

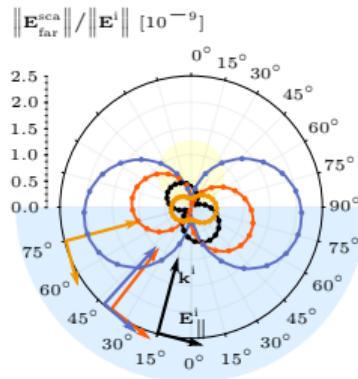
Optical properties of partially embedded nanospheres

Examen de maestría: Propiedades ópticas de nanoesferas parcialmente embebidas

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Antecedentes

Metasuperficies plasmónicas para biosensado

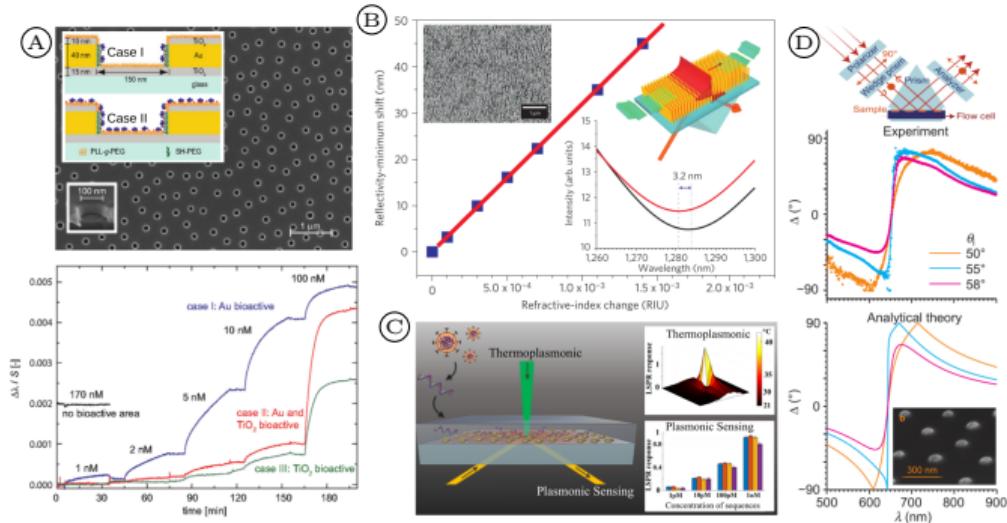
- Arreglos bidimensionales de **nanoestructuras metálicas** (meta-átomos) soportadas por un sustrato.¹

Meta-átomos

- Geometría
- Material
- Distribución
 - Desordenada^{4,5}
 - Periódica^{2,3}
- **Perfecto soporte sobre sustrato**

Respuesta óptica

- Resultados experimentales^{2,3,4,5}
- Simulaciones numéricas^{2,3,4}
- Teorías de medio efectivo⁵



¹ A. K. González-Alcalde et al. *Optics Communications*, **475**:126289, 2020

², A L. Feuz et al. *ACS Nano*, **4**(4):2167-2177, 2010

³, B A. V. Kabashin et al. *Nature Materials*, **8**(11):867-871, 2009

⁴, C G. Qiu et al. *ACS Nano*, **14**(5):5268-5277, 2020

⁵, D M. Svedendahl et al. *Light: Science & Applications*, **3**(11):e220-e220, 2014

Objetivo

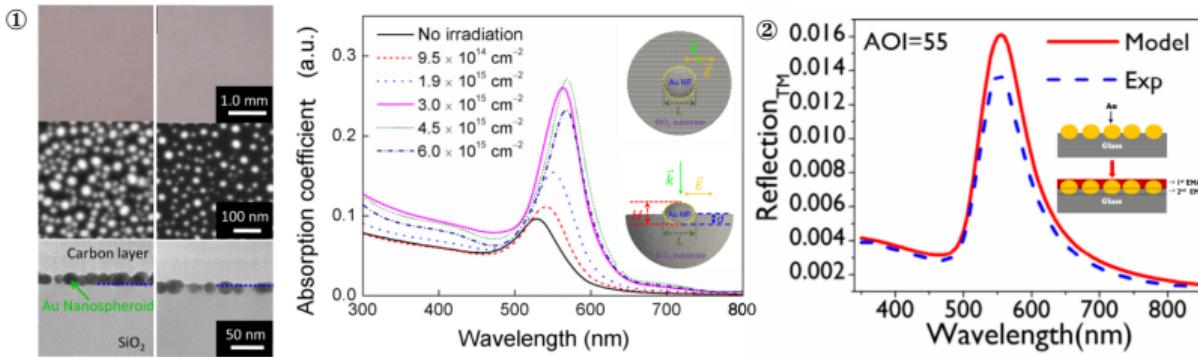
Incrustamiento parcial de meta-átomos en el sustrato

- ▶ Resultados del proceso de fabricación¹
- ▶ Característica deseable para metasuuperficies enfocadas para biosensado (Acoplamiento con sistemas de microfluídica)
- ▶ ¿Cuál es su efecto en la respuesta óptica?

Sistema de estudio

Nanopartícula esférica apta para biosensado en metasuperficies

- ▶ Meta-átomo: 12.5 nm AuNP
- ▶ Matriz: Aire
- ▶ Sustrato: Vidrio



¹ X. Meng et al. *AIP Adv*, 5(2):027112, 2015

² R. S. Moirangthem et al. *Biomedical Optics Express*, 3(5):899, 2012

Contenido

1 Teoría

Esparcimiento por una partícula esférica

Método de elemento finito

Condiciones de frontera abiertas

2 Resultados

Esfera soportada y completamente embebida

 Incidencia normal

 Incidencia oblicua

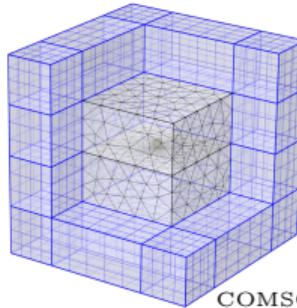
Esfera parcialmente incrustada

 Incidencia normal

 Incidencia oblicua

3 Conclusiones

Fotografía de Gustav Mie alrededor de 1905¹

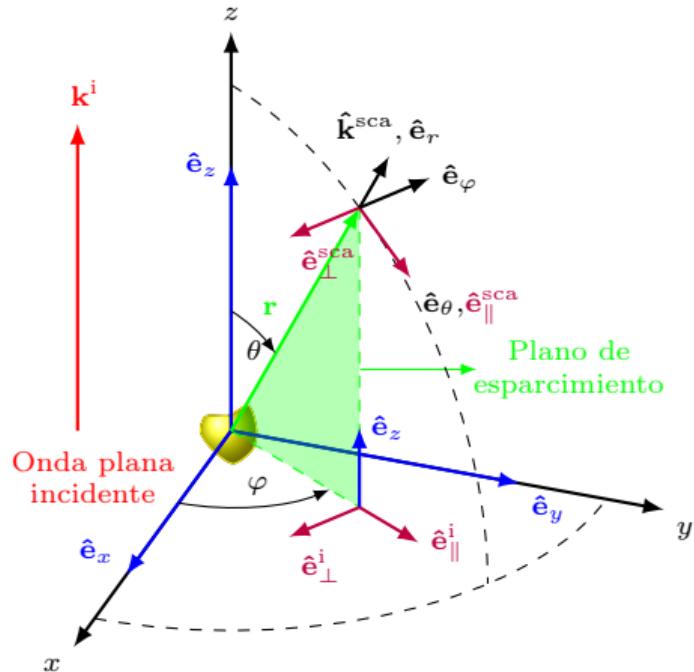


COMSOL Multiphysics™ Ver. 5.4

¹ H. Horvath. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 110(11):787-799, 2009. Number: 11

Esparcimiento por una partícula

Secciones transversales de absorción, esparcimiento y extinción



Teorema óptico¹ y operador de campo lejano²:

$$C_{\text{ext}} = C_{\text{abs}} + C_{\text{sca}}$$

$$\mathbf{E}^{\text{sca}} = \frac{\exp(i\hat{\mathbf{k}}^{\text{sca}} \cdot \mathbf{r})}{r} \mathbb{F}(\hat{\mathbf{k}}^{\text{sca}}, \hat{\mathbf{k}}^{\text{i}}) \mathbf{E}^{\text{i}}$$

$$C_{\text{abs}} = \frac{1}{2} \int_V \frac{\text{Re}(\mathbf{J} \cdot \mathbf{E}^{\text{int}*})}{\|\mathbf{E}_0^{\text{i}}\|^2 / 2Z_{\text{mat}}} dV = \int_V \omega Z_{\text{mat}} \text{Im}(n_p^2) \frac{\|\mathbf{E}^{\text{int}}\|^2}{\|\mathbf{E}_0^{\text{i}}\|^2} dV$$

$$C_{\text{sca}} = \frac{2Z_{\text{mat}}}{\|\mathbf{E}_0^{\text{i}}\|^2} \oint_S \langle \mathbf{S}^{\text{sca}} \rangle_t \cdot d\mathbf{a} = \oint_S \frac{\left\| \mathbb{F}(\hat{\mathbf{k}}^{\text{sca}}, \hat{\mathbf{k}}^{\text{i}}) \mathbf{E}^{\text{i}} \right\|^2}{\|\mathbf{E}_0^{\text{i}}\|^2} da$$

$$C_{\text{ext}} = \frac{4\pi}{k\|\mathbf{E}_0^{\text{i}}\|^2} \text{Im} \left[\mathbf{E}_0^{\text{i}} \cdot \mathbb{F}^*(\hat{\mathbf{k}}^{\text{i}}, \hat{\mathbf{k}}^{\text{i}}) \mathbf{E}^{\text{i}*} \right]$$

