# *Designing plasmon nanoparticles tailored for applications in nanophotonics*


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# *Outline*

- Introduction: Design in plasmonics
- Calculation method: 2D & 3D surface integral equations
  - Formalism
- Design: stochastic methods
  - Genetic algorithm, …
  - SERS: Nanostars
  - SEF: Nanodimers
  - …
- Fano-like resonances on a single rod
- Conclusions

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# *Introduction: Design*

Nano-Optics & Nano-Photonics

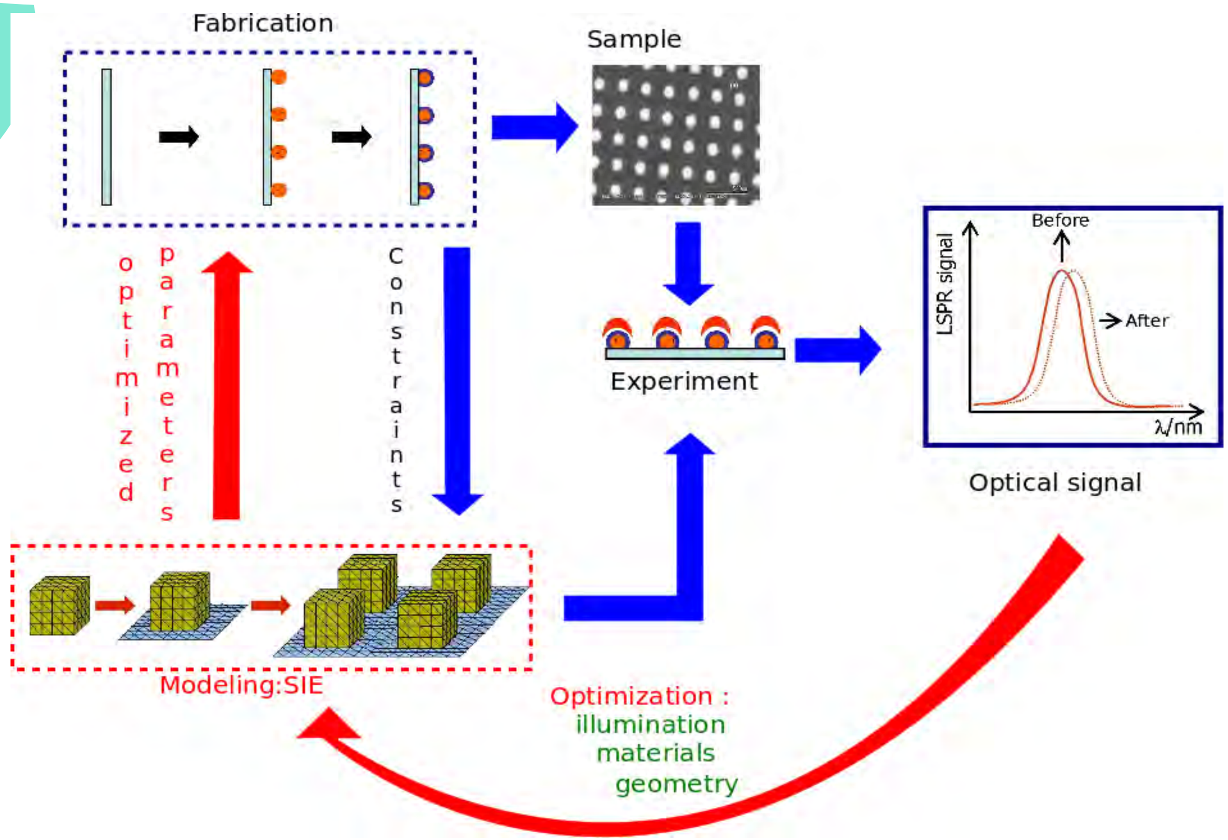
Metamaterials

Sensing

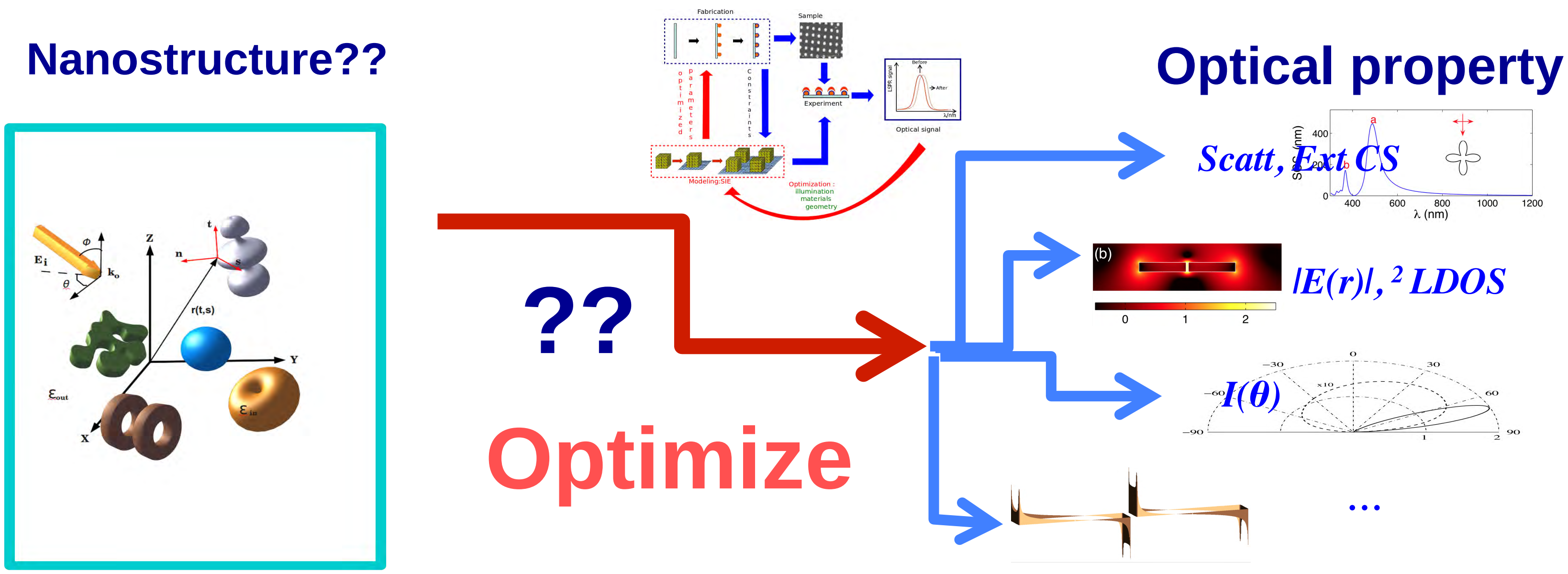
**Plasmonics**

Biomedicine

…



# *Introduction: Design*




➢Direct problem solver: Scattering Equations.
*Rigorous, flexible, numerically efficient.*

➢Optimization method: Stochastic algorithm.
