Supplemental Information

Tuning the Electro-Optical Properties of Nanowire Networks

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In this study, we have performed the spectral characterization of individual nanowires employing Mie light scattering theory (MLST) implemented in MATSCAT[1] software and finite element method (FEM) algorithm implemented in COMSOL® Multiphysics software. Here, we outline how the nanowire model with incident light was built in COMSOL. A FEM analysis using "electromagnetic waves", and "frequency domain" interfaces available in the "radio frequency" module was built to numerically solve Maxwell's equations in the frequency domain. To model the infinite cylinder in COMSOL, we set a two-dimensional (2D) circular disk in the x-y plane which can be illuminated by a plane wave propagating normal to the object with two incident excitation modes as shown in Figure S1, the transverse magnetic (TM) and the transverse electric (TE). In our case, the electromagnetic wave's direction was aligned to the y-axis and its polarizations were along x- and z-axis. The optical extinction coefficients were found by averaging the two perpendicular electric field polarizations. To model the 2D circular disk, we have constructed nanowires with diameters of $30\,nm$ and $50\,nm$. An appropriate thickness for the perfectly matched layer (PML) was chosen to emulate restricted and non-reflecting infinite domains. The surface (2D) and volume (3D) of the object were discretized via meshing. The latter was performed by using physics-controlled mesh refinement, even though we fulfill the custom setting for elements' size by gradually varying the mesh from normal to extra fine. This procedure was employed to ensure that the meshed geometry is suited for spectral identification.

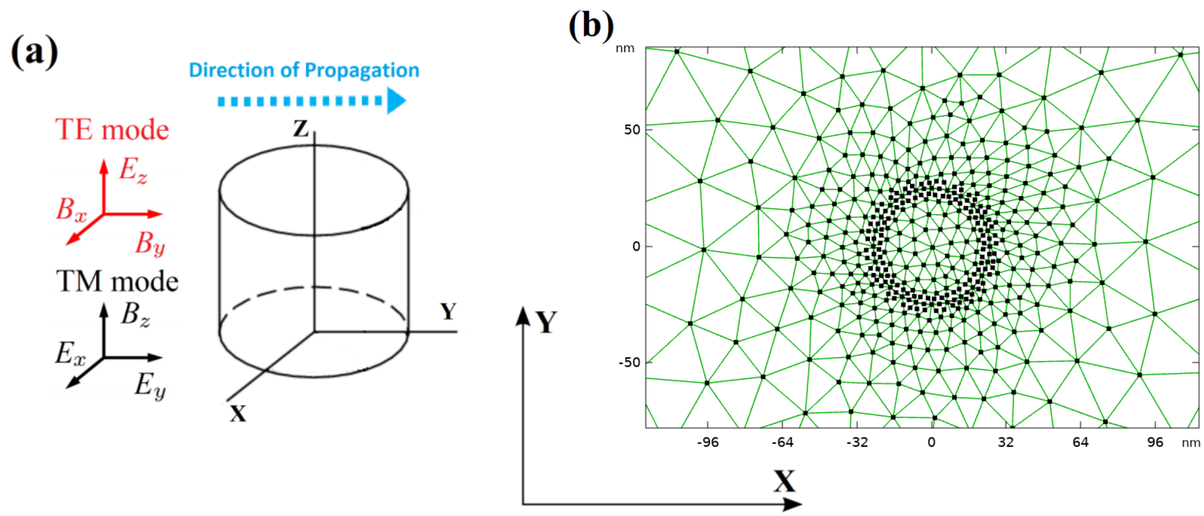

Figure S1. (a) Schematic illustration of a single nanowire viewed as a cylinder when the incident electric field impinges on the surface of the object. The excitation beams were normal to the surface and propagated along the y-direction. The cylinder represents a nanowire with light traveling in the y-direction and its two perpendicular polarizations: TM and TE correspond to the transverse magnetic and the transverse electric polarized waves, respectively (b) The screenshot of a 2D circular disk created to model an infinite cylinder. The circle is the cross-section of the cylinder (top view). The green line segments and dots are the meshing elements distributed everywhere in space.

