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

Supplementary Information for

An insight to metal organic framework derived N-doped graphene towards oxidative degradation of persistent contaminants: Formation mechanism and generation of singlet oxygen from peroxymonosulfate

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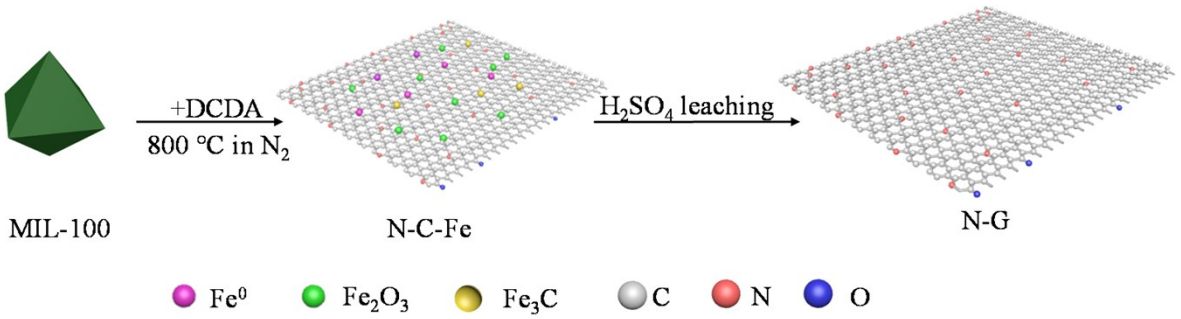


Scheme S1. Synthesis of N-doped graphene samples.

Table S1. Reaction rate constants of quenchers with radicals and $^1O_2$.

Quenching agents	Rate constants ($M^{-1}s^{-1}$)			References
	•OH	$SO_4^{\bullet-}$	$^1O_2$	
Ethanol	$(1.2\text{-}2.8)\times10^9$	$(1.6\text{-}7.8)\times10^7$	-	S1, S2
Tert-butanol	$(3.8\text{-}7.6)\times10^8$	$(4\text{-}9.1)\times10^5$	-	S2
NaN_3	1.2×10^{10}	2.52×10^9	1×10^9	S2, S3

