Supporting Information

Fe-chelated polymer templated graphene aerogel with enhanced Fenton-like efficiency for water treatment

Yuan Zhuang[1], Xuechun Wang[1], Lili Zhang[1], Dionysios D. Dionysiou[2], Baoyou Shi[1,3*]

[1] Key Laboratory of Drinking Water Science and Technology, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing, 100085, China. Tel: 86-10-62922155, Email: byshi@rcees.ac.cn

[2] Environmental Engineering and Science Program, Department of Chemical and Environmental Engineering (ChEE), 705 Engineering Research Center, University of Cincinnati, Cincinnati, OH, USA

[3] University of Chinese Academy of Sciences, Beijing 100049, China

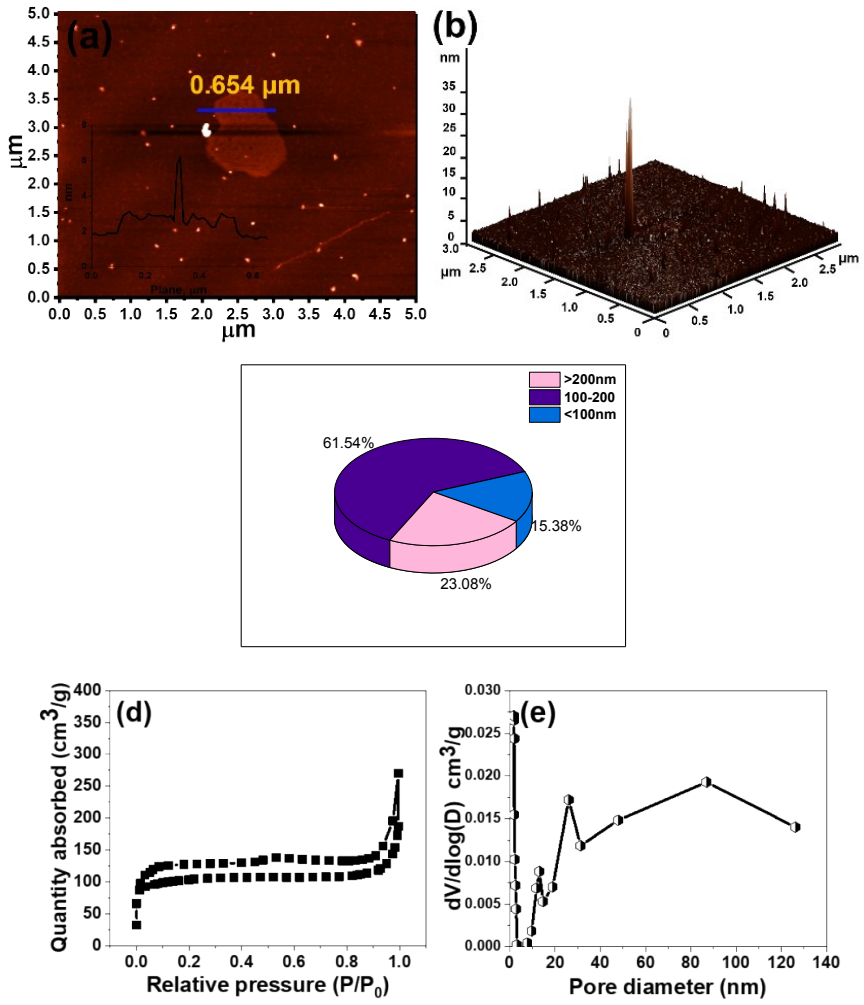


Figure S1 (a) AFM images of MGA (insets show the height profiles), (b) AFM 3D surface images of the MGA, (c) particle size distribution in the MGA, (d) N_2 adsorption and desorption isotherms of MGA, (e) pore size distribution of MGA.

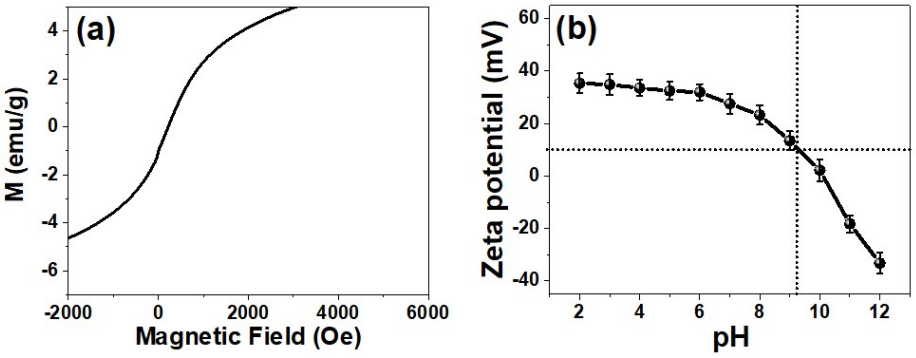


Figure S2 (a) Low field region of magnetization curves, (b) Zeta potential of MGA.

