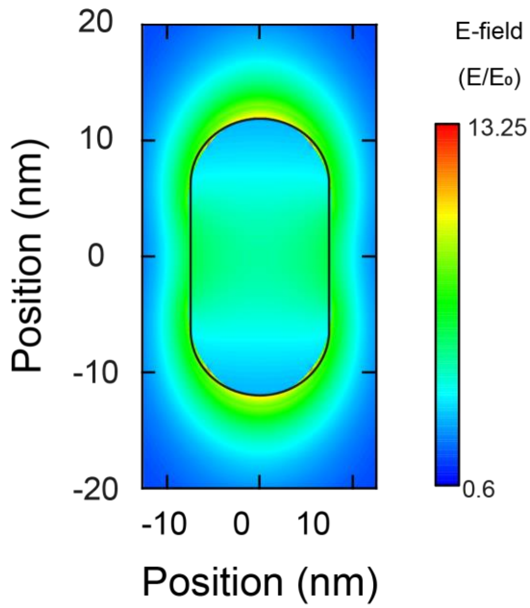
Technical portfolio – Nicola Peruffo

Optical Simulations & Design (Lumerical FDTD, Zemax)



Simulated electromagnetic field of a gold nanorod excited at 590 nm and with polarization parallel to the long nanorod axis

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Technical Focus and Tools

My background combines 7+ years of hands-on experience in optical spectroscopy and nanomaterials, which I am now complementing with training in optical simulation and design tools. I use Lumerical FDTD—learned under expert supervision during a secondment—to model nanoscale light–matter interactions and validate experimental data. More recently, I began to explore basic optical system design: I independently acquired my skills in Zemax and completed the *“Design of High-Performance Optical Systems”* course (University of Colorado Boulder) to build a solid foundation in optics. This portfolio presents two selected projects that demonstrate my ability to bridge experimental work and simulations. The files used to produce this portfolio can be found at https://github.com/Nicola-Peruffo/Technical-Portfolio.

Electromagnetic Simulation of Dye-Capped Gold Nanorods for SERS Applications Using Lumerical FDTD

Context and Motivation

This simulation project began during a two-week secondment at Eindhoven University of Technology (October 2023), funded by a European research grant that I secured. There, I learned to use Lumerical FDTD and performed preliminary simulations on gold nanorods functionalized with organic dyes. I later refined the work in Sweden as part of a broader experimental study on plasmon–dye systems, which was eventually published in a high impact factor journal (Peruffo et al., *ACS Nano*, 2025. DOI: 10.1021/acsnano.4c17571).

Objectives

- Simulate the extinction spectrum and electromagnetic field distribution of individual gold nanorods covered with a polymeric nanolayer. Validate experimental data.
- Extend the model to investigate gold nanorods covered with 16 different dye-capping configurations, involving two dye molecules (PIC and TDBC) and different concentrations.
- Calculate the Surface-Enhanced Raman Scattering (SERS) enhancement factor, using electromagnetic field outputs from FDTD simulations.

Methodology

1. Learning and Setup

Within the first two weeks in Eindhoven, I acquired the essential skills to:
- Build complex 3D geometries in Lumerical (AuNR core + capping layers).
- Define mesh and symmetry conditions suitable for plasmonic nanostructures.
- Set up total-field scattered-field (TFSF) sources, monitor electromagnetic field (DFT monitor, as reported on the first page) and extinction cross sections.

2. Model Design

Gold nanorod geometry was modelled based on transmission electron microscopy data. The refractive index of gold was taken from the Johnson & Christy dataset. The polymeric and dye layers were modelled as shells with defined thicknesses derived from experimental values and literature. The refractive index was set to reproduce the experimental results.

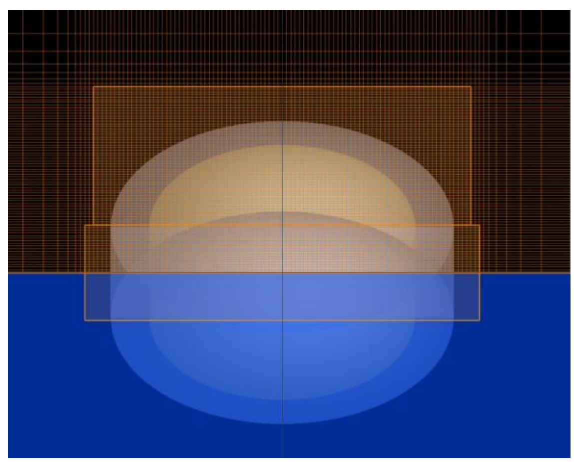


Figure 1: *Simulation of a gold nanorod, composed of the intersection of 2 spheres and a cylinder. The mesh size was set to 0.125 nm close to the surface of the nanorod, and the symmetry boundary conditions were applied.*

