

Online Supporting Information for

Enhanced Catalytic and Supercapacitor Activities of DNA encapsulated β -MnO₂ Nanomaterials

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Instruments.

The synthesized DNA encapsulated β -MnO₂ nanomaterials were characterized using several spectroscopic techniques. The UV-Visible (UV-Vis) absorption spectra were recorded in a Unico (model 4802) UV-Vis-NIR spectrophotometer equipped with a 1 cm quartz cuvette holder for liquid samples. The transmission electron microscopy (TEM) analysis was done with a Tecnai model TEM instrument (TecnaiTM G2 F20, FEI) with an accelerating voltage of 200 KV. The Energy Dispersive X-ray Spectroscopy (EDS) analysis was done with the Field Emission Scanning Electron Microscopy (FE-SEM) instrument (Zeiss ultra FE-SEM instruments) with a separate EDS detector (INCA) connected to that instrument. The X-ray diffraction (XRD) analysis was done using a PAN analytical Advanced Bragg-Brentano X-ray powder diffractometer (XRD) with Cu K α radiation ($\lambda = 0.154$ nm) with a scanning rate of 0.020 s⁻¹ in the 2θ range 10-90°. The LASER Raman measurements were carried out with Renishaw inVia Raman Microscope using an excitation wavelength of 632.8 nm (He-Ne laser). The excitation light intensity in front of the objective was ~10 mW with a spectral collection time of 1 sec for Raman experiment. The integration time for our measurement was set to 10 sec. The X-ray photoelectron spectroscopic (XPS) analysis was done to check the chemical composition and the state of elements present in the outermost

part of materials and analyzed by using Theta Probe AR-XPS System, Thermo Fisher Scientific (U.K). The Fourier Transform Infrared (FT-IR) spectroscopy analysis was done with the model Nexus 670 (FTIR), Centaurms 10X (Microscope) having spectral Range 4,000 to 375 cm^{-1} with a MCT-B detector. The ^1H NMR study was done with Bruker (Germany), 400 MHz, FT-NMR spectrometer. All the electrochemical experiments were examined using an AUTOLAB PGSTAT302N electrochemical work station in 1 M Na_2SO_4 aqueous solution.

Preparation of samples for other characterizations.

The synthesized DNA encapsulated $\beta\text{-MnO}_2$ nanomaterials were characterized using UV-Vis, TEM, EDS, XRD, Raman, XPS and FT-IR analysis studies. The DNA- MnO_2 nanomaterials solution was directly used for the measurement in UV-Vis spectrophotometer. The same liquid solution containing DNA- MnO_2 used for UV-Vis study was used for TEM sample preparation and other thin films preparation. The samples for TEM was prepared by placing a drop of the corresponding DNA- MnO_2 nanomaterials solution onto a carbon coated Cu grid followed by slow evaporation of solvent at ambient conditions. For EDS, XRD, Laser Raman, XPS, and FT-IR analysis, glass slides were used as substrates for thin film preparation. The slides were cleaned thoroughly in acetone and sonicated for about 30 min. The cleaned substrates were covered with the DNA- MnO_2 nanomaterials solution and then dried in air. After the first layer was deposited, subsequent layers were deposited by repeatedly adding more MnO_2 nanomaterials solution and drying. Final samples were obtained after 6-8 depositions and then analyzed using the above techniques. For catalysis study, the reaction procedure is given in the discussion of catalysis reaction section under main text.

