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Supporting information

Synthesis of N-doped porous carbon derived from biomass waste for activating peroxymonosulfate in water decontamination: Mechanism insight and biotoxicity assessment

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Materials

All solvents and chemicals were used as purchased, unless otherwise noted. The deionized water was produced in the laboratory. Dealkali lignin, dicyandiamide, were obtained from Shanghai Yien Chemical Technology Co., Ltd. Peroxymonosulfate (PMS) and L-histidine were purchased from Anhui Zesheng Technology Co., Ltd. Sulfamethoxazole (SMX), *t*-butanol (TBA), sulfadiazine and 3-aminophenol were obtained from Shanghai Aladdin Biochemical Co., Ltd. Bisphenol A was purchased from Shanghai Xushuo Biotechnology Co., Ltd. Ciprofloxacin was bought from Tianjin Xiensi Biochemical Technology Co., Ltd. Tetracycline, melamine and urea were obtained from Shanghai Macklin Biochemical Co., Ltd. Trichloromethane ($CHCl_3$), ethanol (EtOH) was purchased from Shanghai Hushi Laboratory Equipment Co., Ltd. Sodium dihydrogen phosphate dihydrate ($NaH_2PO_4 \cdot 2H_2O$, AR, 99%, Sinopharm Chemical Reagent Co., Ltd.), sodium bicarbonate ($NaHCO_3$, AR, 99.8%, Shanghai Macklin Biochemical Co., Ltd.), Ltd.), sodium chloride (NaCl, AR, Sinopharm Chemical Reagent Co., Ltd.), potassium sulfate (K_2SO_4, AR, 99% Shanghai Macklin Biochemical Co., Ltd.), sodium nitrate ($NaNO_3$, AR, 99%, Tianjin Hengxing Chemical Reagent Manufacturing Co.), and humic acid (HA, 70%, Shanghai Aladdin BioChemical Technology Co., Ltd.) were utilized as received.

Instruments

UV-vis spectra were conducted on Metash UV-8000S. Powder X-ray diffraction (PXRD) analyses were carried out on an Germany-Bruke D8 Advance. Fourier-Transform Infrared Spectrometer (FTIR) spectra of the catalysts were performed on a Thermo Nicolet iS5. Raman was recorded on HORIBA-EVA. N_2 adsorption/desorption isotherms of as-obtained materials were carried out on ASAP-2460. The morphologies of the catalysts were observed by scanning transmission electron microscopy (JEOL-JEM 2100 F) and scanning electron microscopy (Sigma 300). Energy Dispersive Spectrometer (EDS) mapping was conducted with a microscope (Oxford 80T) operated at 200 kV. X-ray photoelectron microscopy (XPS) spectra were measured on a Thermo Scientific

ESCALAB 250Xi using a monochromate Al X-ray resource at a C1s 284.8 eV reference. Electron paramagnetic resonance (EPR) spectroscopy was performed on a Germany-Bruke-A300. High resolution mass spectrometry (HRMS) was collected using Aglient 6540 TOF.

