Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

Facile preparation of MnO_2 doped Fe_2O_3 hollow nanofibers for low temperature SCR of NO with NH_3

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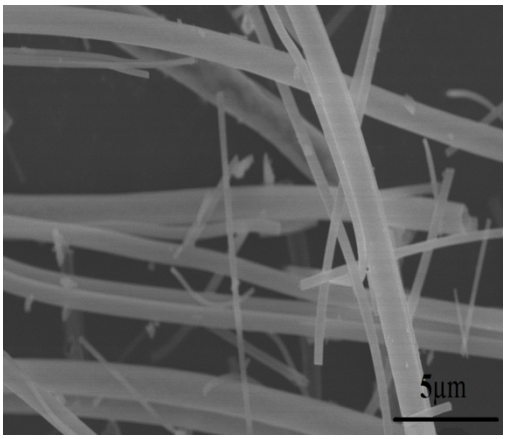

Fig. S1. SEM image of electrospun MnFe (0.05) hollow nanofibers

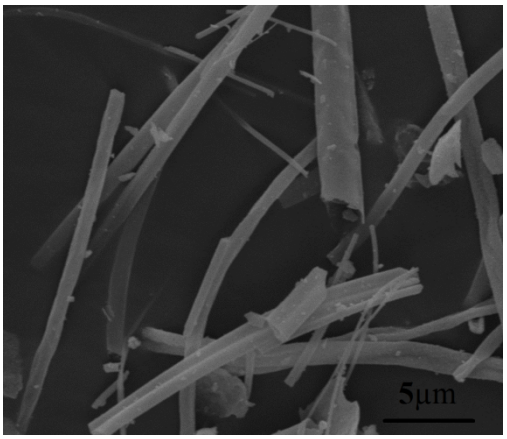

Fig. S2. SEM image of electrospun MnFe (0.20) hollow nanofibers

The stability of MnFe (0.15) under severe hydrothermal treatment (1023 K, 10% H_2O) was tested after being aged for 24h, and the flow rate of N_2 was 100 mL/min. After being aged, the XRD patterns of MnFe (0.15) changed from Fe_2O_3 (PDF#19-0629) to Fe_2O_3 (PDF#79-1741); and the whole catalytic performance decreased obviously and moved to high temperature, the best NO conversion was only 81% at 200 °C; the SEM image showed that there were lots of incomplete tube, some of the hollow tube were damaged. All this results showed that the stability of hollow fibers needed to further improvement in future.

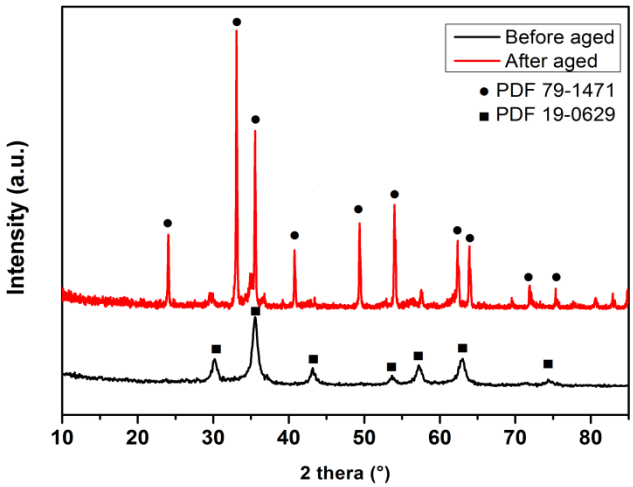

Fig. S3. XRD patterns of MnFe(0.15) hollow nanofibers.

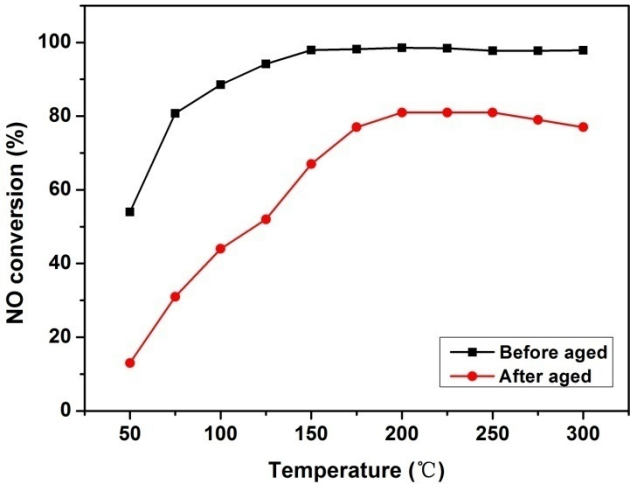

Fig. S4. NO conversion of MnFe(0.15) hollow nanofibers.

