# Online Supporting Information's for

# DNA mediated wire-like clusters of self-assembled $TiO_2$ nanomaterials: Supercapacitor and Dye Sensitized Solar Cell Applications

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**Instruments.**

The synthesized shape-selective DNA-$TiO_2$ 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 (Tecnai$^{TM}$ 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 $K_\alpha$ radiation ($\lambda$ = 0.154178 nm) with a

scanning rate of 0.020 $s^{-1}$ in the $2\theta$ 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 photoluminescence (PL) study was done with Varian (Cary Eclipse Winflr) fluorescence spectrophotometer (serial number el02045776) both in excitation and emission mode using a xenon pump lamps. 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 400 $cm^{-1}$ with a MCT-B detector. The thermal analysis study was recorded with a thermal analyser-simultaneous TGA/DTA instrument with model name SDT Q600 and the analysis was performed in air. A hot air oven (temperature up to 1000 °C) was used to anneal the samples at specific temperature. All the electrochemical experiments were examined using an AUTOLAB PGSTAT302N electrochemical work station in 1 M $Na_2SO_4$ aqueous solution. For DSSC sample preparation, the thickness of working electrode was measured by SJ-301 surface roughness tester. The conductivity (current-voltage, I-V) measurement was performed by using a solar simulator having model number SS80AAA under the light illumination of 1000 $W/m^2$. A spin coater is used for coating the DNA-$TiO_2$ samples and purchased from Spektron Company, Chennai.