*Convergence & time efficiency*

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  - 3D Flexible SIE: Poster Rogelio Rodríguez-Oliveros
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## Theoretical/Numerical Methods

- Real Space
  - Integral
    - ✓Surface: Green's Theorem, MoM, BEM,…
    - ✓Volume: Green's Dyadic, DDA, MMP, CDE, . . .
  - Differential (Volume): FDTD, FEM, . . .
- Reciprocal (*k*) Space
  - Plane wave expansions: Reduced Rayleigh equations,..
  - Others: T-matrix (+EBC),…

- ….Commercial software

# Scattering Formulations

## Theoretical/Numerical Methods

- Real Space
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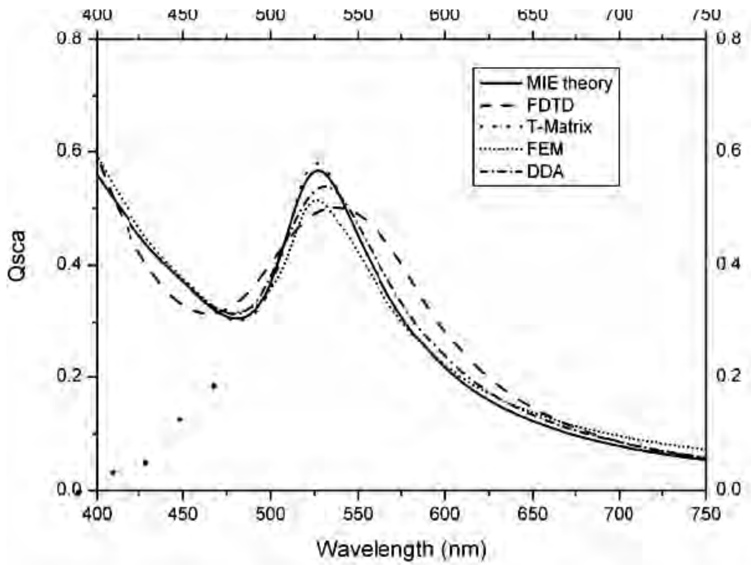
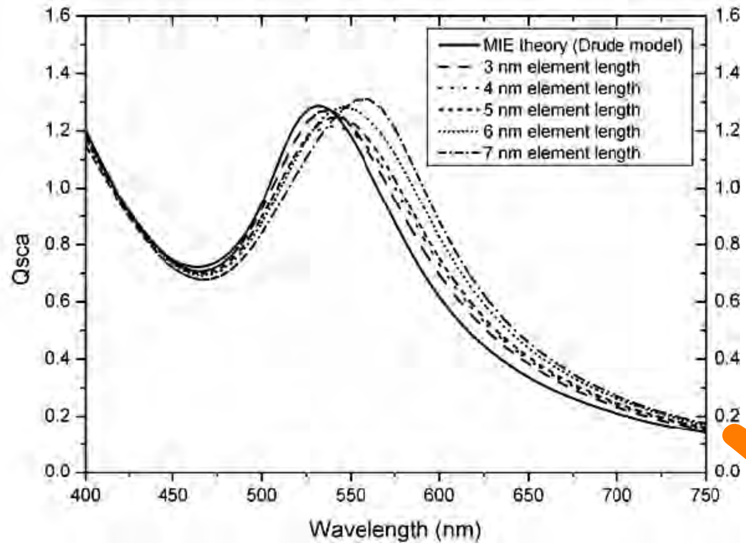
  - – Others: T-matrix (+EBC),…

Warning!!

