

Supplementary information for New Journal of Chemistry

Understanding of 3D hierarchically porous carbon modified electrode based on finite element modeling

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Table S1. Kinetic parameters used in numerical simulation presented in Figure 3a.

Symbol	Value	Definition and units
A	6.49×10^{-6}	Electrode area/ (m^2)
C_{dl}	1.04×10^{-6}	Capacitance/ (F m^{-2})
D_R	6.67×10^{-10}	Diffusion coefficient of ferrocyanide / ($\text{m}^2 \text{s}^{-1}$)
D_O	7.26×10^{-10}	Diffusion coefficient of ferricyanide / ($\text{m}^2 \text{s}^{-1}$)
E_{eq}	0.253	Equilibrium potential/ (V)
k^0	6.91×10^{-5}	Heterogeneous electron transfer rate constant/ (m s^{-1})
T	295 ± 2	Temperature (K)
α	0.51	Charge transfer coefficient/ (-)

Table S2. Kinetic parameters used in numerical simulation presented in Figure 4e.

Symbol	Value	Definition and units
E_{eq}	0.253	Equilibrium potential/ (V)
k^0	1.06×10^{-4}	Heterogeneous electron transfer rate constant/ (m s^{-1})

α	0.51	Charge transfer coefficient/ (-)
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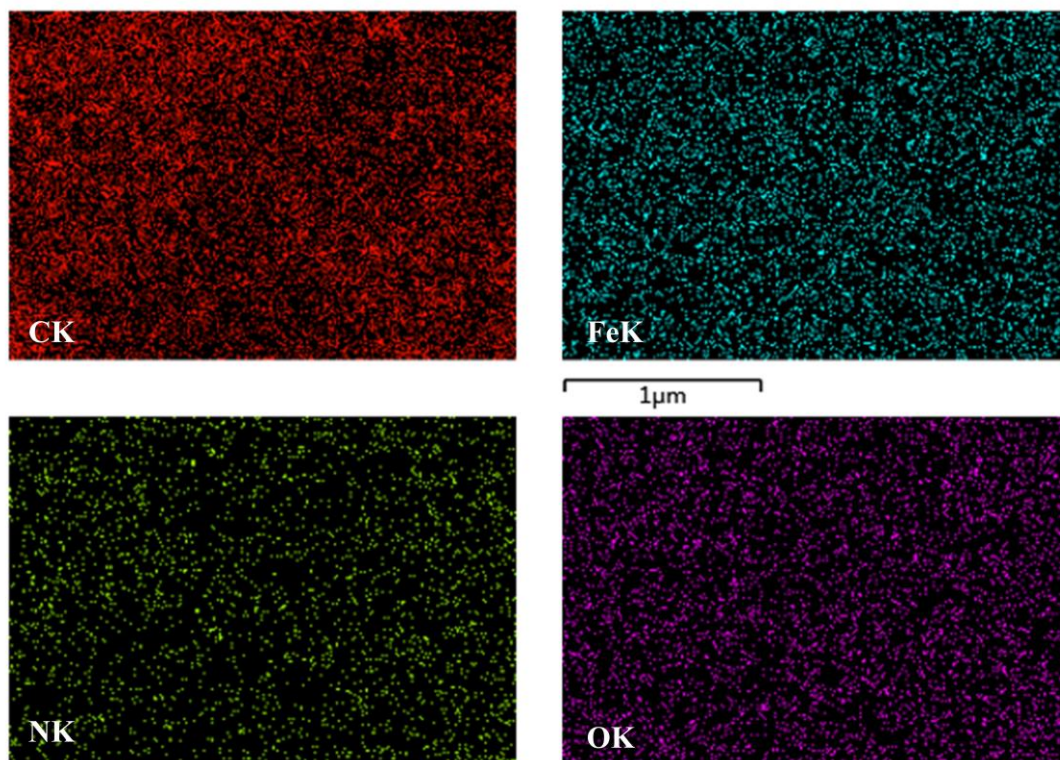


Fig. S1. Distribution of C, Fe, N and O on FeN-HPC via EDS spectrum.