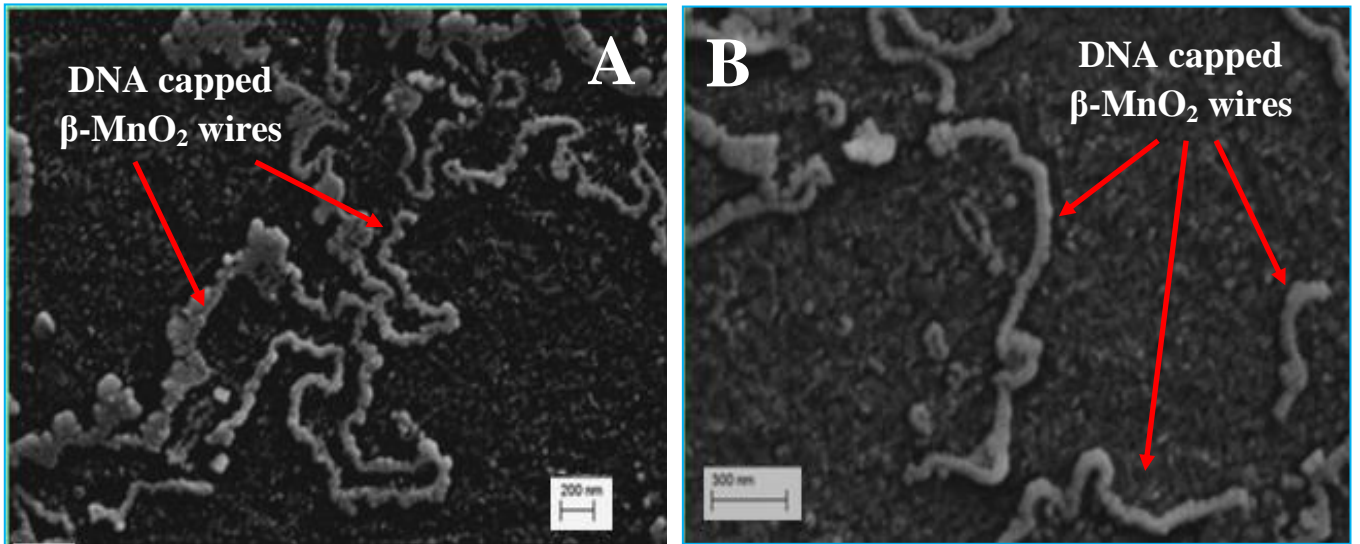


Figure S-1: Low (A) and high (B) magnified FE-SEM image of DNA encapsulated β -MnO₂ nano-wires.

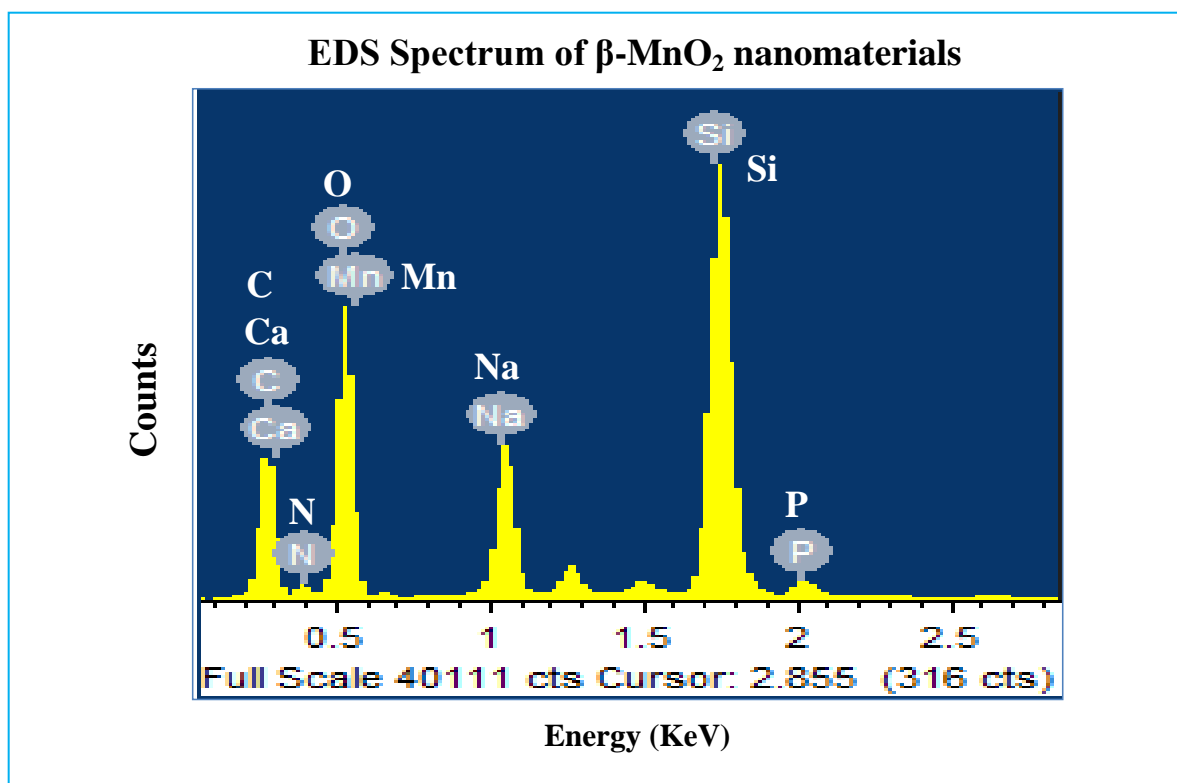


Figure S-2: The energy dispersive X-ray spectroscopic (EDS) analysis of β -MnO₂ nanomaterials on DNA scaffold which consists of the peaks for C, N, O, Si, Mn and P.

