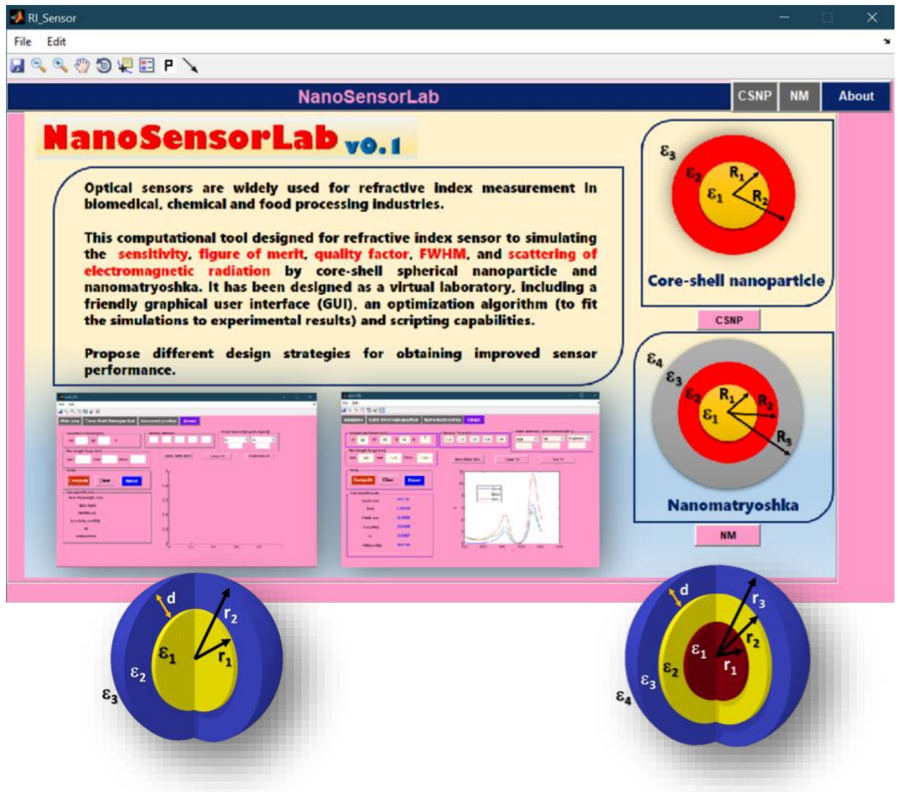
NanoSensorLab

(User Manual)



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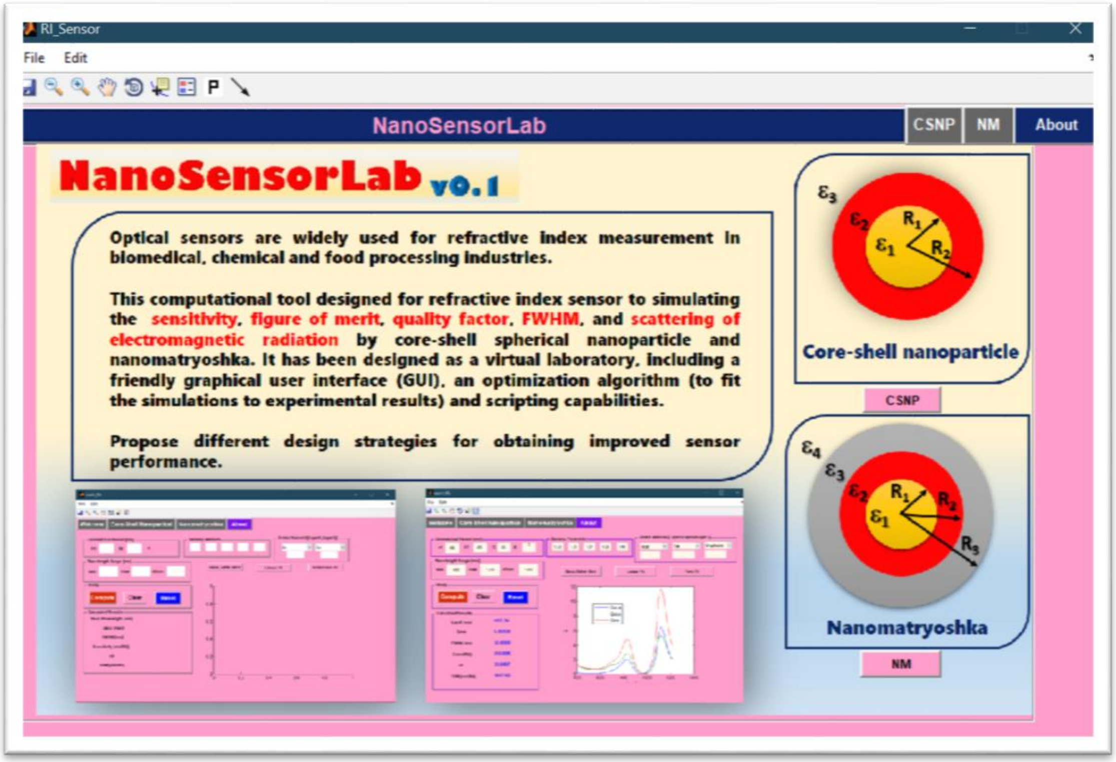
Introduction



Optical sensors are widely used for refractive index measurement in biomedical, chemical and food processing industries.

This computational tool designed for refractive index sensor to simulating the sensitivity, figure of merit, quality factor, FWHM, and scattering of electromagnetic radiation by core-shell spherical nanoparticle and nanomatryoshya. It has been designed as a virtual laboratory, including a friendly graphical user interface (GUI), an optimization algorithm (to fit the

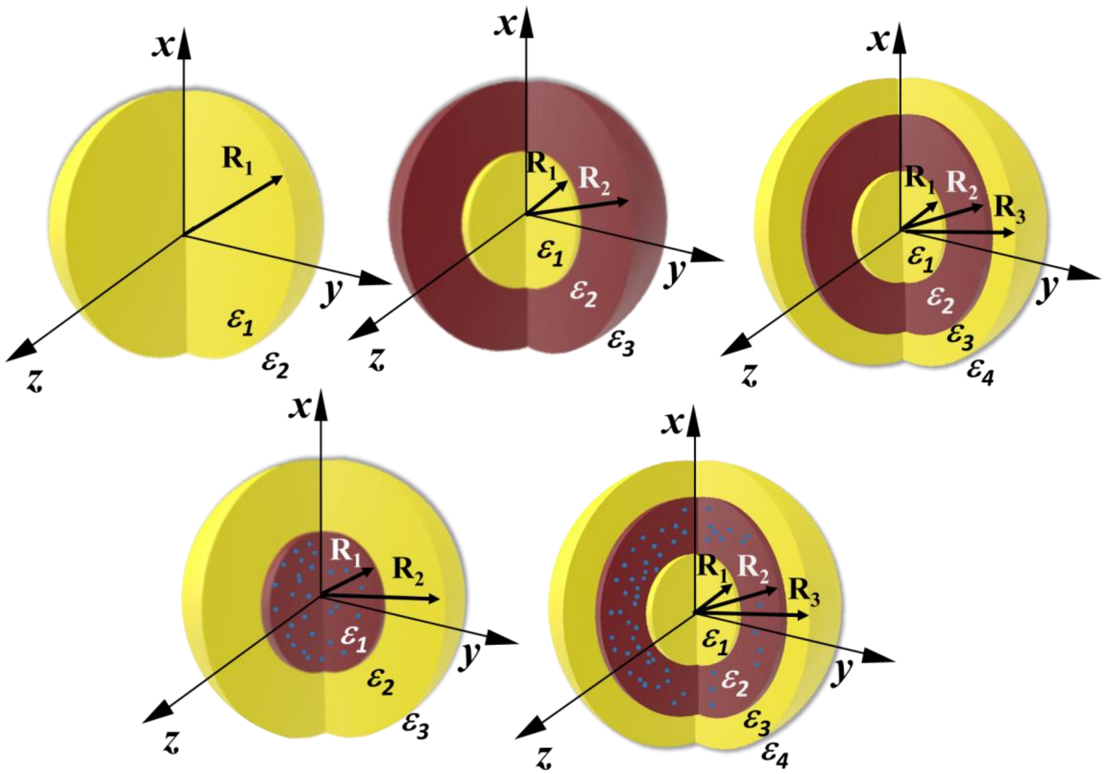
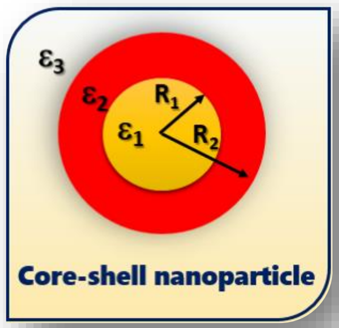


