Designing plasmon nanoparticles tailored for applications in nanophotonics

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Complex metal nanostructures exhibit surface plasmon resonances that play a crucial role in a variety of electromagnetic phenomena relevant to Nanophotonics. We are interested in the electromagnetic properties of metal nanoparticles of complex shape, with localized plasmon resonances (LPR) yielding large local electromagnetic fields or enhanced emission: such as dimers/trimers playing the role of nanoantennas; or nanoparticles of complex shape (nanostars/nanoflowers); both of interest in enhanced optical emission (Raman, fluorescence, photoluminescence,…) [1-5]. In this regard, it is crucial first to fully characterize the **LPR** for a variety of metal nanoparticles of arbitrary shape. To this end, we have developed an advanced numerical formulation to calculate the optical properties of 2D and 3D nanoparticles (single or coupled) of arbitrary shape and lack of symmetry [6,7]. The method is based on the (formally exact) surface integral equation formulation. Thus the 3D version is based on the same equations as that of Ref. [8]; nonetheless, it has been implemented for parametric surfaces describing particles with **flexible shape** through a unified treatment (Gieli's formula), which makes it far more versatile [7,9]. On the basis of these methods, we have indeed calculated the scattering cross sections for nanowires [1-4] and nanoparticles [7] of various shapes (triangles, rectangles, cubes, rods, stars, see i.e. 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-inpired stochastic technique based on genetic algorithms [9], 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 [9]; 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 (SHG, TPL). With regard to the latter, indeed, the occurrence of Fano resonances at the $L{\sim}3\lambda/2$ resonance of the nanorod will also be discussed.

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Figures.

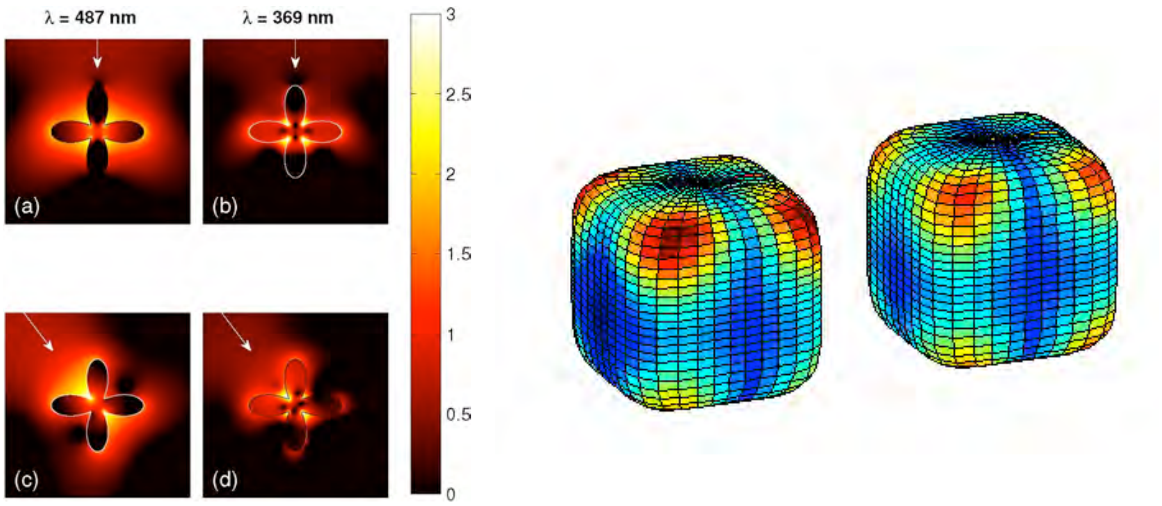

Fig.1. Left-panel: Near-field distributions of the electric field intensities in a log10-scale for the Ag four-petal nanoflower with mean radius ρ=30 nm and deformation parameter β=2/3, illuminated with a monochromatic plane wave with wavelength equal to either one of the two main LPRs (dipolar and quadrupolar, respectively) at λ=487 nm (a,c) and at λ=369 nm (b,d): (a,b) θ_i=0◦; (c,d) θ_i=45^o [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 [7].

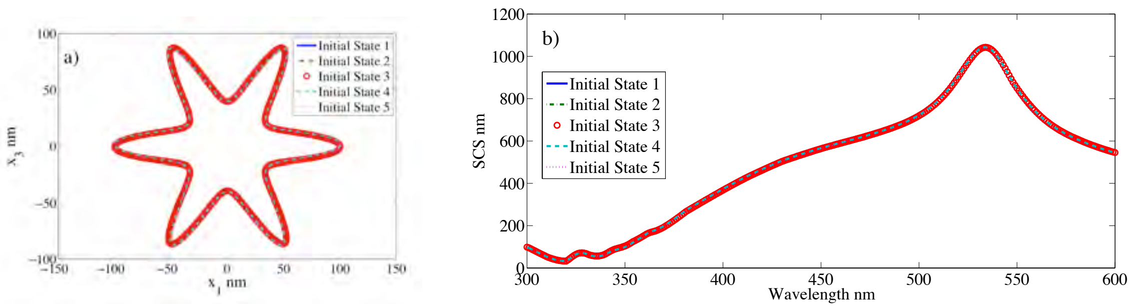

Fig.2. a) Optimized star-like geometries obtained with Gielis' Superformula. Each line corresponds to an initial state of the optimization algorithm. b) SCSs (optimized to yield a maximum at λ=532 nm) for each of the star-like nanostructures depicted in Fig. 2a (same curve styles in both figures) [9].