Our mesh's qualities applying skewness measure were found to be 0.5647 and 0.8303 for minimum element quality and average element quality, respectively. We numerically solved Maxwell's wave equations with respect to the scattered electric field:

$$\nabla \times \mu_r^{-1}(\nabla \times E) - k_0^2\left(\varepsilon_r - \frac{j\sigma}{\omega\varepsilon_0}\right)E = 0, \quad k_0 = \frac{2\pi f}{c} \qquad \text{(Eq. S1)}$$

in which μ_r and ε_r are the relative permeability and permittivity, respectively. In above equations, ε_0, σ, E, ω, f, and c stand for the vacuum permittivity, electrical conductivity, electric field, angular frequency, wave's frequency, and speed of light, respectively. The total extinction cross-section can be defined as $\sigma_{ext} = \sigma_{sca} + \sigma_{abs}$ where σ_{ext}, σ_{sca}, and σ_{abs} are the extinction, scattering and absorption cross-sections (in units of m^2 for 3D and in m for 2D modelling), respectively, as following[2, 3]:

$$\sigma_{abs} = \frac{W_{abs}}{\mathrm{P}_{inc}}, \ \sigma_{sca} = \frac{W_{sca}}{\mathrm{P}_{inc}}, \qquad \text{(Eq. S2)}$$

where W_{abs} and W_{sca} (in units of W) are the absorbed and scattered energy rates by the nanowire, respectively. P_{inc} indicates the incident irradiance, determined as energy flux of the incident wave in units of W/m^2. The absorbed energy rate by the nanowire in Equation S2 can be defined by the integration of energy loss (Q_{loss}) over the volume element (dV) of the nanowire using the following relationship[2, 3]:

$$W_{abs} = \iiint Q_{loss} dV = \frac{1}{2}\iiint Re\{J_{tot}.E^* + j\omega B.H^*\}dV, \ J_{tot} = \sigma E + j\omega D \qquad \text{(Eq. S3)}$$

in which the J_{tot} is the total current density, D is the electric displacement field, and B (H) is the magnetic field (strength). The superscript '*' indicates conjugate gradient. W_{sca} can also be defined as:

$$W_{sca} = \frac{1}{2}\oiint Re\{E_{sca} \times H_{sca}^*\}.nds \qquad \text{(Eq. S4)}$$

In the above surface enclosing nanowire's integration, n is the surface normal unit vector pointing outward, ds is the surface integral element, and the subscript "sca" stands for the corresponding scattering quantity. Because we used plane waves, the flux of the relevant Poynting vector is estimated by ($\hat{k}$ is the incident wave's direction):

$$P_{inc} = \frac{1}{2c\varepsilon_0}|E_{inc}|^2\hat{k} \qquad \text{(Eq. S5)}$$

To obtain the optical efficiency coefficients, $Q = \sigma/A$, ($Q_{ext} = Q_{sca} + Q_{abs}$), the cross-sections ($\sigma_{ext} = \sigma_{sca} + \sigma_{abs}$) for each contribution are divided by their corresponding cross-sectional (A) area of the nanowire. The cross-sectional area for the 2D circular disk model is a line segment of the size of the disk diameter. For the case of the 3D cylinder model, the cross-sectional area is a rectangle outlined by the length and the diameter of the 3D nanowire (cf. Figure S2). We also studied a special case of curved nanowires using a similar 3D model as the one used for straight wires. The cross-sectional area of a 3D curved nanowire can be calculated by subtracting the area confined within two concentric semi-circles as shown in Figure S2.

