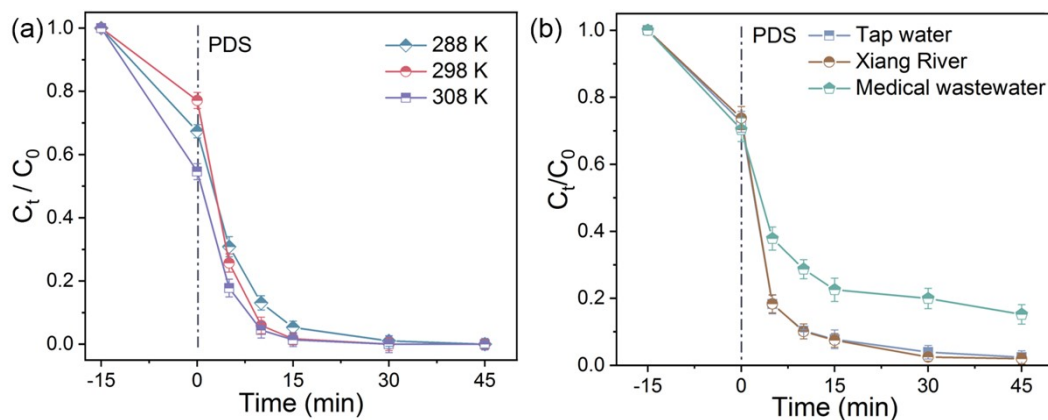


Fig. S9 Removal efficiency of different temperatures (a) and water matrixes (b).

Condition: $C_0=30$ mg/L, $V=50$ mL, catalyst= 0.2 g/L, PDS= 0.3 g/L.

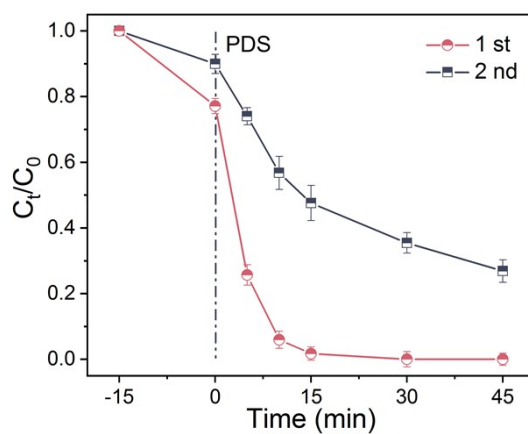


Fig. S10 Removal efficiency of HZC-800 without recovery. Condition: $C_0=30$ mg/L,

$V=50$ mL, catalyst= 0.2 g/L, PDS= 0.3 g/L, $T=298$ K.

Table S1 Detailed information about the involved formulas: removal rate and kinetics

Model	Equation	Parameter
Removal percentage	$R = (C_0 - C_t) / C_0$	C_0 (mg L ⁻¹): initial TC concentration; C_t (mg L ⁻¹): residual TC
Pseudo-first order kinetic	$\ln(C_0/C_t) = kt$	concentration at t (min); k (min ⁻¹) : the rate constants.

Table S2 The element content of HZC-X (700/800/900), ZC-800, used ZC-800, and ZIF-8 form XPS.

Sample	C /%	N /%	O /%	Zn /%
HZC-700	81.46	10.62	6.25	1.68
HZC-800	86.18	7.28	5.76	0.79
HZC-900	90.29	3.19	6.37	0.15
ZC-800	69.24	9.9	19.60	1.26
used ZC-800	69.49	10.94	18.52	1.05
used HZC-800	83.01	5.49	10.84	0.66
carbonized used HZC-800	87.47	4.97	6.72	0.85
ZIF-8	64.62	19.83	6.61	8.94

Table S3 The relative content and actual content of N configurations form N 1s.

Sample	pyridine N %		pyrrole N %		graphite N %		Oxidized N %	
	C _R	C _A	C _R	C _A	C _R	C _A	C _R	C _A
HZC-700	50.60	5.37	36.92	3.92	6.57	0.70	5.90	0.63
HZC-800	47.0	3.42	18.95	1.38	27.66	2.01	6.33	0.46
HZC-900	34.23	1.09	15.45	0.49	38.56	1.23	13.21	0.42
ZC-800	55.35	5.47	29.63	2.93	9.00	0.89	6.02	6.02
used HZC-800	43.92	2.41	25.11	1.37	21.65	1.19	9.32	0.51
carbonized used HZC-800	45.65	2.26	18.14	0.90	24.65	1.22	11.56	0.57

C_R: relative content in N; C_A: actual content in the sample;

Table S4 The intermediate products and their molecular structures during degradation.

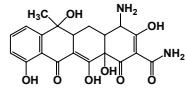
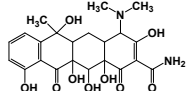
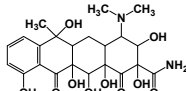
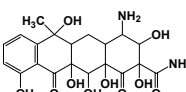
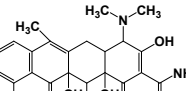
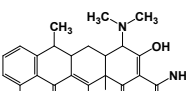
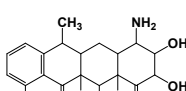
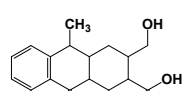
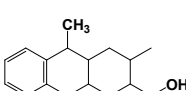
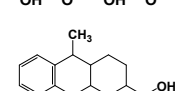
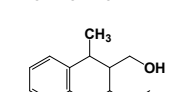
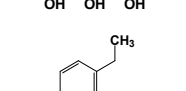
Products	m/z	Molecular formula	Molecular structure
TC	445	C ₂₂ H ₂₄ N ₂ O ₈	
P1	461	C ₂₂ H ₂₆ N ₂ O ₉	
P2	477	C ₂₂ H ₂₈ N ₂ O ₁₀	
P3	453	C ₂₀ H ₂₄ N ₂ O ₁₀	
P4	443	C ₂₂ H ₂₄ N ₂ O ₈	
P5	429	C ₂₂ H ₂₄ N ₂ O ₇	
P6	393	C ₁₉ H ₂₄ NO ₈	
P7	318	C ₁₇ H ₂₀ O ₆	
P8	302	C ₁₇ H ₂₀ O ₅	
P9	274	C ₁₆ H ₂₀ O ₄	
P10	253	C ₁₄ H ₂₀ O ₄	
P11	164	C ₁₀ H ₁₄ O ₂	

Table S5 Quality parameters and removal efficiency in different water matrixes.

Water type	pH	TOC (mg L⁻¹)	Removal efficiency (%)
River water ^a	6.84	23.48	97.62
Medical wastewater ^b	8.54	30.64	87.95
Tap water ^c	7.65	4.44	98.05

^a River water was obtained from Xiang River in Hunan, China.

^b Medical wastewater was obtained from Hunan University Hospital in Changsha, Hunan, China.

^c Tap water was obtained from the laboratory of Hunan University.