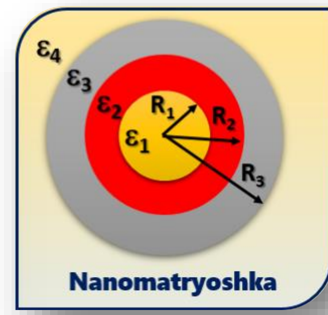
Fig 1. *Schematic representation of the Sphere, Nanoshell, Nanomatryoshya, Nanoshell with gain and Nanomatryoshya with gain, geometries used for calculating the optical properties in NanoSensorLab.*

simulations to experimental results) and scripting capabilities. Propose different design strategies for obtaining improved sensor performance.

Flowchart of Computational Tool



Sensing system Core-shell and Nanomatryoshka (Au, TiN, ZrN, etc.)



Simulation and Optimization Parameters for High Performance Plasmonic Sensor

- **Scattering, Absorption and Extinction**
- **FWHM**
- **Sensitivity**
- **Quality Factor**
- **Figure of Merit**

Theoretical Model

This computational tool is based Mie theory for investigating the optical response of low-dimensional structures for core-shell nanoparticle and nanomatryoshka and the extinction efficiencies, scattering efficiencies and absorption efficiencies are written as [1]

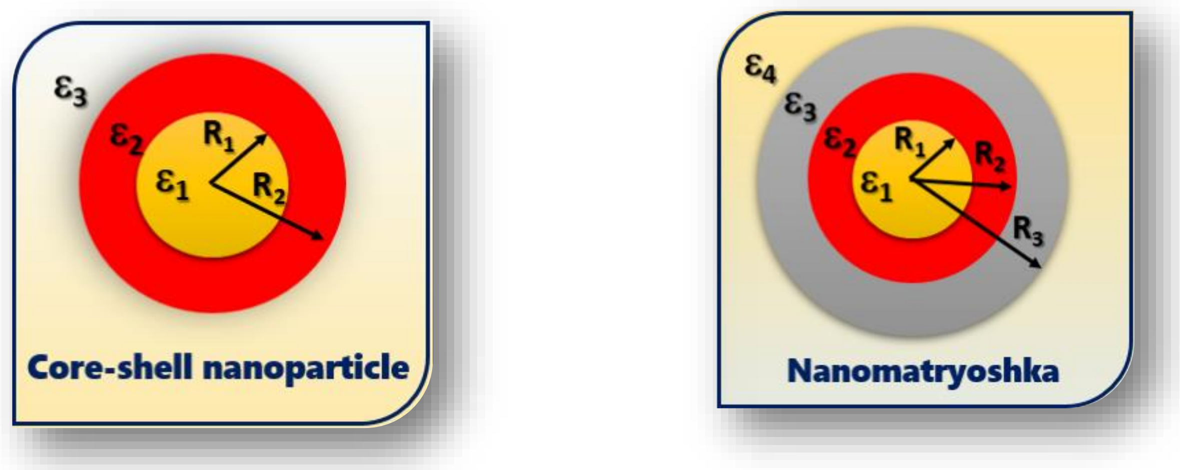


Fig 2. *Schematic representation of the Core-shell nanoparticle and Nanomatryoshka geometries used for calculating the optical properties in computational tool.*

$$Q_{ext} = \frac{2}{x^2} \sum_{l=1}^{\infty} [2l+1] \mathrm{Re}\left(a_l + b_l\right) \tag{1}$$

$$Q_{sca} = \frac{2}{x^2} \sum_{l=1}^{\infty} [2l+1] \left(|a_l|^2 + |b_l|^2\right) \tag{2}$$

$$Q_{abs} = Q_{ext} - Q_{sca} \tag{3}$$

where, x is the size parameter and the coefficients for scattered fields a_n and b_n are defined as [1],

$$a_n = \frac{\psi_n(x_3)H_n^a(u_3x_3) - u_3Z_n^{(1)}(x_3)}{\xi_n(x_3)H_n^a(u_3x_3) - u_3Z_n^{(3)}(x_3)} \tag{4}$$

$$b_n = \frac{\psi_n(x_3)u_3H_n^b(u_3x_3) - Z_n^{(1)}(x_3)}{\xi_n(x_3)u_3H_n^b(u_3x_3) - Z_n^{(3)}(x_3)} \tag{5}$$

where, u_1 and u_2 are the refractive indices of core and the shell,and $u_3 = \varepsilon_3/\varepsilon_4$ is the relative refractive index of outer shell medium relative to surrounding medium. Also, $x_1 = kR_1$, $x_2 = kR_2$ and $x_3 = kR_3$ are size parameters and, Riccati-Bessel functions $\psi_n(x) = xj_n(x)$, $\chi_n(x) = -xy_n(x)$, $\xi_n(x) = xh_n^{(1)}(x)$ of first kind andthe logarithmic derivative of Ricatti-Bessel function like, $Z_n^{(1)}$, $Z_n^{(2)}$, and $Z_n^{(3)}$, are written as, $Z_n^{(1)} = \psi_n^{'}(x)/\psi_n(x)$, $Z_n^{(2)} = \chi_n^{'}(x)/\chi_n(x)$;, $Z_n^{(3)} = \xi_n^{'}(x)/\xi_n(x)$ and $H_n^a(u_3x_3)$, $H_n^b(u_3x_3)$.

