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


# Supplementary material

## Supplementary Methods

**Computational methods.** The distribution of the valence-electron density on the Fe-Mn-$SiO_2$ was investigated through DFT calculation. It was implemented in Vasp (the Vienna ab initio simulation package), with the potential to exchange and correlation Perdew, Burke and Ernzerhof (PBE) within the general apprxiation of the gradinte (GGA). A pseudopotentially engineered wave (PAW) was used to describe the main electrons. For all optimisation calculations, the energy and power conversion criteria are set at 10-5 eV, or 0.01 eV $Å^{-1}$. The energy limit was set to 450 eV, and a 3*3*1 K-point game center was selected to describe the Brilllouin zone. For Hubbard's correction, Ueff's value was set at 3.5 eV for Fe and Mn.

**Table S1**
The structure of the catalysts.

| Samples | BET surface area ($m^2/g$) | Fe (at.%) | | Mn (at.%) | | |
|---|---|---|---|---|---|---|
| | | $Fe^{3+}$ | $Fe^{2+}$ | $Mn^{2+}$ | $Mn^{3+}$ | $Mn^{4+}$ |
| $Fe_2O_3/SiO_2$ | 540 | 38.5 | 61.5 | — | — | — |
| $Mn_2O_3/SiO_2$ | 526 | — | — | 15.0 | 71.6 | 13.4 |
| Fe-Mn-$SiO_2$ | 617 | 73.4 | 26.6 | 9.6 | 56.9 | 33.5 |

**Table S2**
Parameters of the obtained water samples.

| | Deionized Water | Tap Water | Surface Water |
|---|---|---|---|
| pH | 6.98 | 7.65 | 7.87 |
| $UV_{254}(cm^{-1})$ | 0.004 | 0.022 | 0.178 |
| TOC(mg/L) | - | - | 3.53 |
| $Cl^-$(mg/L) | - | 10.63 | 5.94 |
| $SO_4^{2-}$(mg/L) | - | 24.76 | 4.10 |
| $HCO_3^-$(mg/L) | - | 2.52 | 5.71 |

**Table S3**
Analysis method of the pollutants.

| Pollutants | Mobile phase (v/v) |
|---|---|
| Phenol | Water : methanol=60:40 |
| bisphenol A (BPA) | Water : methanol=30:70 |
| 4-chlorophenol (4-CP) | Water : methanol=40:60 |
| Ibuprofen (IBP) | Water : acetonitrile=25:75 |
| Phenytoin (PHT) | Water : acetonitrile=40:60 |

Flow rate of mobile phase using 1.0 mL/min for all experiments.

