Supporting Information

Synthesis of water-soluble phosphonate functionalized single-walled carbon nanotubes and their applications in biosensing

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Molecular dynamics theory

For all simulations presented here, the SPC/E75 water model was used. All molecular dynamics (MD) simulations were performed using the AMBER 9 suite of programs.[1] The charge distributions on all atoms in NYPA-PO_3^{2-} were obtained using the RESP-fit method[2,3] based on B3LYP/cc-pVTZ density functional theory (DFT) calculations.[4-7] The atomic charges used in the simulation are shown in Fig. S1. The atomic charges of carbon atoms of SWNT are set to zero, the force filed for SWNTs were used as σ_{cc}=3.40 Å, ε_{cc}=0.086 kcal.[8] The force field for NYPA-PO_3^{2-} was generated by parmchk.

The simulation and analysis of trajectories of SWNTs were also performed using the AMBER 9.0 program. Boxes of systems were prepared by immersing SWNTs into a cubic box containing 68 NYPA-PO_3^{2-} molecules and 7062 SPC/E water molecules and 68 Na^+ ions were added to neutralize the charge of the system. The resulting final cuboid boxes for pure water, 67×70×77 Å, respectively. The system was minimized with a total of 2500 steps: 1000 of steepest descent, followed by 1500 steps of conjugate gradient minimization. After that, the system was heated to 360 K for 20 ps and equilibrated for 1 ns at 360 K, followed by 200 ps of cooling from 360 to 300 K. The production run of 10 ns was used for data analysis, with the data being collected every 0.5 ps. The atomic coordinates of SWNTs were constrained during MD simulations. All carbon atoms of the CNT were fixed, however NYPA were relaxed.

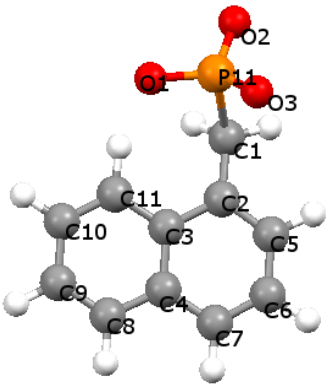

Fig. S1 Structure of NYPA-PO_3^{2-}.

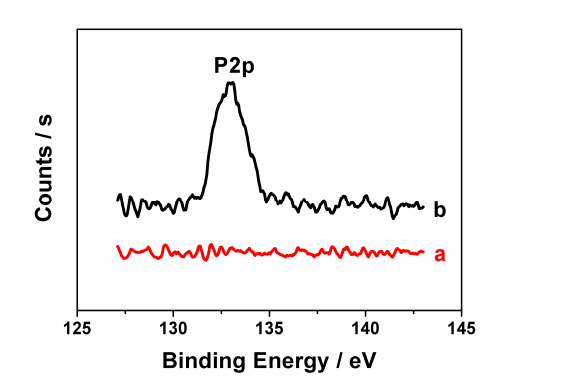

Fig. S2 XPS spectra of (a) pristine SWNTs and (b) NYPA-SWNTs hybrids in the P2p region.

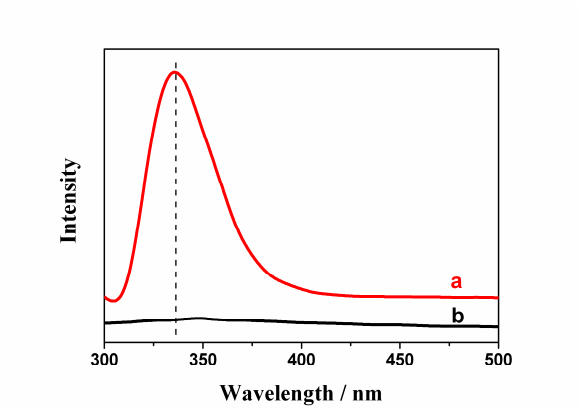

Fig. S3 Normalized fluorescence spectra of (a) NYPA and (b) NYPA-SWNTs hybrids.[9]

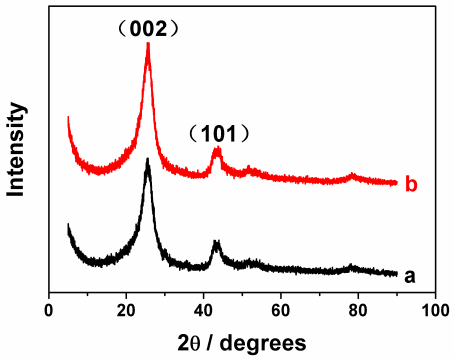

Fig. S4 XRD patterns of (a) pristine SWNTs and (b) NYPA-SWNTs hybrids.

