Electronic Supplementary Information (ESI) for

Zero-valent iron nanomaterial Fe\textsuperscript{0}@Fe\textsubscript{2}MnO\textsubscript{4} for ultrasensitive electroanalysis of As(III): Fe\textsuperscript{0} influenced surficial redox potential

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1. Experimental Section and Discussion

1.1 Chemical Reagents. Fe(acac)₃, Mn(acac)₃, oleic acid (OA, 90%), sodium oleate (SO) and benzyl ether were purchased from Alfa Aesar, China. Anodized aluminum-oxide (AAO) membranes with pore widths of ~300 nm and lengths of ~60 μm were purchased from Shanghai Shangmu Technology Co. Ltd. N₂ (99.999%) was purchased from Chenghong Gas, Nanjing, China. All chemicals were used as received without further purification.

1.2 Synthesis of Fe₂MnO₄ Nanoparticles. We prepared the Fe₂MnO₄ nanoparticles in a similar way as previously reported work, but replaced Co(acac)₂ by Mn(acac)₃.¹ Firstly, 560 mg Fe(acac)₃, 254 mg Mn(acac)₃, 600 mg SO and 4 mL OA were dissolved in 20 mL benzyl ether in a 50 mL three-neck flask at room temperature. Then the mixture was heated to 120 °C for 1 h under N₂ flow. During this time, a process to remove water and oxygen is necessary. After that, the reaction mixture was heated to 290 °C for another 1 h with the protection of N₂. After cooling down to room temperature, the Fe₂MnO₄ nanoparticles was precipitated out by addition of ethanol and then re-dispersed in hexane with a concentration of 20 mg mL⁻¹ for further using.

1.3 Fabrication of Monolayer Tubular Fe⁰@Fe₂MnO₄ Nanoparticles. The self-assembly of nanoparticles into tubes is a reference to the work of Li et al.² In general, the OA-functionalized anodic aluminum oxide (AAO) membrane was immersed in as-prepared Fe₂MnO₄ nanoparticles solution (~ 2 mL) in a small glass vial. Then put the glass vial into an oven with 80 °C. The self-assembly of Fe₂MnO₄ nanoparticles into tubes will proceed with the fast solvent evaporation. After the hexane completely evaporation, the AAO membrane containing the as-assembled monolayer Fe₂MnO₄ nanoparticles was calcined at 500 °C for 2 h in H₂/Ar (5% H₂), which can reduce Fe₂MnO₄ into Fe⁰@Fe₂MnO₄ and carbonize the surface-coating OA ligands to a thin carbon shell. For comparison, the monolayer tubular Fe₂MnO₄ was synthesized under the calcination pure N₂. The final step is to remove the template of AAO using 6 M KOH. The product of carbon-covering monolayer tubular-Fe⁰@Fe₂MnO₄ and -
Fe$_2$MnO$_4$ nanoparticles were obtained after wash with water several times.

**1.4 Apparatus.** Electrochemical measurements were performed with SPCEs (Screen-Printed Carbon Electrode, DeltBio, Shanghai, China). The electrochemical cell consists of a three-electrode arrangement with a SPCE (3 mm diameter) serving as the working electrode; carbon served as the counter electrode. A silver pseudo-reference electrode completes the circuit. All measurements were performed with a CHI 660D computer-controlled potentiostat (ChenHua Instruments Co., Shanghai, China). The SEM images were taken using a field-emission scanning electron microscope (FESEM, Quanta 200 FEG, FEI Company, USA). The transmission electron microscopy (TEM) and high resolution TEM (HRTEM) as well as EDS analyses were performed using a JEM-2010 transmission electron microscope operating at 200 kV (Quantitative method: Cliff Lorimer thin ratio section). The high angle annular dark field scanning transmission electron microscopy (HAADF-STEM) is operated on aberration-corrected scanning transmission electron microscope (Ac-STEM, JEOL ARM-200F). The X-ray diffraction (XRD) patterns of the samples were obtained with a Philips X’Pert Pro X-ray diffractometer with Cu Kα radiation (1.5418Å). X-ray photoelectron spectroscopy (XPS) measurements were operated using a VG ESCALAB MKII spectrometer with an Mg Ka X-ray source (1253.6eV, 120W) at a constant analyzer.