3. Parameter Sweep and EM Analysis

Simulations were run for each of the 16 dye configurations. From each simulation:
- The extinction spectrum was extracted;
- The electromagnetic field maps were recorded at the excitation and emission wavelengths retrieved from experimental data. Using a custom script written in Lumerical's scripting language, I automatically extracted the $|E|^2$ values at $\lambda_{excitation}$ and $\lambda_{emission}$, necessary for the calculation of the SERS enhancement factor.

Results and data interpretation

Extinction Spectra and Validation

The simulated extinction spectra show good agreement with experimental data obtained for gold nanorods coated with polymeric and dye shells. The experimental unpolarized extinction spectrum of nanorods coated with a polymer (black line in Figure 2a) displays both transverse and longitudinal plasmon resonances. The longitudinal plasmon resonance can be reproduced in simulations with excitation light polarized along the nanorod's long axis (green line), while the simulation with excitation along the short axis (red line) reproduces the transverse plasmon.

The concentration of the PIC dye was gradually increased from 0 to 7.4 µM (Figure 2a to 2d). Since the absorption peak of PIC (indicated by the green vertical line) overlaps with the longitudinal plasmon resonance, strong exciton–photon coupling occurs. This leads to the emergence of two new peaks flanking the PIC absorption, separated by an energy known as Rabi splitting. Both the experimental and simulated extinction spectra under longitudinal polarization (black and green lines) clearly show this splitting effect, which increases increasing the PIC concentration.

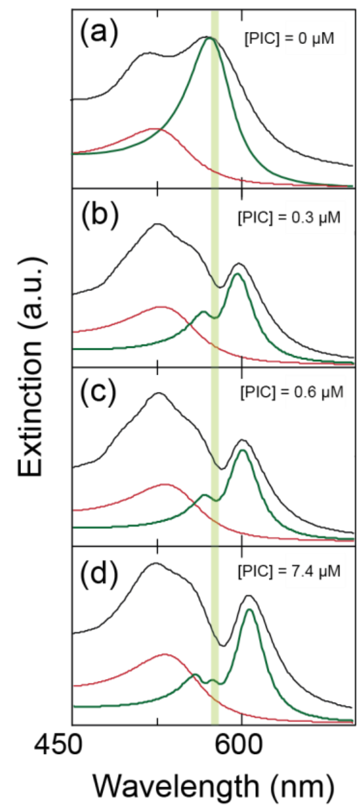


Figure 2: *Gold nanorods experimental (black lines) and simulated extinction spectra (green and red lines for polarization along the long and short nanorod axes, respectively). PIC concentrations increase along the panels from 0 to 7.4 µM. The green vertical line indicates the main absorption of the PIC dye.*

SERS Enhancement Factor Calculation

The SERS EF (EF_{SERS}) was calculated using the formula:

$$EF_{SERS} = \left|\frac{E(\lambda_{excitation})}{E_0}\right|^2 \cdot \left|\frac{E(\lambda_{emission})}{E_0}\right|^2 ,$$

where $E(\lambda_{excitation})$ and $E(\lambda_{emission})$ are the maximum electric field values at the excitation and emission wavelengths, respectively, extracted from the electromagnetic field profiles, and E_0 is the incident field amplitude (normalised to 1). These values were retrieved via an automated Lumerical script I developed, enabling consistent and reproducible EF calculations across all samples.

The EF_{SERS} was calculated for 16 samples that differ in dye molecule (PIC or TDBC) and concentration. Moreover, for each sample, I calculated the SERS enhancement factor for two molecular vibrations, specifically for the vibration at 675 cm^{-1} and 1427 cm^{-1} for TDBC (blue and light blue lines in Figure 3, respectively). The green and light green lines in Figure 3 represent instead the enhancement for the vibration of PIC at 590 cm^{-1} and 1410 cm^{-1}, respectively. The EF_{SERS} were plotted as a function of the ratio between the Rabi splitting and the energy of the vibration. When this ratio is one, the EF_{SERS} peaks, which leads to important conclusions about SERS and strong exciton-photon coupling, as discussed in more detail in the published article (DOI:10.1021/acsnano.4c17571).