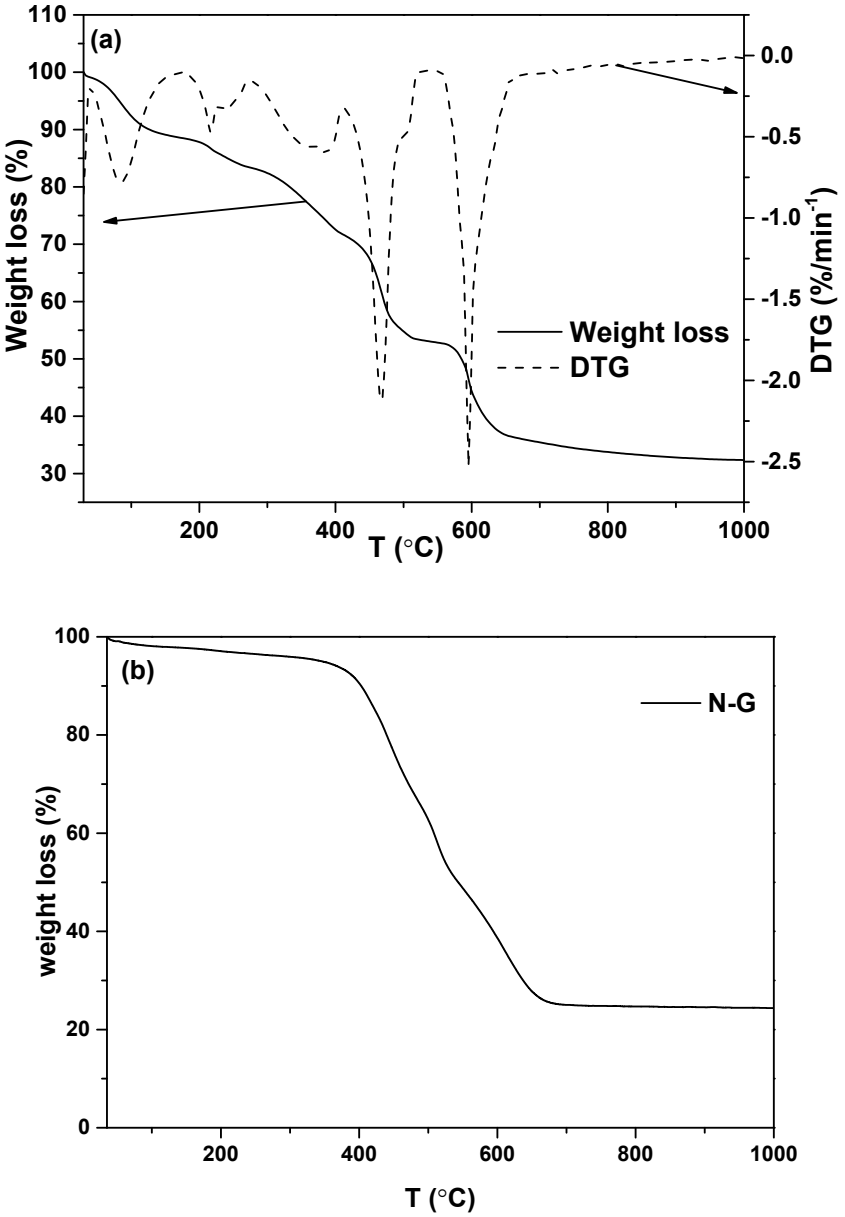


Figure S1. TG-DTG curves of MIL-100 (Fe) in argon (a) and N-G in air (b).