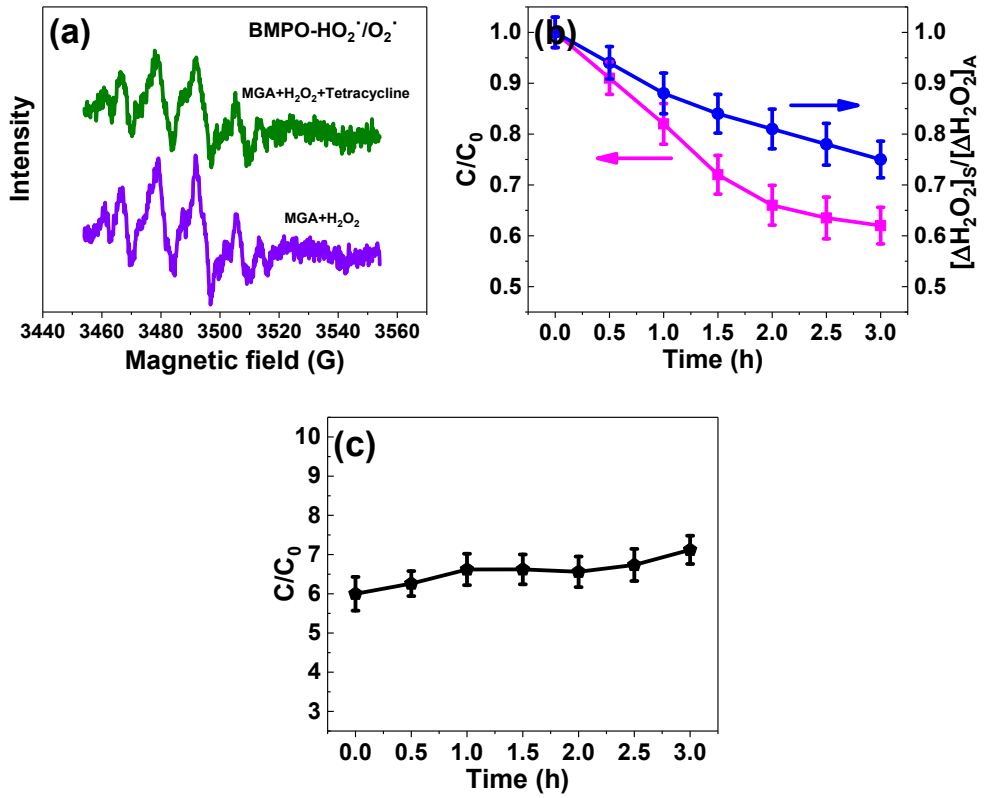
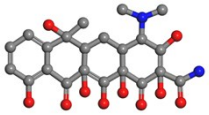
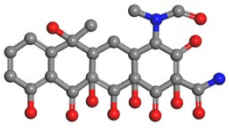
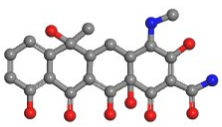
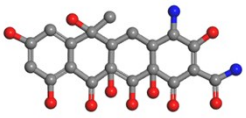
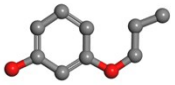
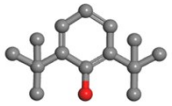
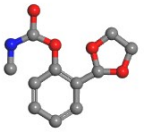
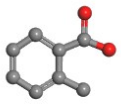
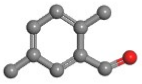
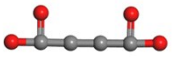
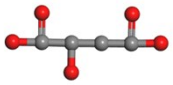
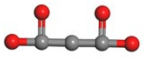
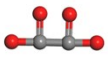
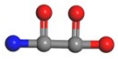


Figure S3 (a) BMPO spin-trapping EPR spectra for $HO_2^{\bullet}/O_2^{\bullet}$ of MGA, (b) The decomposition and utilization efficiency of H_2O_2 during tetracycline degradation by MGA, (c) pH changes of the solution during tetracycline degradation by MGA.

Table S1 Intermediate products identified using HPLC–MS and GC–MS during tetracycline degradation.

Time (min)	Molecular mass (g/mol)	Molecular structure
5	476	
5	490	
10	430	

10	448	
15	152	
15	206	
15	223	
15	138	
15	134	
20	118	
20	134	
20	104	
20	90	
20	89	
20	60	

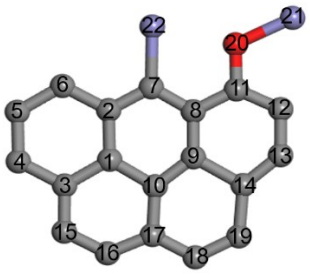


Figure S4 DFT optimized structure of MGA.

$$\mu = (E_{HOMO+}E_{LUMO})/2 \quad \text{(S1)}$$

$$\eta = (E_{LUMO-}E_{HOMO})/2 \quad \text{(S2)}$$

$$\omega = \mu^2/2\eta \quad \text{(S3)}$$

$$\chi = -\mu \quad \text{(S4)}$$

Table S2 Parameter of chemical activity analysis.

Molecule	**MGA**
E_{HOMO}	-0.62450
E_{LUMO}	-0.60713
$\Delta E_{LUMO-HOMO}$	0.01737
μ	-0.61582
χ	0.61582
η	0.00869
ω	21.82015

Table S3 Fukui function of MGA.

Atom	f_k^+	f_k^-
C(1)	0.034	0.034
C(2)	0.035	0.034
C(3)	0.035	0.034
C(4)	0.049	0.05
C(5)	0.049	0.05
C(6)	0.047	0.048
C(7)	0.035	0.036
C(8)	0.035	0.034
C(9)	0.039	0.04
C(10)	0.034	0.033
C(11)	0.037	0.038
C(12)	0.046	0.047
C(13)	0.049	0.049
C(14)	0.044	0.044
C(15)	0.048	0.049
C(16)	0.047	0.048
C(17)	0.036	0.034
C(18)	0.048	0.049
C(19)	0.05	0.05
O(20)	0.037	0.037

Fe(21)	0.084	0.083
Fe(22)	0.081	0.078