The most relevant sensing parameters are: (I). quality factor (QF) of scattering resonance peak, (II). sensitivity (S) and (III). figure of merit (FOM). The quality factor of resonant peak is defined as the ratio of resonant wavelength of peak to the full width at half maximum of the resonant peak as [2]

$$\mathrm{QF} = \frac{\lambda_\mathrm{R}}{\mathrm{FWHM}} \tag{6}$$

This suggests that the resonant peak with smaller FWHM corresponds to the higher quality factor. The sensitivity (S) of the sensor is defined as the rate of shift of resonant peak wavelength 56 with the variation in the refractive index (n) of surrounding medium, and the same is mathematically written as

$$\mathrm{S} = \frac{\mathrm{d}\lambda_\mathrm{R}}{\mathrm{dn}} \tag{7}$$

The Figure of Merit (FOM) of the sensor is directly proportional to the quality factor of the resonant peak and the sensitivity, and the same is expressed as

$$\mathrm{FOM} = \frac{\lambda_R}{\mathrm{FWHM}} \times S \tag{8}$$

Example/Demonstrate (Sphere)

In this section, our investigations concerning design considerations for spherical nanoparticle based simulater panel are presented in Fig. 3-5. We can calculate the scattering, absorbstion and extention efficiency. For these calculation follow the steps and enter the parameters

1. In geometrical panel R_1=50nm;
2. Select wavelength range between min 400 nm max 1200 nm and steps 1000.
3. In material section select inbuild Au data and plot.
4. Import data is optional and requires wavelength [nm], real part of the dielectric, and imaginary part of the dielectric. it is user define material data. Please make sure to take one option inbuild or user define data.
5. Take Sensing parameter ‘n=1.33’.
6. In study section press Compute and wait for few moment.
7. Calculated results will display.