¹ C. F. Bohren et al. *Absorption and Scattering of Light by Small Particles*. Wiley Science Paperbk Series. John Wiley & Sons, 1.^a edición, 1983

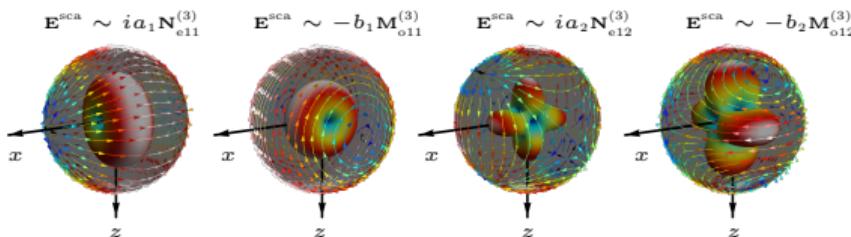
² L. Tsang et al. *Scattering of Electromagnetic Waves: Theories and Applications*. John Wiley & Sons, Inc., New York, USA, 2000

Solución de Mie^{1,2}

Espaciamiento por partículas esféricas embebidas en medios infinitos

$$\mathbf{E}^i(\mathbf{r}) = E_0 \sum_{\ell=1}^{\infty} \frac{i^\ell (2\ell+1)}{\ell(\ell+1)} \left(\mathbf{M}_{o1\ell}^{(1)} - i\mathbf{N}_{e1\ell}^{(1)} \right)$$

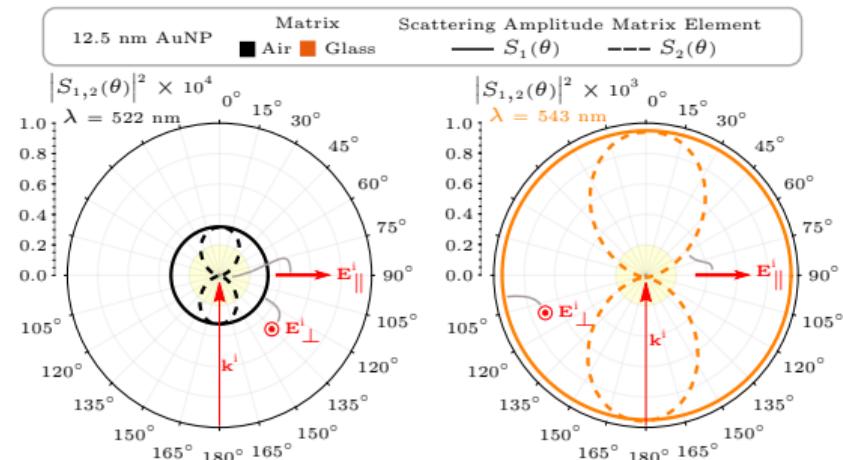
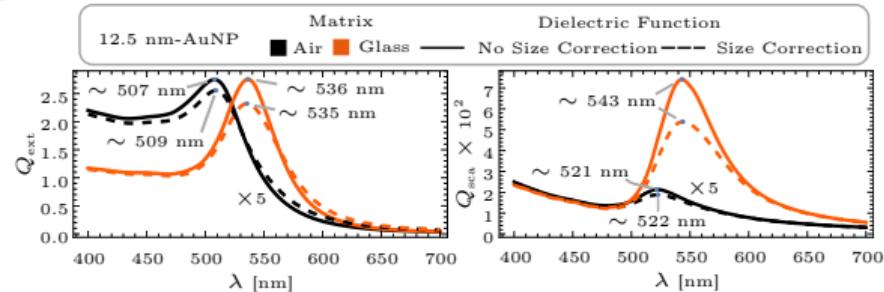
$$\mathbf{E}^{sca}(\mathbf{r}) = E_0 \sum_{\ell=1}^{\infty} \frac{i^\ell (2\ell+1)}{\ell(\ell+1)} \left(ia_\ell \mathbf{N}_{e1\ell}^{(3)} - b_\ell \mathbf{M}_{o1\ell}^{(3)} \right)$$



$$\mathbb{F}(\hat{\mathbf{k}}^{sca}, \hat{\mathbf{k}}^i) = \begin{pmatrix} \frac{i}{k} S_2(\theta) & 0 \\ 0 & \frac{i}{k} S_1(\theta) \end{pmatrix}$$

$$S_1(\theta) = \sum_{\ell=1}^{\infty} \frac{2\ell+1}{\ell(\ell+1)} [a_\ell \tau_\ell(\cos \theta) + b_\ell \pi_\ell(\cos \theta)]$$

$$S_2(\theta) = \sum_{\ell=1}^{\infty} \frac{2\ell+1}{\ell(\ell+1)} [a_\ell \pi_\ell(\cos \theta) + b_\ell \tau_\ell(\cos \theta)]$$



¹ C. F. Bohren et al. *Absorption and Scattering of Light by Small Particles*. Wiley Science Paperbk Series. John Wiley & Sons, 1.^a edición, 1983

² L. Tsang et al. *Scattering of Electromagnetic Waves: Theories and Applications*. John Wiley & Sons, Inc., New York, USA, 2000

Problema de valores propios de Maxwell

Formulación fuerte y débil del problema de esparcimiento de luz en un volumen Ω

Formulación fuerte¹: Ecuación diferencial

$$\nabla \times [\mu^{-1} \nabla \times \mathbf{E}] - \kappa^2 \mathbf{E} = \mathbf{0}, \quad \text{donde} \quad \kappa^2 = (i\omega\sigma + \omega^2 \epsilon)$$

- ▶ Condiciones de frontera de Dirichlet (D) y de Neumann (N)

$$\hat{\mathbf{n}} \times \mathbf{E}(\mathbf{r}) \Big|_{\partial\Omega} = \mathbf{E}_D \quad \mu^{-1} \nabla \times \mathbf{E} \times \hat{\mathbf{n}} \Big|_{\partial\Omega} = \mathbf{E}_N$$

Formulación débil^{1,2}: Ecuación integral con el uso de la función de prueba $\boldsymbol{\eta}(\mathbf{r})$

- ▶ Simplificación mediante integración por partes y teorema de Gauss

$$\int_{\Omega} \left\{ (\mu^{-1} \nabla \times \mathbf{E}) \cdot (\nabla \times \boldsymbol{\eta}) - \kappa^2 \cdot \mathbf{E} \cdot \boldsymbol{\eta} \right\} d\Omega - \oint_{\partial\Omega} (\boldsymbol{\eta} \times \mathbf{E}_N) \cdot \hat{\mathbf{n}} d(\partial\Omega) = 0$$

- ▶ Condiciones de frontera

$$\hat{\mathbf{n}} \times \mathbf{E}(\mathbf{r}) \Big|_{\partial\Omega} = \mathbf{E}_D.$$

¹ G. Dhatt et al. *Finite element method*. Numerical methods series. ISTE ; Wiley, London : Hoboken, N.J, 2012

² J.-M. Jin. *Theory and Computation of Electromagnetic Fields*. Wiley & Sons, 2010

Aproximación de elemento finito y método de Galerkin

Conceptos fundamentales

Sistema de ecuaciones diferenciales en Ω : $\mathcal{L}[u(\mathbf{r})] - f_\Omega = 0 \iff \int_\Omega \{\mathcal{L}[u(\mathbf{r})] - f_\Omega\} \psi(\mathbf{r}) d\Omega = 0$

Aproximación nodal^{1,2}

- ▶ Combinación lineal:

$$u(\mathbf{r}) \approx \sum_i^N u_i \phi_i(\mathbf{r})$$

- ▶ Funciones de interpolación :

$$\{\phi_i\}_{i \leq N}$$

- ▶ Nodos con valores exactos:

$$u_i = u(\mathbf{r}_i), \quad \mathbf{r}_i \in \Omega$$

Elemento finito¹⁻⁴ Ω_k

- ▶ Geometría

$$\bigcup_{k=1}^M \Omega_k = \Omega \quad \bigcap_{k=1}^M \Omega_k = \emptyset$$

- ▶ Espacio de funciones polinomiales

$$\{\phi_{i_k}\}_{i_k \leq N_k}$$

- ▶ Funcional lineal

$$\mathcal{F}_{\ell_k}[\phi_{i_k}] = \delta_{\ell_k i_k}$$

Método de Galerkin⁴

- ▶ Formulación débil del problema en Ω_k

- ▶ Funciones de prueba:

$$\{\psi_{i_k}\}_{i_k \leq N_k} = \{\phi_{i_k}\}_{i_k \leq N_k}$$

- ▶ Sistema de ecuaciones algebráicas:

$$\mathbf{A}\mathbf{u} = \mathbf{f}$$

donde

$$A_{i_k j_k} = \int \phi_{i_k}(\mathbf{r}) \mathcal{L}[\phi_{j_k}(\mathbf{r})] d\Omega,$$
$$u_{i_k} = u(\mathbf{r}_{i_k}) \text{ y}$$
$$f_{j_k} = \int f_\Omega \phi_{j_k}(\mathbf{r}) d\Omega.$$

¹ G. Dhatt et al. *Finite element method*. Numerical methods series. ISTE ; Wiley, London : Hoboken, N.J, 2012

² M. G. Larson et al. *The Finite Element Method: Theory, Implementation, and Applications*. Volumen 10 de *Texts in Computational Science and Engineering*. Springer Berlin Heidelberg, Berlin, Heidelberg, 2013