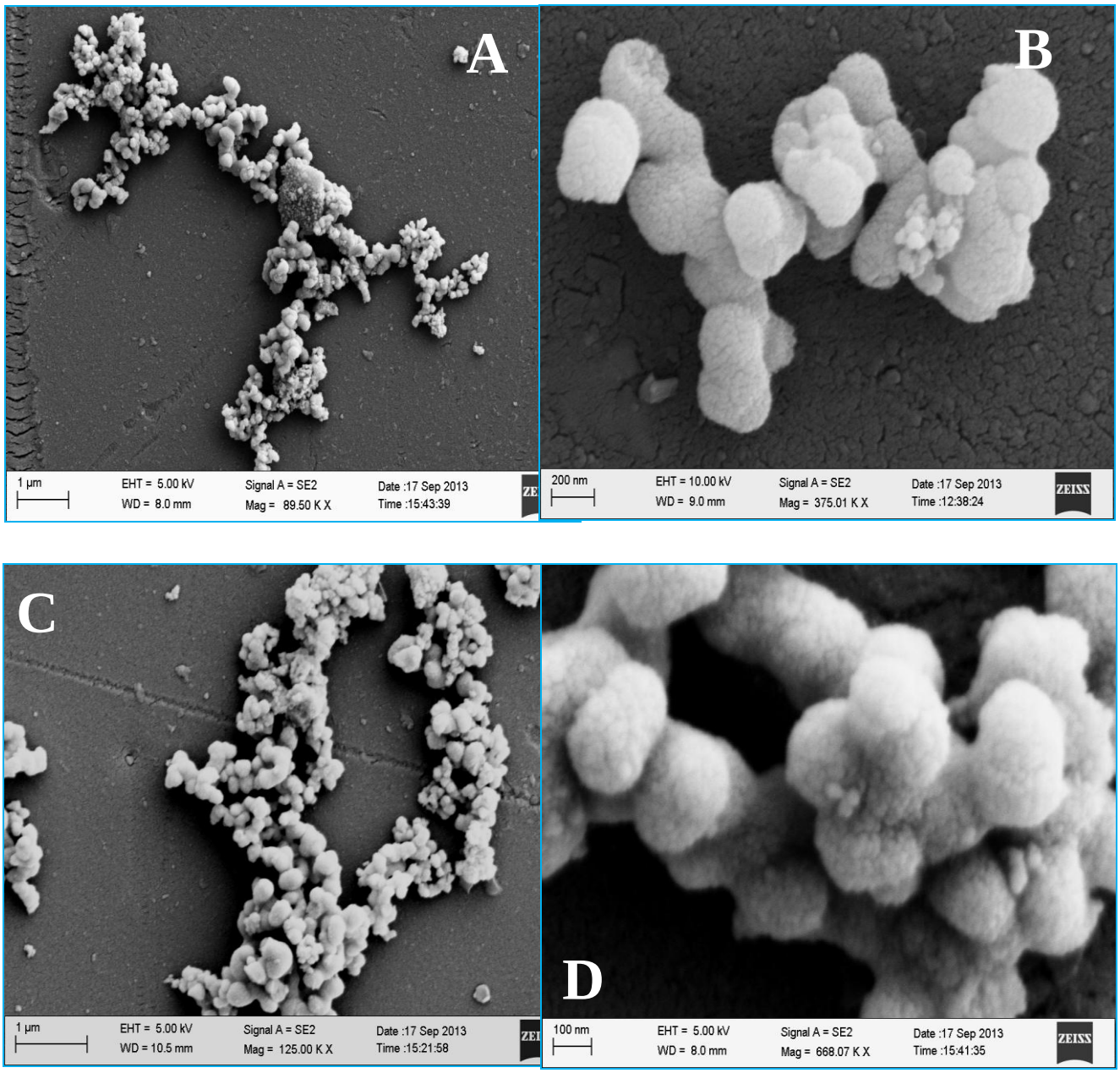


**Figure S-1:** Low and high magnified FE-SEM image of the larger size $TiO_2$ nanomaterials (A and B) and smaller size $TiO_2$ nanomaterials (C and D) self-assembled to wire-like shape in DNA.

**Energy Dispersive X-ray Spectroscopy (EDS) analysis.**

Figure S-2 shows the energy dispersive X ray spectroscopy (EDS) analysis of our synthesized DNA-$TiO_2$ nanomaterials. The EDS spectrum consists of different peaks for Ti, O, Si and P. The high intense Ti and O peak came from the $TiO_2$ nanomaterial sample where as the small intense Si peak came from the glass substrate which is used to deposit the $TiO_2$ sample for EDS analysis. A small intense P peak also appeared that came from the DNA which is used during synthesis and acts as a capping agent and template for the growth of the $TiO_2$ particles.