**1.5 Fabrication of Fe$_0$@Fe$_2$MnO$_4$ Modified Screen-Printed Carbon Electrode.**
The synthesized Fe$_0$@Fe$_2$MnO$_4$ were added to water and ultrasonicated for 1 min to obtain a 0.3 mg mL$^{-1}$ suspension. To fabricate the modified electrode, 7 μL of the suspension was pipetted onto the surface of the carbon working electrode in SPCE and evaporated under room temperature to obtain the Fe$_0$@Fe$_2$MnO$_4$ SPCE. For comparison, the Fe$_2$MnO$_4$ SPCE were prepared in the same way.

**1.6 Electrochemical Test.** The Fe$_0$@Fe$_2$MnO$_4$ nanoparticles modified screen-printed carbon electrode (SPCE) served as the working electrode for arsenic detection with square wave anodic stripping voltammetry (SWASV) under optimized conditions. The as-prepared Fe$_0$@Fe$_2$MnO$_4$ SPCE was dipped in a stirred analyte solution of 0.1
M HAc-NaAc (pH 5.0) containing As(III) and kept at −1.0 V for 120 s. The anodic stripping was performed from −0.5 to 0.6 V. After each measurement, the modified electrode was regenerated in a freshly stirred supporting electrolyte by desorption at 0.6 V for 120 s to remove the previous residual As(0) from the electrode surface. For comparison, other modified electrodes were used with the same processes and conditions.

1.7 Adsorption Experiments. The physical adsorption experiments: in order to be consistent with electrochemical sensing conditions, all the adsorption measurements were performed in 0.1 M HAc-NaAc (pH 5.0 ± 0.2). To start the experiment, 10 mg of the individual sorbent was introduced into 10 mL aqueous solution containing As(III) using a 15 mL centrifuge tube, and then the solutions were shaken at 298 K for 24 h to ensure the sorption process reach equilibrium. The water used here were all operated with the process of deoxygenated by N₂. The solid and liquid phases were separated by centrifugation at 4000 rpm for 3 min, and the solid was dried using freezing dryer with high vacuum for further XPS and HRTEM analysis. The adsorption experiments with negative potential (electro-adsorption): the process of electro-adsorption is the same as the electrochemical concentration process of detection. The modified electrodes were immersed in 0.1 M HAc-NaAc (pH 5.0) containing As(III) with applying −1.0 V for 120 s. Then take out of the electrode for further characterization of XPS analysis.

1.8 Evidence of Fe⁰ Promoted Surface Fe(II)/Fe(III) Experiments. We study the structural differences between the Fe⁰@Fe₂MnO₄ and Fe₂MnO₄ nanoparticles in detail by high-angle annular dark field-scanning transmission electron microscopy (HAADF-STEM). The adsorption experiments of As(III) on both Fe⁰@Fe₂MnO₄ and Fe₂MnO₄ nanoparticles are all performed, including simple adsorption, adsorption with potential and stripping during the detection. We further show the valence and binding states change of As(III), O and Fe(III) on adsorption samples by X-ray photoelectron spectroscopy (XPS).
1.9 Simulation Method. The electrocatalytic reactions of A/B mediated by X/Y is expressed as Eqn. (1)-(4):

\[ A^{\text{sol}} \xleftrightarrow{k_{\text{ads}}^{\text{sol}}} A^{\text{ads}} \quad \text{\textcopyright MERGEFORMAT (1)} \]

\[ A^{\text{ads}} + 3e^{-} \xleftrightarrow{k_{\text{AB,lat}}^{\text{ads}}} B^{\text{ads}}, E_{\text{LAB}} \quad \text{\textcopyright MERGEFORMAT (2)} \]

\[ A^{\text{ads}} + X \xrightarrow{k_{\text{on}}} B^{\text{ads}} + Y \quad \text{\textcopyright MERGEFORMAT (3)} \]

\[ Y + e^{-} \xleftrightarrow{k_{\text{xy}}} X, E_{\text{LXY}} \quad \text{\textcopyright MERGEFORMAT (4)} \]