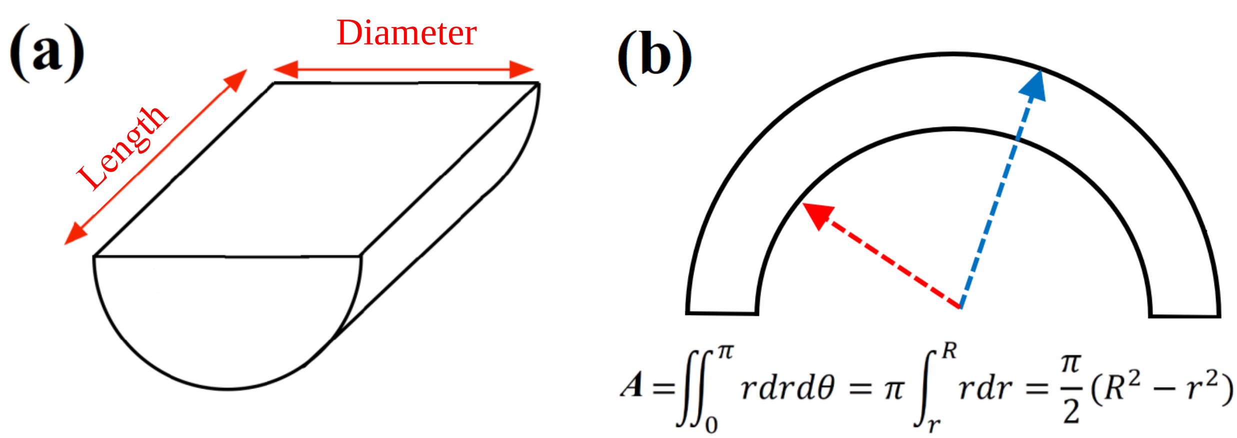

Figure S2. Sliced view of a (a) straight and (b) a curved nanowire. (a) A half cylinder surface area outlining a rectangular area $A = Length \times Diameter$. (b) Sliced view of a 3D curved nanowire. The cross-sectional area A is determined by integrating the surface integral element scanning radial (r) and angular (θ) degrees of freedom. θ is integrated from $[0, \pi]$ and the radial variable is integrated from the inner radius (red arrow) r up to the outer radius (blue arrow) R.

The extinction, scattering, and absorption efficiency coefficients obtained from COMSOL for the 2D modeling scheme are presented in Figure S3. The results are for four materials including Ag, Al, Au, and Cu and of cylindrical shape with a diameter of 50 nm. The relatively high Q_{ext} values exhibited by Al over the wavelength range indicate that Al may offer lower transparencies in comparison to the other materials, making Al less attractive for transparent conductors' applications. These results are in good agreement with those obtained via MATSCAT as illustrated in Figure 2 of the main manuscript.