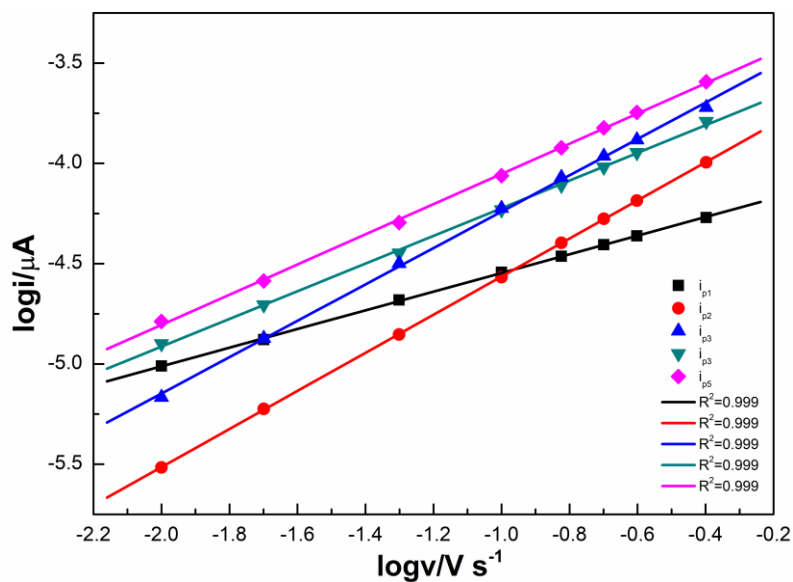


Fig. S2. Linear relationship between $\log i$ and $\log v$ of 2 mM ferrocyanide for i_{pa} on bare GC (black); $i_{0.1V}$ on 4 μg FeN-HPC modified electrode (red); $i_{0.1V}$ on 8 μg FeN-HPC modified electrode (blue); i_{peak} on 4 μg FeN-HPC modified electrode (dark cyan) and i_{peak} on 4 μg FeN-HPC modified electrode (magenta).

Table S3. Redox peak potential comparison between bare GC electrode and FeN-HPC modified electrode.

Symbol	Value	Definition and units
E_{pa}	0.29 ± 0.01	Anodic peak potential on GC electrode/ (V)
$E_{pa'}$	0.29 ± 0.02	Anodic peak potential on FeN-HPC electrode/ (V)
E_{pc}	0.21 ± 0.01	Cathodic peak potential on GC electrode/ (V)
$E_{pc'}$	0.21 ± 0.02	Cathodic peak potential on FeN-HPC electrode/ (V)

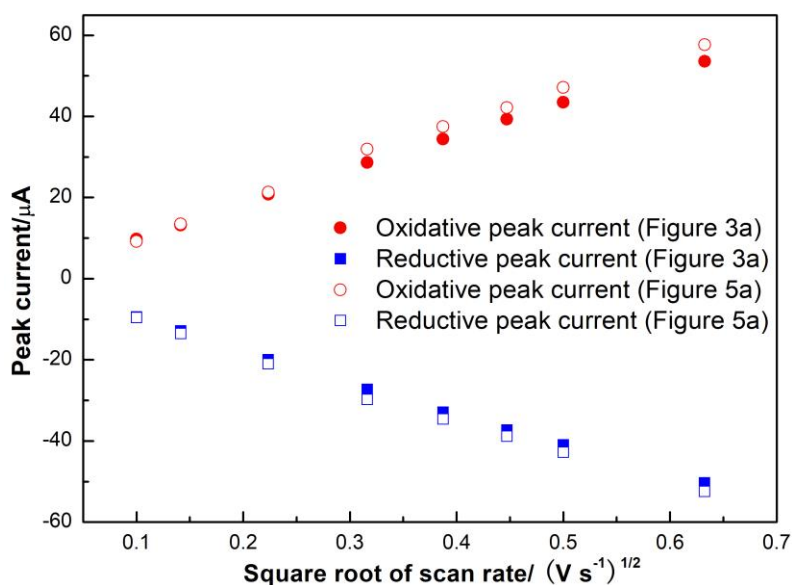


Fig. S3. Redox peak currents on bare GC electrode and FeN-HPC modified GC electrode.