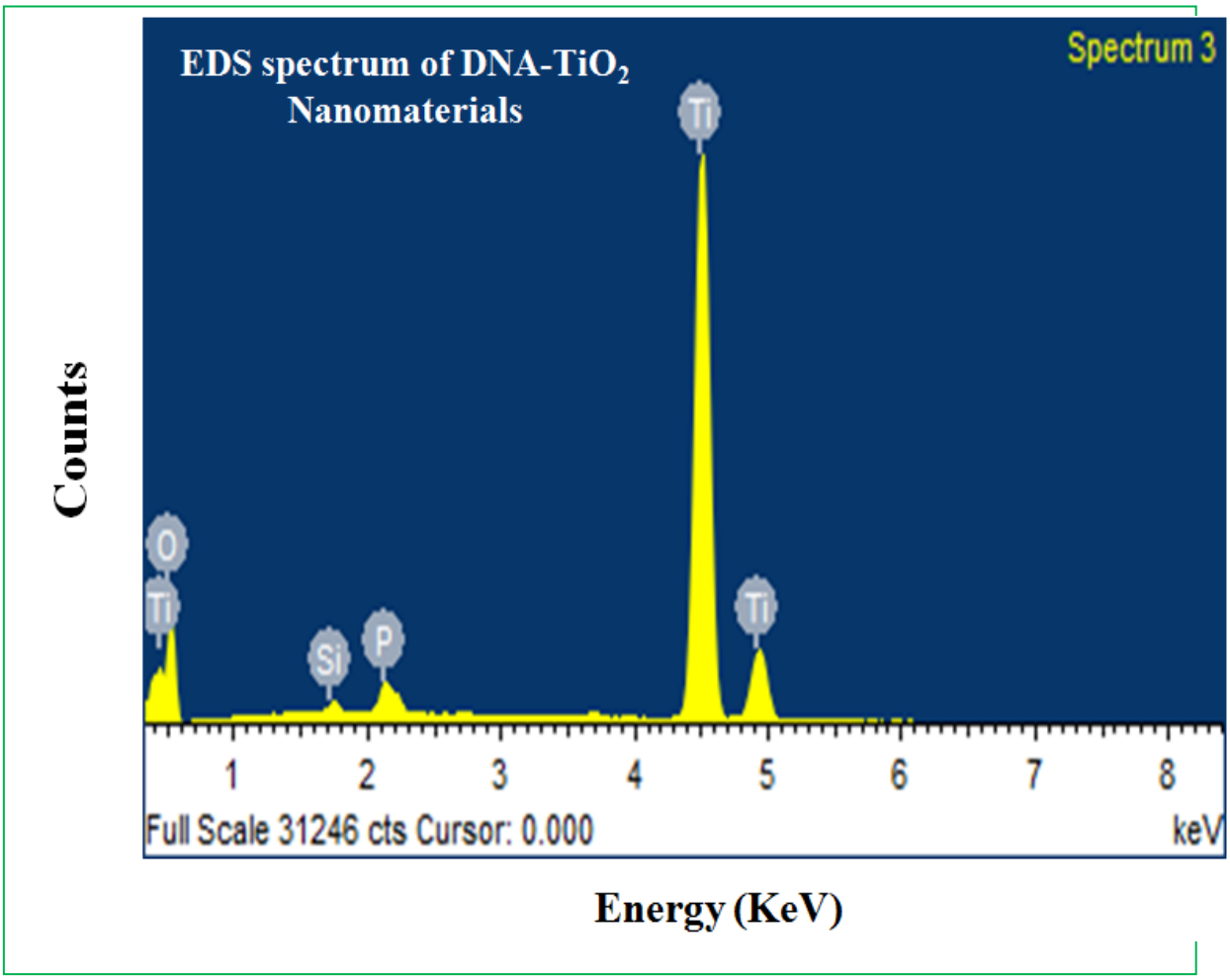


**Figure S-2:** Energy dispersive X ray spectroscopy (EDS) analysis of DNA-$TiO_2$ nanomaterial and the spectrum consists of different peaks for Ti, O, Si and P.