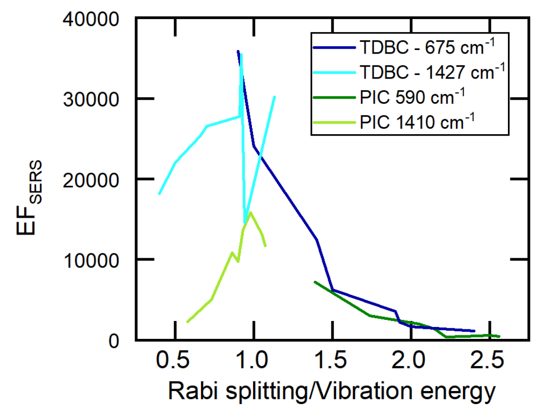


Figure 3: *Simulated SERS enhancement factor (EF_{SERS}) plotted for different Rabi splitting / Vibration energy ratios. The different colored lines refer to different molecular vibration enhanced by SERS.*

Key competencies applied

- Use of Lumerical FDTD for plasmonic nanostructure modelling;
- Custom scripting in Lumerical for field extraction and batch simulations;
- Understanding of electromagnetic field enhancement, nanoparticle photonics, and correlation with experimental data;
- Experience in interpreting optical properties of functionalized nanoparticles.

Conclusion

This project demonstrated the potential of numerical simulations to validate experimental data of nanomaterials. It also enabled me to quantify SERS enhancements and explore structure-function relationships of complex nanostructures. This work supported a deeper understanding of exciton–plasmon interactions and guided experimental design, demonstrating how simulations can accelerate the development of SERS-based optical sensors.

Design and Optimization of a Two-Lens Microscope in Zemax

Objective

Design a simple microscope using only two catalog lenses, with a 40× magnification (8× objective and 5× tube lens). The system was evaluated for three standard wavelengths (F-d-C lines) using a field height of Hy = 1mm and an entrance pupil diameter of 3 mm.

Optical layout

Approach

1. Paraxial Design (Baseline)

Initial distances between lenses were calculated using paraxial optics.

→ Result: Magnification = 40×, but spot RMS ≈ 4 mm: poor image quality due to aberrations.

2. Geometrical Optimization

Lens-to-object and tube distances were optimized while keeping M = 40×.

→ Result: spot RMS reduced to 565 µm, with an Airy radius of 575 µm. The system achieved near-diffraction-limited performance.

3. Full Optimization (Lens Shapes)

Lens curvatures and thicknesses were also optimized within reasonable mechanical limits.

→ Final result: RMS = 389 µm, Airy radius = 203 µm. The resolution is significantly improved.

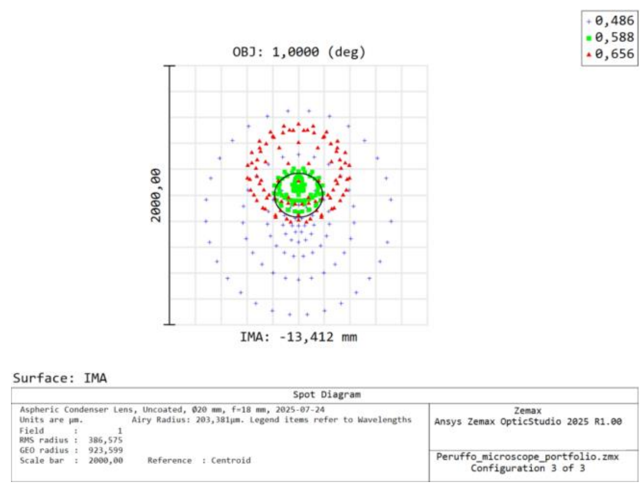
→ The tube length is 397 mm, longer than the standard (160–180 mm), but achieved using only two simple lenses.

Zemax Merit Function

Used to simultaneously:

- Set the wavelengths magnification to 40×;
- Minimize both RMS spot size and Airy disk radius;
- Keep lens parameters within practical values.

Spot diagram



Summary Table of Key Results

Config.	RMS Spot [µm]	Airy Radius [µm]	Magn.	Tube Length [mm]
1	4000	12	40×	180
2	566	575	40×	169
3	389	203	39×	397

Key competencies and conclusion

- Optical system design from scratch;
- Paraxial analysis and ray tracing;
- Merit Function-based optimization;
- Evaluation of diffraction-limited performance.

This project represents my first step into optical system design, complementing my expertise in photonics and spectroscopy.