

Electronic Supporting Information for

Ferric carbide nanocrystals encapsulated in nitrogen-doped

carbon nanotubes as an outstanding environmental catalyst

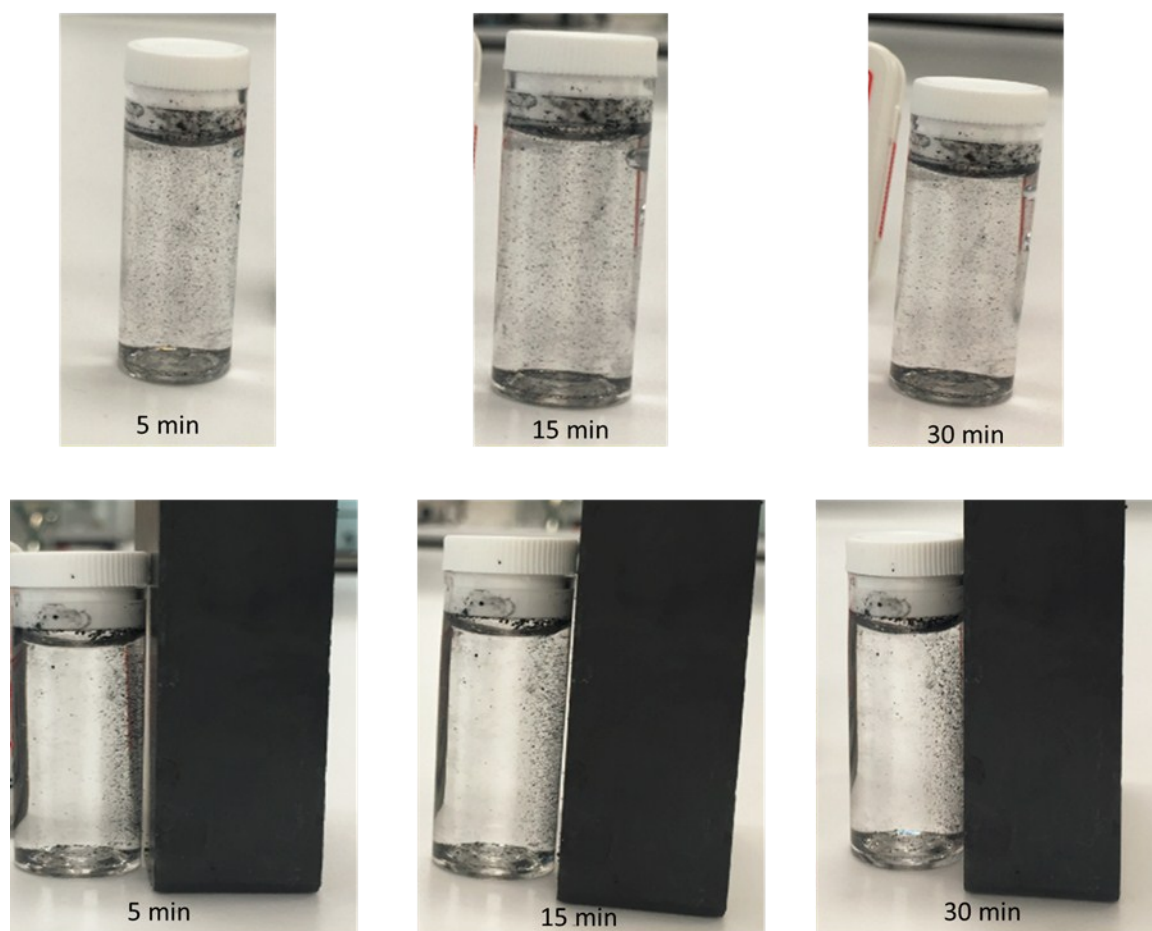
Chen Wang ^a, Jian Kang ^a, Ping Liang ^a, Huayang Zhang ^a, Hongqi Sun ^{b*}, Moses O. Tadé ^a,
and Shaobin Wang^{a*}