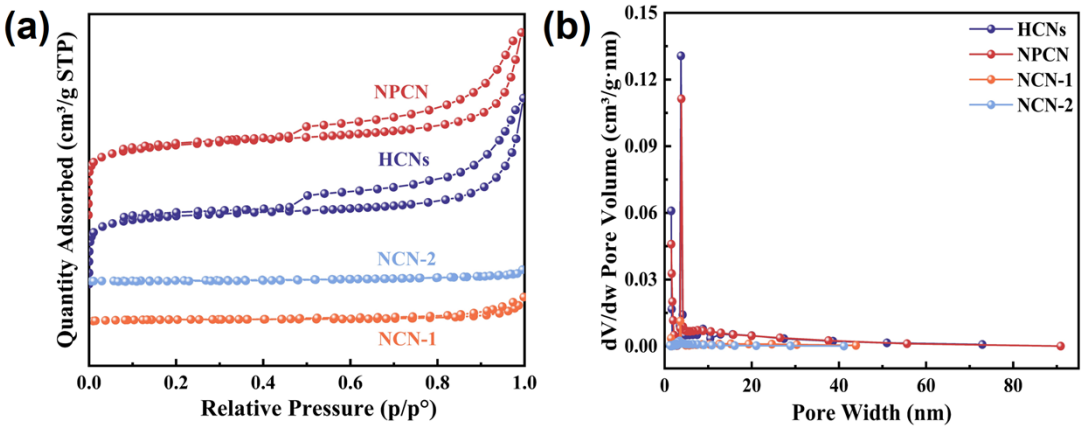


Fig. S1. (a) N_2 adsorption-desorption isotherms and (b) corresponding Barrett-Joyner-Halenda curve of the as-obtained catalysts.

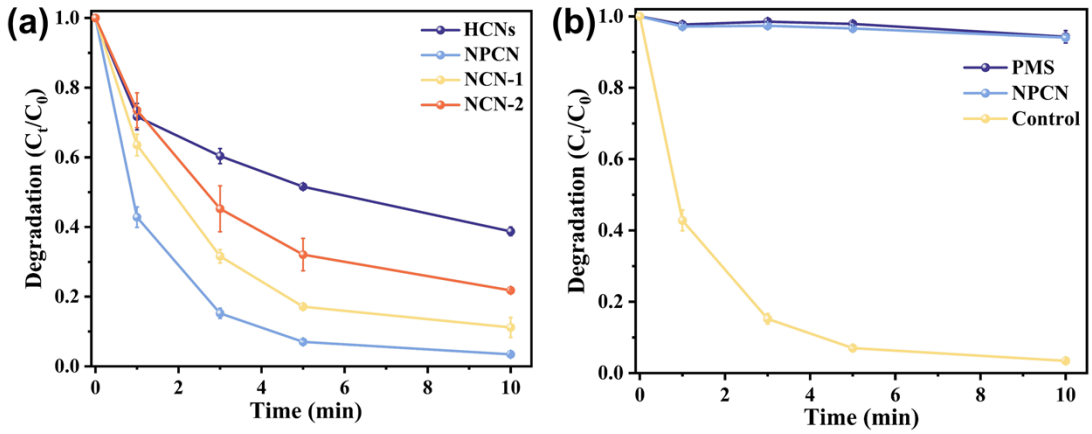
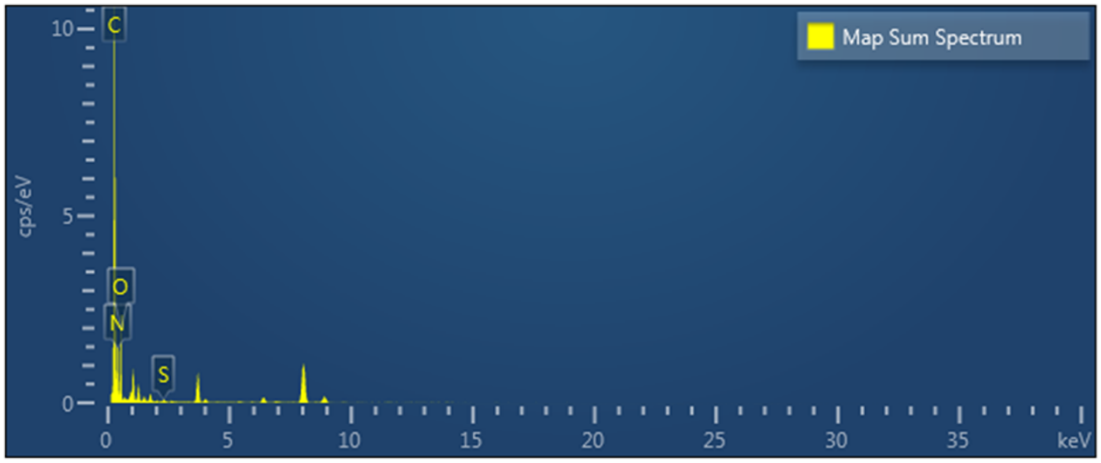


Fig. S2. (a) SMX degradation catalyzed by as-obtained catalysts, (b) SMX absorption effect of NPCN and oxidation effect of PMS alone. Standard conditions: 50 mL SMX (20 mg/L), 25 mg Catalyst, and 25 mg PMS at 30 °C.