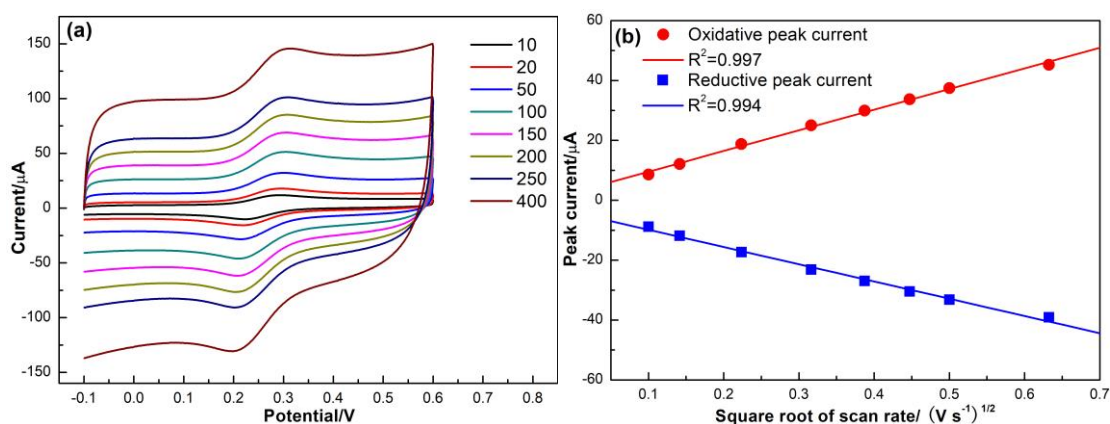


Fig. S4. Cyclic voltammograms of 2 mM potassium ferrocyanide on a FeN-HPC (4 μ g) modified working electrode immersing in a 0.5 M KCl solution for 48 h at various scan

rates (10-400 mV s^{-1}); (b) Plots of corresponding anodic and cathodic peak currents as a function of the square root of scan rates.

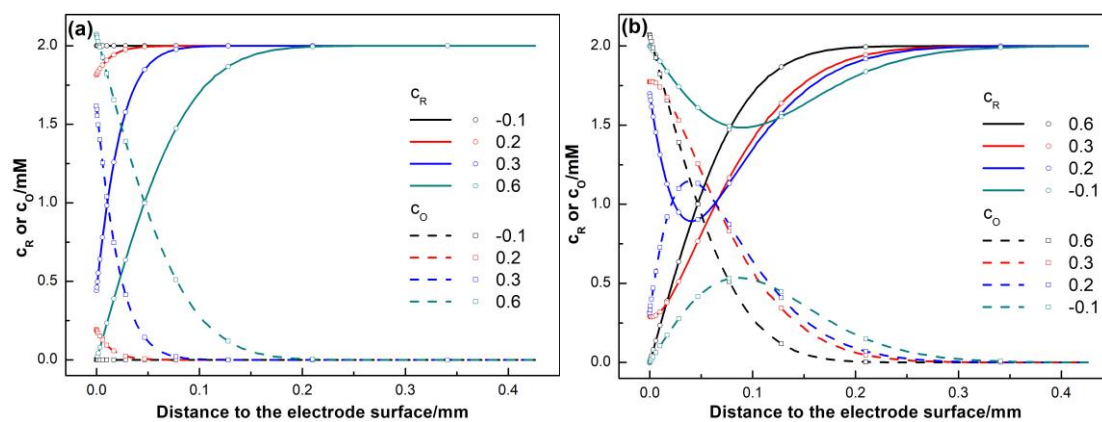


Fig. S5. Comparison of concentrations of both the ferrocyanide (solid lines) and ferricyanide (dashed lines) on bare GC electrode (dot lines) and FeN-HPC modified electrode (solid/dashed lines) at (a) the forward and (b) reversed scan of cyclic voltammetry at different potentials applied ($v=100 \text{ mV s}^{-1}$).