³ J.-M. Jin. *Theory and Computation of Electromagnetic Fields*. Wiley & Sons, 2010

⁴ C. A. J. Fletcher. *Computational Galerkin Methods*. Springer Berlin Heidelberg, Berlin, Heidelberg, 1984

Implementación numérica del problema de esparcimiento de luz

Familia de elementos finitos de Nédélec^{1,2}

Para geometrías triangulares:

Aproximación nodal

$$\mathbf{E}(\mathbf{r}) \approx \sum_{i_k} e_{i_k} \boldsymbol{\eta}_{i_k}(\mathbf{r}) \quad e_i = \hat{\mathbf{t}}_{i_k} \cdot \mathbf{E}(\mathbf{r} \in E_{i_k})$$

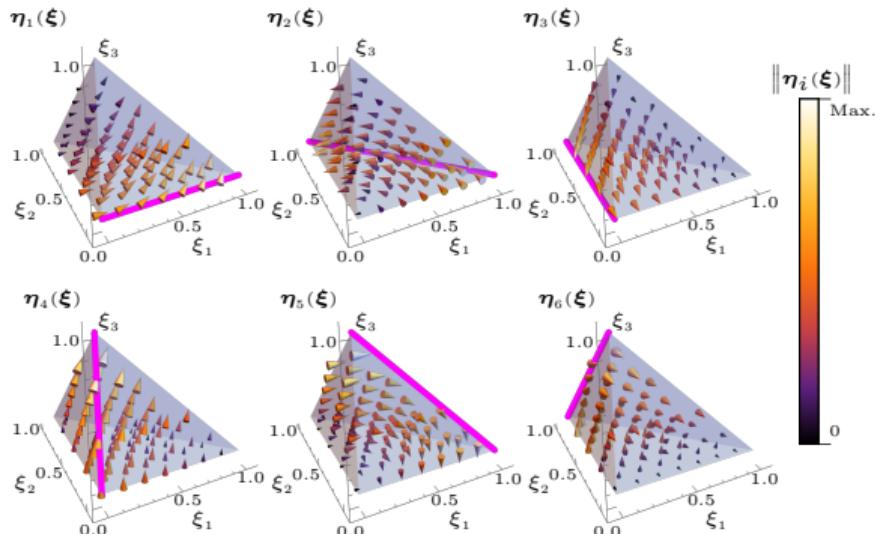
Método de Galerkin

$$\mathbb{A}\mathbf{e} = \mathbf{0}$$

$$A_{ij} = \int_{\Omega_k} \left\{ (\mu^{-1} \nabla \times \boldsymbol{\eta}_i) \cdot (\nabla \times \boldsymbol{\eta}_j) - \kappa^2 \cdot \boldsymbol{\eta}_i \cdot \boldsymbol{\eta}_j \right\} d\Omega_k + \\ - \oint_{\partial\Omega} (\boldsymbol{\eta}_j \times \mathbf{E}_N) \cdot \hat{\mathbf{n}} d(\partial\Omega)$$

Funcional de Nédélec de menor orden

$$\mathcal{F}_{i_k}^N[\boldsymbol{\eta}_{\ell_k}(\xi)] = \frac{1}{|E_{i_k}|} \left(\int_{E_{i_k}} \hat{\mathbf{t}}_{i_k} \cdot \boldsymbol{\eta}_{\ell_k}(\xi) d(\partial\Omega_k) \right)^{1/2}$$



¹ J.-M. Jin. *Theory and Computation of Electromagnetic Fields*. Wiley & Sons, 2010

² M. G. Larson et al. *The Finite Element Method: Theory, Implementation, and Applications*. Volumen 10 de *Texts in Computational Science and Engineering*. Springer Berlin Heidelberg, Berlin, Heidelberg, 2013

Condiciones de frontera abiertas

Simulando medios infinitos

Condición de radiación de Sommerfeld¹: Comportamiento en el campo lejano

$$\lim_{r \rightarrow \infty} \left(\hat{\mathbf{e}}_r \times \mathbf{E} - \sqrt{\frac{\mu}{\epsilon}} \mathbf{H} \right) = \lim_{r \rightarrow \infty} r(\nabla \times \mathbf{E} - ik\hat{\mathbf{e}}_r \times \mathbf{E}) = 0$$

Perfect Matching Layer²: Película (Ω_{PML}) sin impedancia y absorbente basada en su geometría:

$$\left. \begin{array}{l} \epsilon_\Omega = \epsilon_{\text{PML}}, \quad \mu_\Omega = \mu_{\text{PML}} \\ s_x^{(\Omega)} = s_x^{(\text{PML})}, \quad s_y^{(\Omega)} = s_y^{(\text{PML})} \end{array} \right\} \implies r_s = r_p = 0.$$

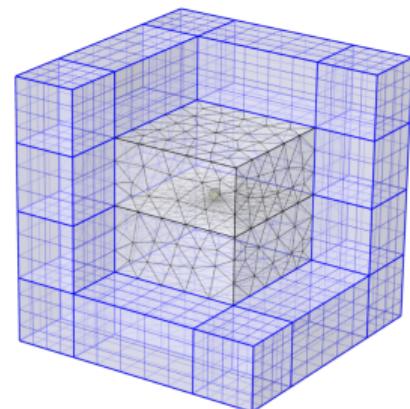
Método de Galerkin³

$\mathbb{A}\mathbf{e} = \mathbf{0}$ con \mathbb{A} y \mathbf{e} definidas anteriormente,

$\mathbb{A} = \text{diag}(s_z, s_z, s_z^{-1})$, con $s_z = 1$ en Ω y $\text{Im}[s_z] < 0$ en Ω_{PML} ,

$(\mu^{-1} \nabla \times \boldsymbol{\eta}_i) \cdot (\nabla \times \boldsymbol{\eta}_j) \rightarrow (\mathbb{A}^{-1} \mu^{-1} \nabla \times \boldsymbol{\eta}_i) \cdot (\nabla \times \boldsymbol{\eta}_j)$,

$\boldsymbol{\eta}_i \cdot \boldsymbol{\eta}_j \rightarrow \boldsymbol{\eta}_i \cdot \mathbb{A} \boldsymbol{\eta}_j$,



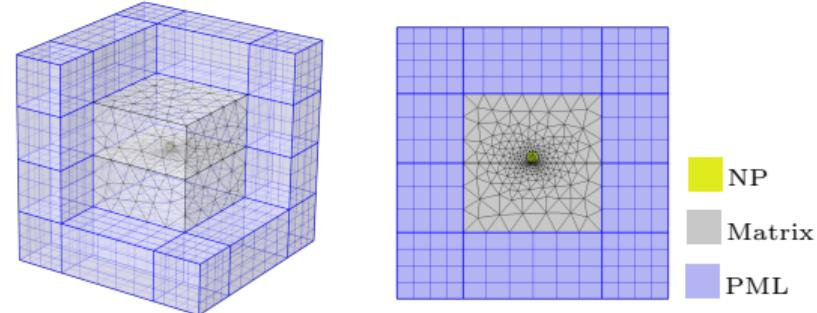
¹ S. Silver. *Microwave Antenna Theory and Design*. The Institution of Engineering and Technology, 1984. 640 páginas

² W. C. Chew et al. *Microwave and Optical Technology Letters*, 15(6):363-369, 1997

³ J.-M. Jin. *Theory and Computation of Electromagnetic Fields*. Wiley & Sons, 2010

Análisis de convergencia

Comsol vs Mie: 12.5 AuNP@Aire y 12.5 AuNP@BK7

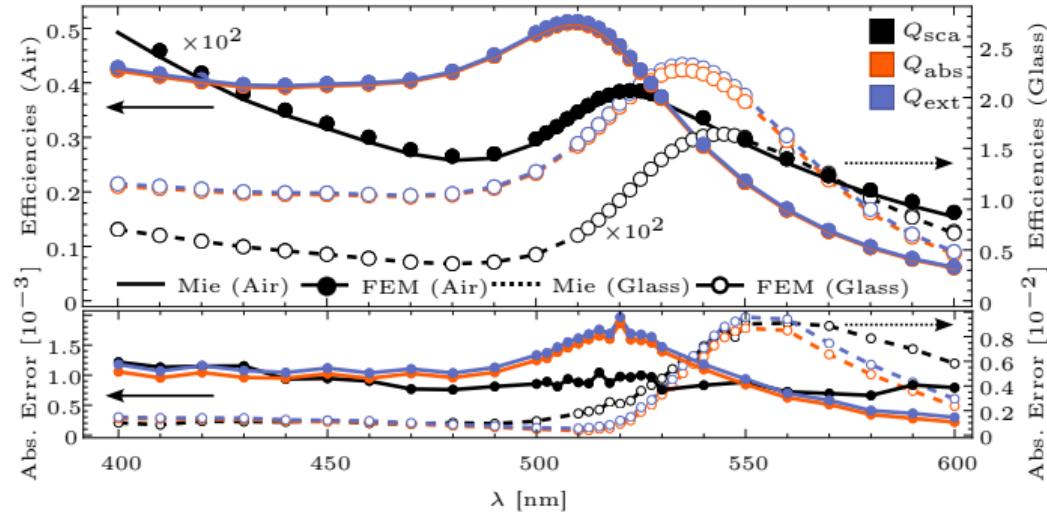


Tamaño del elemento (matriz): $\lambda/(6n_m)$

Tamaño del elemento (esfera): $a/5$

Tamaño de la matriz: $2(15 + 1)a n_m$

Grosor PML: $\lambda/4$



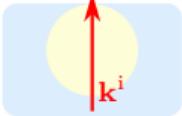
Esfera soportada y completamente embebida