- ….Commercial software

# *Scattering calculations*




**Barnes, J. Opt. A: Pure Appl. Opt. 2009**

**Theoretical/Numerical Methods:**

**80 nm Au sphere**

**Comparison with**

**Mie Scattering:**

- **inaccurate!!**
- **($10^2$-$10^4$ times) slower!!**

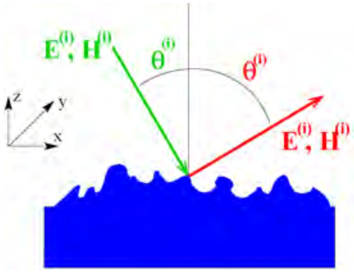
**Warning!!**

**FDTD vs Mie**

# *Scattering calculations*

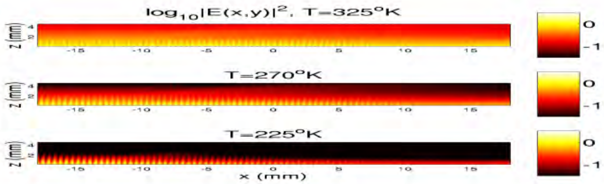
## 2D SIE

### Rough surface scattering



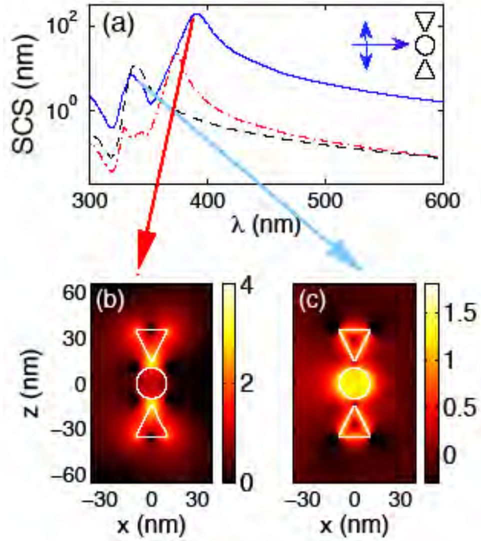

80s, 90s : Maradudin, Mendez, and co.
Nieto-Vesperinas, Soto-Crespo, S-G
Maystre & Saillard

### SPP scattering

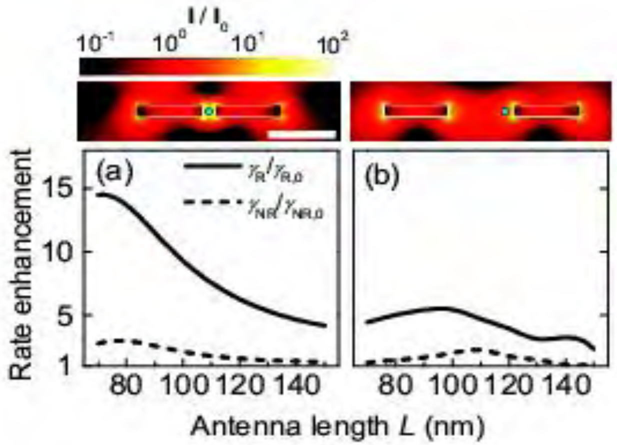



Gomez Rivas et al, PRL 2004, PRB 2006, APL 2008
Muskens et al, Opt. Express. 2007

### Nano-antenna enhanced fluorescence



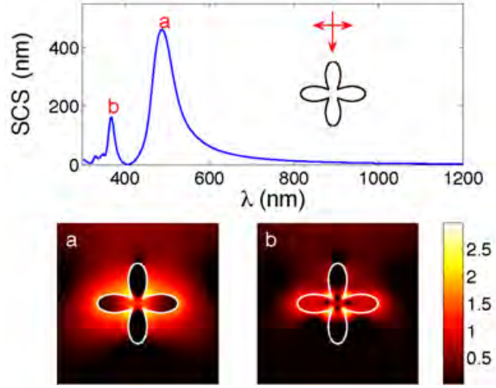

Giannini, Sánchez-Gil, Opt. Lett. 2008




Muskens, Giannini, Sánchez-Gil , Gómez Rivas, Nano Letters 2007

### LSP resonances, SERS, ...

Giannini, Rodriguez-Oliveros, Sánchez-Gil, JOSAA 2007, Plasmonics 2010
Muskens et al, Opt. Express. 2007



# 2D/3D SIE: features

- Surface-integral representation of Maxwell equations (Stratton-Chu equations) ➔ Exact EM scattering theory
- System of SIE for the unknown sources ➔ surface EM fields **E**,**H** (or **J**,ρ)
- 2D/3D Surface mesh (*N*) ➔ ***System of linear equations 2Nx2N/6Nx6N***
- 2D/3D Surface in parametric coordinates➔ ***Gielis' Superformula***