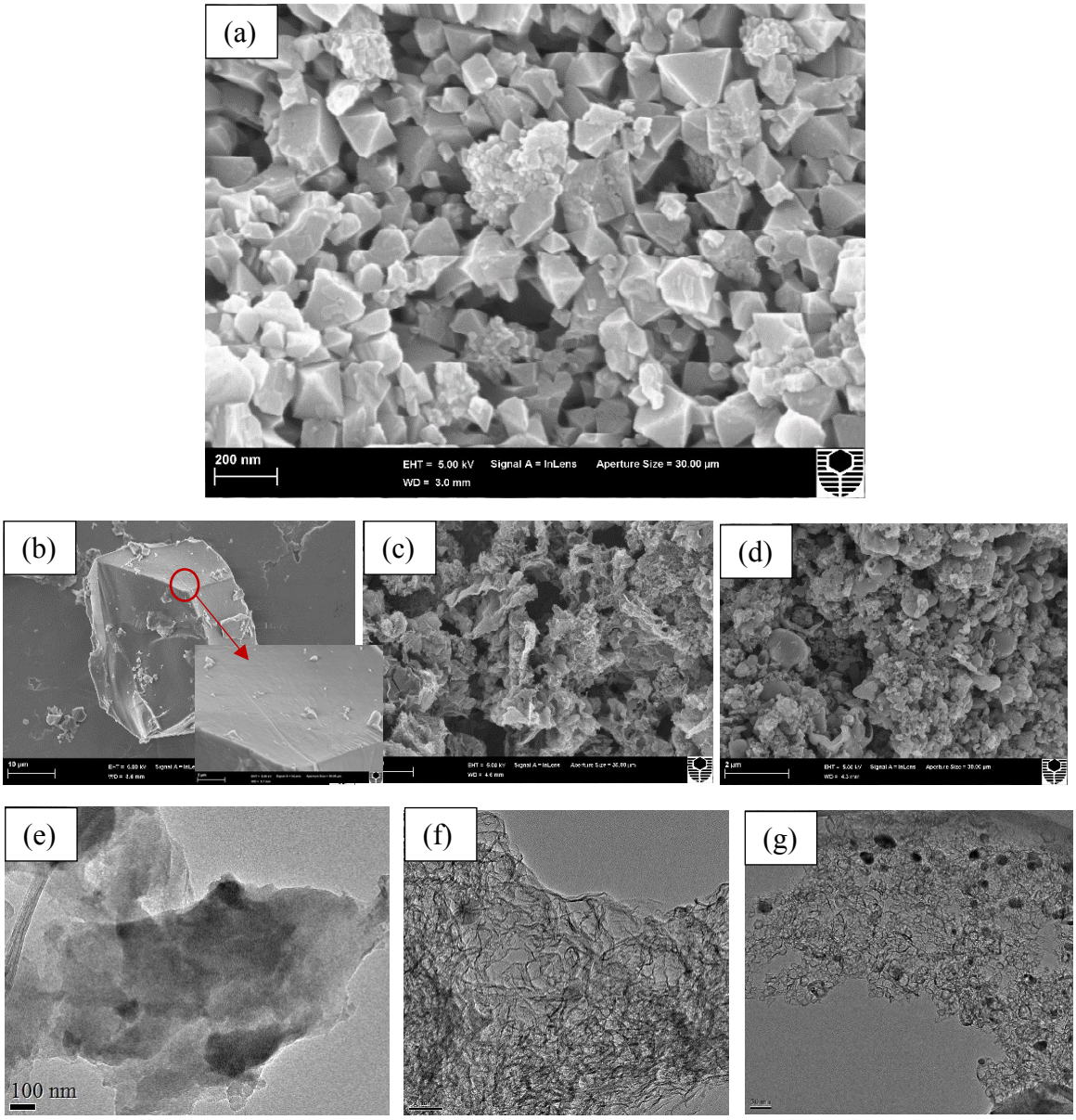
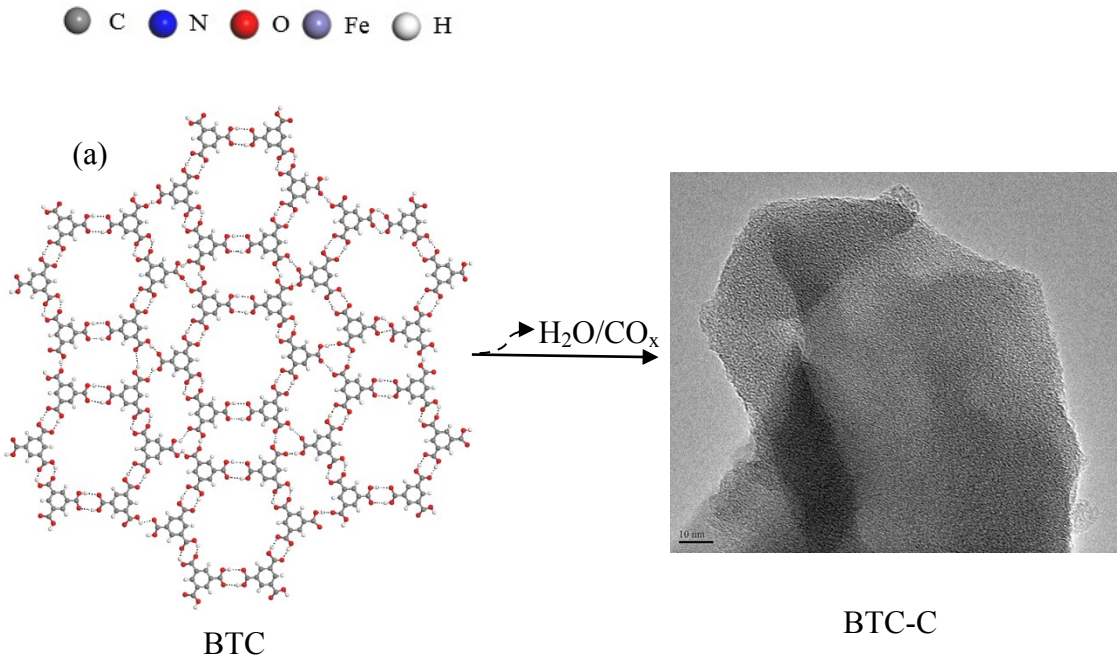
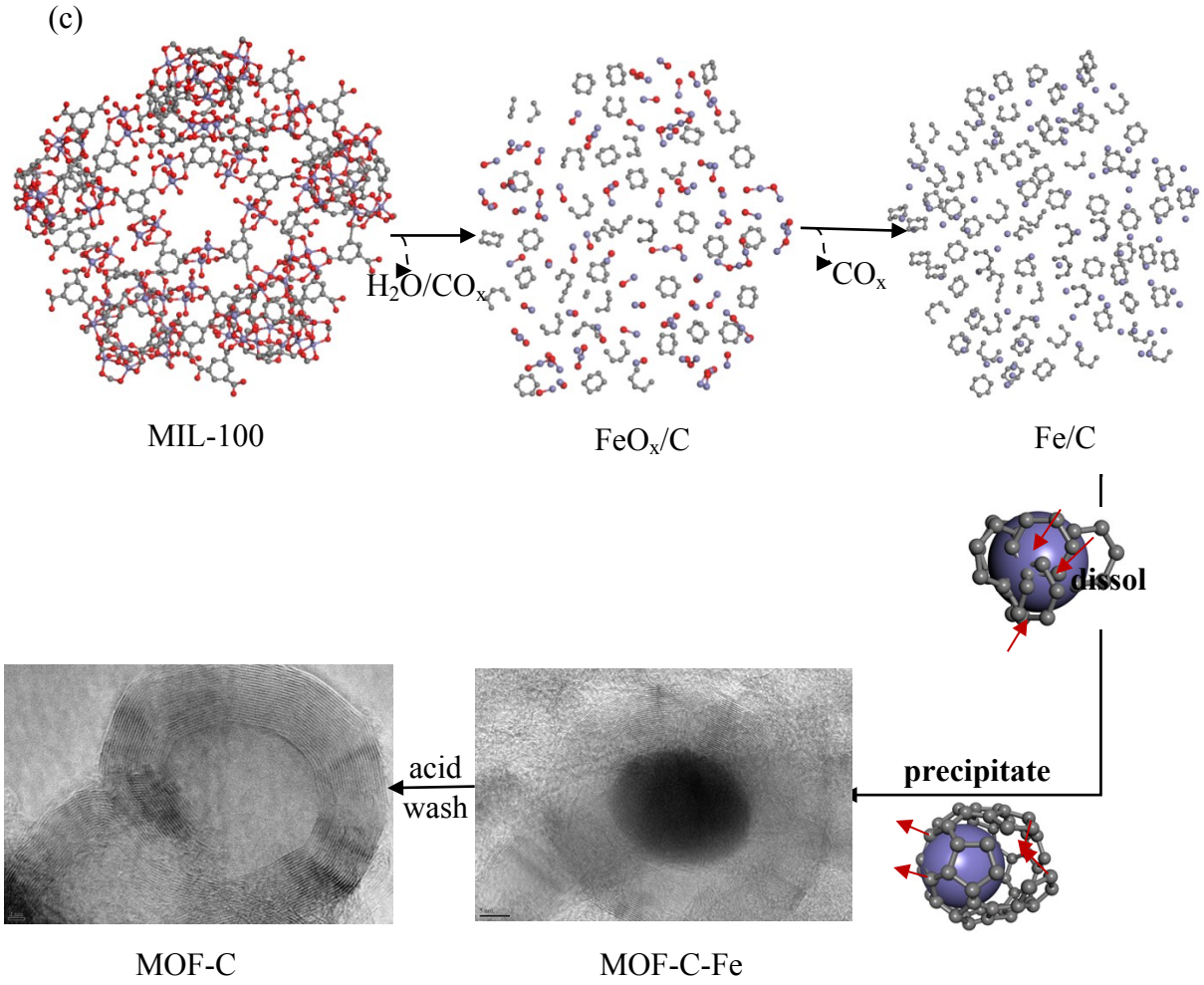