Incidencia normal: 12.5 AuNP@Aire/BK7

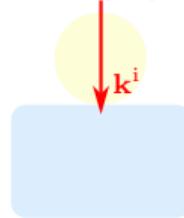
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External (EE)



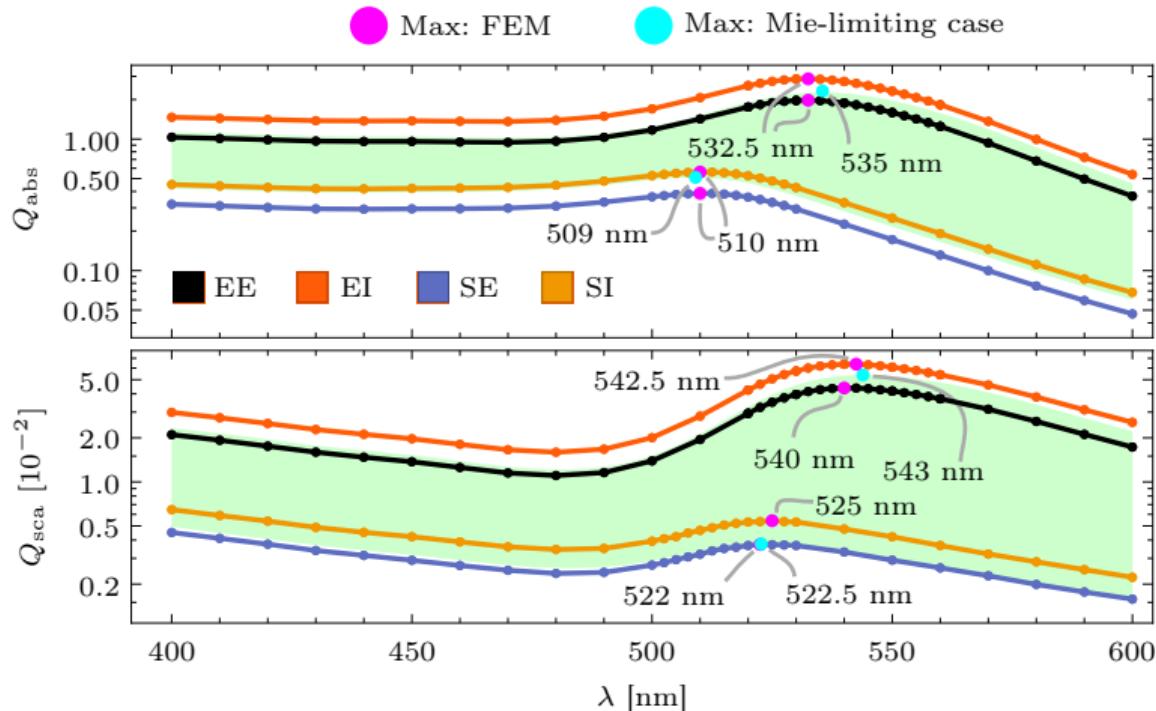
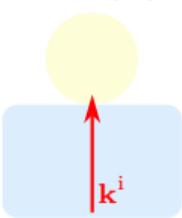
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Internal (EI)



Supported
External (SE)

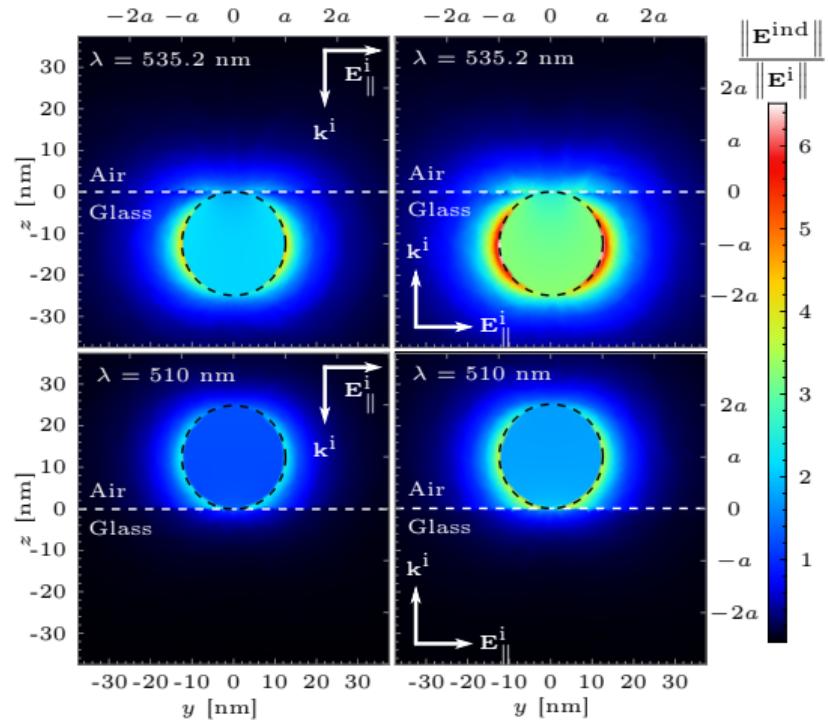
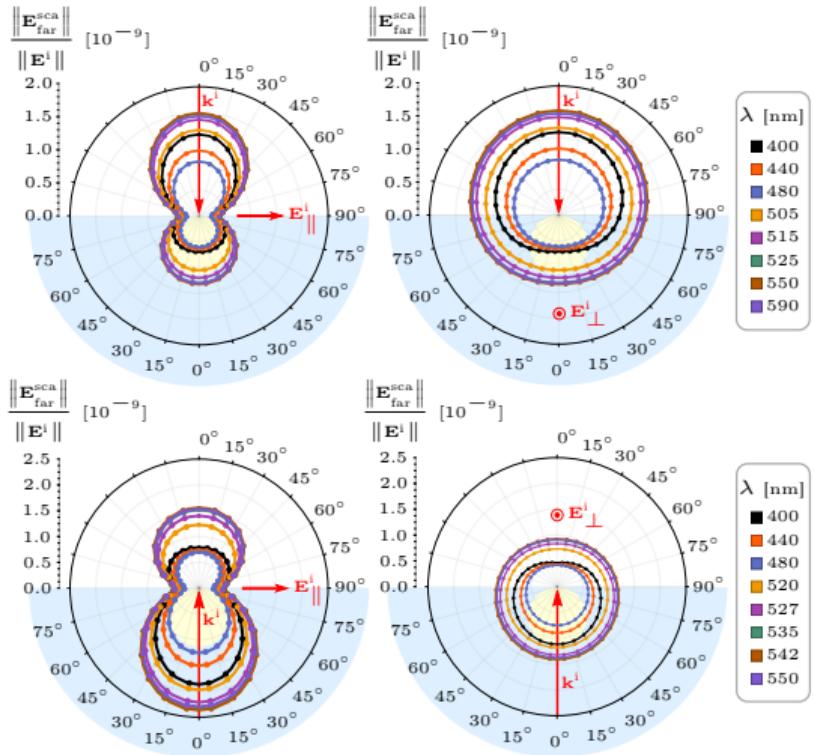


Supported
Internal (SI)



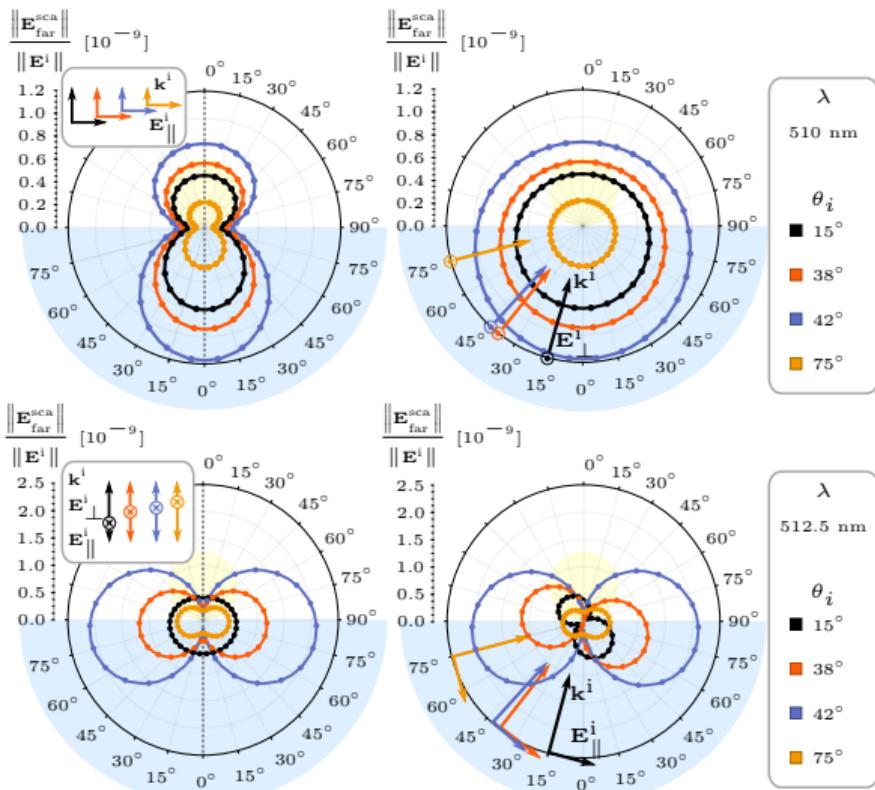
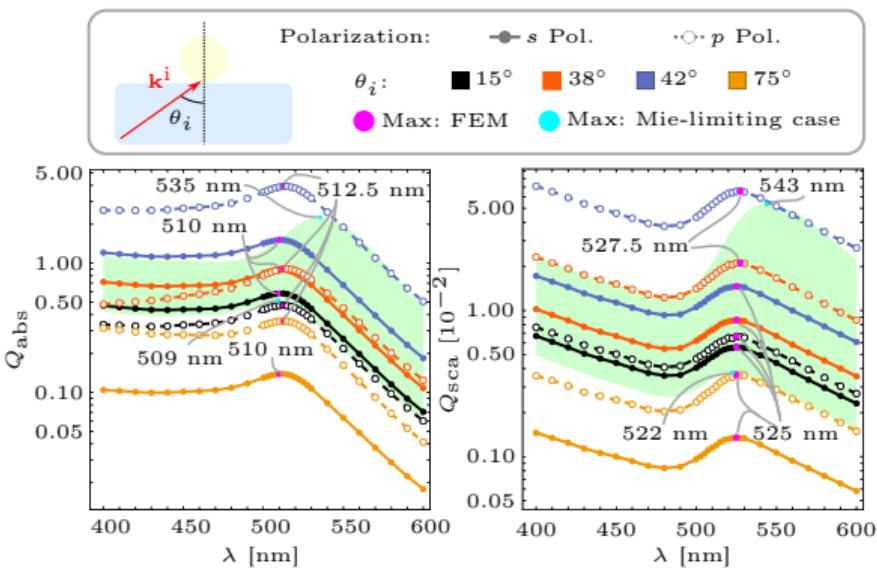
Esfera soportada y completamente embebida