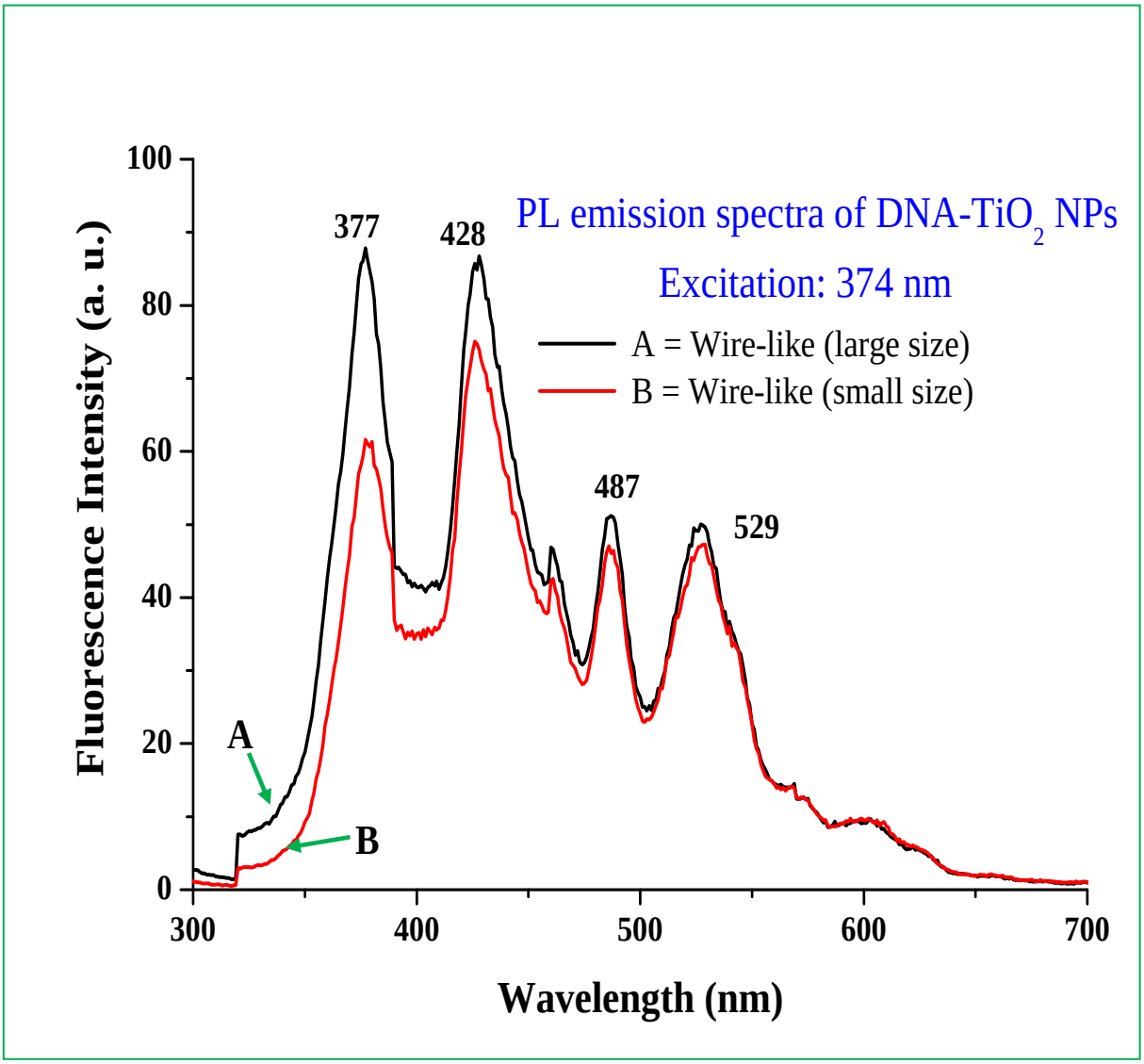


**Figure S-3:** The photoluminescence (PL) emission spectra of $TiO_2$ nanomaterials on DNA. Curve A and B denotes the emission spectra of wire-like $TiO_2$ nanomaterials having large and small sizes respectively.