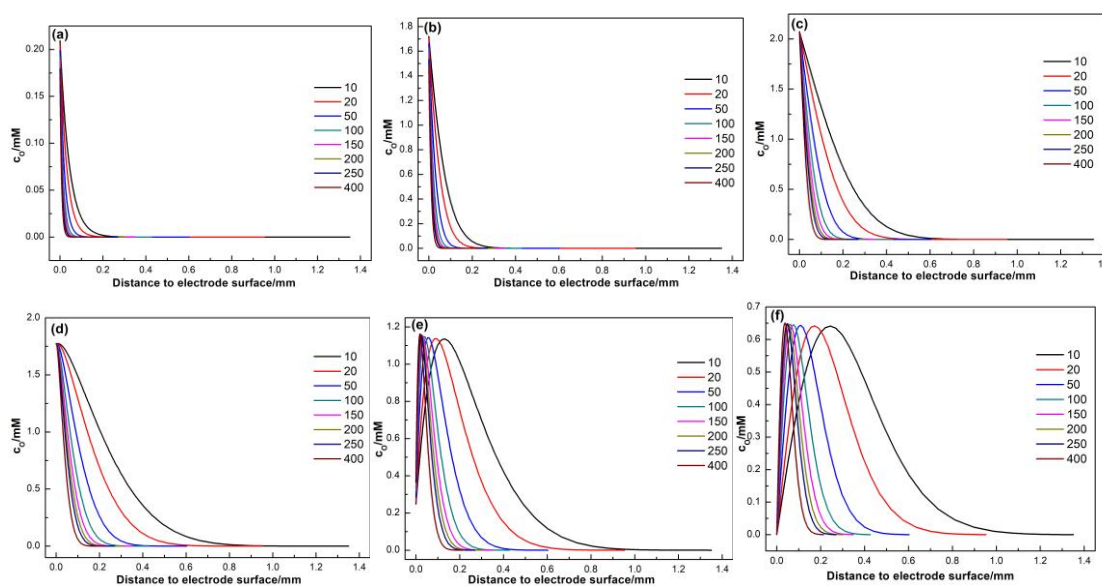


Fig. S6. Concentrations of ferricyanide (c_O) at various potentials applied at (a) 0.2 V; (b) 0.3 V; (c) 0.6 V; (d) 0.3 V (reversed scan); (e) 0.2 V (reversed scan) and (f) 0.0 V (reversed scan) along the distance to the working electrode surface at different scan rates (400-10 mV s^{-1}).

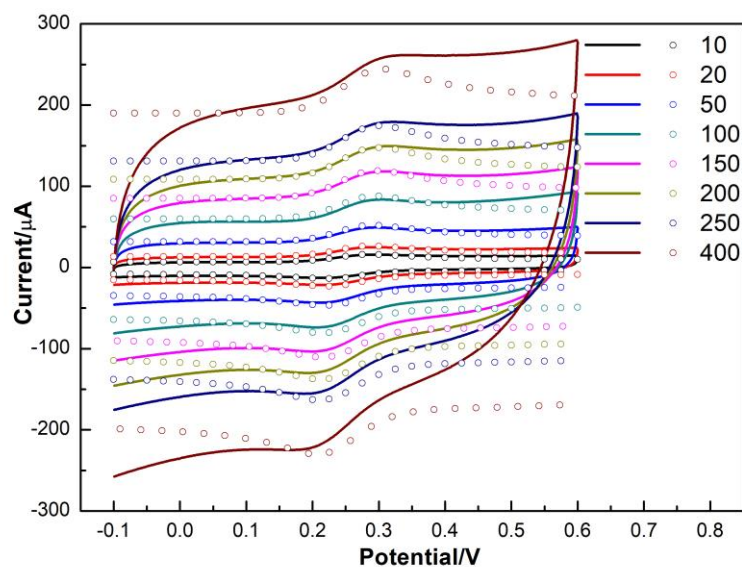


Fig. S7. Cyclic voltammograms (– Experimental data; ○ Simulated data) of 2 mM potassium ferrocyanide on a FeN-HPC (8 μg) modified working electrode immersing in a 0.5 M KCl solution for 48 h at various scan rates (10–400 mV s^{-1}).