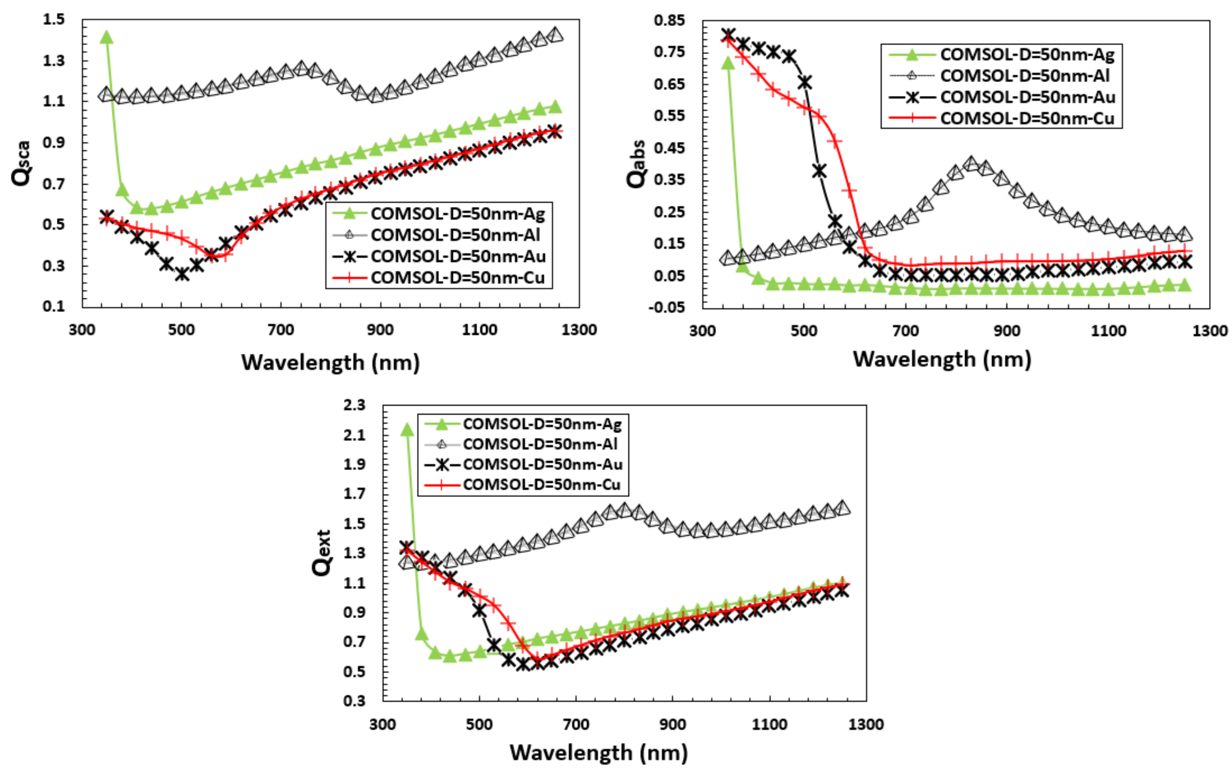

Figure S3. (top-left) Scattering, (top-right) absorption, and (bottom) extinction efficiency coefficients obtained using COMSOL for different materials (Ag, Al, Au, Cu) and of cylindrical shape with a diameter of 50 nm. The wavelength was varied from $\sim 300 - 1300$ nm. These results were taken with the 2D circular disk model.

In a further investigation for the optical spectra modeling in COMSOL, we have plotted the results found from the 2D modeling scheme for an infinite Ag cylinder and the 3D modeling scheme for an Ag straight and curved nanowires as shown in Figure S4. The geometrical features (diameter and length) of the Ag straight and curved nanowires are $D = 50\ nm$ and $L = 7\ \mu m$. Comparing the efficiency coefficients of an infinite cylinder (2D circular disk) and straight nanowire (3D cylinder) suggests that they both follow a similar trend, yet the 3D straight nanowire model displays peaks above wavelengths of $620\ nm$.

