

# Tailoring plasmon resonances for applications in nanophotonics

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## Abstract

Complex metal nanostructures exhibit surface plasmon resonances that play a crucial role in a variety of electromagnetic phenomena. By means of the surface integral equation formulation, we have calculated the scattering properties of nanoparticles with different shapes, either isolated or interacting. Furthermore, we have made use of a bio-inspired stochastic technique in order to optimize particle design for some configurations of interest in nanophotonics.

## 1. Introduction

Complex metal nanostructures exhibit surface plasmon resonances that play a crucial role in a variety of electromagnetic phenomena. We are interested in the properties of metal nanoparticles with localized plasmon resonances (LPRs) yielding large local electromagnetic fields or enhanced emission. More precisely, we have focused our efforts on dimers/trimers composed of nanoparticles of various shapes (triangles, rectangles, cubes, rods) playing the role of nanoantennas, as well as on single more complex nanoparticles (nanostars/nanoflowers), because of their interest in enhanced optical emission processes (Raman, fluorescence, photoluminescence,...) [1-5].

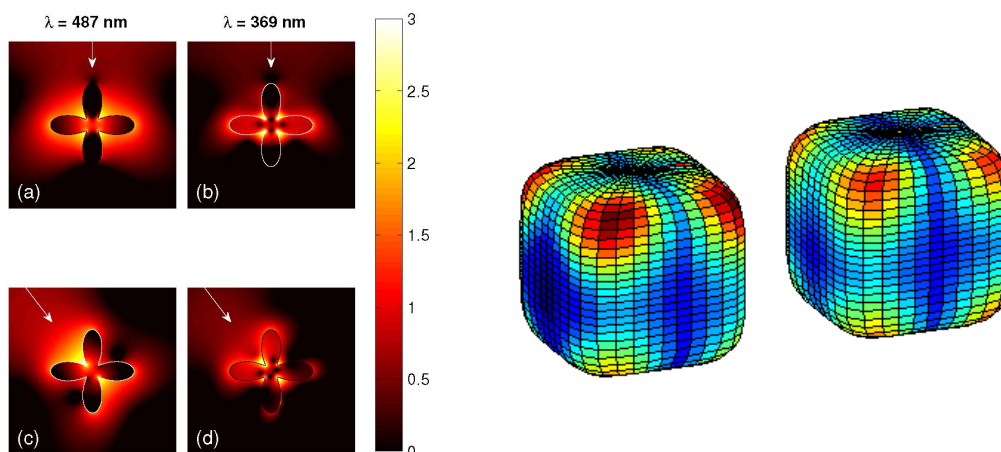


Fig.1. Left-panel: Near-field distributions of the electric field intensities in a log10-scale for the Ag four-petal nanoflower with mean radius  $\rho=30$  nm and deformation parameter  $\beta=2/3$ , illuminated with a monochromatic plane wave with wavelength equal to either one of the two main LPRs (dipolar and quadrupolar, respectively) at  $\lambda=487$  nm (a,c) and at  $\lambda=369$  nm (b,d): (a,b)  $\theta_i=0^\circ$ ; (c,d)  $\theta_i=45^\circ$ . Adapted from [3]. Right-panel: Electric field intensity on the surface of a Ag rounded-cube dimer ( $L=30$  nm, gap=20 nm) with plane wave illumination matching the longitudinal LPR. Adapted from [7].

## 2. Surface integral formulation of light scattering by small nanoparticles

From the theoretical side, the calculation of light scattering by small nanoparticles in the optical regime is a well-defined but difficult problem that requires a trade-off between ambition and numerical cost, as well as between quantitative and qualitative descriptions of the system under consideration. In the last few years, we have developed an advanced numerical formulation to calculate the optical properties of 2D and 3D nanoparticles of arbitrary shape and lack of symmetry [6, 7]. The method is based on the well-known Green's theorem surface integral equations for scattering [8], but it has been implemented for parametric surfaces describing particles with flexible shape through a unified treatment (Giel's formula [9]), which makes it remarkably versatile [7,10].

## 3. Tailoring plasmon resonances

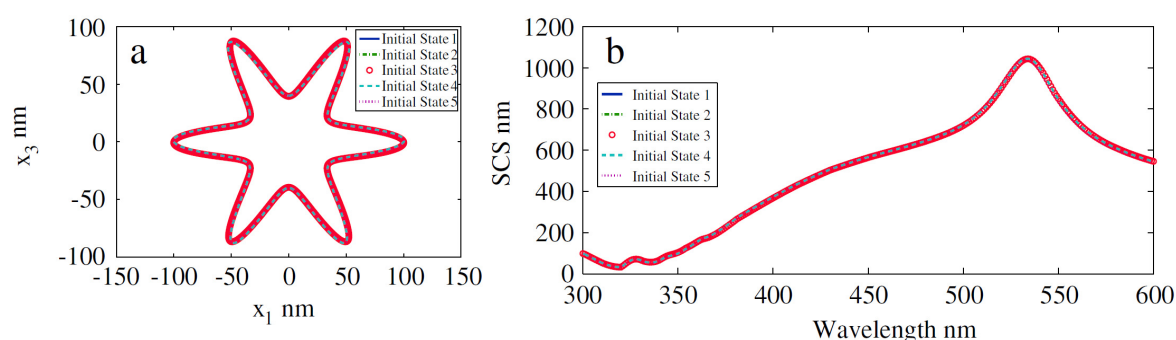


Fig. 2: a) Optimized star-like geometries obtained with Giel's Superformula. Each line corresponds to an initial state of the optimization algorithm. b) SCSs for each of the star-like nanostructures depicted in Fig. 2a, optimized to yield a maximum at  $\lambda=532$  nm. Adapted from [10].

On the basis of the above-mentioned method, we have calculated the scattering cross sections for nanowires [1-4] and nanoparticles [7] of various shapes (see Fig. 1), either isolated or interacting, including far-field patterns and spectra, near-field intensity maps (with corresponding enhancement factors), decay rates, and surface charge distributions. Furthermore, the optimal design of nanoantennas with specific properties is an aspect of the inverse problem that has not received too much attention until recently, despite being crucial from the point of view of applications. In order to find the optimal nanoparticle geometry that maximizes/minimizes a given optical property, we have made use of a bio-inspired stochastic technique based on genetic algorithms [10], which exploits the above mentioned formulations for flexible surfaces [6,7] to solve the direct scattering problem.

We show how this stochastic procedure converges to optimized nanoparticles in some configurations of interest in nanophotonics: nanoflower/nanostar geometry that exhibits a LPR at or near a given wavelength (see Fig. 2) for SERS (surface-enhanced Raman scattering) substrates [10]; dimer nanoantennas that yield maximum field enhancements and radiative decay rates within the gap for enhanced fluorescence/photoluminescence; long nanoantennas with third-order resonances at given wavelengths for non-linear optical processes, such as second harmonic generation and two-photon luminescence. With regard to the latter, the occurrence of Fano resonances [11] at the  $L \sim 3\lambda/2$  resonance of the nanorod will also be discussed.



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