Incidencia normal: 12.5 AuNP@Aire/BK7



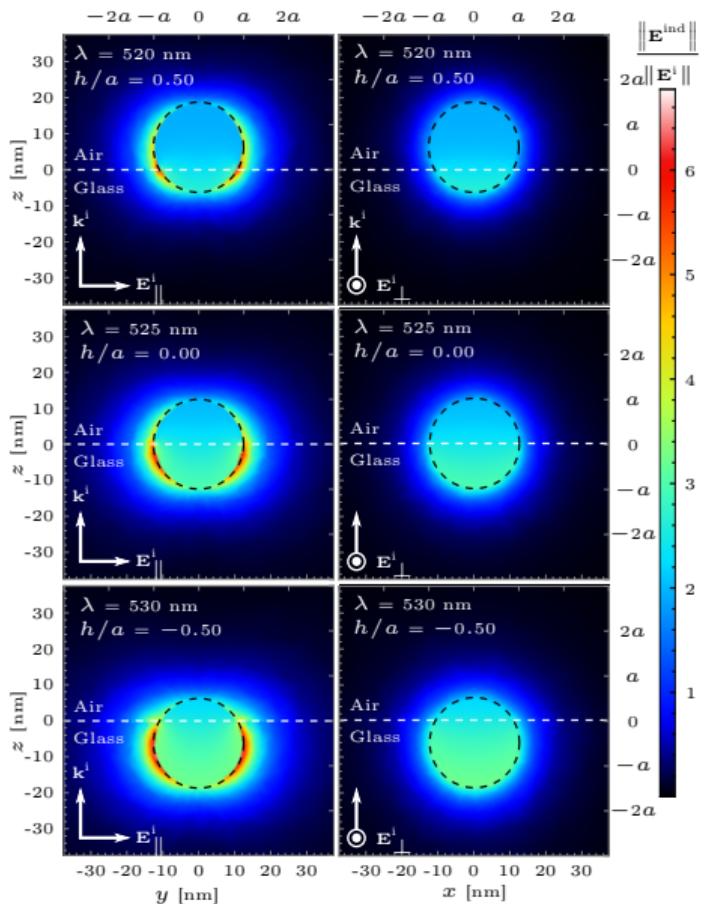
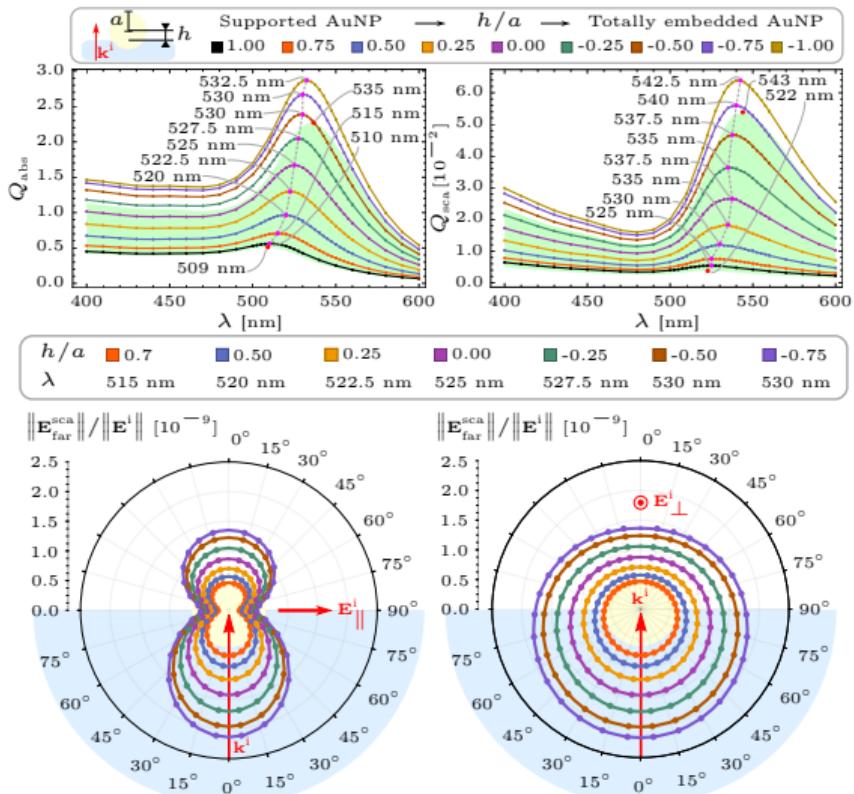
Esfera soportada en incidencia interna