Figure S2. SEM (a-d) and TEM images (e-g) of MIL-100 (Fe) (a), BTC-C (b,e), C-N (c,f), MOF-C (d,g).


C
N
O
Fe
H
(a)
H_2O/CO_x
10 nm
BTC
BTC-C
(b)
H_2O/NO_x
CO_x/NH_x
10 nm
BTC + DCDA
C-N



Scheme S2. The formation mechanisms of BTC-C (a), C-N (b) and MOF-C (c).

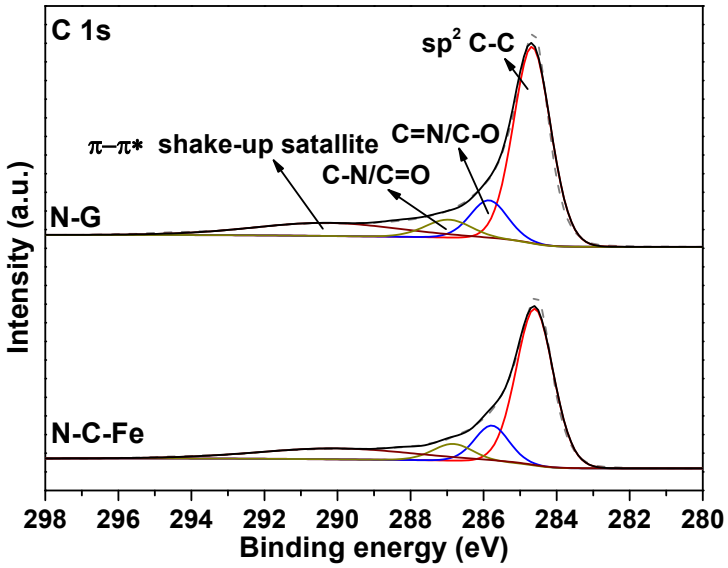


Figure S3. De-convoluted C1s XPS spectra of N-C-Fe and N-G.

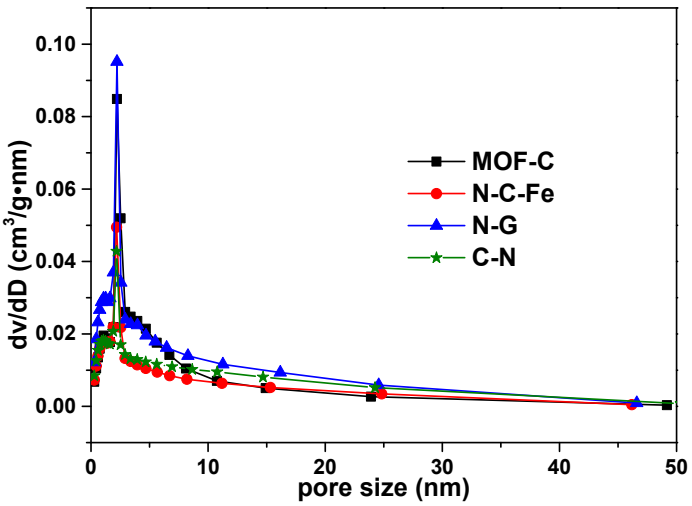


Figure S4. Pore size distribution curves of the synthesized materials.