Element	Line Type	k factor	Absorption Correction	wt%	wt% Sigma
C	K series	2.50675	1.00	77.52	0.43
N	K series	3.14061	1.00	11.49	0.41
O	K series	1.86867	1.00	10.75	0.23
S	K series	0.95908	1.00	0.23	0.04
Total:				100.00	

Fig. S3. Sum EDS spectrum (up) and corresponding elemental proportions (down) of NPCN.

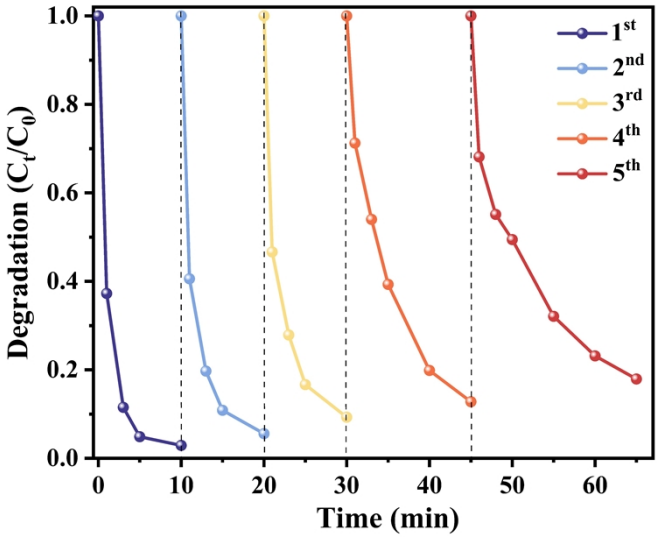


Fig. S4. Recycling test for the NPCN catalyst in SMX degradation.

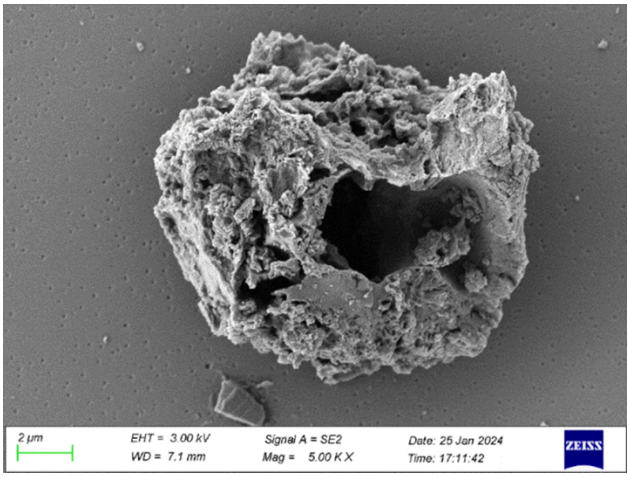


Fig. S5. SEM image of the NPCN after 5 times recycling.