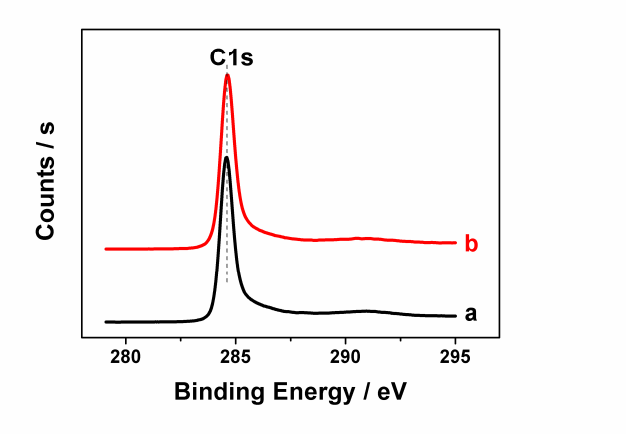

Fig. S5 XPS spectra of (a) pristine SWNTs and (b) NYPA-SWNTs hybrids in the C 1s region.

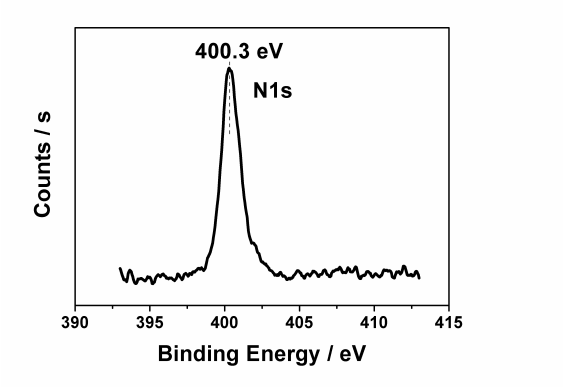

Fig. S6 XPS spectrum of Mb/NYPA-SWNTs hybrids in the N 1s region.

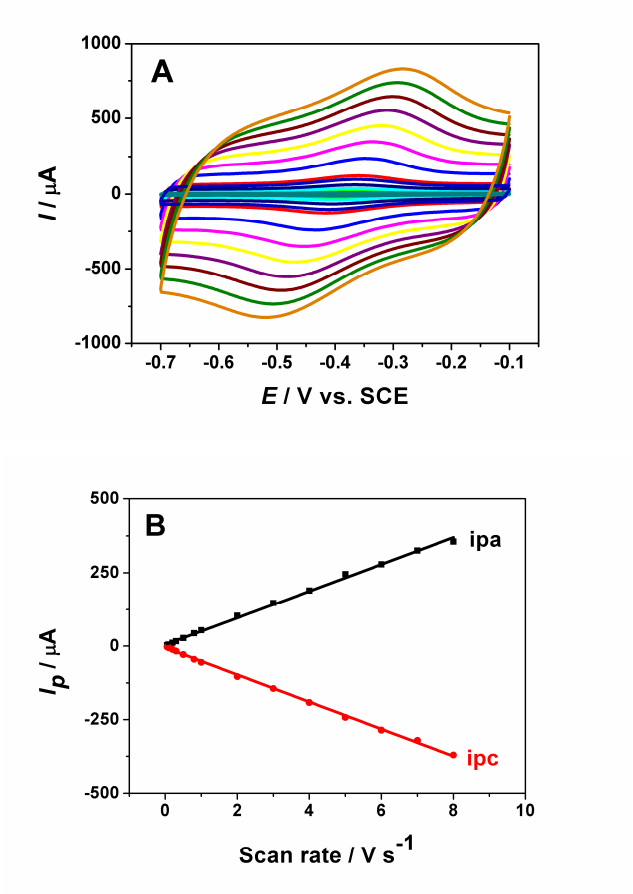

Fig. S7 (A) Cyclic voltammograms of the Nafion/Mb/NYPA-SWNTs/GC electrode in a 0.1 M PBS (pH 7.0) at scan rates of 50, 80, 100, 200, 300, 500, 800, 1000, 2000, 3000, 4000, 5000, 6000, 7000 and 8000 mVs^{-1} (from inner to outer), respectively. (B) Plots of the corresponding cathodic and anodic peak currents vs. scan rate.