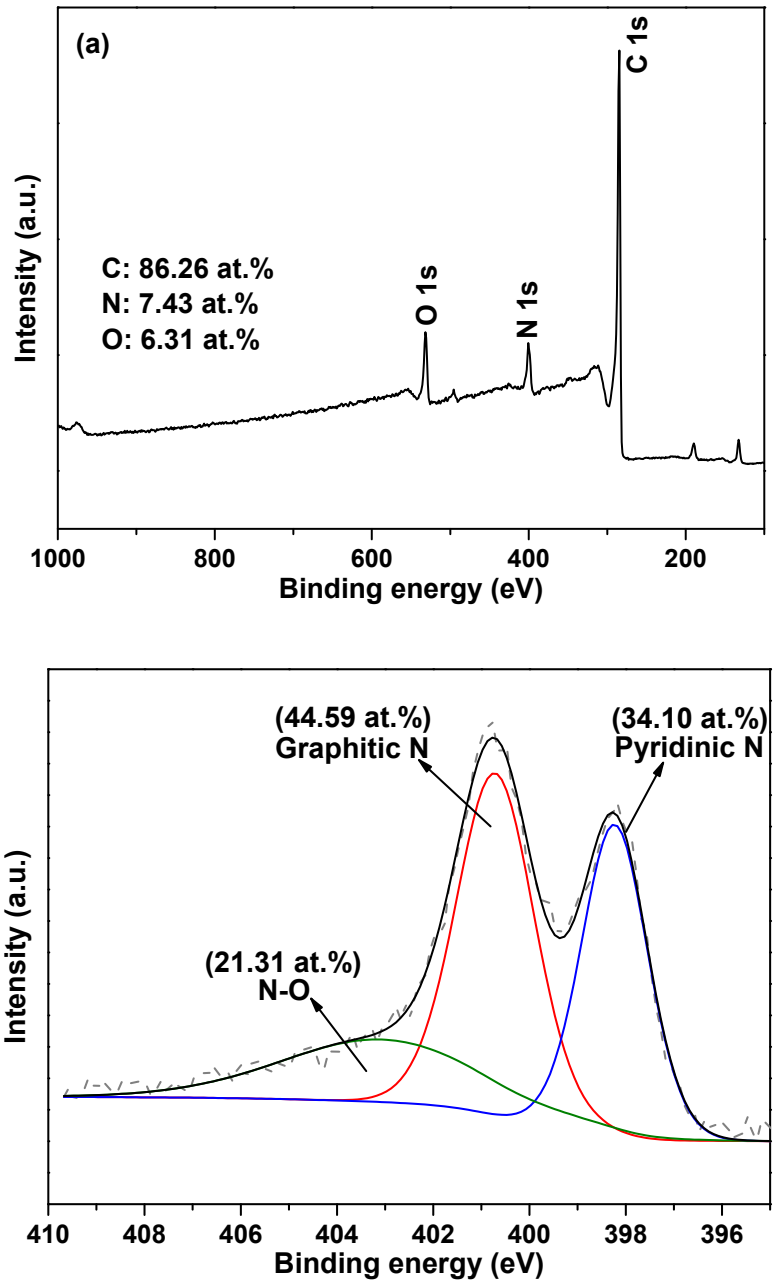


Figure S5. (a) XPS survey and (b) N 1s spectra of C-N.

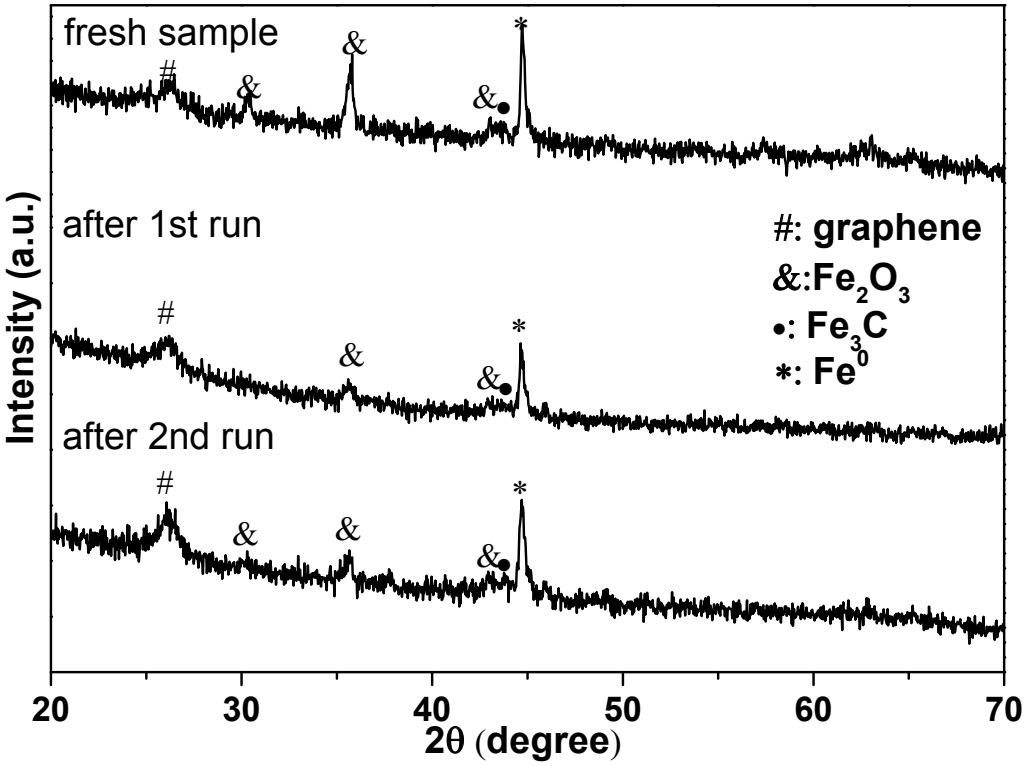


Figure S6. XRD patterns of fresh and used N-C-Fe.