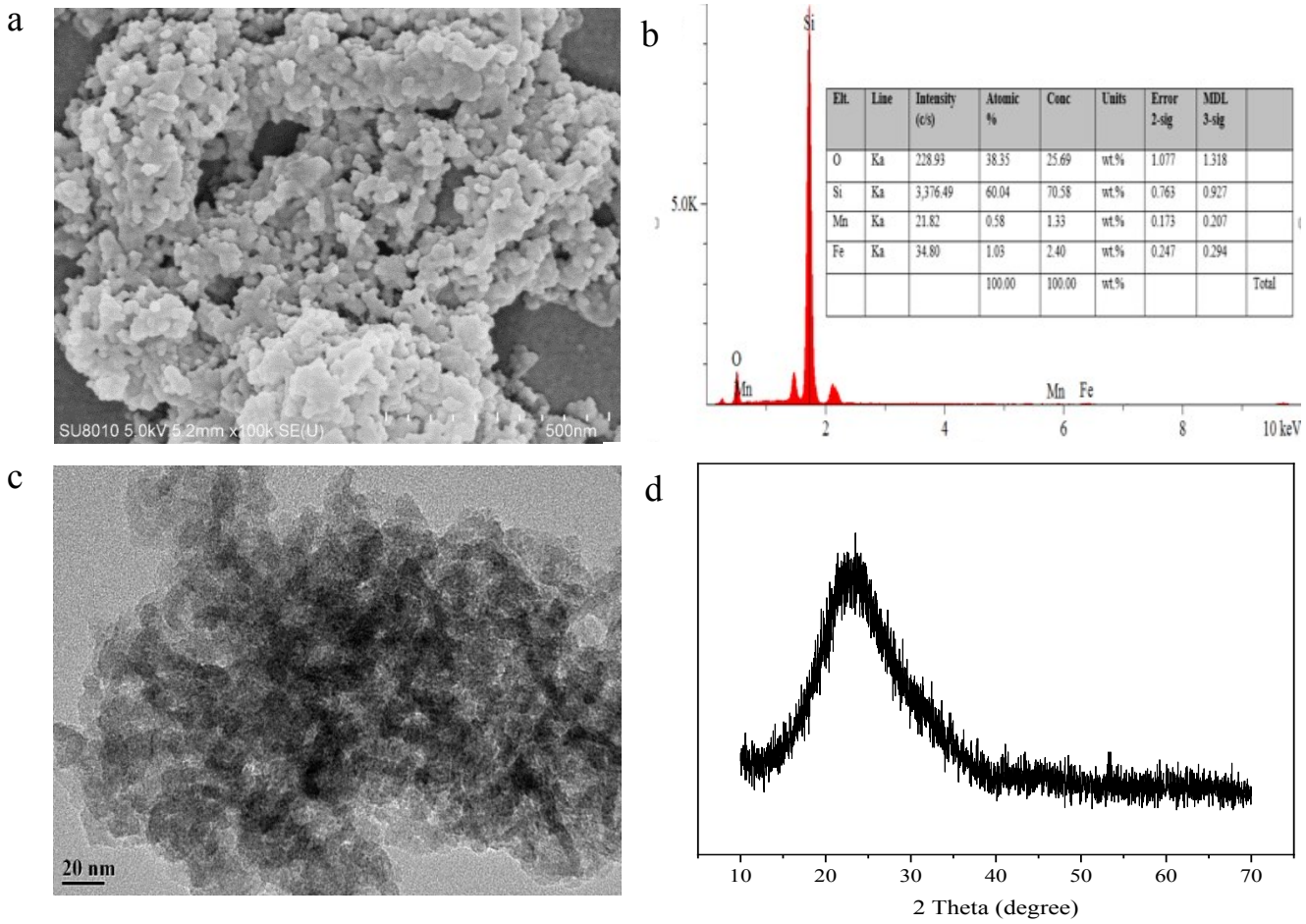


**Figure S1** The structure of the Fe-Mn-$SiO_2$ catalyst.
(a. SEM image; b. SEM-EDX image; c. TEM image; d. XRD spectrum)

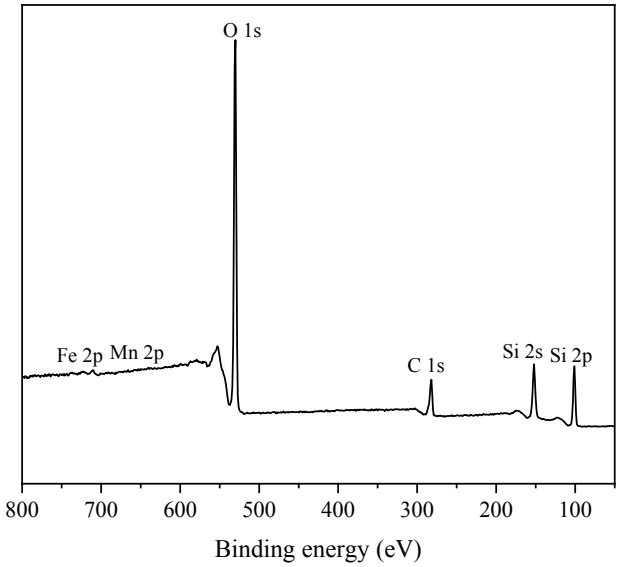


**Figure S2** The survey scan spectrum of the Fe-Mn-$SiO_2$ catalyst.

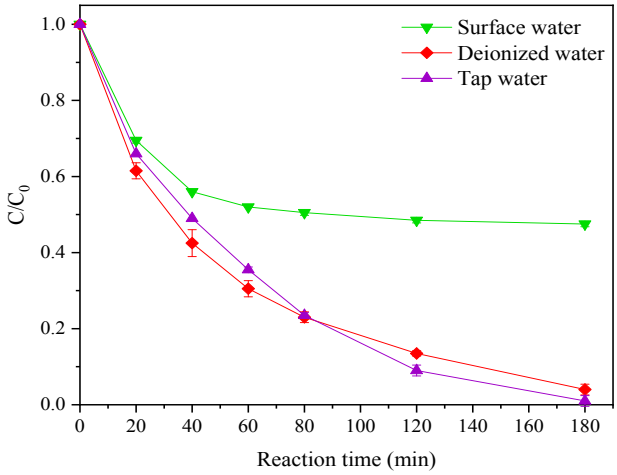


**Figure S3** The SMT removal by the Fe-Mn-$SiO_2$/$H_2O_2$ system in the different water matrices. ($[SMT]_0$=20mg/L, $[H_2O_2]_0$=60mM, [Catalyst]=1g/L, T=25°C)