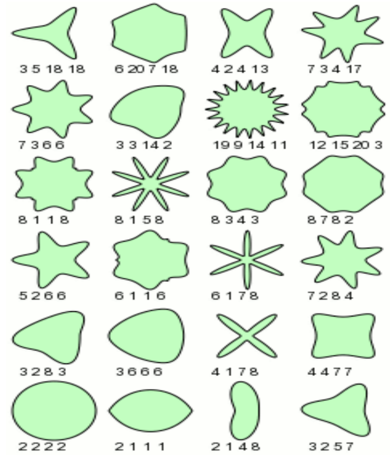
3D: Rodríguez-Oliveros Poster

# *Scatterers: Flexible 2D/3D Surfaces*

## Gielis' supershape+3D superformula

- 2D

$r(\varphi)=[|a^{-1}\cos(m\varphi/4)|^{n2}+b^{-1}\sin(m\varphi/4)|^{n3}]^{1/n1}$

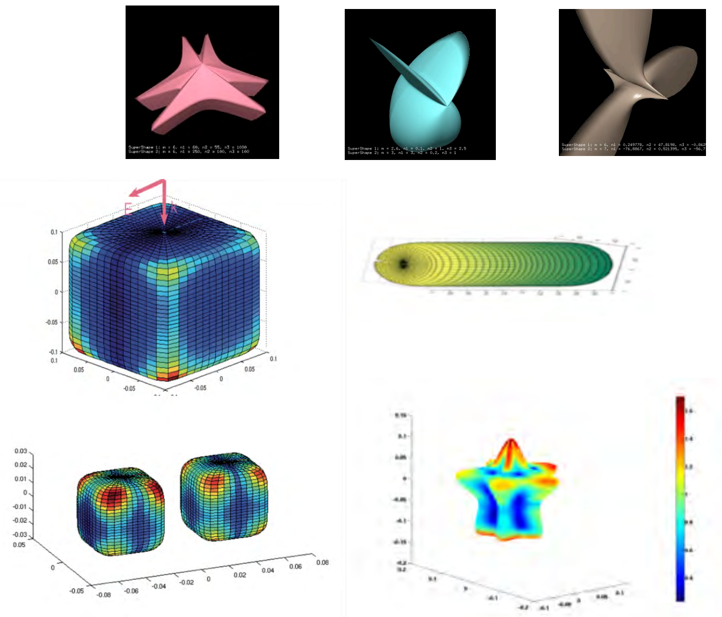



- 3D

$x=r_1(\theta)\cos\theta\ r_2(\varphi)\cos\varphi$

$y=r_1(\theta)\sin\theta\ \ r_2(\varphi)\cos\varphi$

$z=r_1(\varphi)\sin\varphi$



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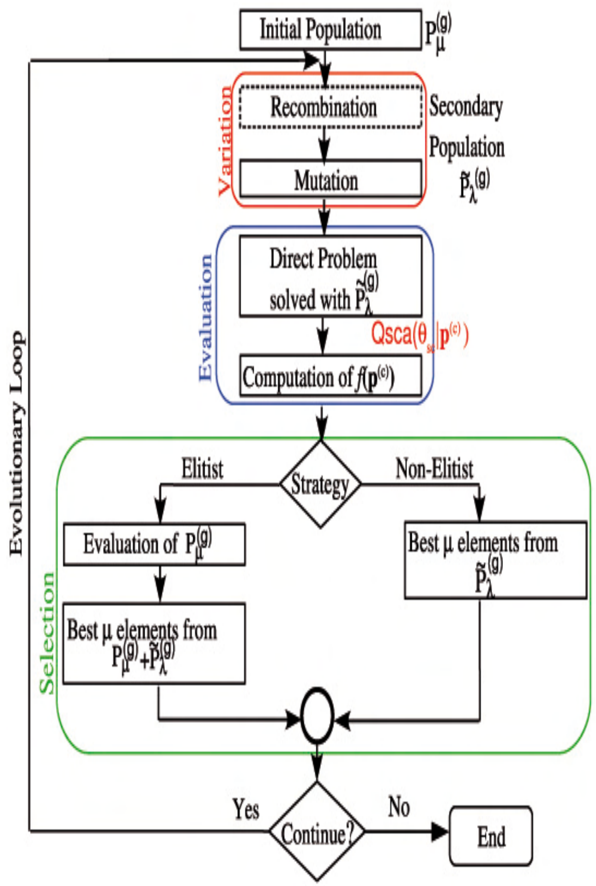
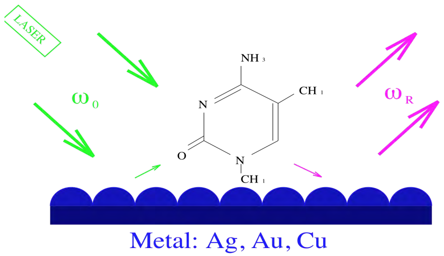
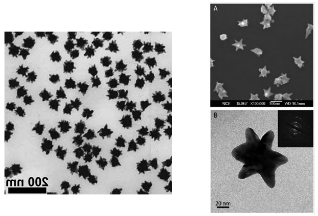
## Genetic algorithm

- Define ***objective function***
  ► SCS σ(ω), Near-field E(**r**), Far-field I(θ), LDOS, …
- Define ***parameters*** to be optimized ► SUPERSHAPE
- Initial random ***population*** of parameters
- ***Recombination & mutation***
- Evaluation method
  ► (2D/3D-SIE)
- Strategy
- Convergence