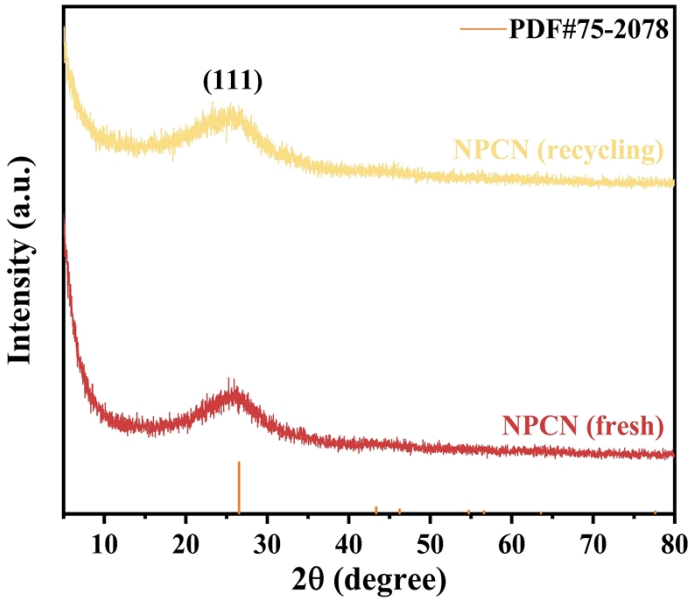


Fig. S6. PXRD of NPCN before and after 5 times recycling.

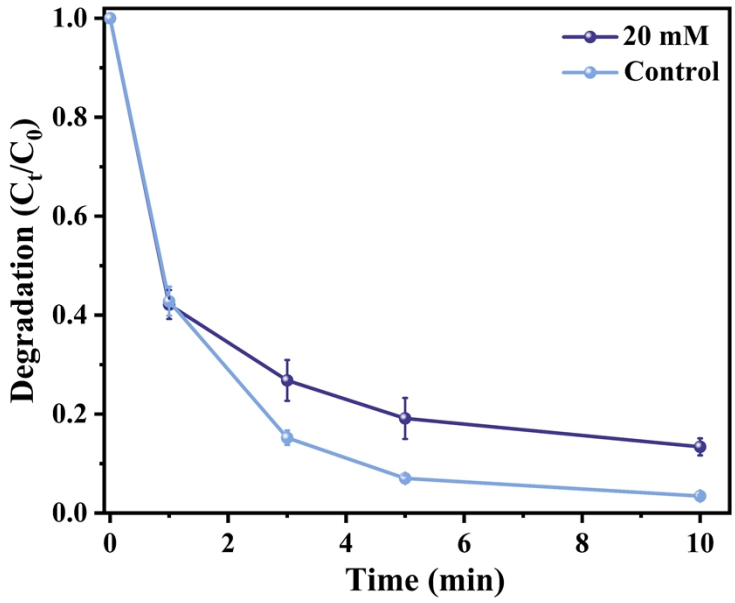


Fig. S7. Electronic quenching experiment in the NPCN/PMS system using $AgNO_3$ as electron scavenger.

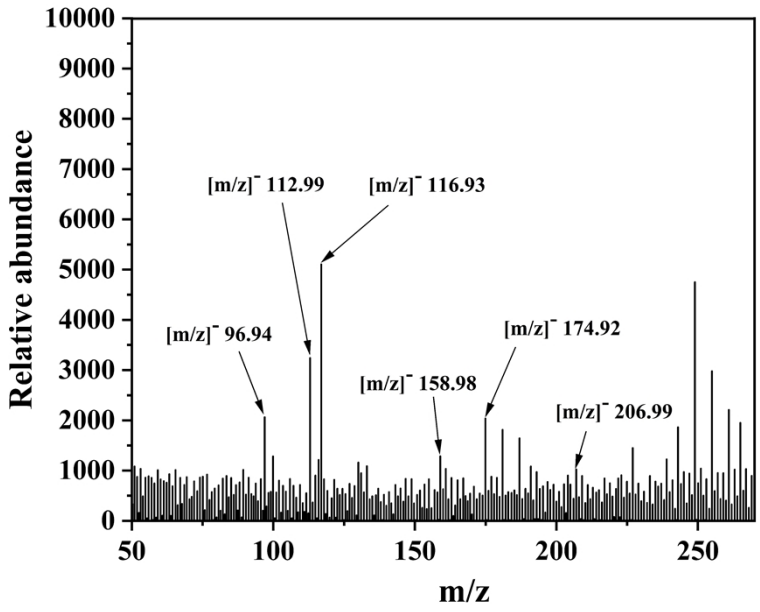


Fig. S8. Negative HR-MS analysis of the final productions catalyzed by the NPCN/PMS system.