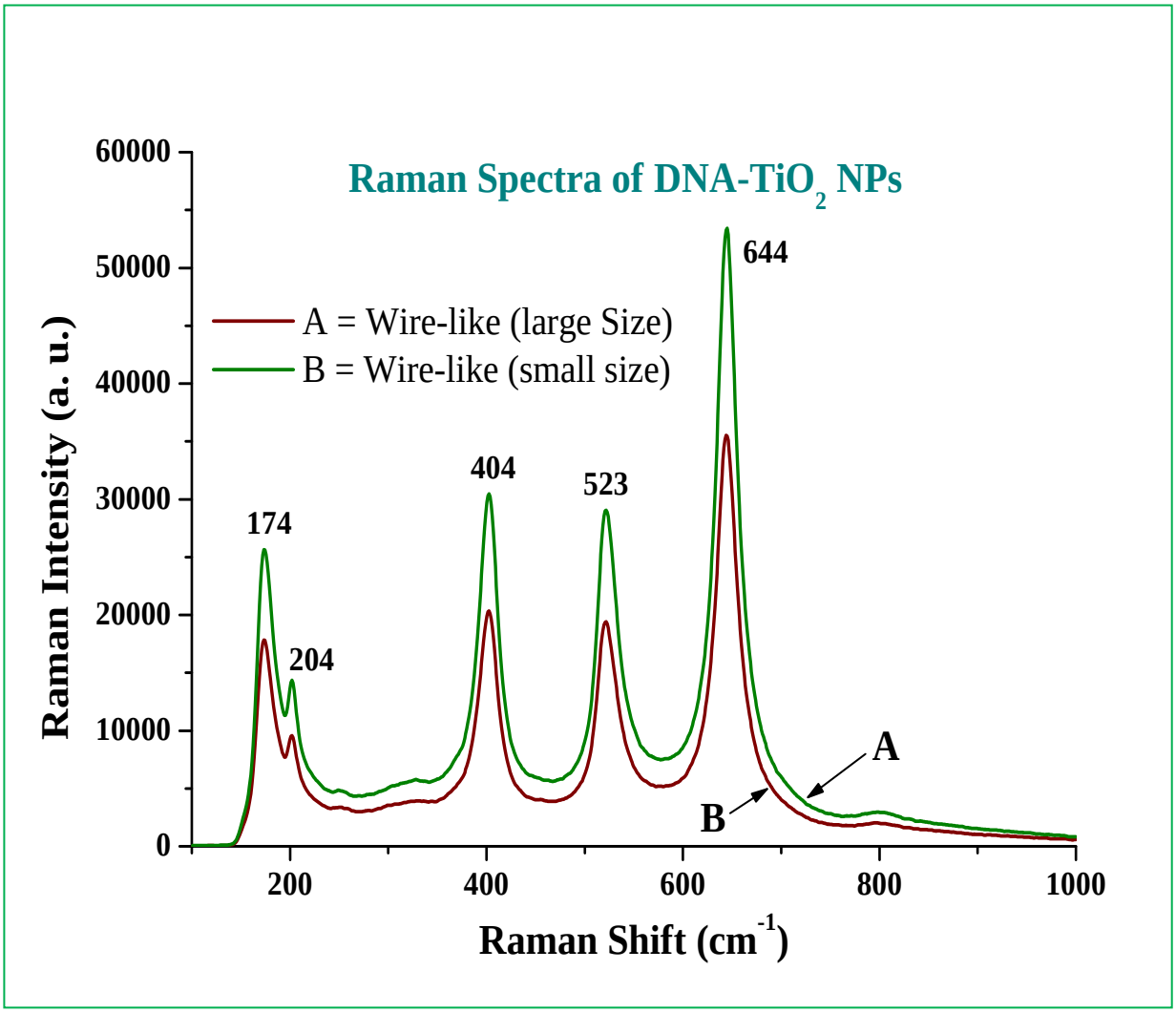


**Figure S-4:** The Raman spectra of the wire-like $TiO_2$ nanomaterials in DNA using 632.8 nm He-Ne LASER as an excitation source. Curve A and B shows the spectra for large and small sizes DNA-$TiO_2$ nanomaterials respectively.

**Table T-1:** The experimentally observed FT-IR bands of DNA, reported bands from literature and the assignments of different peaks are summarized.

| **Experimental and Reported FT-IR bands for DNA** | | |
|---|---|---|
| **FT-IR bands ($cm^{-1}$) (experimentally observed)** | **FT-IR frequency range ($cm^{-1}$) (reported value)[58]** | **Absorbing bonds/vibration types** |
| 3615 | 3100-3750 | ν (OH group in DNA/water) |
| 2812 | 2800-2950 | Symmetric stretching vibration (C-H bonds in $–CH_2$ group) |
| 1723 | 1732-1595 | C=O, C-N, N-H |
| 1494 | 1496-1480 | Bending (δ) of C-H bond in $CH_2$[46] |
| 1240 | 1170-1300 | Asymmetric stretching of $PO_2^-$ group |
| 1129 | 1150-990 | ν (C-O-C, C-C)[58] |
| 924, 979 | 800-1000 | De-oxyribose region |