The mass transport of A(sol) is simply modelled by Fick’s Second Law:

\[ \frac{\partial c_{A^{\text{sol}}}}{\partial t} = D_{A^{\text{sol}}} \nabla^2 c_{A^{\text{sol}}} \quad \text{\textcopyright MERGEFORMAT (5)} \]

Where \( c \) is the concentration, \( t \) is the reaction time and \( D_{A^{\text{sol}}} \) is the diffusion coefficient. \( D_{A^{\text{sol}}} \) is set as \( 10^{-7} \text{ m}^2\text{s}^{-1} \) considering that the solution is under stirring during the pre-concentration. As the aim of this model is to explore the influence of X/Y and it is seen from experimental data that the mass transport of A(sol) is not the rate-determining step, we set \( D_{A^{\text{sol}}} \) a relatively large value.

The reaction rate equations determined by the adsorption of A(sol), the direct electron transfer of A/B, the mediated reduction of A and the electron transfer of X/Y are described as following:

\[ -D_{A^{\text{sol}}} \nabla c_{A^{\text{sol}}} = -k_{\text{ads}} c_{A^{\text{sol}}} + k_{\text{des}} \Gamma_{A^{\text{ads}}} \quad \text{\textcopyright MERGEFORMAT (6)} \]

\[ \frac{\partial \Gamma_{A^{\text{ads}}}}{\partial t} = k_{\text{ads}} c_{A^{\text{sol}}} - k_{\text{des}} \Gamma_{A^{\text{ads}}} - k_{\text{AB,lat}} \exp\left(-0.5 \frac{F (E - E_{\text{LAB}})}{RT}\right) \Gamma_{A^{\text{ads}}} \]

\[ + k_{\text{AB,ox}} \exp\left(0.5 \frac{F (E - E_{\text{LAB}})}{RT}\right) \Gamma_{B^{\text{ads}}} - k_{\text{cat}} \Gamma_{A^{\text{ads}}} \Gamma_{X} \quad \text{\textcopyright MERGEFORMAT (7)} \]
\[
\frac{\partial \Gamma_{\text{B(ads)}}}{\partial t} = -k_{\text{ads}} c_{\text{A(sol)}} + k_{\text{des}} \Gamma_{\text{A(ads)}} + k_{\text{AB,red}} \exp\left(-0.5 \frac{F(E - E_{\text{LA}})}{RT}\right) \Gamma_{\text{A(ads)}} - k_{\text{AB,ox}} \exp\left(0.5 \frac{F(E - E_{\text{LA}})}{RT}\right) \Gamma_{\text{B(ads)}} + k_{\text{cat}} \Gamma_{\text{A(ads)}} \Gamma_{\text{X}} \]
\]
MERGEFORMAT (8)

\[
\frac{\partial \Gamma_{\text{X}}}{\partial t} = -\frac{\partial \Gamma_{\text{Y}}}{\partial t} = -k_{\text{cat}} \Gamma_{\text{A(ads)}} \Gamma_{\text{X}} + k_{\text{el,XY}} \exp\left(-0.5 \frac{F(E - E_{\text{LY}})}{RT}\right) \Gamma_{\text{Y}} - k_{\text{el,XY}} \exp\left(0.5 \frac{F(E - E_{\text{LY}})}{RT}\right) \Gamma_{\text{X}} \]
\]
MERGEFORMAT (9)

\[E\] is the applied potential (V), \(F\) is the Faraday constant, \(R\) is the gas constant and \(T\) is the room temperature which we set as 298.15 K. The meaning of other parameters has been explained in the main text. We simulated the overall reaction procedure including a pre-concentration step and a stripping step. The electrochemical conditions set to the simulation model is the same as the optimum experimental conditions. Here we set the initial surface coverage of \(X\) to be \(10^{-7}\) mol m\(^{-2}\) and during reaction the sum of \(X\) and \(Y\) is always \(10^{-7}\) mol m\(^{-2}\). Previous study reported that a 4 nm \(\text{Fe}_3\text{O}_4\) nanoparticle has ca. 30 active iron sites.\(^3\) The assumption of a \(10^{-7}\) mol m\(^{-2}\) \(X\) in Figure 7b corresponds to a very low density of active sites (only 1 active site on a 4 nm-diameter nanoparticle).