Incidencia oblicua: 12.5 AuNP@Aire/BK7



Esfera parcialmente incrustada

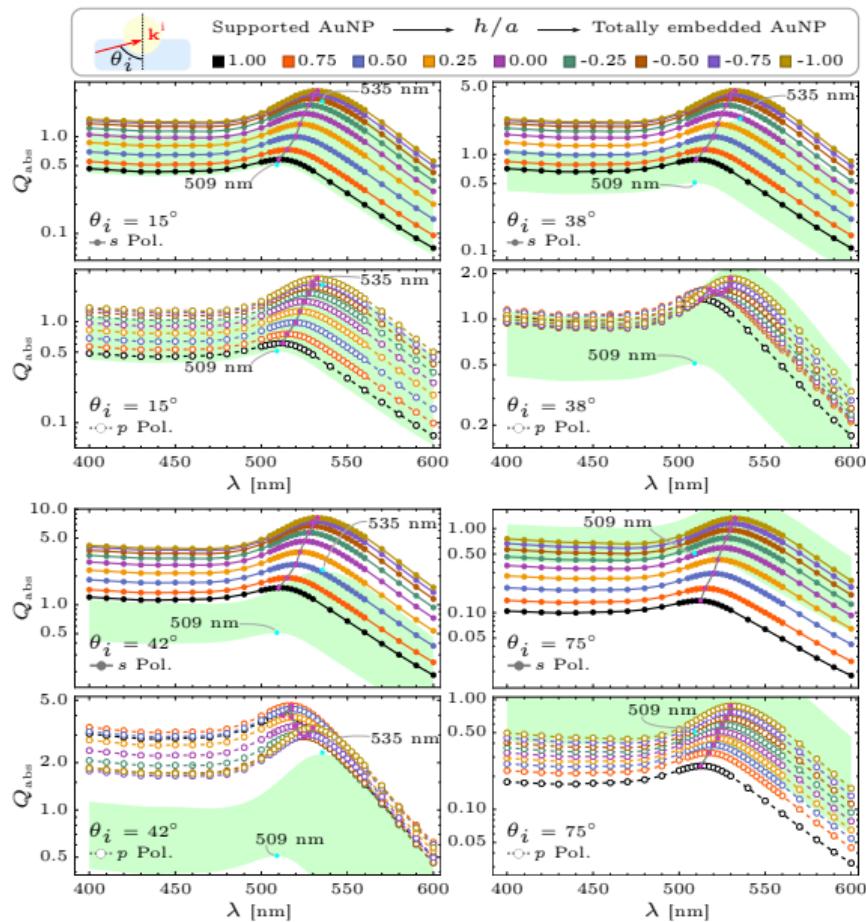
Incidencia normal: 12.5 AuNP@Aire/BK7



Esfera parcialmente incrustada

Incidencia oblicua: 12.5 AuNP@Aire/BK7

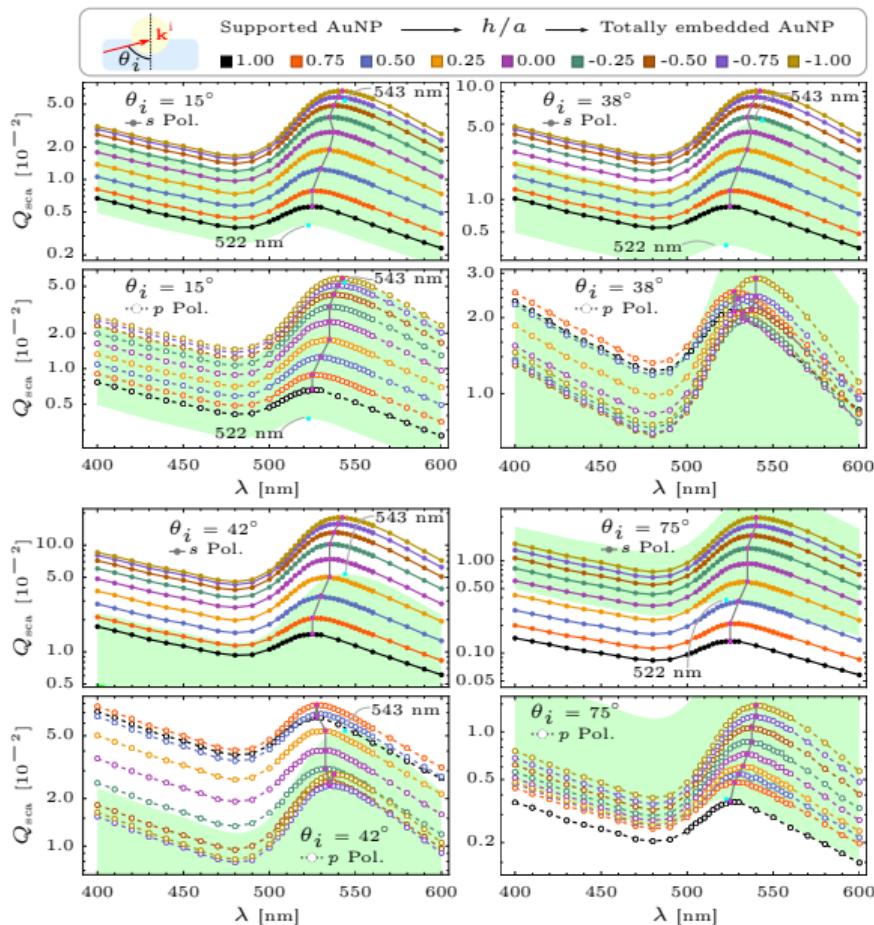
		$\lambda_{\text{res}}^{\text{abs}}$ [nm]				
	h/a	0°	15°	38°	42°	75°
s Polarization	1.00	510	510	510	510	512.5
	0.75	515	515	515	515	515
	0.50	520	520	520	520	520
	0.25	522.5	522.5	522.5	522.5	522.5
	0.00	525	525	525	525	525
	-0.25	527	527	527	527	527
	-0.50	530	530	530	530	530
	-0.75	530	530	530	530	530
	-1.00	532.5	532.5	532.5	532.5	532.5
p Polarization	1.00	510	512.5	512.5	512.5	512.5
	0.75	515	515	517.5	517.5	517.5
	0.50	520	520	517.5	517.5	520
	0.25	522.5	525.5	520	517.5	525.5
	0.00	525	525	522.5	520	522.5
	-0.25	527	527	525	522.5	525
	-0.50	530	530	527	525	527
	-0.75	530	530	530	527	530
	-1.00	532.5	532.5	530	530	530



Esfera parcialmente incrustada

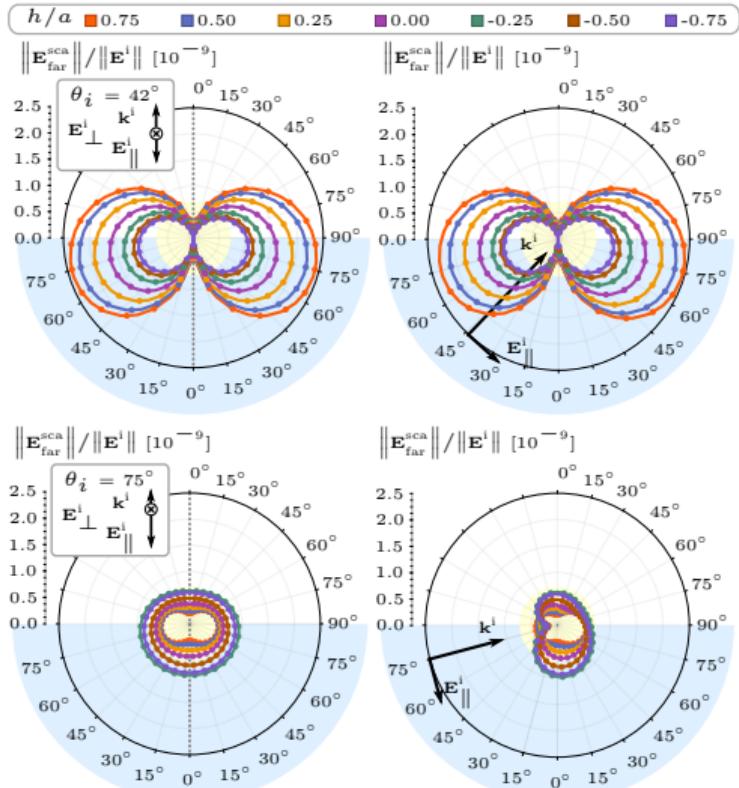
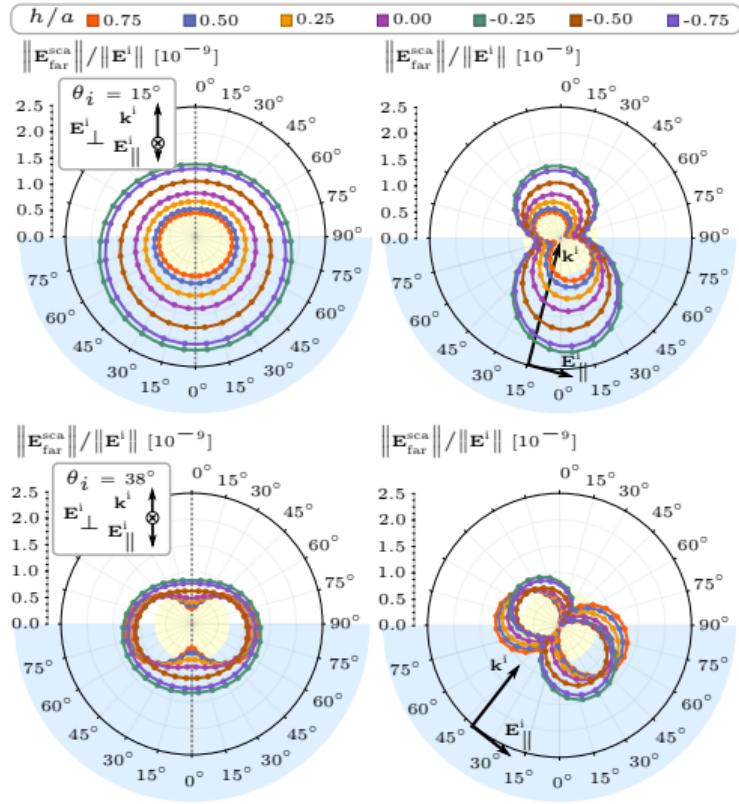
Incidencia oblicua: 12.5 AuNP@Aire/BK7

		$\lambda_{\text{res}}^{\text{sca}}$ [nm]				
	h/a	0°	15°	38°	42°	75°
s Polarization	1.00	525	525	525	525	525
	0.75	525	525	525	525	525
	0.50	530	530	530	530	530
	0.25	535	535	535	535	535
	0.00	537.5	537.5	537.5	535	535
	-0.25	535	535	535	535	535
	-0.50	537.5	537.5	537.5	537.5	537.5
	-0.75	540	540	540	540	540
	-1.00	542.5	542.5	542.5	542.5	540
p Polarization	1.00	525	525	527.5	527.5	525
	0.75	525	525	527.5	527.5	527.5
	0.50	530	530	530	527.5	530
	0.25	535	535	532.5	532.5	532.5
	0.00	537.5	535	535	535	535
	-0.25	535	535	532.5	535.5	537.5
	-0.50	537.5	537.5	537.5	535	537.5
	-0.75	540	540	540	535	540
	-1.00	542.5	542.5	540	537.5	540