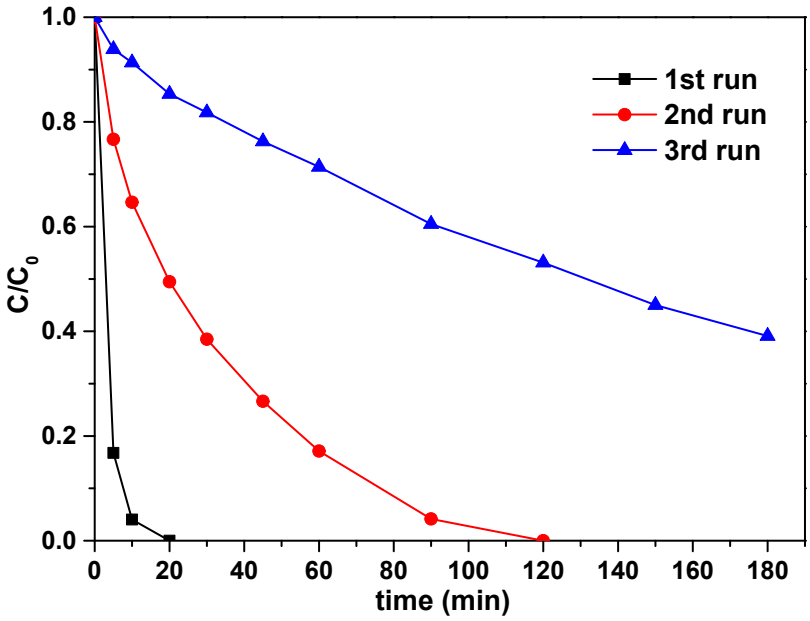


Figure S7. Stability tests of N-G.

[C (N-G): 0.1 g/L; C (phenol): 20 ppm; C (PMS): 1 g/L; T: 25 °C]

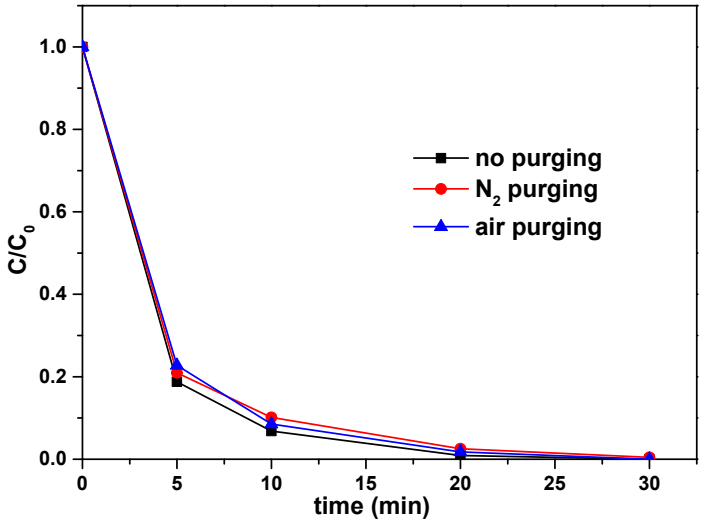


Figure S8. Phenol degradation in the N-G/PMS system under ambient condition, nitrogen gas purging and air purging. Reaction conditions: catalyst: 100 mg/L, PMS: 3.25 mM, phenol: 50 ppm, temperature: 25 °C.

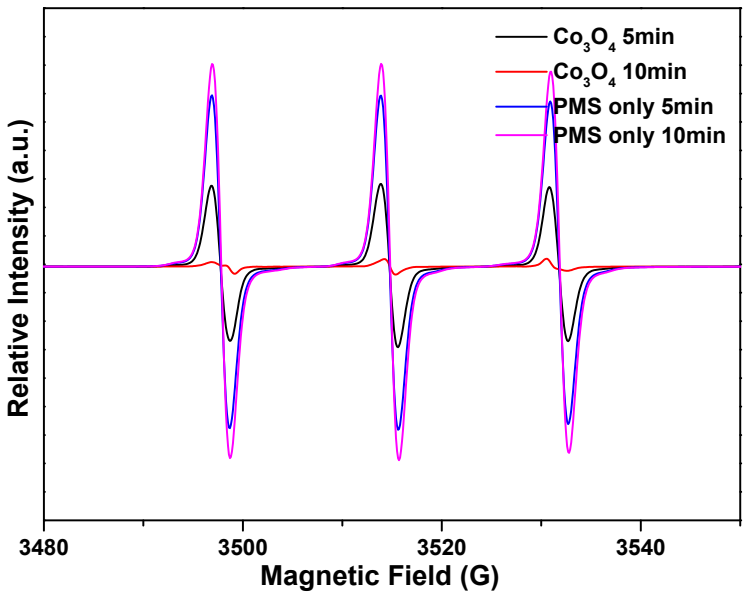


Figure S9. EPR spectra of TMPN on Co_3O_4 (catalyst: 200 mg/L, PMS: 6.5 mM, phenol: 50 ppm, temperature: 25 °C, reaction time: 5-10 min; TMP: 1.16 g/L)