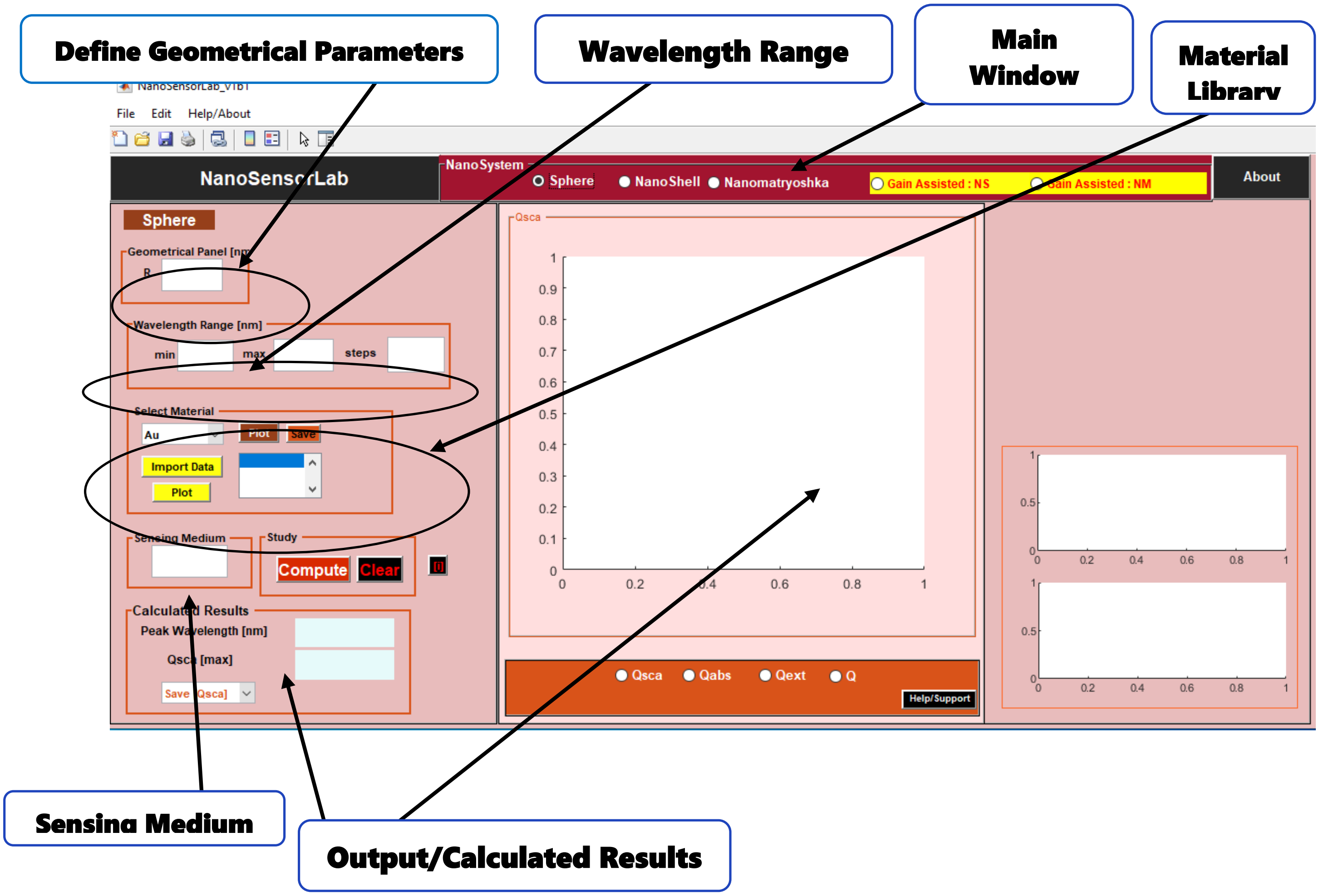


Fig. 3 *Main panal of the sphere based system.*

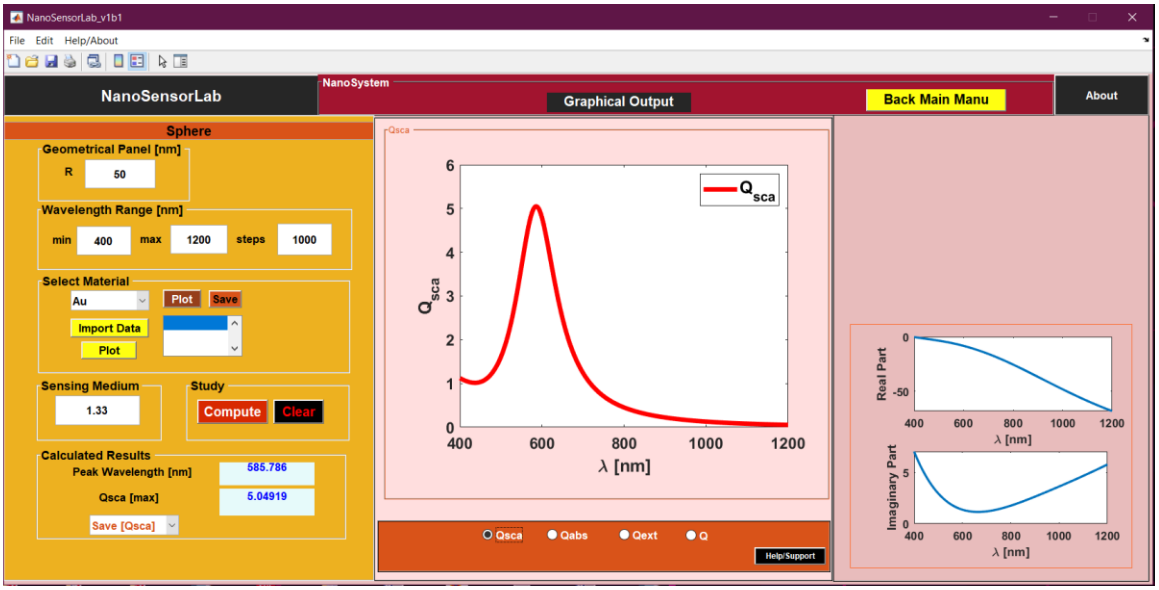


Fig. 4 *Example of calculated scattering efficiency of sphere nanoparticle.*

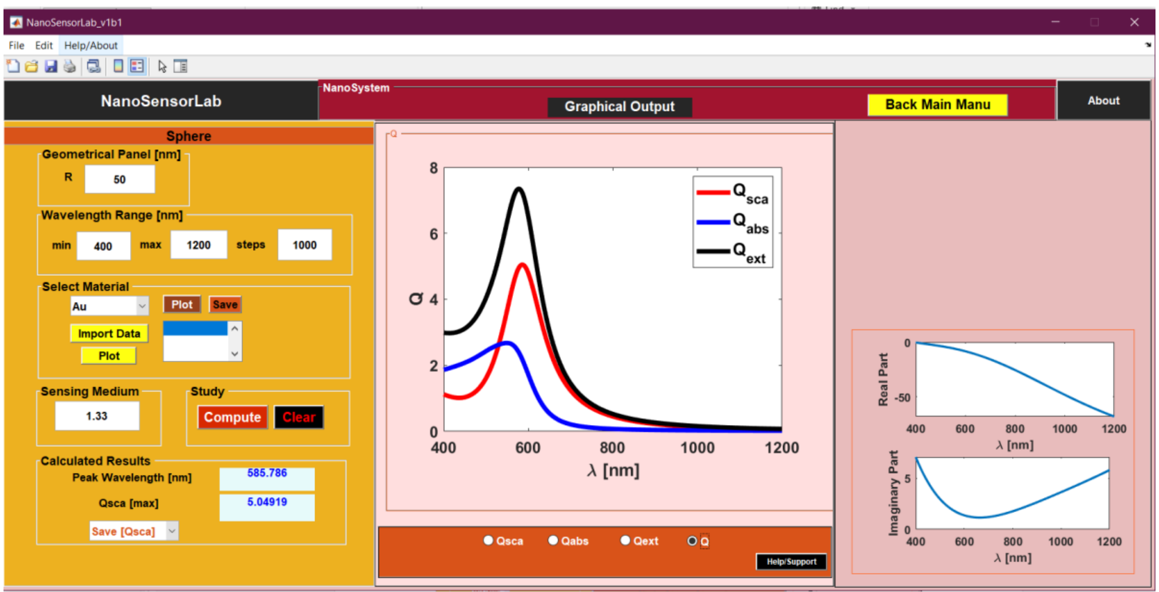


Fig. 5 *Example of calculated the scattering, absorbstion and extention efficiency of sphere nanoparticle.*

Example/Demonstrate (Nanoshell)

In this section, our investigations concerning design considerations for the nanoshell nanoparticle based simulator panel are presented in Fig 6-10. We can calculate the scattering efficiency, absorption efficiency, extention efficiency, full width half maximum, sensitivity, and figure of merit. For these calculations follow the steps and enter the parameters (Case: SiO_2/Au)

1. In geometrical Panel R_1=30nm; R_2=40nm
2. Take Sensing parameter ‘n=1.33, 1.34, 1.35, 1.36, 1.37’.
3. Select wavelength range between min 400 nm max 1230 nm and steps 1000.
4. In material section select inbuild SiO_2 /Au data and plot.
5. Import data is optional and requires wavelength [nm], real part of the dielectric, and imaginary part of the dielectric. it is user define material data. Please make sure to take one option inbuild or user define data.
6. In study section press compute and wait for few moment.
7. Calculated results will display.

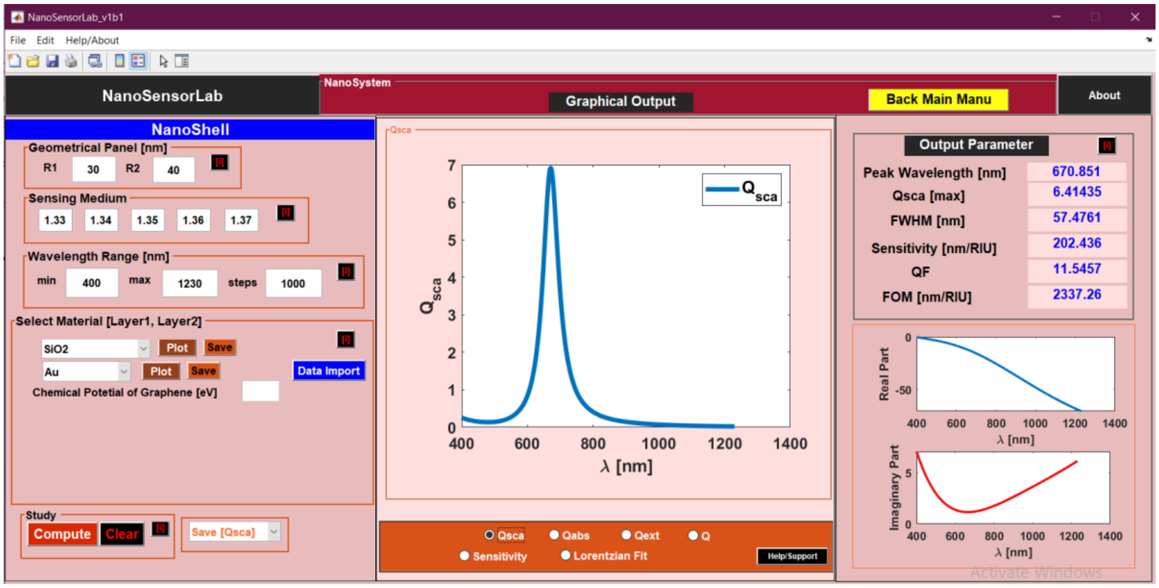


Fig.6 Example of calculated scattering efficiency of nanoshell nanoparticle (SiO_2/Au)