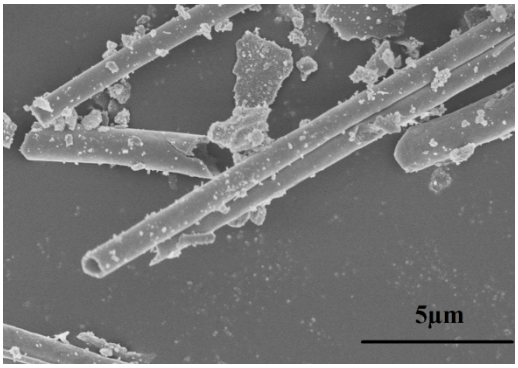

Fig. S5. SEM image of MnFe(0.15) hollow nanofibers after being aged

Table. S1 the TOF analysis of MnFe (0.05) and MnFe (0.15)

Sample	temperature/℃	conversion/%	TOF(10^{-4} s^{-1})
MnFe(0.05)	50	38.2	0.243
	75	47.8	0.304
	100	55.8	0.355
MnFe(0.15)	50	54	0.262
	75	80.7	0.392
	100	88.5	0.430

The turnover frequency (TOF) was a basic parameter to evaluate catalyst's activities. As shown in Table. S1, the TOF value was almost constant at a certain temperature. This directly proved that the Mn^{4+} species were the active sites of catalysts for the NH_3-SCR reaction.

TOF calculation formula:

$$TOF = \frac{Converted\ NO\ (mol/s)}{Active\ sites\ number\ (mol)}$$

$$Converted\ NO\ (mol/s) = \frac{500 ppm \times conversion\ (\%) \times flow\ rate\ (L/s)}{22.4\ L/mol}$$

where flow rate=200 mL/min=1/300 (L/s).

$$Active\ sites\ number\ (mol) = (m_{MnO2}/M_{MnO2}) \times \eta$$

where m_{MnO2} stands for the mass of the grown MnO_2 on the hollow fibers, M_{MnO2} represents the molecular weight of MnO_2 (86.9 g/mol) and is the portion of Mn^{4+}, which is determined by XPS analysis.

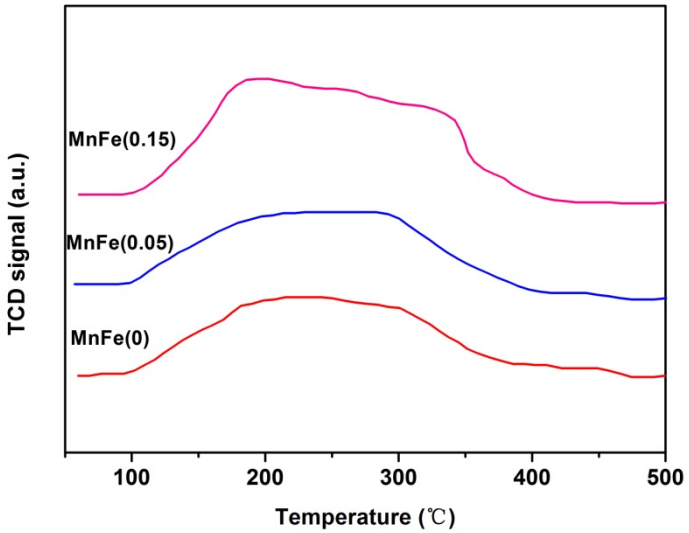

Fig. S6. NH_3-TPD profiles of MnFe(0), MnFe(0.05) and MnFe(0.15).

Fig. S6 showed the NH_3-TPD results over FeMn(0), FeMn(0.05) and FeMn(0.15) catalysts in the range of 100-500 °C. NH_3 desorption was observed over a wide temperature range, the peaks at lower temperature were caused by the desorption of physisorbed NH_3; while the peaks centered at 180-230 °C were caused by the desorption of coordinated NH_3 bound to Lewis acid sites, at the higher temperature were assigned to NH_3 strongly adsorbed on the Brønsted acid sites.[4-6] Besides all the desorption peaks slightly moved to the low temperature edge, it seemed that the Mn substitution of Fe did not obviously influence the NH_3 adsorption ability of these catalysts, but the amount of NH_3 adsorption increased gradually, which may be due to the increase of BET surface area and strong adsorption for NH_3 of the Mn species. In SCR reaction, chemical adsorbed NH_3 species were considered to be the important intermediates, so the increase of them at higher Mn content had a positive effect on NO conversion.

References:

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