1.10 Electrochemical Characterization and the Optimized Experimental Conditions. Before the detection, the electrochemical characterization and the optimized experimental conditions of the \(\text{Fe}^0@\text{Fe}_2\text{MnO}_4\) SPCE are studied as presented in Fig. S8 and S9 (ESI†). Probing by cyclic voltammetry and electrochemical impedance spectra (Fig. S8, ESI†), the \(\text{Fe}^0@\text{Fe}_2\text{MnO}_4\) SPCE exhibits a better conductivity than bare SPCE and \(\text{Fe}_2\text{MnO}_4\), which benefits from the core \(\text{Fe}^0\). The optimal conditions are determined as 0.1 M HAc-NaAc (pH 5.0) with -1.0 V for 120 s pre-concentration time and the electrode modified with 7 \(\mu\)L volume of 0.3 mg mL\(^{-1}\) \(\text{Fe}^0@\text{Fe}_2\text{MnO}_4\) suspension (Fig. S9, ESI†).
1.11 Investigate on Stability and Reproducibility. Besides, the stability of \( \text{Fe}^0@\text{Fe}_2\text{MnO}_4 \) nanoparticles is tested with 10 ppb As(III) for 15 consecutive and repetitive stripping (Fig. S14a). The relative standard deviation (RSD) is only 1.41%, which proves the stability of the fabricated electrode. We also examine three different \( \text{Fe}^0@\text{Fe}_2\text{MnO}_4 \) SPCE, the peak shape shows slight shift and the peak current is almost identical (Fig. S14b), indicating that the fabricated sensor has excellent reproducibility.

2. Figures

![Cross section images](image1.png)

**Fig. S1** Cross section images of the anodic aluminum oxide (AAO) template a) without and b) with self-assembled monolayer \( \text{Fe}_2\text{MnO}_4 \). c) Low-magnification scanning electron microscope (SEM) and d) high-resolution scanning electron microscope (HRSEM) images of as-synthesized \( \text{Fe}^0@\text{Fe}_2\text{MnO}_4 \). e) TEM and f) HAADF-STEM images of monolayer tubular \( \text{Fe}_2\text{MnO}_4 \).
Fig. S2 a) HAADF-STEM image and b-f) the corresponding elemental energy dispersive spectrometer (EDS) mapping images of as-synthesized Fe@Fe₂MnO₄ nanoparticles.

Fig. S3 EDS pattern of prepared Fe@Fe₂MnO₄.

Fig. S4 HRTEM image of Fe@Fe₂MnO₄ nanoparticles.
Fig. S5 a) HAADF-STEM image and b) the corresponding EDS elemental overlay image of Fe@Fe₂MnO₄ nanoparticles after adsorption of 1 ppm As(III). c) EDS spectra of core (i.e. the area in curve I of Figure j) and shell (curve II in Figure j) on Fe@Fe₂MnO₄ nanoparticles, inset is the atomic ratio of Fe and O.

Fig. S6 a), b) HRTEM and c) HAADF-STEM image of Fe₂MnO₄ nanoparticles. Insets in c) is the corresponding X-ray diffraction (XRD) pattern.

Fig. S7 High-resolution XPS spectra of Mn on the Fe@Fe₂MnO₄ and Fe₂MnO₄.
Fig. S8  a) Cyclic voltammograms and b) Nyquist diagram of electrochemical impedance spectra of the bare, Fe$^0$@Fe$_2$MnO$_4$ and Fe$_2$MnO$_4$ SPCE, respectively.

Fig. S9  Optimum the detection experimental conditions. Influence of a) supporting electrolytes; b) pH value; c) deposition potential; d) deposition time and e) modified volume on the response to 10 ppb As(III) on Fe$^0$@Fe$_2$MnO$_4$ SPCE.