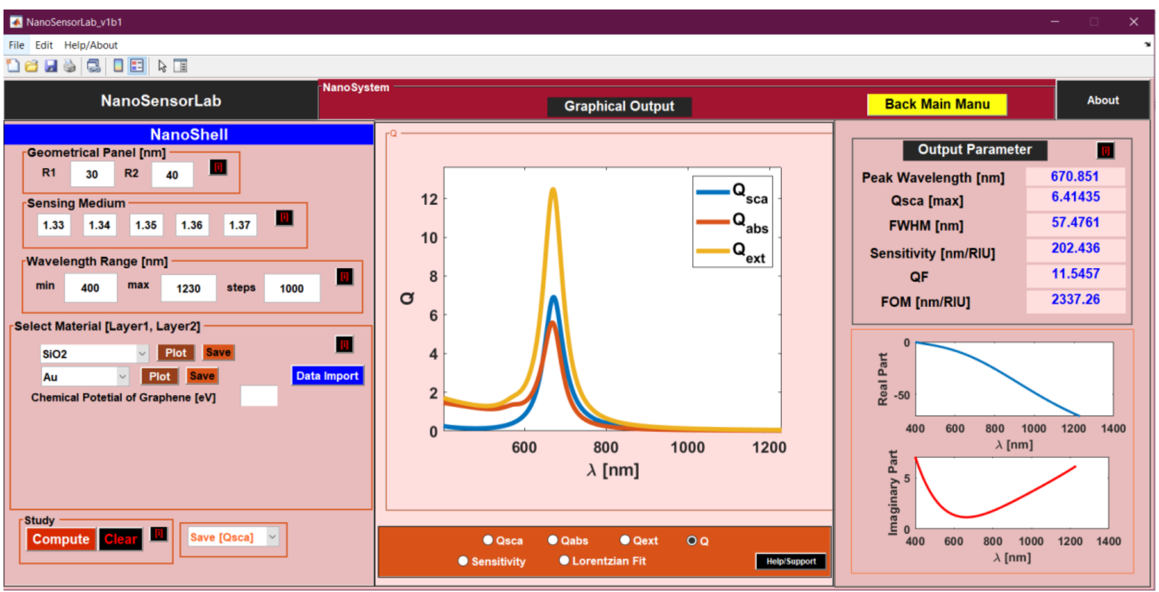


Fig. 7 *Example of calculated scattering, absorbstion and extention efficiency of nanoshell nanoparticle (SiO_2/Au)*

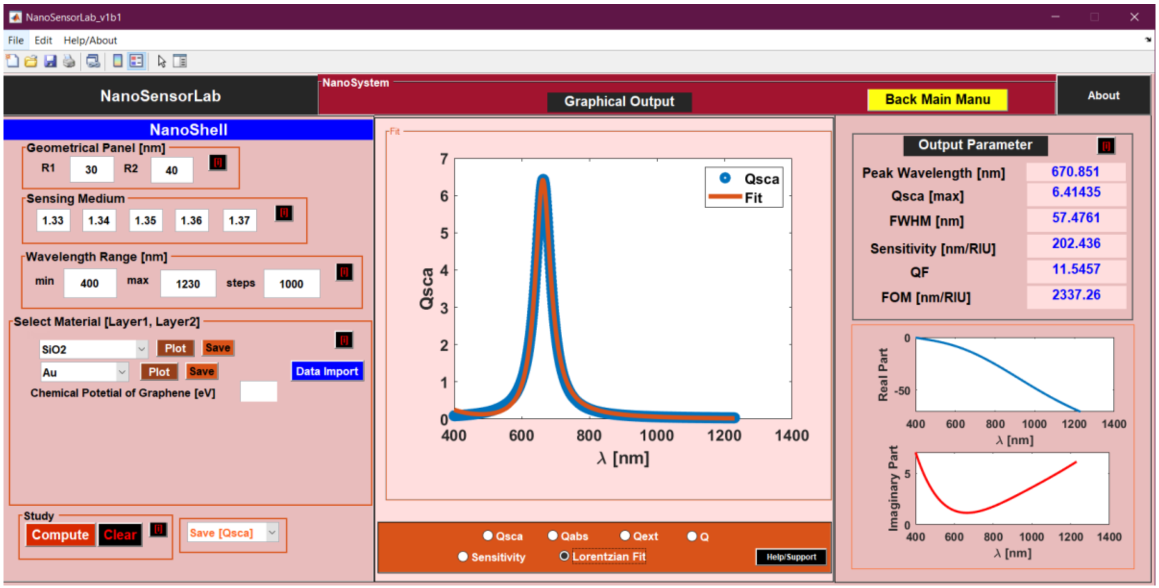


Fig. 8 *Calculated FWHM using Lorentzian fitting of scattring efficiency for nanoshell nanoparticle (SiO_2/Au)*

Fig. 9 *Calculated Sensitivity of nanoshell nanoparticle (SiO_2/Au) with different sensing medium.*

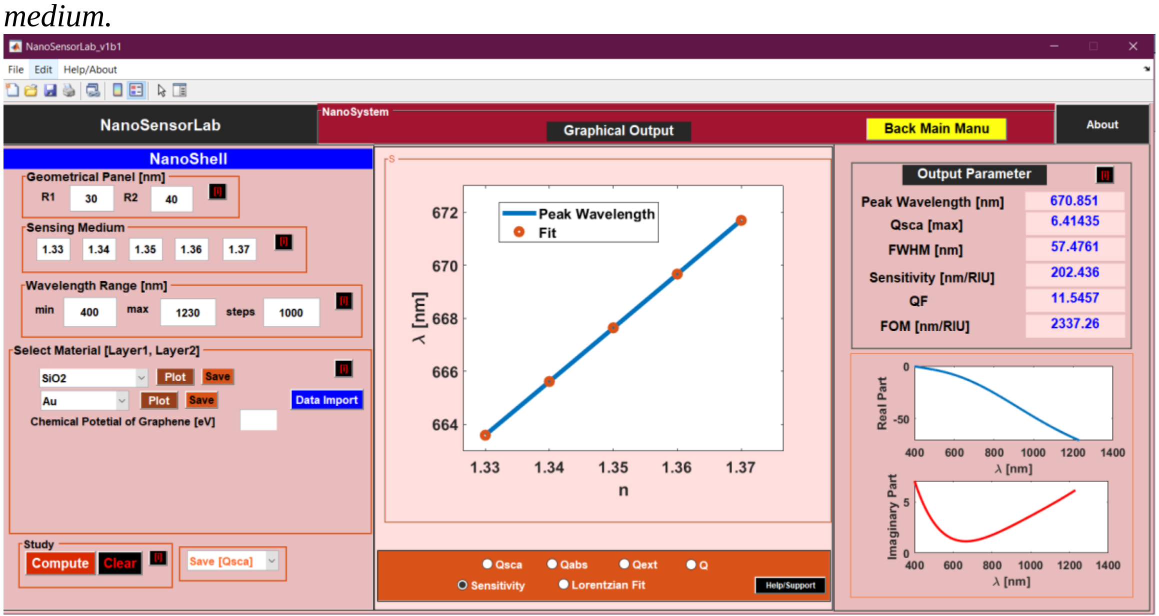


Fig. 10 *Case of user define option for nanoshell nanoparticle system.*

Example/Demonstrate (Nanomatryoshka)

In this section, our investigations concerning design considerations for the nanomatryoshka nanoparticle based simulater panel are presented in Fig 11-14. We can calculate the scattering efficiency, absorbstion efficiency, extention efficiency, full width half maximum, sensitivity and figure of merit. For these calculation follow the steps and enter the parameters (Case: SiO_2/Au/ SiO_2)

1. In geometrical Panel R_1=40nm; R_2=45nm; R_3=50
2. Take Sensing parameter ‘n=1.21, 1.22, 1.23, 1.24, 1.25’.
3. Select wavelength range between min 400 nm max 1230 nm and steps 2000.
4. In material section select inbuild SiO_2/Au/SiO_2 data and plot.
5. Import data is optional and requires wavelength[nm], real part of the dielectric, and imaginary part of the dielectric. it is user define material data. Please make sure to take one option inbuild or user define data.
6. In study section press Compute and wait for few moment.
7. Calculated results will display.

