Supporting Information for

Fe-doped α-MnO$_2$ nanorods for catalytic removal of NO$_x$ and chlorobenzene: The relationship between lattice distortion and catalytic redox properties

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Table S1 Basic properties of the samples.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Fe:Mn molar ratio&lt;sup&gt;a&lt;/sup&gt;</th>
<th>Specific surface area (m²·g⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MnFe₀</td>
<td>&lt; 0.001</td>
<td>45.0</td>
</tr>
<tr>
<td>MnFe₀.4</td>
<td>0.370</td>
<td>122.0</td>
</tr>
<tr>
<td>MnFe₀.7</td>
<td>0.650</td>
<td>124.3</td>
</tr>
<tr>
<td>MnFe₀∞</td>
<td>&gt; 1000</td>
<td>1.9</td>
</tr>
</tbody>
</table>

<sup>a</sup> Measured by ICP-OES

![Fig.S1 XRD patterns of MnFe<sub>x</sub> samples.](image)

To identify whether a single crystalline phase is formed after Fe-doping, XRD measurements are performed on the four samples. As shown in Fig. S1, a typical α-MnO₂ phase (JCPDS:42-1348) is observed for MnFe₀, indicating a generation of pure α-MnO₂. Nevertheless, for Fe-doped catalysts, characteristic peaks of KFe₃(SO₄)₃(OH)₆ (JCPDS: 36-0427) are detected, which verify the formation of a secondary phase.
Fig. S2 Initial H\textsubscript{2} consumption rate of as-prepared MnFe\textsubscript{x} samples.

The initial H\textsubscript{2} consumption rate is an effective method to investigate the reducibility of the catalyst. Fig. S2 clearly shows that the order of initial hydrogen consumption rate is MnFe\textsubscript{0.4} \approx MnFe\textsubscript{0.7} > MnFe\textsubscript{0} > MnFe\textsubscript{∞}, indicating the reducibility of MnFe\textsubscript{0.4} and MnFe\textsubscript{0.7} is obviously strengthened compared to MnFe\textsubscript{0}\textsuperscript{[1, 2]}.

Fig. S3 Raman spectra of MnFe\textsubscript{x} samples.

In order to further verify Jahn-Teller distortion, Raman spectra are analysed as shown in Fig. S3. The Raman spectrum of α-MnO\textsubscript{2} displays a sharp band at around 630 cm\textsuperscript{-1}, which is a total symmetric vibration mode\textsuperscript{[3]}. The sharpness of this band indicates the lattice structure is highly symmetric. However, a splitting and/or broadening of this peak is observed after Fe doping, considering the full width at half maxima (FWHM)
of MnFe$_0$ (55.5 cm$^{-1}$) is much smaller than that of MnFe$_{0.4}$ (99.1 cm$^{-1}$) and MnFe$_{0.7}$ (143.4 cm$^{-1}$), which suggests the 630 cm$^{-1}$ peak is highly degenerated and the vibration symmetry is broken. Therefore, the Jahn-Teller distortion induced by Fe doping is proved, and a stronger distortion effect is observed on the high Fe-loaded sample.

Reference