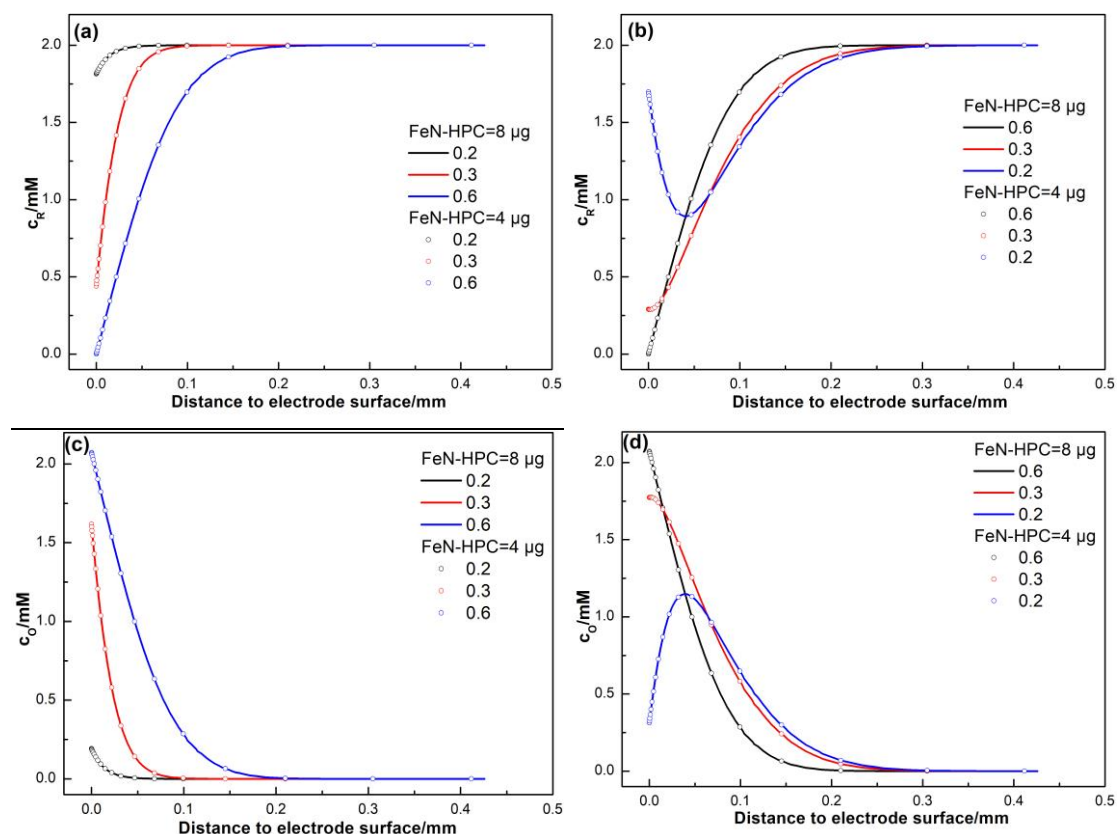


Fig. S8. Comparison of theoretical concentrations of ferrocyanide (c_R) on different FeN-HPC loads at (a) the forward and (b) reversed scan of cyclic voltammetry at different potentials applied ($v=100 \text{ mV s}^{-1}$); Comparison of theoretical concentrations

of ferricyanide (c_0) on different FeN-HPC loads at (c) the forward and (d) reversed scan of cyclic voltammetry at different potentials applied ($\nu=100 \text{ mV s}^{-1}$).