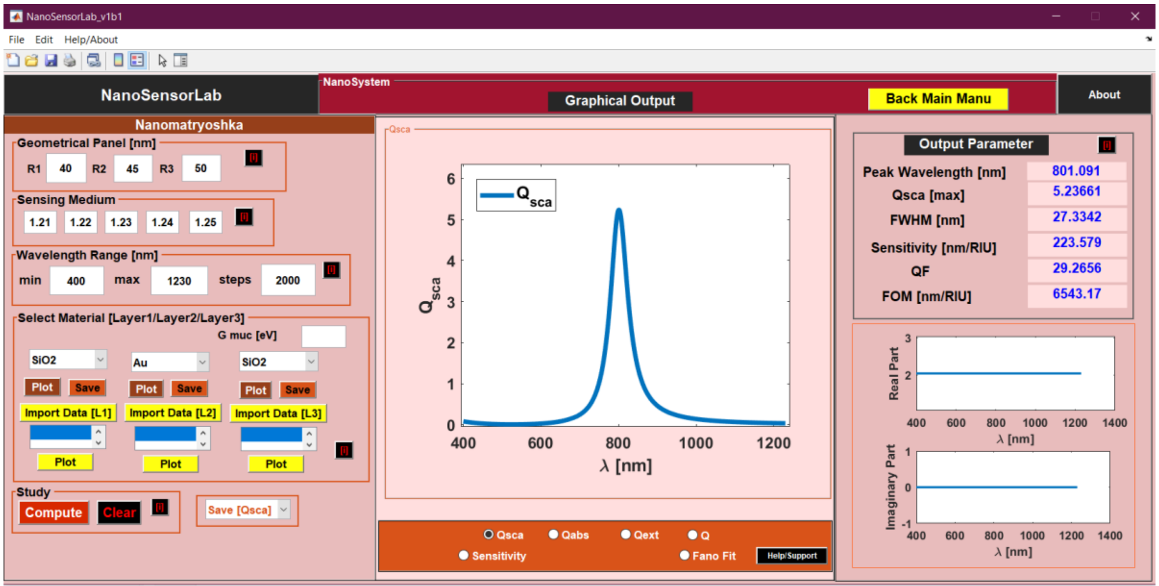


Fig. 11 *Example of calculated scattering efficiency of nanomatryoshka nanoparticle (SiO_2/Au/SiO_2)*

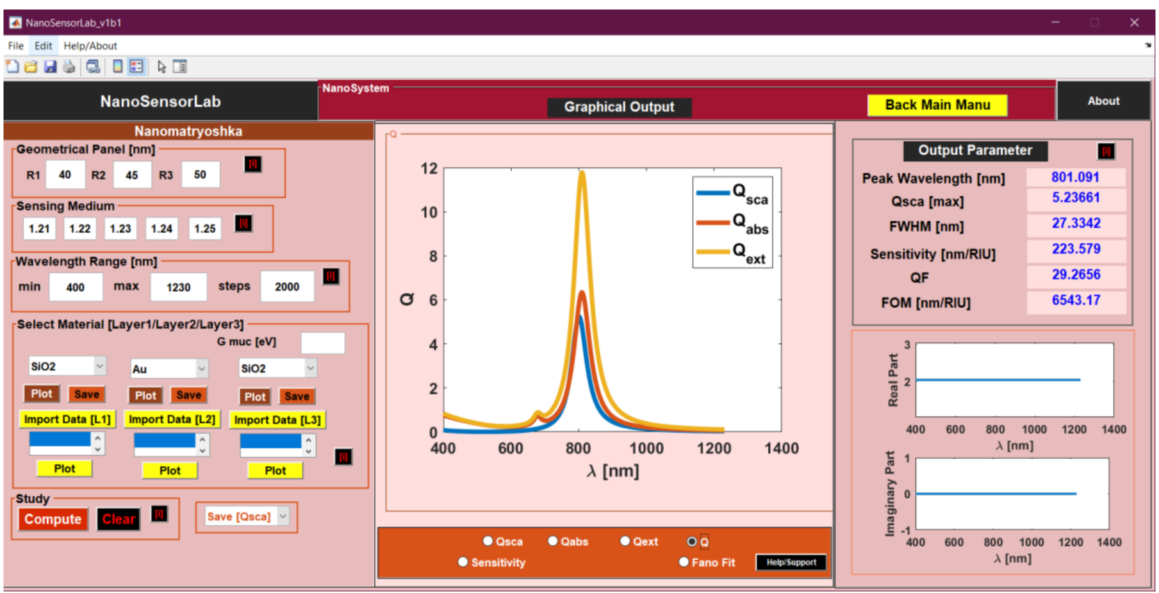


Fig. 12 *Example of calculated scattering, absorbstion and extention efficiency of nanomatryoshka nanoparticle (SiO_2/Au/SiO_2).*

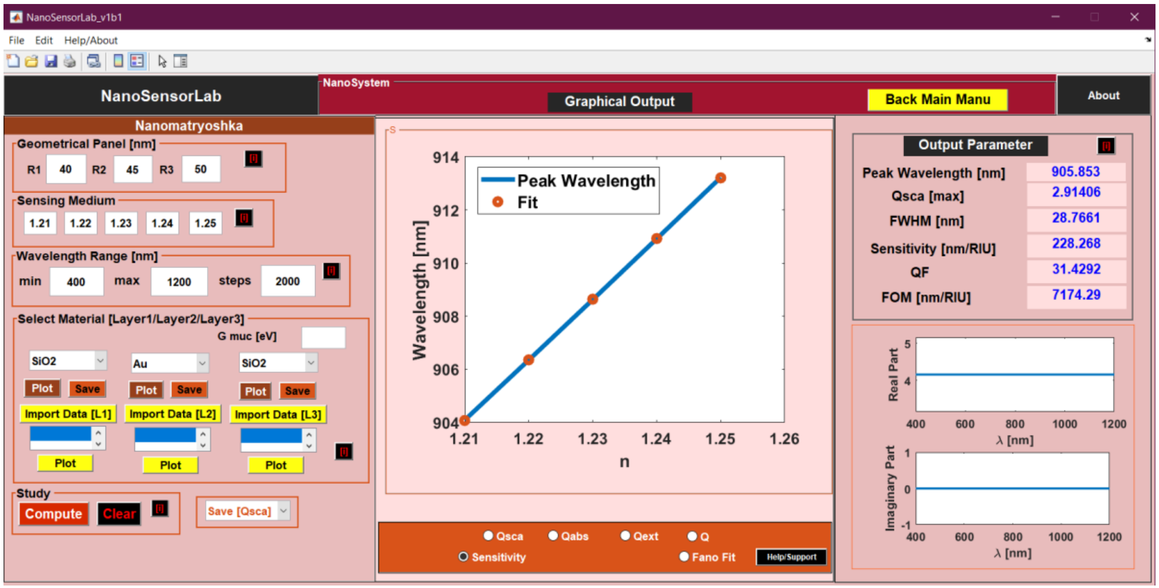


Fig. 13 *Calculated Sensitivity of nanomatryoshka nanoparticle (SiO_2/Au/SiO_2) with different sensing medium.*