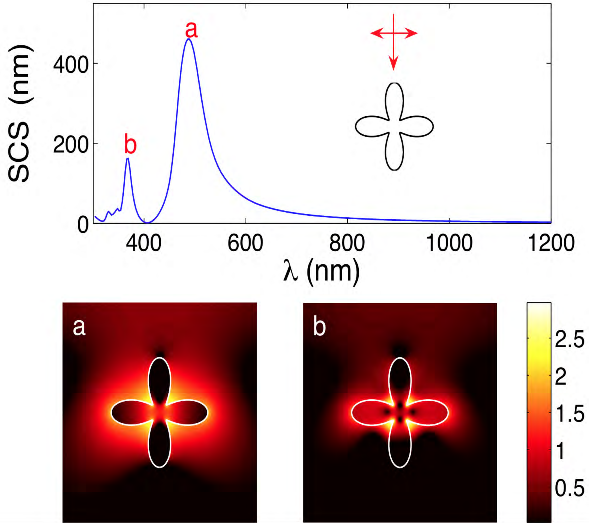


## Nanostars/Nanoflowers: SERS

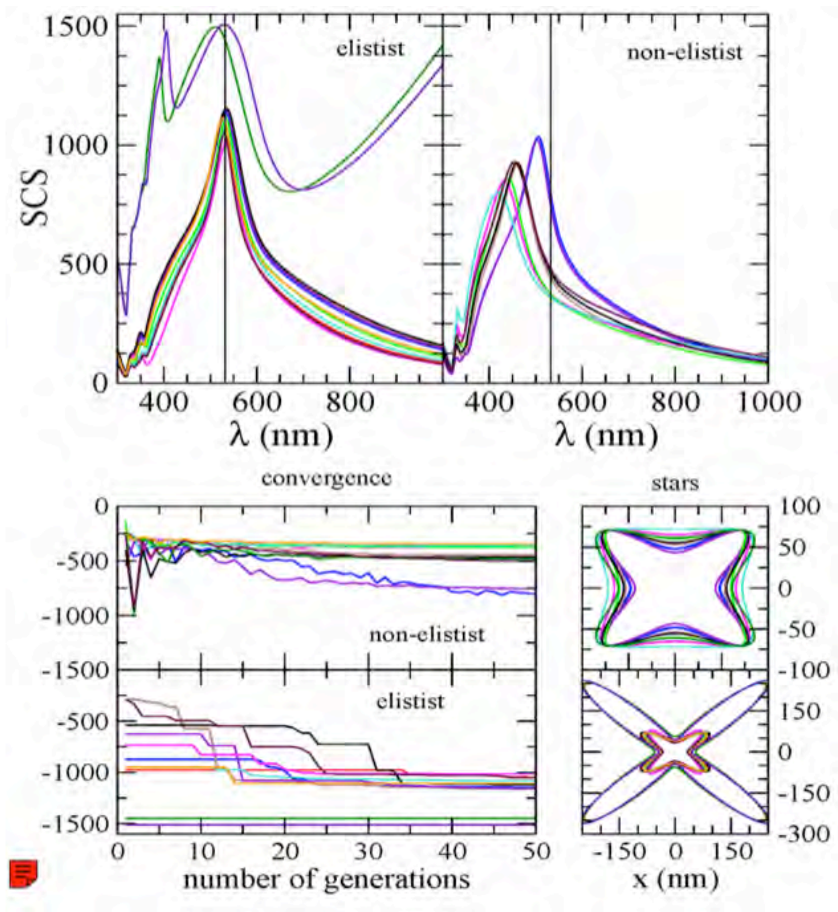



Kumar et al, Nanotech 2008
Nehl et al, Nano Lett. 2010

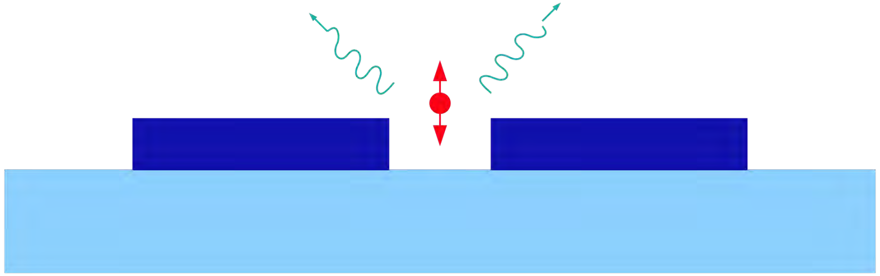


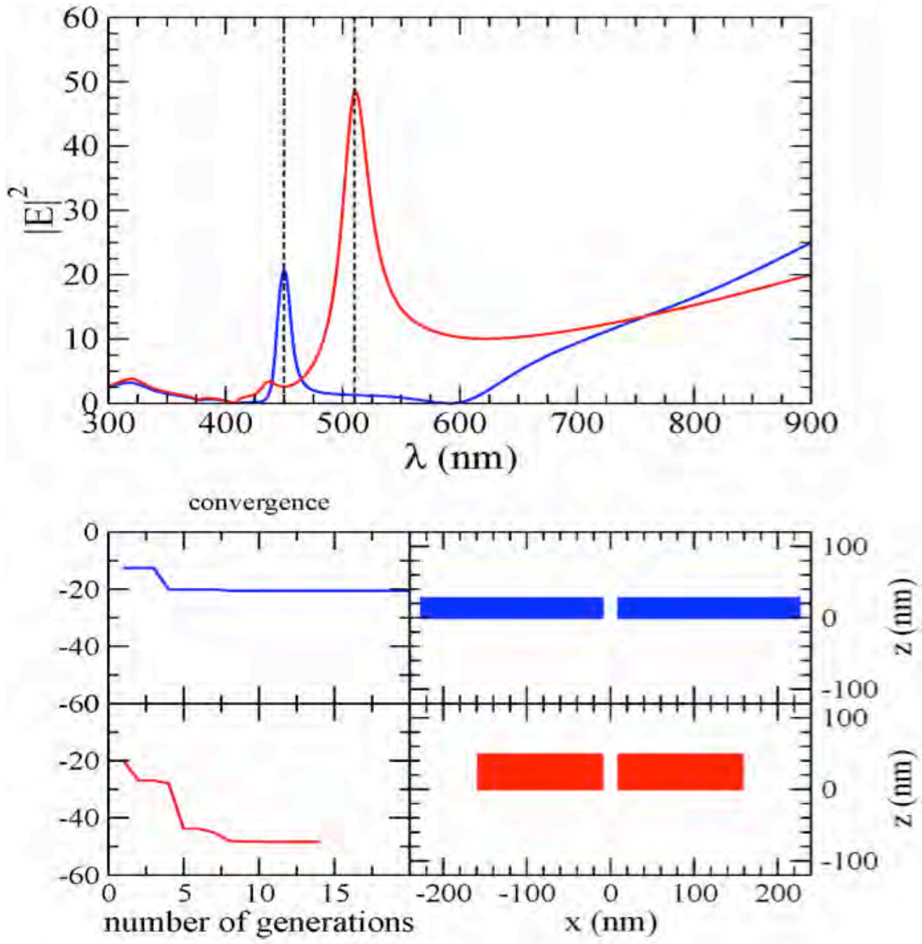

Giannini, Rodriguez-Oliveros, Sánchez-Gil, JOSAA 2007, Plasmonics 2010




Tassadit, Macías, Sánchez-Gil, Adam, Rodriguez-Oliveros, Superlattices & Microstructures 2011

