Nanohub Tool Supplementary Information

**Methodology**

The CS NWs are modeled as cylinders with infinite length and with the incident light perpendicular to the axis. To calculate the local density of states (LDOS) and Purcell factor (PF), a Green’s function approach has been utilized1,2. As the emission is due to the recombination of an electron and a hole at the band gap of the semiconductor, the emission can be described as arising due to the electric and magnetic fields emitted by a dipole. The electric field due to a dipole is the Green’s function solution to Maxwell’s equations. The complete solution account for the orientation of the dipole is defined as a 2D Green’s tensor3,4. This tensor can be used to calculate the local density of states, and consequently, the PF. The PF calculated here is obtained starting from Fermi’s golden rule and is in the low coupling regime5.

The dielectric constants as a function of wavelength have been obtained from nanohub6. The LDOS is calculated by:

$ρ\left(r\_{s},ω\right)=-\frac{2ω}{πc^{2}}Im\left\{Tr\left(G^{E}\left(r,r\_{s},ω\right)\right)\right\}\#\left(1\right) $

where rs is the position of the dipole source, and the 2-D Green’s tensor GE(r,rs,ω) is given by7,8:

 $G^{E}\left(r,r\_{s},ω\right)=\left[G\_{xx} G\_{xy} 0 G\_{yx} G\_{yy} 0 0 0 G\_{zz} \right]=-\frac{1}{iωμ}\left[E\_{x}^{S\_{x}} E\_{y}^{S\_{x}} 0 E\_{x}^{S\_{y}} E\_{y}^{S\_{y}} 0 0 0 E\_{z}^{S\_{z}} \right]\#\left(2\right) $

where $E\_{y}^{S\_{x}}$ is defined as the electric field due to a x-oriented dipole in the ŷ-direction. The emission rate is:

$γ=q\_{i}\frac{2ω}{ℏε}\left|μ\right|^{2}ρ\left(r\_{s},ω\right)\#\left(3\right) $

where we are using the total dielectric functions ε and hence including the optical absorption losses which are occurring, through the imaginary part of the dielectric constant. Therefore, the PF can be defined as:

 $PF=\frac{γ}{γ\_{0}}=\frac{ρ\left(r\_{s},ω\right)}{ρ\_{0}\left(r\_{s},ω\right)} (4)$

**Tool User Guide**

The current version of the tool is limited to only up to two shells and has pre-chosen materials options. The number of shells can be selected from a dropdown menu; the options are core-only, core with a shell (core-shell), and core with 2 shells (core-multishell). Depending on the selection of number shells, the core radius, and shell thicknesses can be input between 1 and 500 nanometers. The material for the core and each of the shells can be selected from dropdown menus. The medium the nanowire is in can be selected from a drop down menu to be air/vacuum, water, glass or other where the dielectric constant of the desired medium can be input (a number between 1 and 50).

Currently there are three options for the type of calculation the tool can do, one at a time.

Option 1: LDOS and Purcell Factor along the Nanowire Radius

For this calculation wavelength can be entered between 300 and 1400 nm. Some materials options are limited to 800 nm or 1000 nm. This option will generate 2 graphs, one for the Purcell Factor along the nanowire radius, and one for the local density of states along the nanowire radius.

Option 2: Purcell Factor of Selected Nanowire Layer

 For the calculation select a Wavelength Range, between 300 and 1400 nm. If you are doing a CS or CSS you will have the option of what section(s) of the nanowire you want to see the PF of. For CSS don't choose non adjacent sections, or the results you get back won’t be what you’ve chosen. This option will generate one graph, which will give you the Purcell Factor of the nanowire over the wavelength range you’ve selected.

Option 3: Purcell Factor Contour Plot for Varying Nanowire Thickness

 For this option the core and shell sizes become ranges that you can change. You will have to enter the initial and final core radius or shell thicknesses for the nanowire, and the interval that they should change at. If you choose CSS you will have to choose a section of the nanowire to be a constant, as this is only a 2D contour plot. The contour plot will only be viewable as a image file, so you will not be able to interact with it.

When the calculations are completed, graphical representations of results appear on the right side of the screen. Through the drop down menu, the desired graph can be chosen. By clicking on the graphing plane and dragging the mouse and clicking, an area can be chosen to zoom in on. To zoom back out, double click anywhere on the graph. Clicking on the button next to the drop down menu downloads either the data or the image of the currently being viewed graph. Images can be saved as a PDF, PS, EPS, JPEG, or PNG.