^aDepartment of Chemical Engineering and CRC for Contamination Assessment and Remediation of the Environment (CRC CARE), Curtin University, GPO Box U1987, Western Australia, Australia

^bSchool of Engineering, Edith Cowan University, 270 Joondalup Drive, Joondalup, WA 6027, Australia

*Corresponding Authors

Email: shaobin.wang@curtin.edu.au (S. Wang), h.sun@ecu.edu.au (H. Sun)



FigureS1 Photographs of magnetic separation tests of $\text{Fe}_3\text{C}@\text{NCNT-800}$ after different time

Figure S1 shows photographs of $\text{Fe}_3\text{C}@\text{NCNT-800}$ dispersion in water and their response under an external magnetic field. As illustrated in the photograph, by sonicating for 2 min, $\text{Fe}_3\text{C}@\text{NCNT-800}$ can be well dispersed in the deionized water and form a stable suspension before magnetic separation. If a magnet was placed close to the vial, $\text{Fe}_3\text{C}@\text{NCNT-800}$ nanoparticles were attracted towards the magnet very quickly and accumulated to the side wall of the vial near the magnet. And the solution became clear and transparent with the presence of the magnet. After removing the magnet and repeating the above sonicating procedure, $\text{Fe}_3\text{C}@\text{NCNT-800}$ was rapidly redispersed in water. Therefore, from the above simple experiments, the attraction and dispersion processes can be readily altered by placing or removing an external magnetic field, indicating good water dispersion and magnetic separation for effective water-solid separation.^{1, 2}