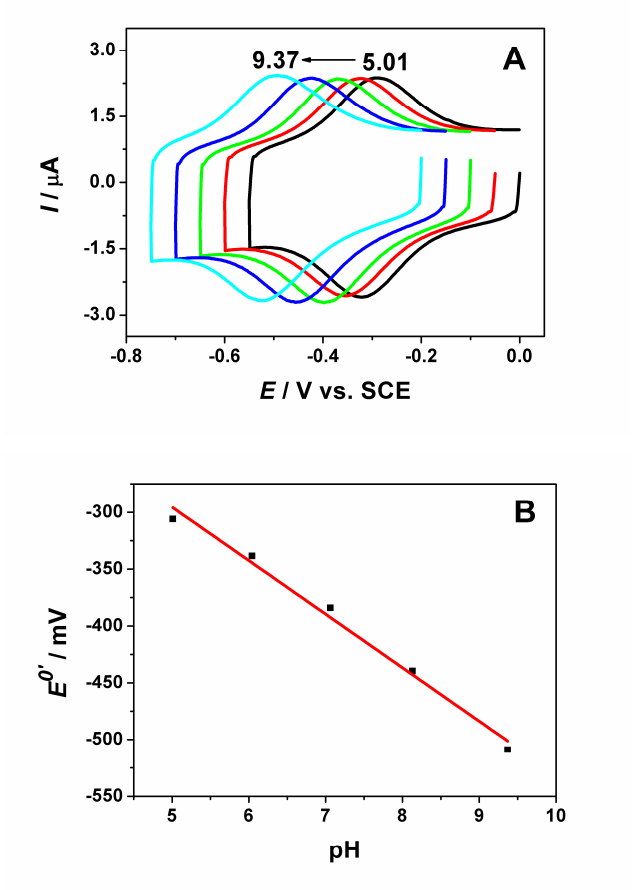

Fig. S8 (A) Cyclic voltammograms of the Nafion/Mb/NYPA-SWNTs/GC electrode in a 0.1 M PBS at different pH value of 5.01, 6.04, 7.06, 8.13 and 9.37 (from right to left) at a scan rate of 50 mVs^{-1}. (B) Effect of pH on the formal potential ($E^{0'}$).

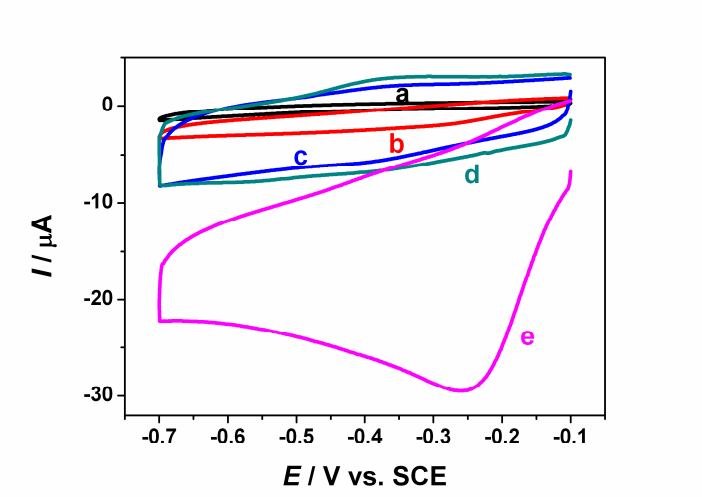

Fig. S9 Cyclic voltammograms of (a) GC, (b) Nafion/Mb/GC, (c) Nafion/Mb/SWNTs/GC, (d) Nafion/NYPA-SWNTs/GC and (e) Nafion/Mb/NYPA-SWNTs/GC electrodes in a 0.1 M PBS (pH 7.0) containing 1.98 mM H_2O_2 at a scan rate of 50 mV s^{-1}.

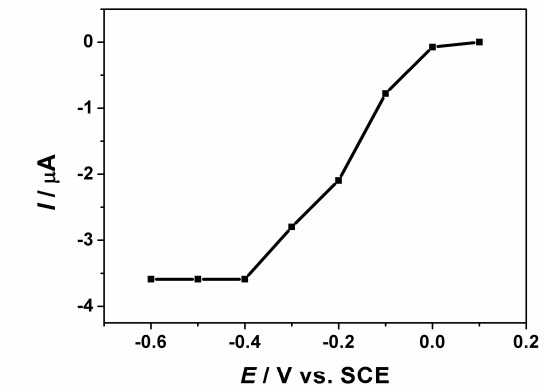

Fig. S10 Dependence of the current response of Nafion/Mb/NYPA-MWCNTs/GC electrode to 5.0×10^{-5} M H_2O_2 on the applied potentials (pH 7.0).

Notes and references

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