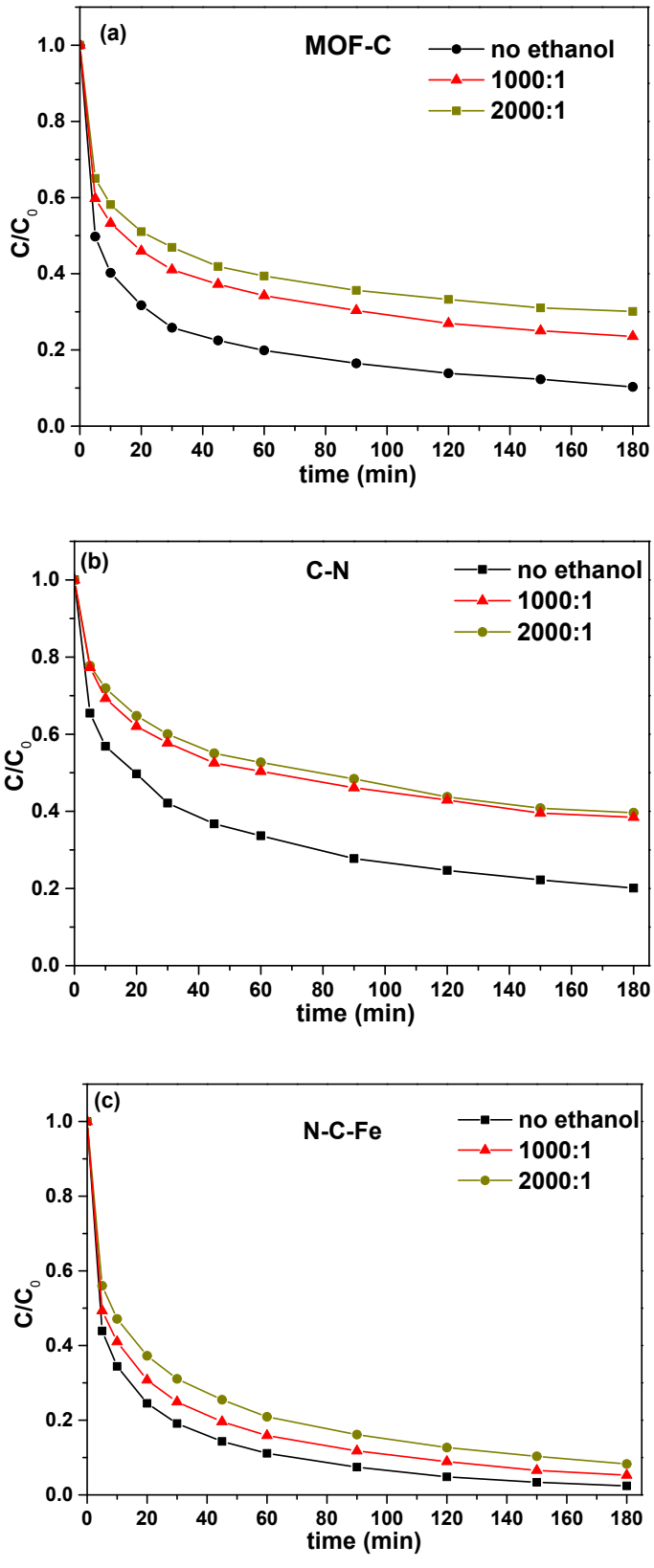


Figure S10. Effect of ethanol on phenol degradation: (a) MOF-C/PMS; (b) C-N/PMS; (c) N-C-Fe/PMS. Reaction conditions: catalyst: 100 mg/L, PMS: 3.25 mM, phenol: 50 ppm, temperature: 25 °C, molar ratio (ethanol *vs.* PMS): 1000:1 (2000:1).