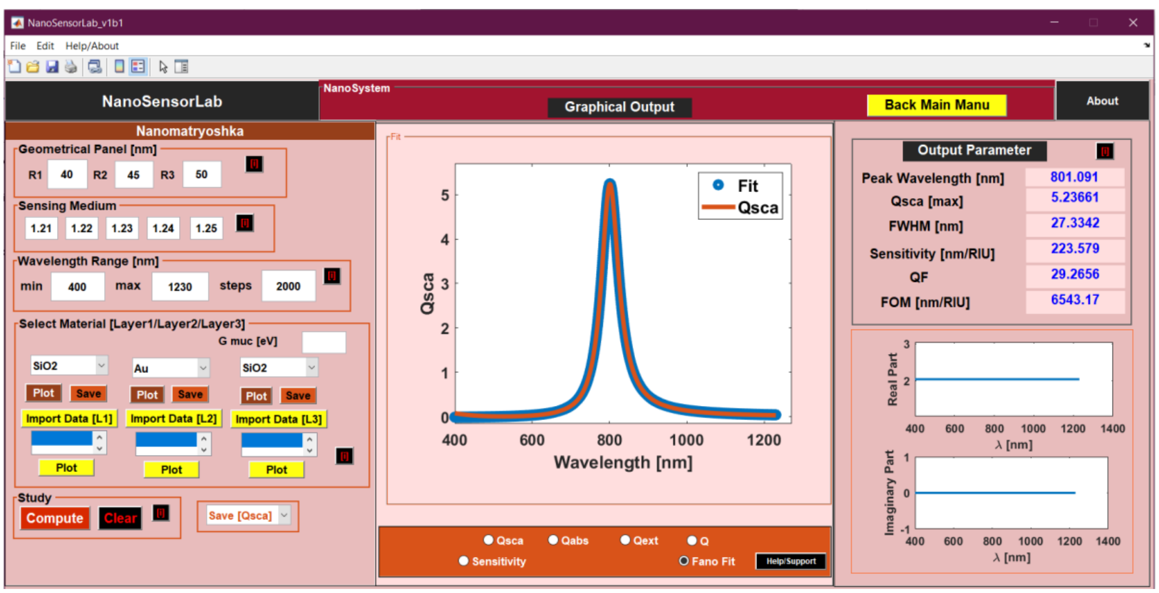


Fig. 14 *Calculated FWHM using Lorentzian fitting of scattring efficiency for nanomatryoshka nanoparticle (SiO_2/Au/SiO_2).*

Example/Demonstrate (Nanoshell with Gain)

In this section, our investigations concerning design considerations for SiO_2/Aubased plasmonic structure as shown in Fig 15-16. are presented.

Enter the following parameters

1. In geometrical Panel R_1=17; R_2=20;
2. Take Sensing parameter '1.333'.
3. Select wavelength range between min 500 nm max 900 nm and steps .1.
4. In material section select SiO_2 ($\varepsilon_1 = 2.04$)/Au.
5. Case 1: Gain=0; Case 2: Gain=0.539.
6. In study section press Compute and wait for few moment.
7. Calculated results will display.

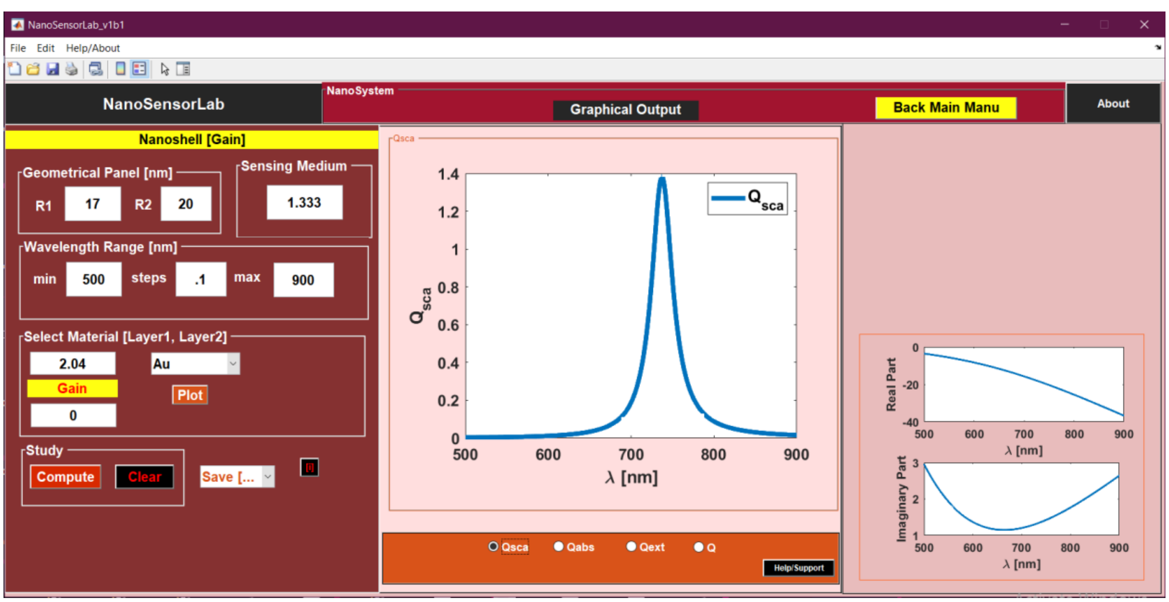


Fig 15. *The calculated scattering efficiency of (case 1: Gain =0) Nanoshell nanoparticle*

SiO_2/Au (17, 20).

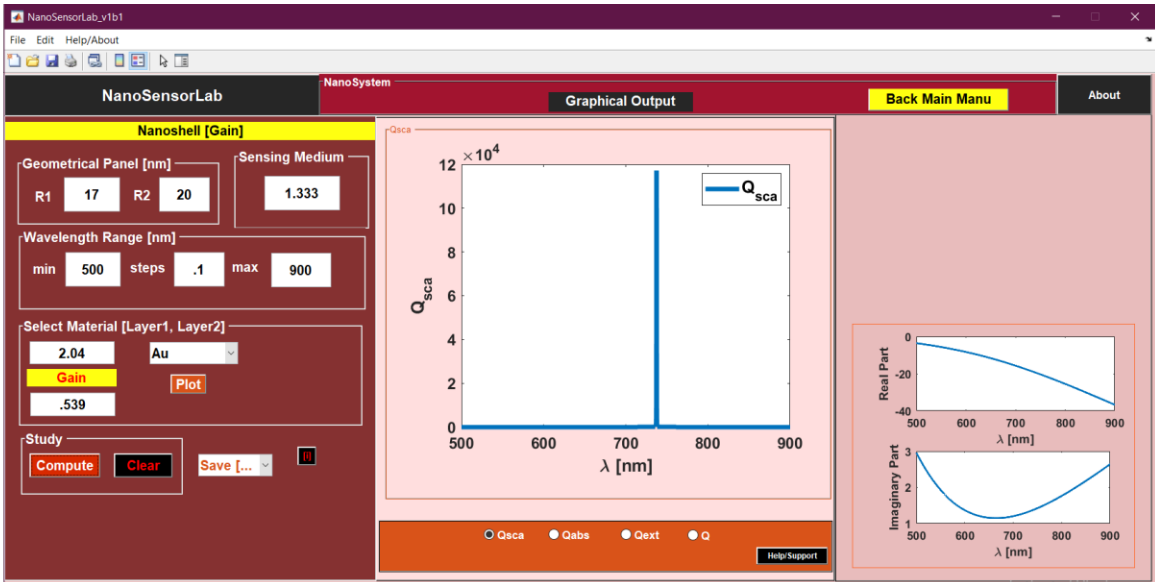


Fig 16. *The calculated scattering efficiency of (case 2: Gain=0.539) Nanoshell nanoparticle SiO_2/Au (17, 20).*

Example/Demonstrate (Nanomatryoshka with Gain)

In this section, our investigations concerning design considerations for the nanomatryoshka nanoparticle based simulater panel are presented in Fig 17-14. We can calculate the scattering efficiency, absorbstion efficiency, extention efficiency. For these calculation follow the steps and enter the parameters (Case: Au/SiO_2/Au)

1. In geometrical Panel R_1=30nm; R_2=40nm; R_3=50.
2. Take Sensing parameter ‘n=1.1545’
3. Select wavelength range between min 400 nm max 1230 nm and steps 2000.