# Nanodimers: Enhanced fluorescence, SHG, TPPL, THG



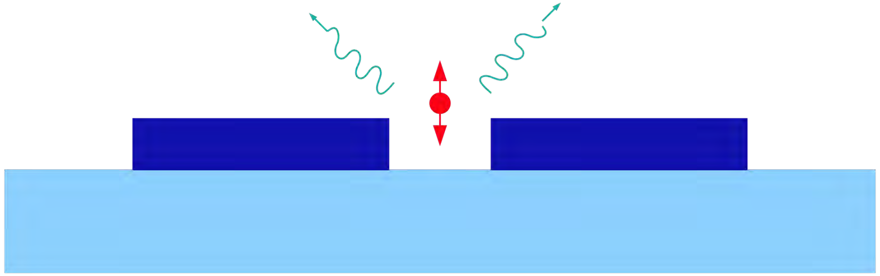


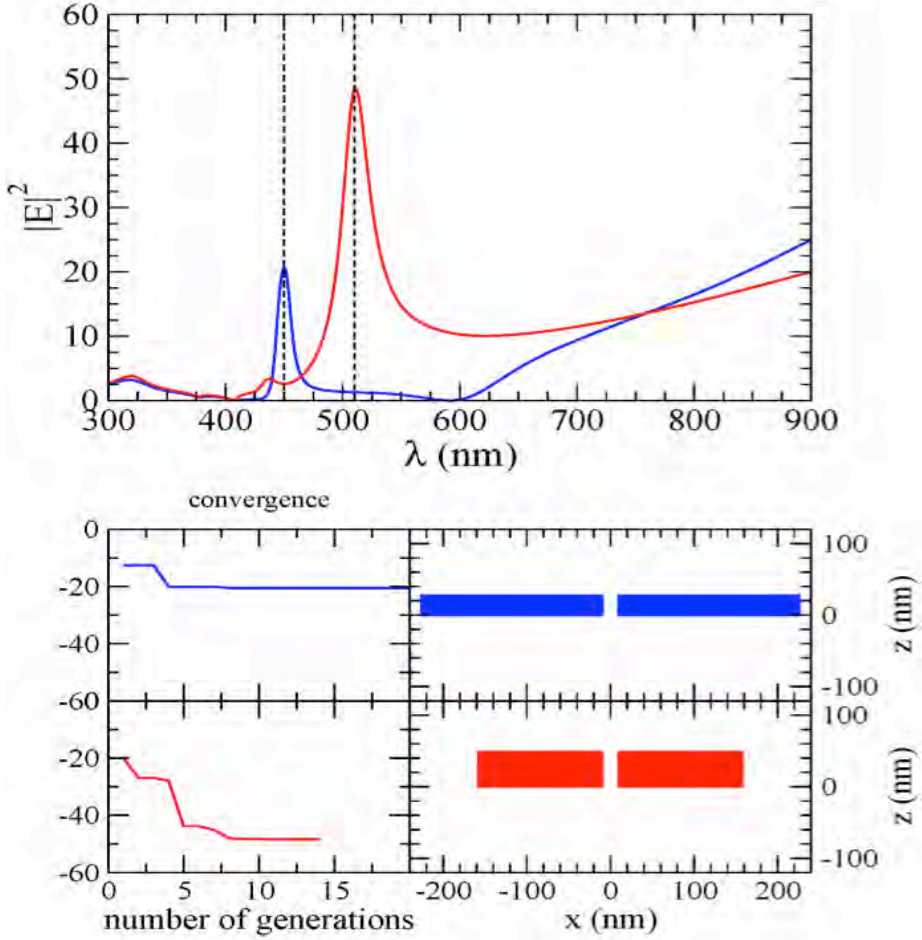

Tassadit, Macías, Sánchez-Gil, Adam, Rodriguez-Oliveros, preprint

# *Design*

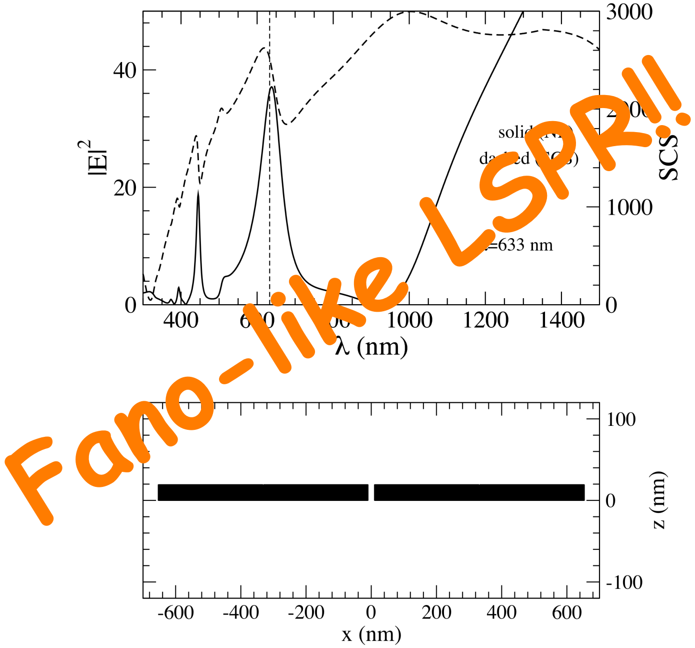