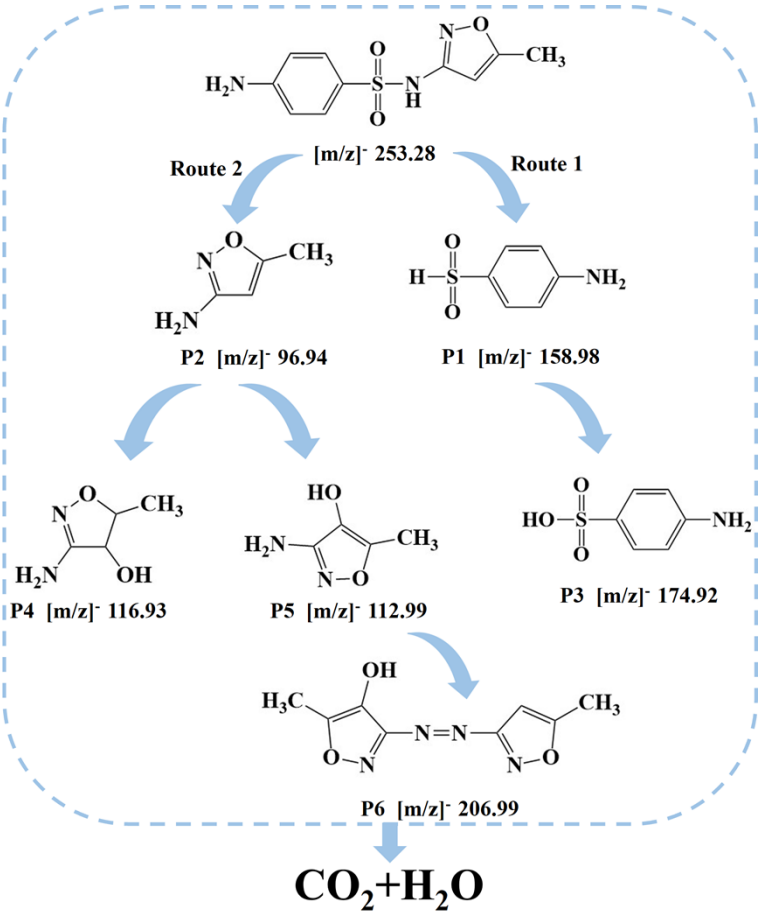


Fig. S9. The possible degradation pathways of SMX in the NPCN/PMS system.

