Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Geometrical modifications and tuning of optical and surface plasmon resonance behaviour of Au and Ag coated TiO_2 nanotubular arrays

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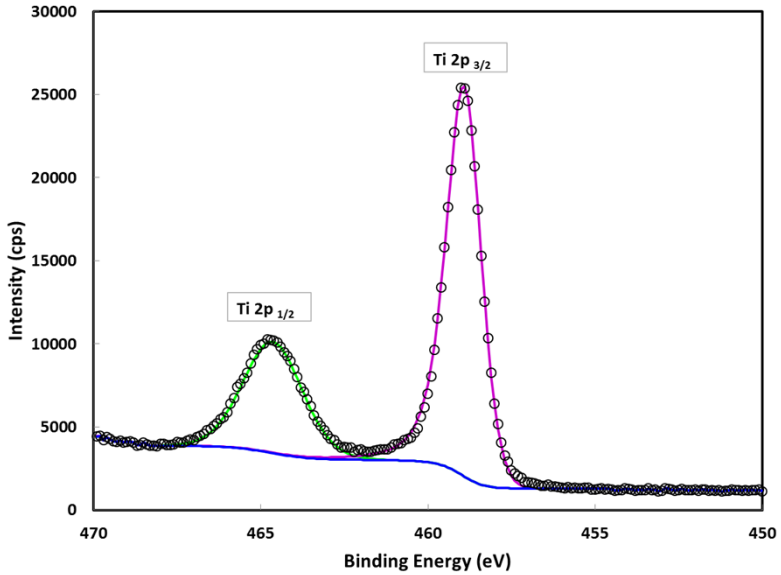
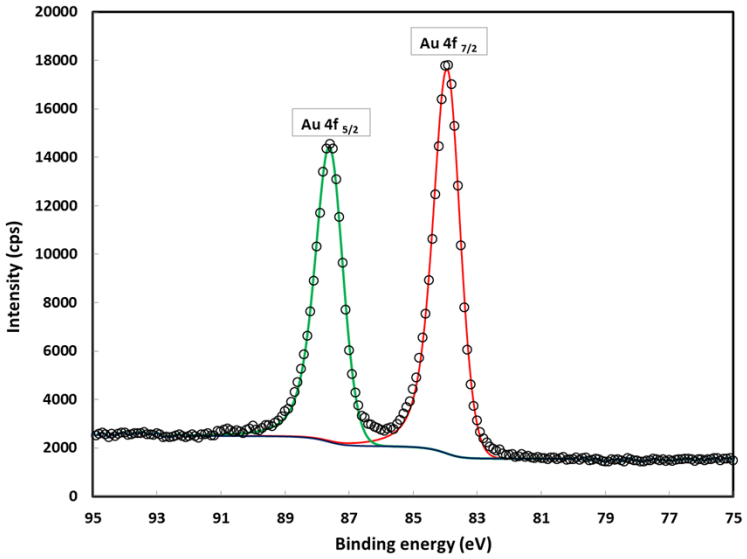
1. X-Ray Photoelectron spectroscopy results:

The Ti 2p level x-ray photoelectron spectra of TNA depicted in Figure S1a, illustrate the distinct $2p_{1/2}$ and $2p_{3/2}$ peaks at 464.2 and 458.5 eV, respectively, with a separation of ~5.7 eV between the $2p_{1/2}$ and $2p_{3/2}$ peaks. These distinct peak positions and separation corresponds to Ti^{4+} oxidation state, which is consistent with the TiO_2 nanotube lattice. The XPS core level spectra of Au from the gold coated TNA is depicted in Figure S1b. The Au 4f level x-ray photoelectron spectra depict the distinct $4f_{5/2}$ and $4f_{7/2}$ peaks at 87.6 and 83.9 eV, respectively, with a separation of 3.7 eV between the $4f_{5/2}$ and $4f_{7/2}$ peaks arising from the spin–orbit interaction.



(a)



(b)

Figure S1: XPS core level spectra of (a) Ti reveals the Ti2p1/2 and Ti2p3/2 peaks at 464.2 and 458.5 eV, respectively and (b) gold reveals the $Au4f_{5/2}$ and $Au4f_{7/2}$ peaks at 87.6 and 83.9 eV, respectively, thereby further confirming the presence of gold in its native oxidation state on the TNA.

2. Energy bandgap measurements from UV-Vis spectroscopy

Diffuse reflectance data from UV-Vis spectroscopy were utilized for band gap energy measurements. Figure S2 shows Tauc plots of vertically-oriented nanotubes with uniform diameter, tilted nanotubes, tapered nanotubes, and dumbbell-shaped nanotubes. A remarkable increase in absorbance was observed when the shape of nanotubes was altered. Band gap energy was calculated using Tauc plots. The Tauc plot exhibits the relation between the energy of incident photons ($h\nu$) on the material (abscissa) against $(\alpha h\nu)^{1/n}$ on the ordinate axis, where 'α' is the absorption coefficient of the material and is directly related to the measured absorbance. The exponent 'n' denotes the nature of the transition and for titania nanotubes, $n = 1/2$ for direct allowed transitions. A considerable increase in absorbance begins at 390nm and a peak centered at 334nm appears. The wavelength, at which the increase in absorbance starts in the annealed samples, indicates the formation of band tail due to incorporation of impurity states. The intersection between the linear fit and the photon energy axis gives the value of the band gap.

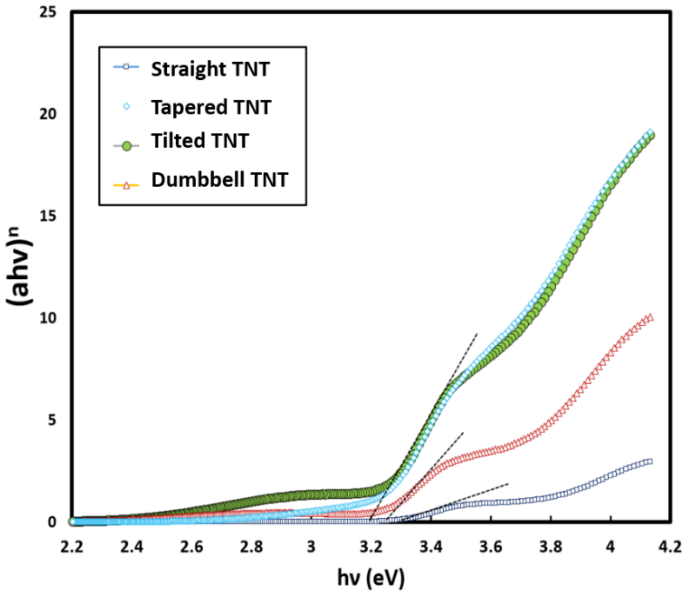


Figure S2: Tauc plots for the different TNA morphologies reveal a decreasing trend in the band gap as the geometry deviates from the straight nanotube due to induced strain effect.