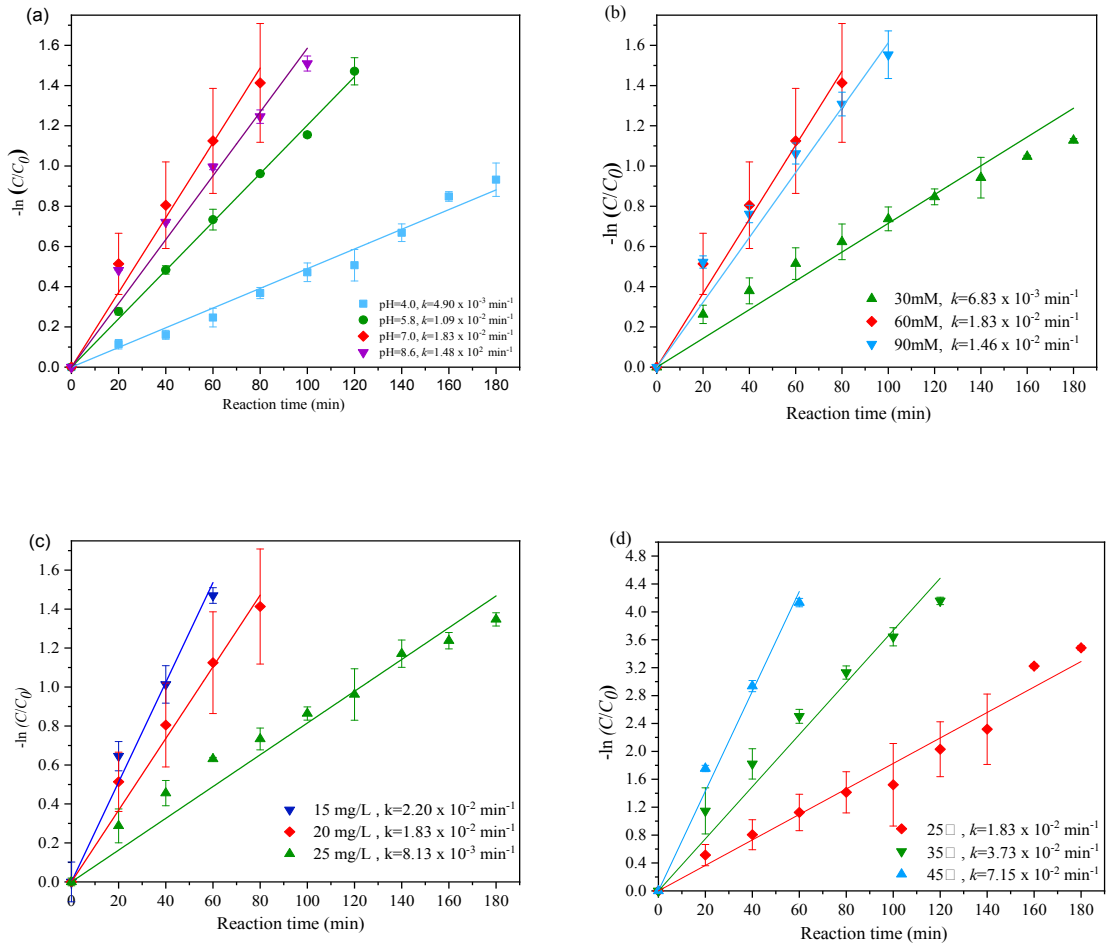


**Figure S4** The kinetics curves for the SMT degradation in the Fenton-like reaction over the Fe-Mn-$SiO_2$ catalyst under the different operating conditions. ((a) pH value: $[SMT]_0$=20mg/L, $[H_2O_2]_0$=60mM, [Catalyst]=1g/L, T=25°C; (b) $H_2O_2$ dosage: $[SMT]_0$=20mg/L, pH=7.0, [Catalyst]=1g/L, T=25°C; (c) SMT concentration: pH=7.0, $[H_2O_2]_0$=60mM, [Catalyst]=1g/L, T=25°C; (d) reaction temperature: $[SMT]_0$=20mg/L, pH=7.0, $[H_2O_2]_0$=60mM, [Catalyst]=1g/L).