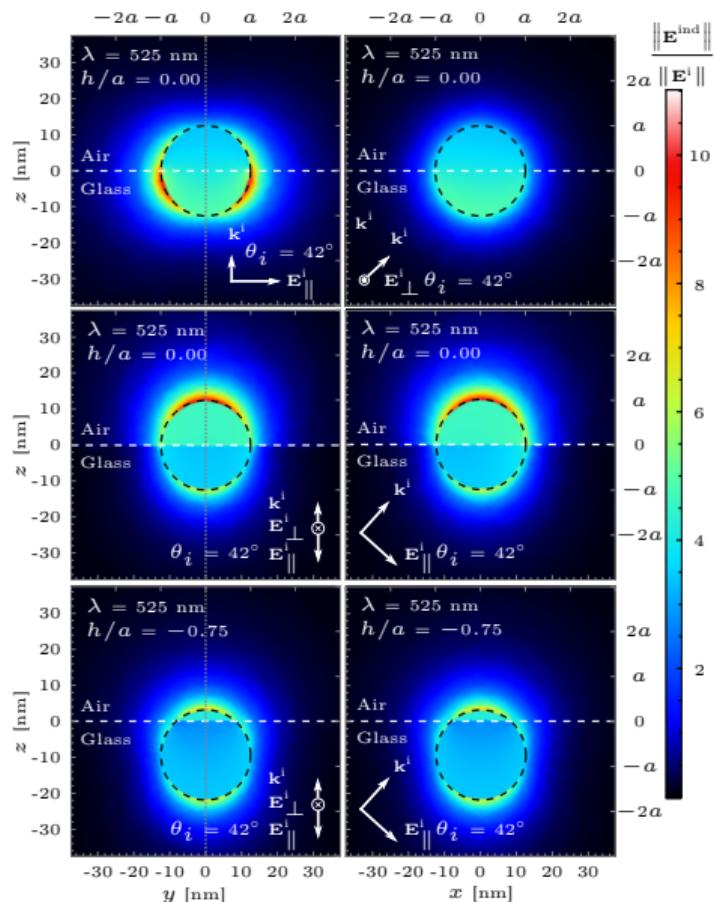
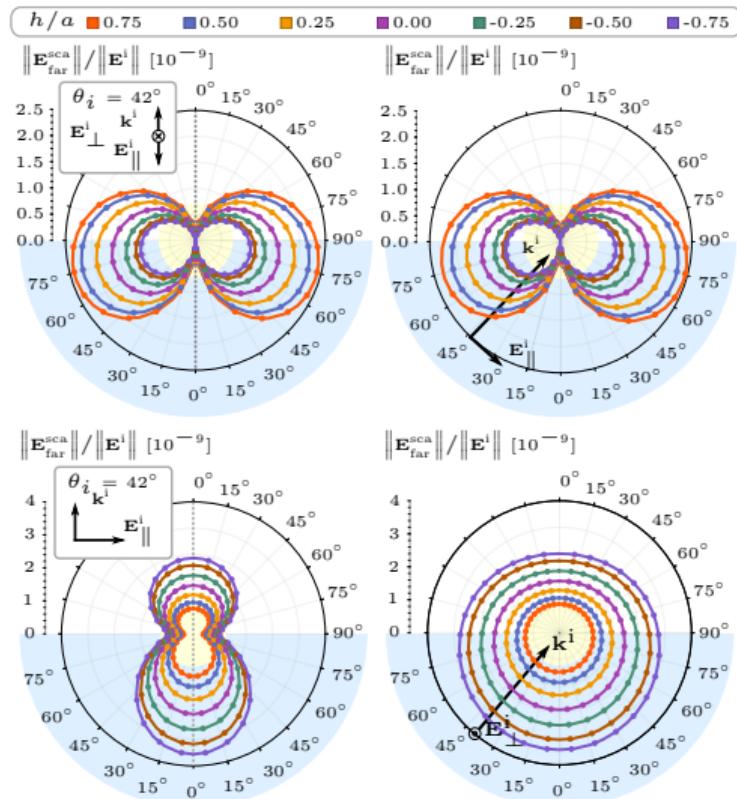
Esfera parcialmente incrustada

Incidencia oblicua en polarización p : 12.5 AuNP@Aire/BK7



Esfera parcialmente incrustada

Incidencia después del ángulo crítico: 12.5 AuNP@Aire/BK7

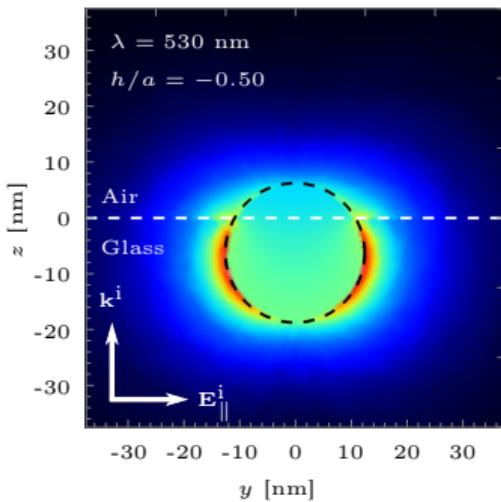


Resumen

Efecto del sustrato

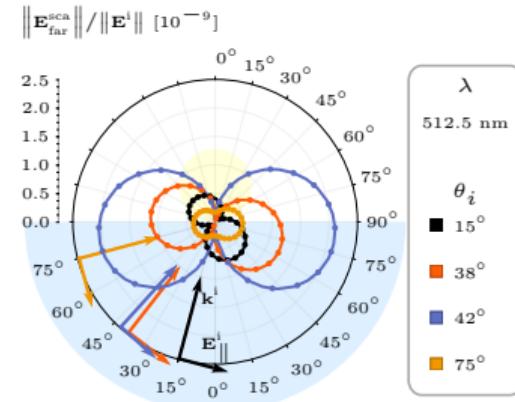
Anisotropía:

- ▶ Campo cercano
- ▶ Patrón de radiación



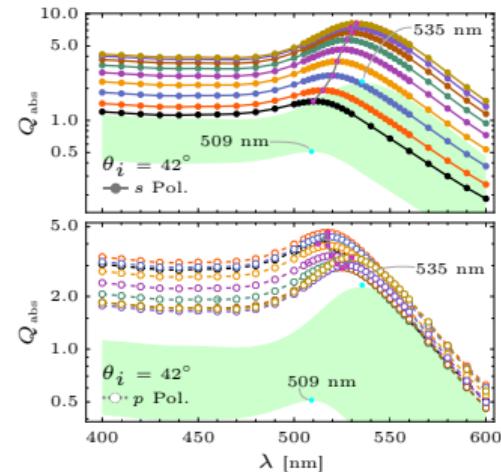
Efecto de la iluminación

- ▶ Partícula parcialmente embebida e incidente interna
 - ▶ Onda plana $\theta_i < \theta_c$
 - ▶ Onda evanescente $\theta_i > \theta_c$
- ▶ Maximización de propiedades ópticas $\theta_i \approx \theta_c$



Efecto de la incrustación

- ▶ Corrimiento al rojo (LSPR)
- ▶ Aumento de la extinción
- ▶ Pol. *s*:
 - ▶ Proceso homogéneo
- ▶ Pol. *p*:
 - ▶ h/a y θ_i

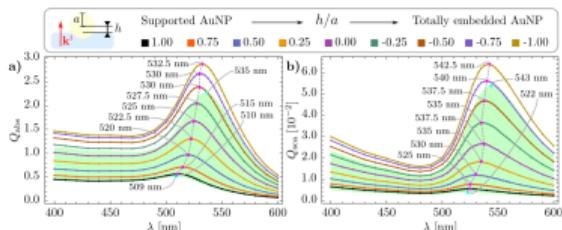


Conclusiones y trabajo a futuro

Para una 12.5 nm AuNP parcialmente embebida entre un sustrato plano y una matriz

Transición

- ▶ Contribución mayormente dipolar.
 - ▶ Transición *suave* entre los dos casos límites de Mie.



Incrustación

A lo más un octavo del volumen en

- ▶ Sustrato → AuNP soportada
 - ▶ Matriz → AuNP totalmente embebida

Iluminación

Resonancia y la distribución espacial del campo eléctrico

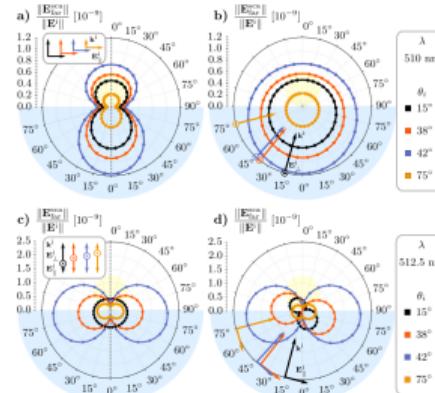
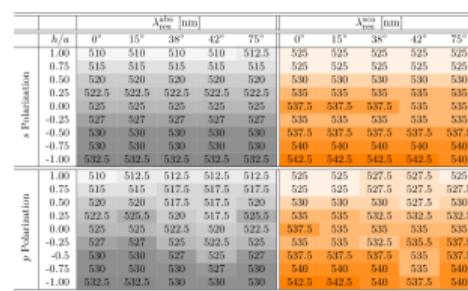
- ▶ Pol. s : no dependen de el ángulo de incidencia.
 - ▶ Pol. p : sí dependen de el ángulo de incidencia.