4. Case 1: Gain=0; Case 2: Gain=0.539.
5. In material section select inbuild Au/SiO_2/Au data and plot.
6. Import data is optional and requires wavelength[nm], real part of the dielectric, and imaginary part of the dielectric. it is user define material data. Please make sure to take one option inbuild or user define data.
7. In study section press Compute and wait for few moment.
8. Calculated results will display.

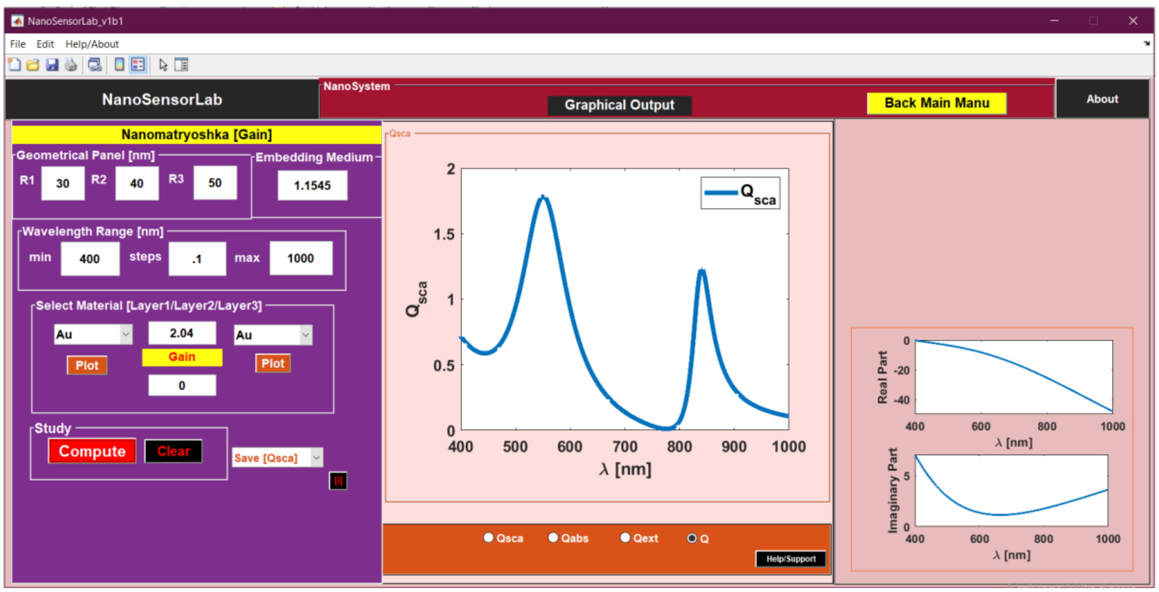


Fig 17. The calculated scattering efficiency of (case 1: Gain =0) Nanomatryoshka nanoparticle Au/SiO_2/Au (30, 40, 50).

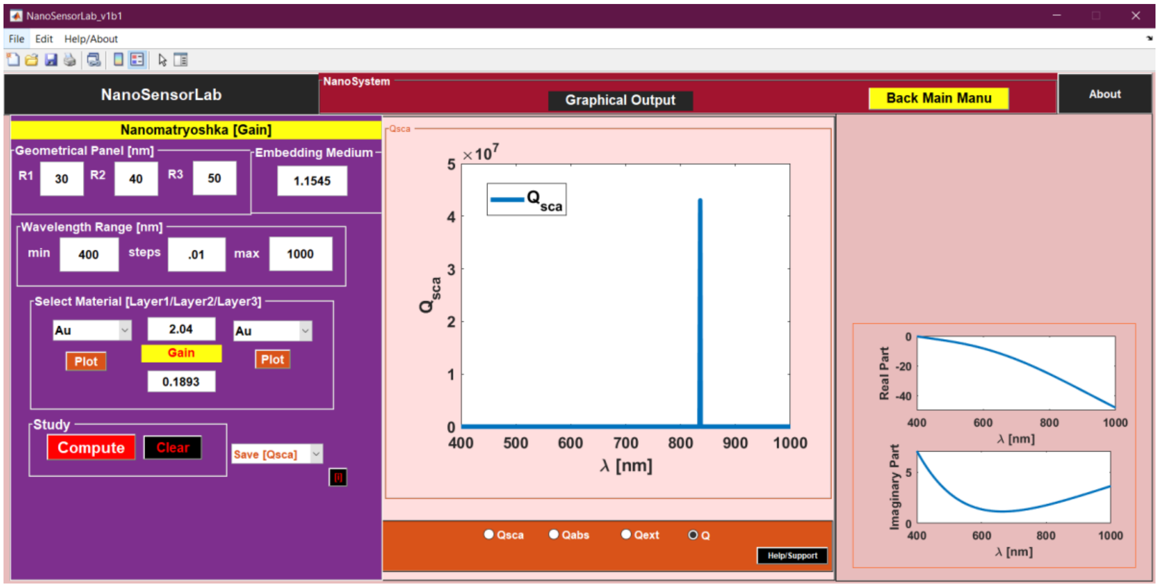


Fig 17. *The calculated scattering efficiency of (case 2: Gain=0.1893) Nanomatryoshka nanoparticle Au/SiO_2/Au (30, 40, 50).*

Limitations/Conditions

- Particle size should be in range of 15nm-120nm. Makesure for radius should be $R_1(\text{core})<R_2(\text{shell})$, $R_1(\text{core})<R_2(\text{inner shell})<R_3(\text{outer shell})$.

- Spectral range should be in 400nm-1225nm.

- Case of Graphene thickness should in 1nm-3nm.

- Sensing medium should be equal interval like .01 or.1 (1.33, 1.34, 1.35, 1.36, 1.37).

- Please select combination Dielectric/Metal or Metal/Dielectric for Nanoshell only and for Nanomatryoshka Dielectric/Metal/ Dielectric or Metal/ Dielectric/Metal only.

Computation requirements

- 64-bit Windows Operating System
- At least 1 GB memory, but 4 GB per processor core or more is recommended.
- 2-5 GB of disk space required for installation.

References

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2. P. Rajput, and M. S. Shishodia, **“Förster Resonance Energy Transfer and Molecular Fluorescence near Gain Assisted Refractory Nitrides Based Plasmonic Core-Shell Nanoparticle”,** Plasmonics **15**, 2081 **(2020).**

3. A. Singh, and M. S. Shishodia, **“Graphene vs. silica coated refractory nitrides based core-shell nanoparticles for nanoplasmonic sensing”,** Physica E Low Dimens. Syst. Nanostruct. **124**, 114288 **(2020).**