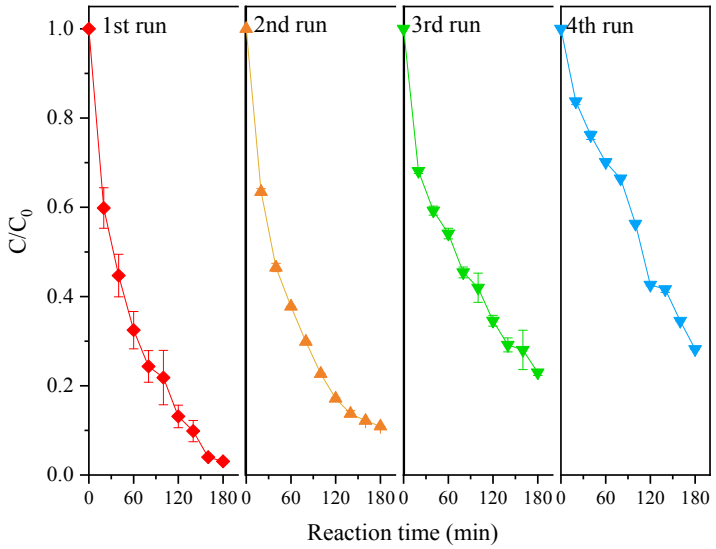


**Figure S5** The catalytic stability of the Fe-Mn-$SiO_2$ catalyst in the Fenton-like reaction for the SMT degradation. ($[SMT]_0$=20mg/L, pH=7.0, $[H_2O_2]_0$=60mM, [Catalyst]=1g/L, T=25°C)

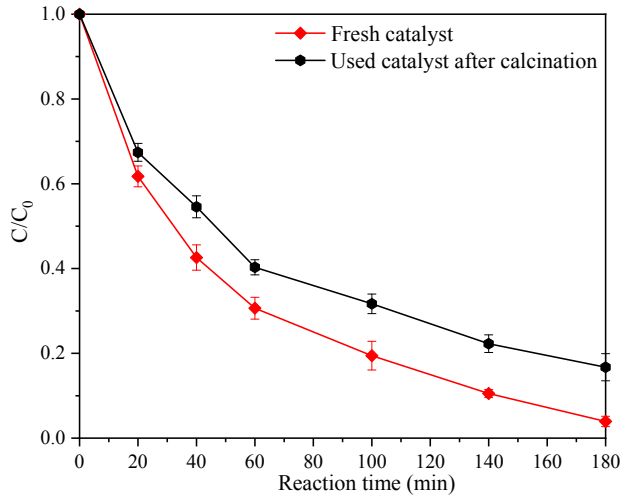


**Figure S6** The SMT removal in the Fenton-like reaction over the fresh Fe-Mn-$SiO_2$ catalyst and the used Fe-Mn-$SiO_2$ after calcination. ($[SMT]_0$=20mg/L, pH=7.0, $[H_2O_2]_0$=60mM, [Catalyst]=1g/L, T=25$^o$C).

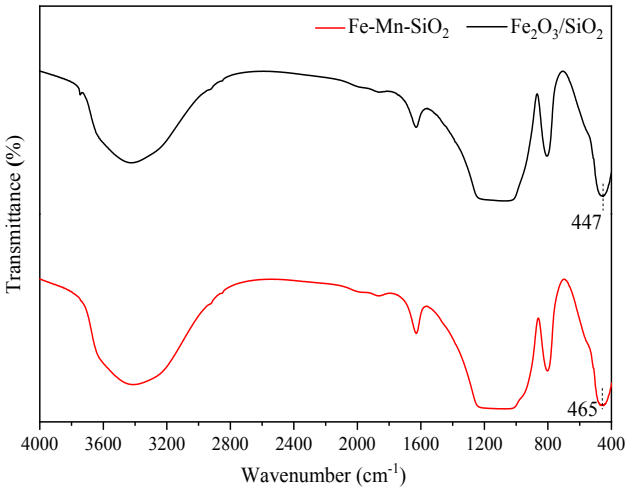


**Figure S7** FTIR spectrum of $Fe_2O_3/SiO_2$ and Fe-Mn-$SiO_2$ catalysts.