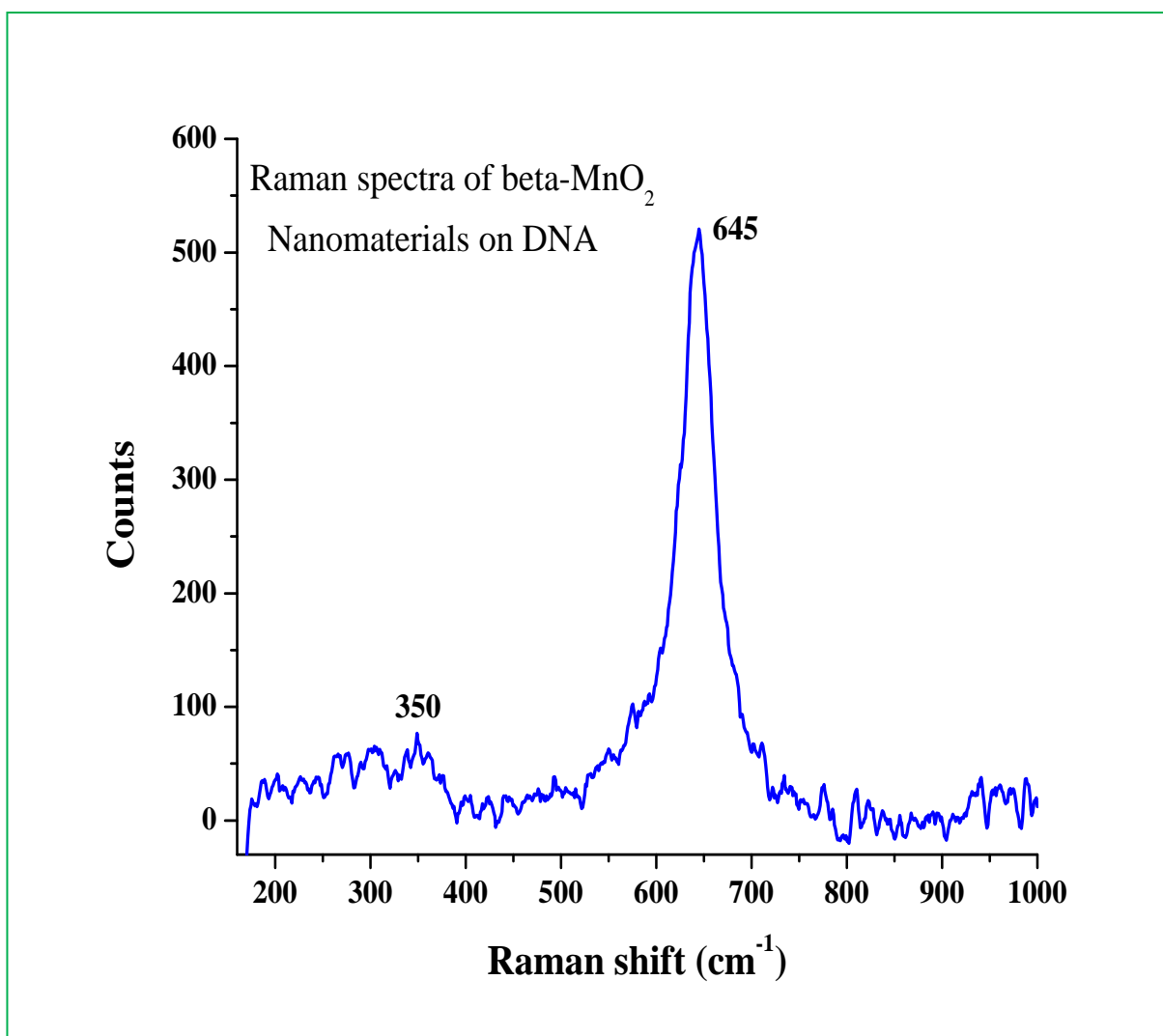


Figure S-3: The Laser Raman spectra of the β -MnO₂ nanomaterials on DNA scaffold.

FT-IR bands - de-oxyribo nucleic acid (DNA)-Experimental and Reported values		
FT-IR bands (cm⁻¹) (experimentally observed)	FT-IR frequency range (cm-1) (reported value)⁴¹	Absorbing bonds/vibration types
3611	3100-3750	v (OH group in DNA/water)
2987-2890	2800-2950	Symmetric stretching vibration (C-H bonds in -CH ₂ group)
1683, 1750	1732-1595	C=O, C-N, N-H ⁴¹
-	1492-1480	Bending (δ) of C-H bond in CH ₂ ⁴¹
1108-1213, 1281	1170-1300	Asymmetric stretching of PO ₂ - group
1108-1213	1140-990	v (C-O-C, C-C) ⁴¹
821	800-1000	De-oxyribose region

Table T-1: The experimentally observed FT-IR bands of herring testes DNA, the comparison with the reported value and the corresponding peak assignments of different peaks are elaborated.