## Nanodimers: Enhanced fluorescence, SHG, TPPL, THG






Enhanced 3rd-order resonance




Tassadit, Macías, Sánchez-Gil, Adam, Rodriguez-Oliveros, preprint

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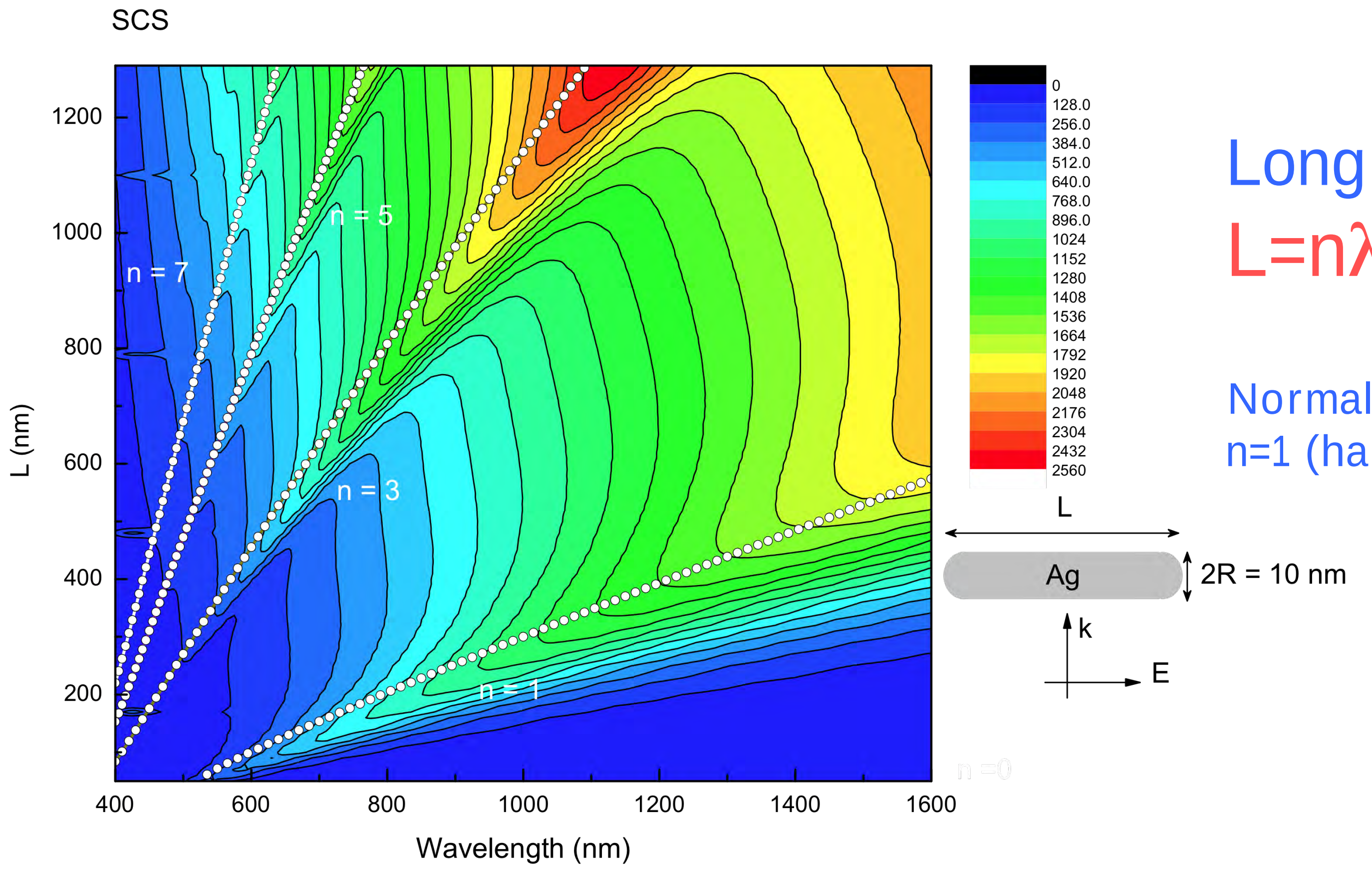
## 2D Nanorods: LSPR resonances