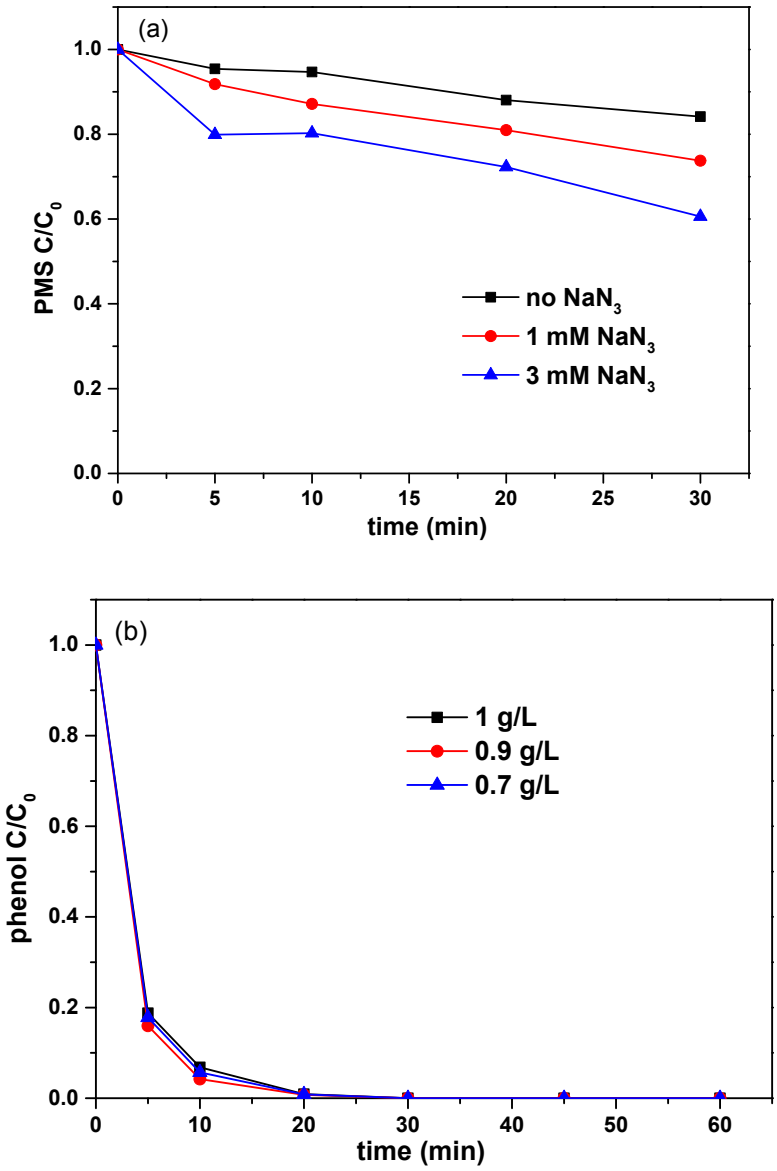


Figure S11. (a) Effect of NaN_3 on PMS decomposition in the phenol solution (catalyst: 100 mg/L, PMS: 1 g/L, phenol: 50 ppm, T: 25 °C). (b) Phenol degradation with different PMS concentrations (catalyst: 100 mg/L, PMS: 1 (0.9 or 0.7) g/L, phenol: 50 ppm, T: 25 °C).

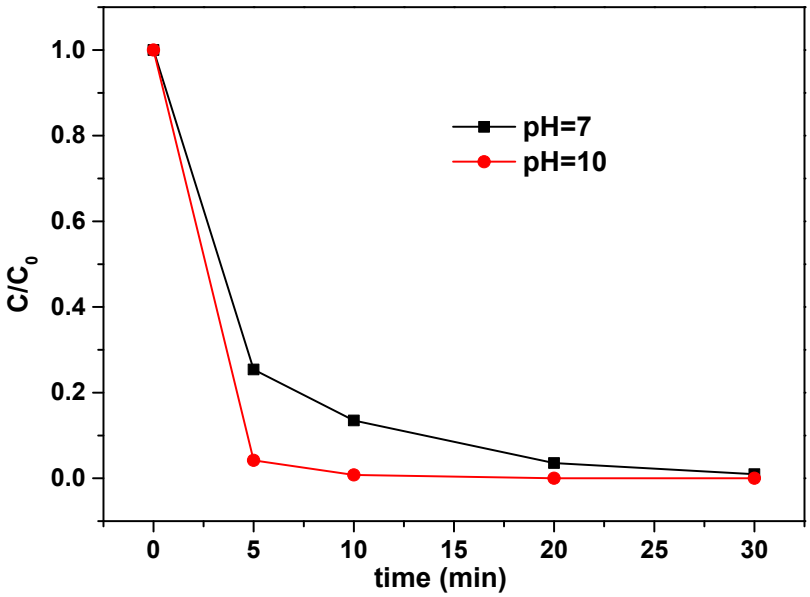


Figure S12. Influence of pH on phenol degradation. Reaction conditions: catalyst: 100 mg/L, PMS: 3.25 mM, phenol: 50 ppm, temperature: 25 °C, buffer (sodium borate): 20 mM.

References

(S1) G. V. Buxton; C. L. Greenstock; W. P. Helman; A. B. Ross, J. Phys. Chem. Ref. Data, 1988, **17**, 513-886.

(S2) G. P. Anipsitakis; D. D. Dionysiou, Environ. Sci. Technol. 2004, **38**, 3705-3712.

(S3) R. E. Huie; C. L. Clifton, J. Phys. Chem. 1990, **94**, 8561-8567.