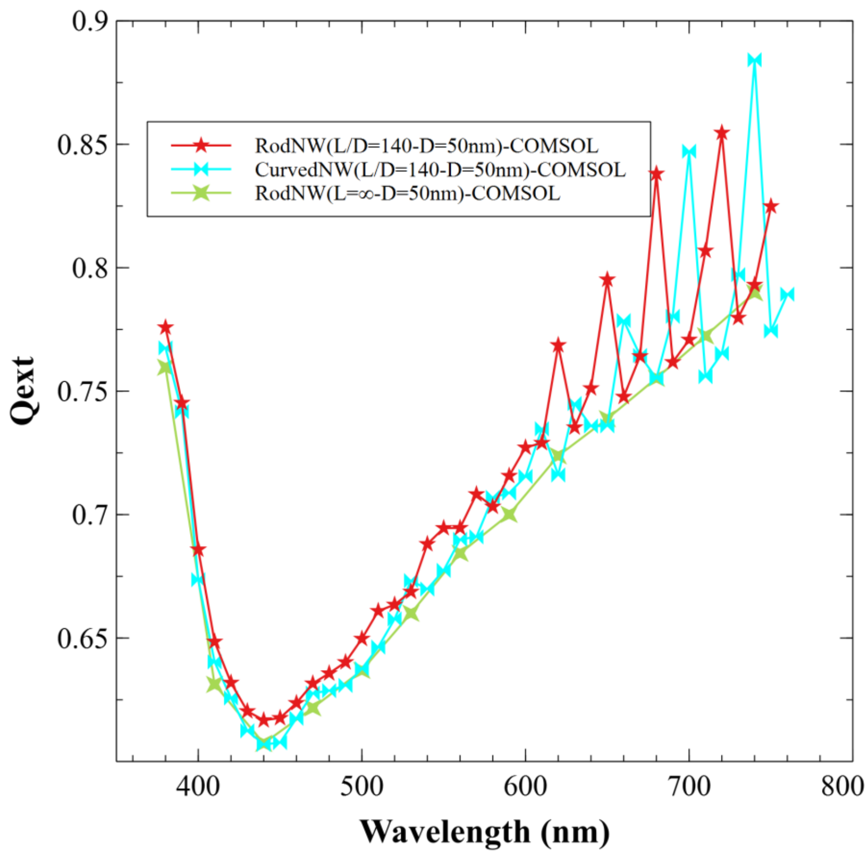

Figure S4. Extinction efficiencies as a function of wavelength from $350\ nm$ to $750\ nm$ of an Ag single nanowire calculated using COMSOL. The red, cyan, and green color curves refer to straight/finite, curved/finite and infinite nanowire (2- dimensional circular disk), respectively. In all simulations, the nanowires have the same diameter of $D = 50\ nm$ and the finite nanowires (straight and curved) have the same (arc) length of $L = 7\ \mu m$.

Similarly, curved and straight Ag nanowires exhibit similar Q_{ext} behavior, except that the peaks are somehow shifted. This is something to keep in mind when studying the optical properties of curved and straight nanowires, particularly for wavelength ranges above $630\, nm$. It is worth emphasizing that this is a trade-off analysis between optical and electrical properties in nanowire network systems which requires the consideration and tunning of many other degrees of freedom as detailed in the main manuscript.

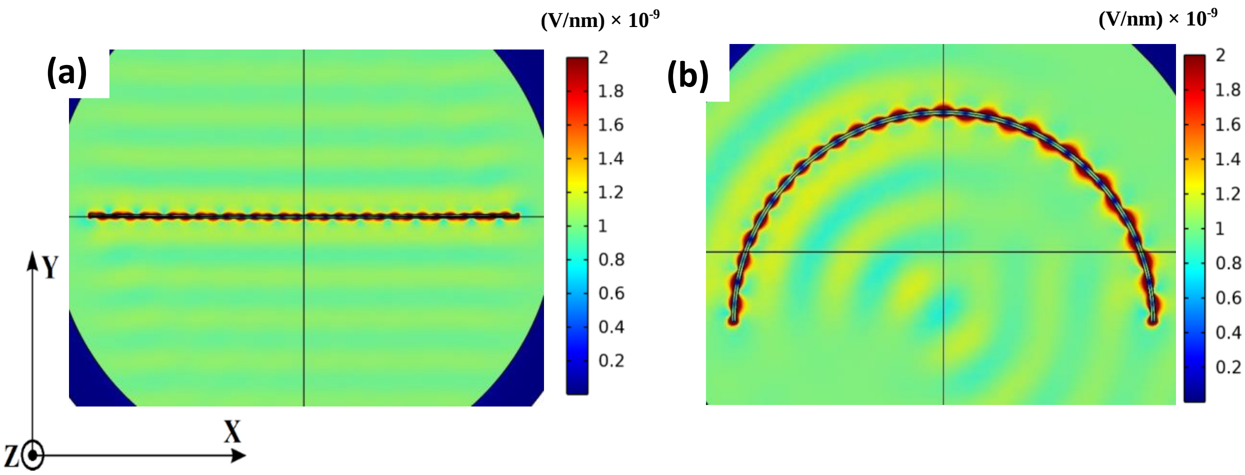

Figure S5. Electric field color map around an Ag (a) straight and (b) curved nanowire. The structural characteristics of the nanowire are a diameter of $D = 50\, nm$ with a finite arc/straight length of $L = 7\, \mu m$. The electric field wave propagates along z-axis with two polarizations along x- and y-axis. The color bar displays the electric field strength in each panel. Color maps depict the illumination of an Ag (a) straight nanowire by a $680\, nm$ light wave and a (b) $700\, nm$ light wave on an Ag curved nanowire. These wavelength values correspond to peaks in Q_{ext} as shown in Figure S4.

The optical characterizations of 3D Ag straight and curved nanowires are shown in Figure S5 Figures S5(a) and S5(b) present the simulated electric field strength around the Ag nanowires at the wavelengths of $680\, nm$ (straight) and $700\, nm$ (curved) where each of these wavelengths corresponds to Q_{ext} peaks in Figure S4. The 'hot spots' (ripples in the electric field strength around the wires) created around each nanowire can be due to localized surface plasmon resonance[4-7] which is observed at specific ratios between the incident wavelength and the object aspect ratio ($Wavelength/aspect\ ratio$).

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