Longitudinal LSPR

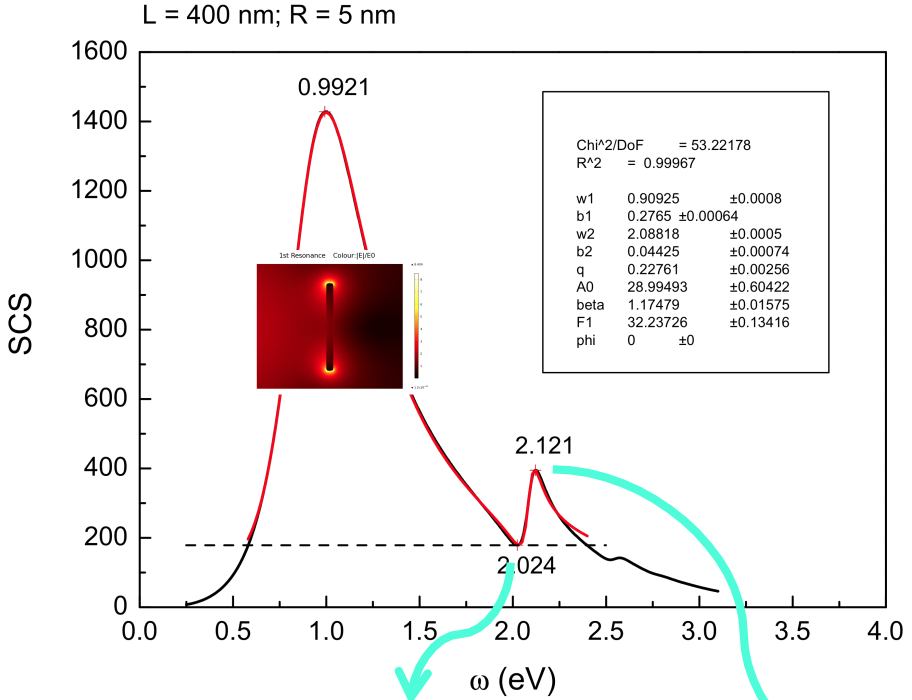
$L = n\lambda_{eff}/2[1-R]$

Normal incidence: odd modes
n=1 (half-wavelength), 3,...

López-Tejeira, Rodriguez-Oliveros, Paniagua-Domínguez, Sánchez-Gil, preprint

# *Fano-like LSPR/Nanorod*

## LSPR Interference: broad, bright & narrow, dark

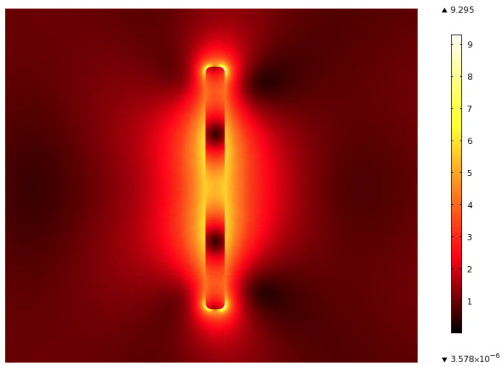


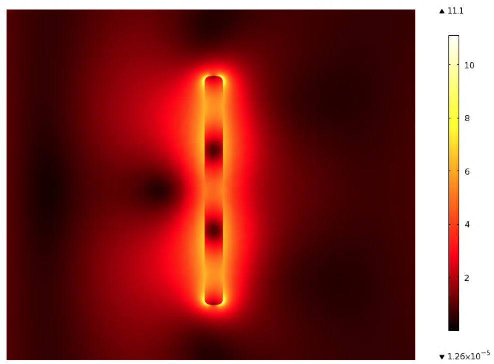

n=1 (HW) ▶ Broad, Bright

n=3 (HW) ▶ Narrow, Dark

2 Lorentzian fit:

$$I \sim |c_1 f(\omega-\omega_1) + c_3 f(\omega-\omega_3)|^2$$




López-Tejeira, Rodriguez-Oliveros, Paniagua-Domínguez, Sánchez-Gil, preprint

# *Conclusions*

► Two powerful theoretical/numerical methods

2D/3D-Surface integral Eqs+ Flexible Surfaces

Stochastic methods (genetic algorithm)

Plasmonics,
Nanophotonics, Metamaterials,
…EM

**PS: Brute-force tools, useful to explore new physics & guide experiments**

► Fano-like LSPR on a single nanorod

# *Applications*

2D/3D-SIE + (2D-3D) stochastic optimization

- ***Plasmon resonances***: Nanocube dimers, nanostars, nanoprisms,…
- ***Nano-antenna enhanced emission***:
  - QD/Dye photoluminescence (Nano-dimers & nanotrimers)
  - SERS (nanostars, nanocrosses, nanodisk dimers)
- Light coupling into ***nanowires***
- ***Metamaterials***: (nanorings) building blocks…

Paniagua-Domínguez Poster

⟶Extend 3D-SIE: periodic boundary conditions, homogeneization

# *Acknowledgements*

## Coworkers


*Instituto de Estructura de la Materia (CSIC), Madrid (Spain)*

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**Ramón  Paniagua-Domínguez**

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**Demetrio Macías** *(ICD-LNIO),  Université de Technologie de Troyes (France)*

# *Acknowledgements*

## Funding agencies

*…Thank you*

# Surface integral equations: Brief (incomplete) overview

Optical regime: metals

***70s***: Sein; Pattanayak & Wolf;

de Goede & Mazur

. . .

***90s***: Rough (dielectric/metal) surface scattering…

***1994*: 3D rough metal surfaces**:

Tran/Maradudin (UCI) and

Tsang et al (UWA)

…

***2010***: IBC Simonsen/Maradudin/ Leskova PRL.

Low frequency regime: PEC

***Late 60's***: MoM

**…**

***1982***: RWG+Galerkin

…

***2009***: Kern/Martin extended to 3D metal/ dielectric scatterers

# *Scattering Calcs.: 2D/3D-SIE*

*Pros*

*Cons*

Physics

*N-volumes with:*
*Arbitrary ε,μ*
*Complex (Flexible) shape*

*ALL easily from SF:*
*FF, NF, SCS, LDOS,*

Scatterers

Magnitudes

*Homogeneous*

*Time domain*

Calcs

*Scales with surface,*
*Matrix inversion:*
*Memory & Time*

*~~Configuration setup~~*
*(user friendly)*

3D: Rodríguez-Oliveros Poster