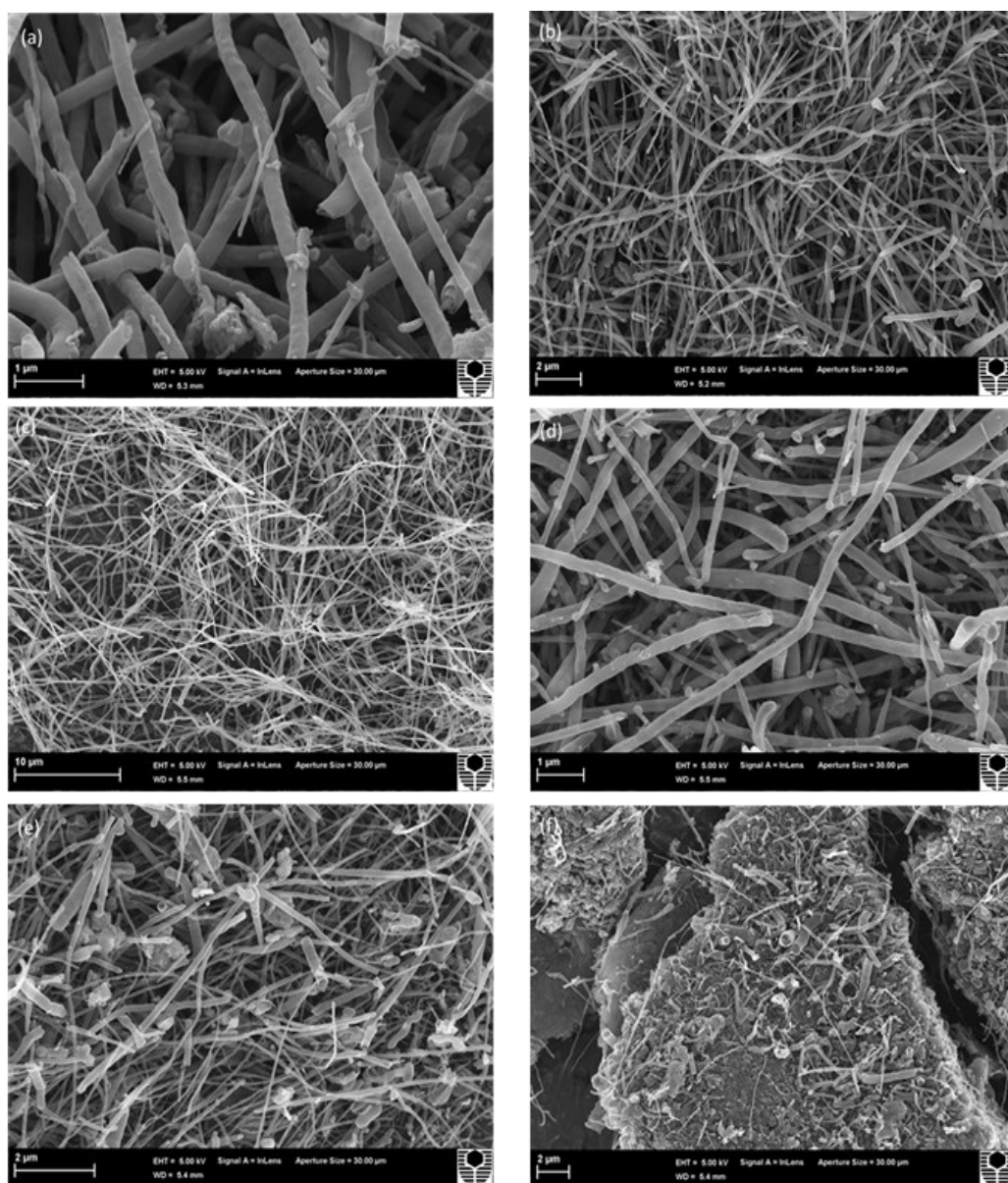


Fig.S2 SEM images for $\text{Fe}_3\text{C}@\text{NCNT}$ catalysts prepared at (a) (b) 700 °C, (c) (d) 800 °C and (e) (f) 900 °C.

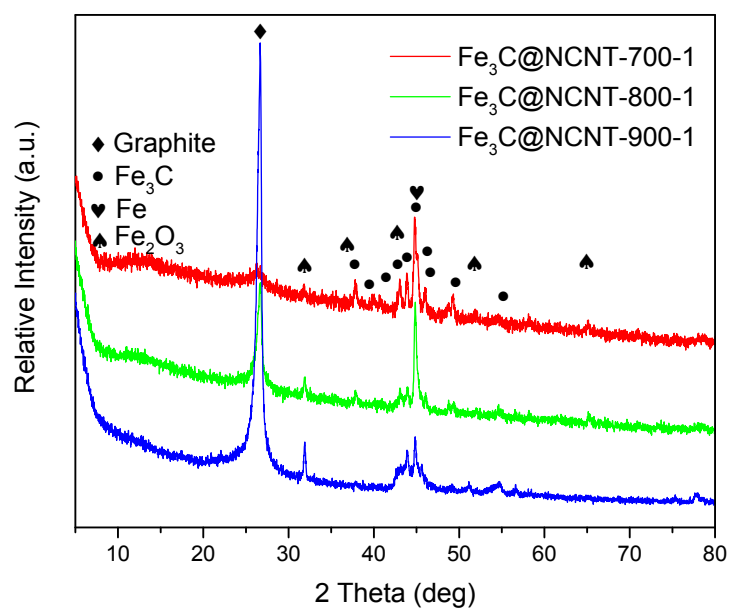


Fig. S3 XRD patterns of $\text{Fe}_3\text{C@NCNT}$ after the first run.

Table S1 The content of iron ions detected by ICP

	Fe ₃ C@NCNT-700	Fe ₃ C@NCNT-800	Fe ₃ C@NCNT-900
Iron ions (mg/L)	0.13	0.23	0.11

As shown in Table S1, after 3 h phenol degradation, the metal ion concentrations remained in the solution were very low and can be neglected. Therefore, iron ions were not the reasons for excellent catalytic degradation of Fe₃C@NCNT catalysts.