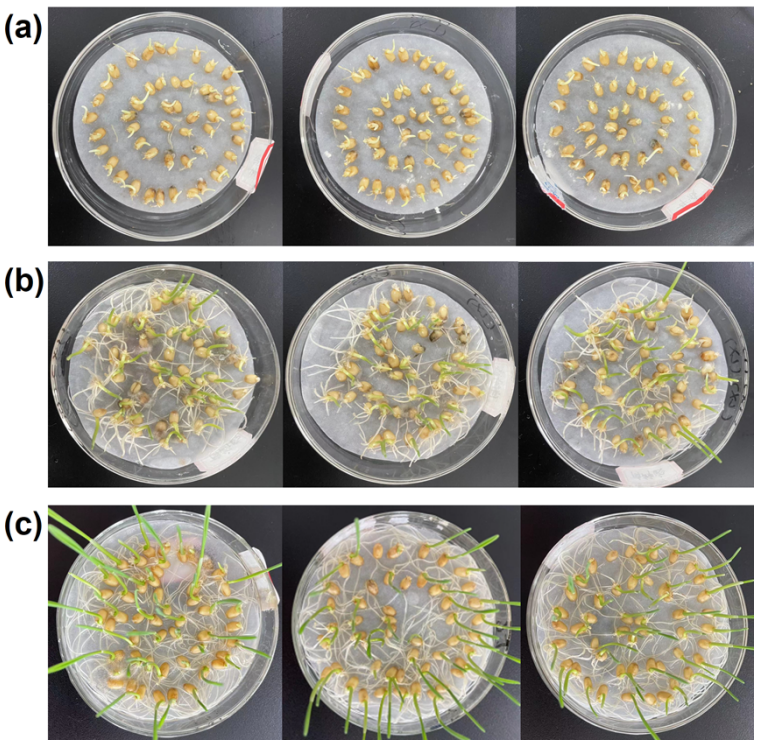


Fig. S10. Phenotype of representative wheat seeds cultivated by (a) SMX aqueous solution, (b) degraded SMX aqueous solution, and (c) deionized water at three days.

Table S1. Brunauer-Emmett-Teller (BET) results of the as-prepared samples.

Samples	Surface Area (m^2g^{-1})	Pore Volume (cm^3g^{-1})	Pore Size (nm)
HCNs	358.46	0.42	4.63
NCN-1	16.62	0.06	13.37
NCN-2	6.76	0.02	14.60
NPCN	369.92	0.42	4.58

Table S2. Comparison of previous reports on SMX degradation activated by PMS.

Entry	Contaminant	Catalyst	Oxidant	Degradation efficiency	Time	Ref.
1	SMX (20 mg/L)	NPCN (0.5 g/L)	PMS (0.5 g/L)	96.6%	10 min	This work
2	SMX (10 mg/L)	C-N-M (0.1 g/L)	PMS (0.5 mM)	95.0%	30 min	[S1]
3	SMX (10 mg/L)	BMNSBC (0.4 g/L)	PMS (1 mM)	100%	60 min	[S2]
4	SMX (5 mg/L)	Fe-DA-CN (50 mg/L)	PMS (0.5 mM)	99%	30 min	[S3]
5	SMX (20 mg/L)	CoNi-600@NC (25 mg/L)	PMS (0.3 mM)	100%	25 min	[S4]
6	SMX (10 mg/L)	CN@FeMn-10-800 (0.15 g/L)	PMS (0.2 g/L)	91.2%	60 min	[S5]
7	SMX (0.04 mM)	Fe0 @Fe3O4-MC (0.1 g/L)	PMS (3 mM)	100%	120 min	[S6]
8	SMX (5 mg/L)	BOSBC (0.14 g/L)	PMS (1 mM)	98.6%	60 min	[S7]
9	SMX (10 mg/L)	BNSBC (0.4 g/L)	PMS (1 mM)	92.1%	60 min	[S8]
10	SMX (20 mg/L)	CoS/BBC (0.02 g/L)	PMS (0.3 g/L)	99.12%	10 min	[S9]

Table S3. Toxicity classification according to the Globally Harmonized System of Classification and Labelling of Chemicals (GHS).

Toxicity range (mg L^{-1})	**Class**
LC_{50}/ChV ≤1	Very toxic
1< LC_{50} /ChV ≤10	Toxic
10< LC_{500}/ChV ≤100	Harmful
LC_{50}/ ChV >100	Not harmful

Table S4. Acute and chronic toxicity of SMX and its degraded intermediates to aquatic organisms estimated using ECOSAR.

Compound	Acute toxicity (mg L^{-1})			Chronic toxicity (mg L^{-1})		
	Fish (LC_{50}-96 h)	Daphind (LC_{50}-48 h)	Green algae (LC_{50}-96 h)	Fish (ChV)	Daphind (ChV)	Green algae (ChV)
SMX	267.00	6.43	21.80	5.00	0.068	11.10
P1	1330.00	9.05	39.00	44.00	0.084	35.40
P2	270.00	3.63	13.80	6.59	0.036	9.16
P3	11200.00	5220.00	1740.00	868.00	296.00	295.00
P4	1990.00	168.00	274.00	331.00	9.85	70.90
P5	646.00	5.61	23.10	19.20	0.054	18.80
P6	954.00	502.00	272.00	85.20	39.50	60.10

Reference

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