Fig. S10  High-resolution XPS spectra of As on Fe$_2$MnO$_4$ nanoparticles under different condition: a) with 1 ppm As(III) in solution, b) with applying negative potential, c) stripping after electro-adsorption.
**Fig. S11** a) HAADF-STEM image and corresponding EDS element maps of b) Fe, c) Mn, d) O and e) As of Fe$^0$@Fe$_2$MnO$_4$ nanoparticles after adsorption of 1 ppm As(III).

**Fig. S12** a) HAADF-STEM image and corresponding EDS element mappings of b) Fe, c) Mn, d) O and e) As of Fe$_2$MnO$_4$ nanoparticles after adsorption of 1 ppm As(III). f) HAADF-STEM image and g) the corresponding EDS elemental overlay image of the four elements of Mn, Fe, As and O of Fe$_2$MnO$_4$ after adsorption of 1 ppm As(III). h) EDS spectra of core (i.e. the area in curve I of Figure g) and shell (curve II in Figure g) on Fe$_2$MnO$_4$, inset is the atomic ratio of Fe and O.

**Fig. S13** High-resolution XPS spectra of Mn on Fe$^0$@Fe$_2$MnO$_4$, Fe$^0$@Fe$_2$MnO$_4$ in
HAc-NaAc for three days, with 1 ppm As(III) in solution, with applying negative potential and stripping after electro-adsorption.

Fig. S14 a) Current change of 10 ppb of As(III) for 20 consecutive and repetitive stripping voltammetric measurements on the Fe@Fe$_2$MnO$_4$, inset is the corresponding SWASV response. b) The response of 10 ppb As(III) at three Fe@Fe$_2$MnO$_4$ SPCE after storage at room temperature for 30 days.
Fig. S15 a) The current change of 10 ppb As(III) in the addition of 50-400 ppb Cu(II) on Feₐ@Fe₃MnO₄ SPCE, inset is the corresponding SWASV response. b) The detection of As(III) in real sample with standard additions in the presence of 10 ppb Cu(II), inset is the corresponding linear calibration plot.
3. Table

**Table S1.** A comparison of detection performance of the Au-based (electro)chemical sensors for the analysis of As(III).

<table>
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<tr>
<th>Electrode</th>
<th>Electrolyte (pH)</th>
<th>Linear range (ppb)</th>
<th>Sensitivity (μA ppb⁻¹)</th>
<th>LOD (ppb)</th>
<th>Ref.</th>
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<tr>
<td>Au-coated BDD</td>
<td>1 M HCl</td>
<td>0.1–40</td>
<td>–</td>
<td>0.005</td>
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<tr>
<td>Au-UMEA</td>
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<td>Au-NEE</td>
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<td>sonically assisted gold microdisk electrode</td>
<td>0.1 M HNO₃</td>
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<td>0.363</td>
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<td>Au(111)-like polycrystalline gold electrode</td>
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<td>0–1125</td>
<td>0.3636</td>
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<td>MWCN Ts/gold electrode</td>
<td>0.1 M acetic bu Luna (pH 4.0)</td>
<td>10–50</td>
<td>0.236</td>
<td>–</td>
<td>9</td>
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<tr>
<td>Au NPs/GCE</td>
<td>1 M HNO₃</td>
<td>0.5–15</td>
<td>0.024</td>
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<td>Au NPs/GCE</td>
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<td>0.1–15</td>
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<td>0.002</td>
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<td>Au NPs/GCE</td>
<td>1 M HCl</td>
<td>0–7.5</td>
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<td>Au NPs-SPE</td>
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<td>0–250</td>
<td>–</td>
<td>0.4</td>
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<td>3D Au nanodendrite network</td>
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<td>AuNPs-CNTs</td>
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<td>CNT/Au NPs-GC/GCE</td>
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<td>Au/Fe₃O₄-RTIL/SPCE</td>
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Table S2. Simulation parameters used in Figure 4

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4. References

2944-2951.