Table S2 Elemental analysis of N element of Fe₃C@NCNT samples

	Fe ₃ C@NCNT-700	Fe ₃ C@NCNT-800	Fe ₃ C@NCNT-900
N (wt%)	5.19	1.47	0.62

As shown in Table S2, N content in Fe₃C@NCNT-700 was 5.19 wt%, higher than that obtained by XPS (2.08 wt%). However, Fe₃C@NCNT-800 and Fe₃C@NCNT-900 had N contents at 1.47 wt% and 0.62 wt%, respectively, lower than those obtained by XPS (3.15 wt% and 4.22 wt%, respectively). These results implied that N doping of Fe₃C@NCNT-700 mainly occurred in the bulk. On the contrary N dopants of Fe₃C@NCNT-800 and Fe₃C@NCNT-900 were mainly agglomerated on the surfaces. The doped N profiles further suggested that Fe₃C@NCNT-800 and Fe₃C@NCNT-900 had better catalytic performances than Fe₃C@NCNT-700 because of the more pyridinic and pyrrolic N on the surfaces.

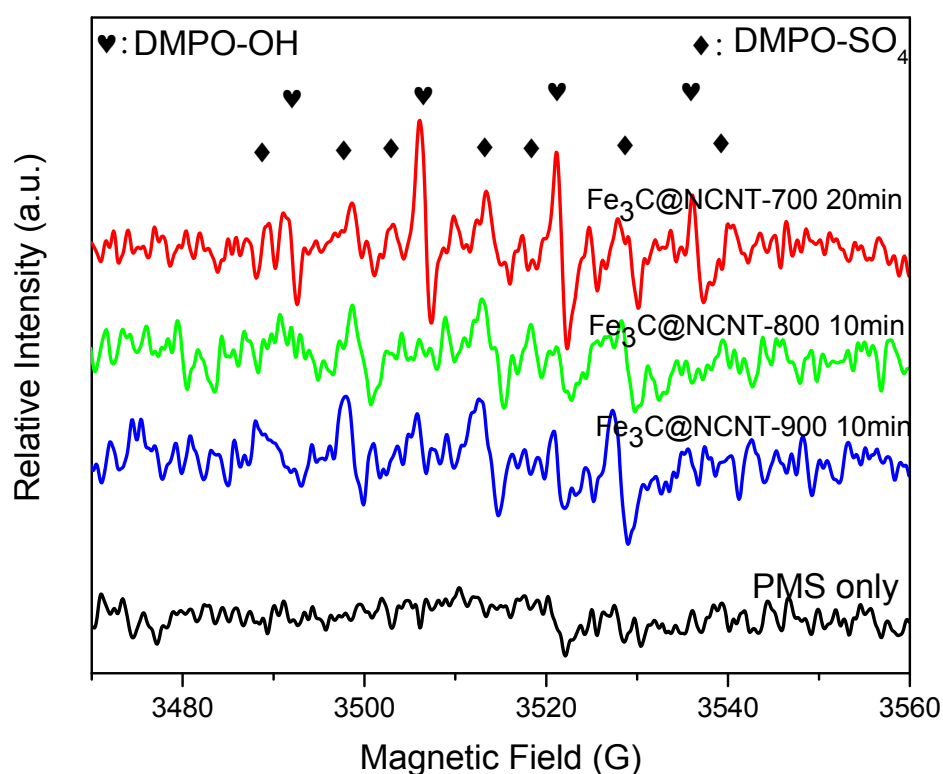


Fig.S4 EPR spectra of PMS activation with $\text{Fe}_3\text{C}@\text{NCNT}$ composites at different time.

We employed electron paramagnetic resonance (EPR) to probe the generation and evolution of reactive radicals using 5,5-dimethyl-1-pyrroline (DMPO) as a radical spin trapping agent.³

Notes and references

1. Y. Wang, H. Sun, H. M. Ang, M. O. Tadé and S. Wang, *J. Colloid Interface Sci.*, 2014, **433**, 68-75.
2. Y. Wang, H. Sun, H. M. Ang, M. O. Tadé and S. Wang, *Chem. Engin. J.*, 2014, **245**, 1-9.
3. X. Duan, H. Sun, Y. Wang, J. Kang and S. Wang, *ACS Catal.*, 2015, **5**, 553-559.