$\theta_i \approx \theta_c$: Maximización de la extinción

Trabajo a futuro: Incrustación + Polarización

Metasuperficies de AuNP parcialmente incrustadas

- ▶ Descripción de su respuesta óptica mediante teorías de medio efectivo
 - ▶ Metodología para medir su grado de incrustación promedio

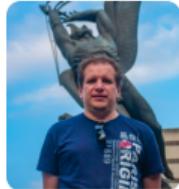


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Dirección General de Asuntos
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PAPIIT IN107122

Secciones de apoyo

4 Armónicos esféricos vectoriales

5 Solución de Mie

6 Elemento finito

7 Condiciones de frontera abierta

Condición de radiación de Sommerfeld

Perfect Matching Layer

8 Función dieléctrica: Corrección por tamaño

9 Análisis de convergencia: Mie vs. COMSOL

Armónicos esféricos vectoriales¹: $\{\mathbf{L}, \mathbf{M}, \mathbf{N}\}$

Base de campos vectoriales que son solución a la ecuación de Helmholtz

$$\mathbf{L} = \nabla\psi$$

$$\mathbf{M} = \nabla \times (\mathbf{r}\psi)$$

$$\mathbf{N} = \frac{1}{k} \nabla \times \mathbf{M}$$

$$\text{Función generadora } \psi : \quad \nabla^2\psi + k^2\psi = 0$$

Considerando el sistema coordenado esférico:

$$\psi_{\text{o}}^{\text{e}}{}_{\ell m}(r, \theta, \varphi) = \frac{\sin(m\varphi)}{\cos(m\varphi)} P_{\ell}^m(\cos\theta) z_{\ell}(kr),$$

$$\begin{aligned} \mathbf{L}_{\text{o}}^{\text{e}}{}_{\ell m} &= \frac{\cos(m\varphi)}{\sin(m\varphi)} k P_{\ell}^m(\cos\theta) \frac{dz_{\ell}(kr)}{d(kr)} \hat{\mathbf{e}}_r + \frac{\cos(m\varphi)}{\sin(m\varphi)} k \frac{z_{\ell}(kr)}{kr} \frac{dP_{\ell}^m(\cos\theta)}{d\theta} \hat{\mathbf{e}}_{\theta} + \\ &\quad - \sin(m\varphi) km \frac{P_{\ell}^m(\cos\theta)}{\sin\theta} \frac{z_{\ell}(kr)}{kr} \hat{\mathbf{e}}_{\varphi} \\ &\quad + \cos(m\varphi) km \frac{P_{\ell}^m(\cos\theta)}{\sin\theta} \frac{z_{\ell}(kr)}{kr} \hat{\mathbf{e}}_{\varphi} \end{aligned}$$

$$\begin{aligned} \mathbf{M}_{\text{o}}^{\text{e}}{}_{\ell m} &= -\sin(m\varphi) m z_{\ell}(kr) \frac{P_{\ell}^m(\cos\theta)}{\sin\theta} \hat{\mathbf{e}}_{\theta} - \frac{\cos(m\varphi)}{\sin(m\varphi)} z_{\ell}(kr) \frac{dP_{\ell}^m(\cos\theta)}{d\theta} \hat{\mathbf{e}}_{\varphi} \end{aligned}$$

$$\begin{aligned} \mathbf{N}_{\text{o}}^{\text{e}}{}_{\ell m} &= \frac{\cos(m\varphi)}{\sin(m\varphi)} \frac{z_{\ell}(kr)}{kr} \ell(\ell+1) P_{\ell}^m(\cos\theta) \hat{\mathbf{e}}_r + \frac{\cos(m\varphi)}{\sin(m\varphi)} \frac{1}{kr} \frac{d[kr z_{\ell}(kr)]}{d(kr)} \frac{dP_{\ell}^m(\cos\theta)}{d\theta} \hat{\mathbf{e}}_{\theta} + \\ &\quad - \sin(m\varphi) m \frac{1}{kr} \frac{d[kr z_{\ell}(kr)]}{d(kr)} \frac{P_{\ell}^m(\cos\theta)}{\sin\theta} \hat{\mathbf{e}}_{\varphi} \\ &\quad + \cos(m\varphi) m \frac{1}{kr} \frac{d[kr z_{\ell}(kr)]}{d(kr)} \frac{P_{\ell}^m(\cos\theta)}{\sin\theta} \hat{\mathbf{e}}_{\varphi} \end{aligned}$$

P_m^{ℓ} : Funciones asociadas de Legendre

z_{ℓ} : Funciones esféricas de Bessel (Hankel)

Comportamiento asintótico² de $h_{\ell}^{(1)} = j_{\ell} + iy_{\ell}$:

$$h_{\ell}^{(1)}(\rho) \approx (-i)^{\ell} \frac{\exp(i\rho)}{i\rho}$$

$$\frac{dh_{\ell}^{(1)}(\rho)}{d\rho} \approx (-i)^{\ell} \frac{\exp(i\rho)}{\rho},$$

¹ L. Tsang et al. *Scattering of Electromagnetic Waves: Theories and Applications*. John Wiley & Sons, Inc., New York, USA, 2000

² C. F. Bohren et al. *Absorption and Scattering of Light by Small Particles*. Wiley Science Paperbak Series. John Wiley & Sons, 1.^a edición, 1983

Solución de Mie^{1,2}

Esparcimiento de luz por partículas esféricas embebidas en medios infinitos

$$\mathbf{E}^i(\mathbf{r}) = E_0 \sum_{\ell=1}^{\infty} \frac{i^\ell (2\ell+1)}{\ell(\ell+1)} \left(\mathbf{M}_{o1\ell}^{(1)} - i\mathbf{N}_{e1\ell}^{(1)} \right)$$

$$(1) \implies z_\ell(\rho) = j_\ell(\rho)$$

$$\mathbf{E}^{\text{sca}}(\mathbf{r}) = E_0 \sum_{\ell=1}^{\infty} \frac{i^\ell (2\ell+1)}{\ell(\ell+1)} \left(ia_\ell \mathbf{N}_{e1\ell}^{(3)} - b_\ell \mathbf{M}_{o1\ell}^{(3)} \right)$$

$$(3) \implies z_\ell(\rho) = h_\ell^{(1)}(\rho) = j_\ell(\rho) + iy_\ell(\rho)$$

- ▶ Funciones angulares: $\pi_\ell(\cos \theta) = \frac{P_\ell^1(\cos \theta)}{\sin \theta}$ $\tau_\ell(\cos \theta) = dP_\ell^1(\cos \theta)/d\theta$
- ▶ Funciones de Riccati-Bessel: $\psi_\ell(\rho) = \rho j_\ell(\rho)$ $\xi(\rho) = \rho h^{(1)}(\rho)$
- ▶ Parámetro de tamaño: $x = ka = 2\pi n \frac{a}{\lambda}$
- ▶ Coeficientes de Mie: $a_\ell = \frac{\psi_\ell(x)\psi'_\ell(mx) - m\psi_\ell(mx)\psi'_\ell(x)}{\xi_\ell(x)\psi'_\ell(mx) - m\psi_\ell(mx)\xi'_\ell(x)}$ $b_\ell = \frac{m\psi_\ell(x)\psi'_\ell(mx) - \psi_\ell(mx)\psi'_\ell(x)}{m\xi_\ell(x)\psi'_\ell(mx) - \psi_\ell(mx)\xi'_\ell(x)}$
- ▶ Secciones transversales: $C_{\text{ext}} = \frac{2\pi}{k^2} \sum_{\ell=1}^{\infty} (2\ell+1) \operatorname{Re}(a_\ell + b_\ell)$ $C_{\text{sca}} = \frac{2\pi}{k^2} \sum_{\ell=1}^{\infty} (2\ell+1) (|a_\ell|^2 + |b_\ell|^2)$
- ▶ Resonancia de plasmón de superficie localizada (LSPR):
 - $\xi_\ell(x)\psi'_\ell(mx) - m\psi_\ell(mx)\xi'_\ell(x) \rightarrow 0$ (LSPR eléctrica)
 - $m\xi_\ell(x)\psi'_\ell(mx) - \psi_\ell(mx)\xi'_\ell(x) \rightarrow 0$ (LSPR magnética)

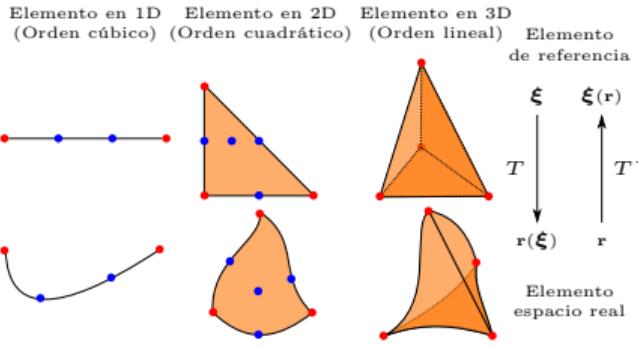
¹ C. F. Bohren et al. *Absorption and Scattering of Light by Small Particles*. Wiley Science Paperbak Series. John Wiley & Sons, 1.^a edición, 1983

² L. Tsang et al. *Scattering of Electromagnetic Waves: Theories and Applications*. John Wiley & Sons, Inc., New York, USA, 2000

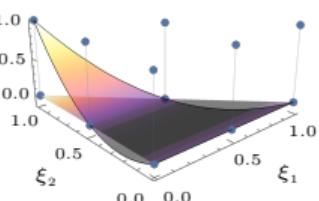
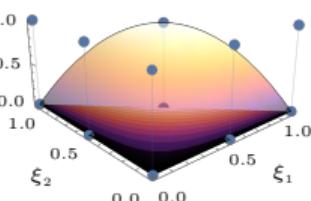
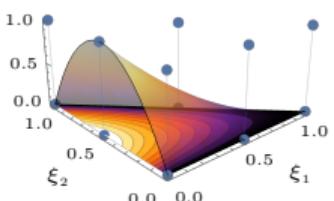
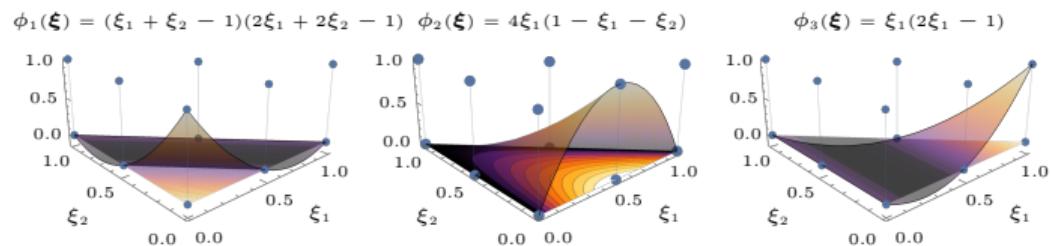
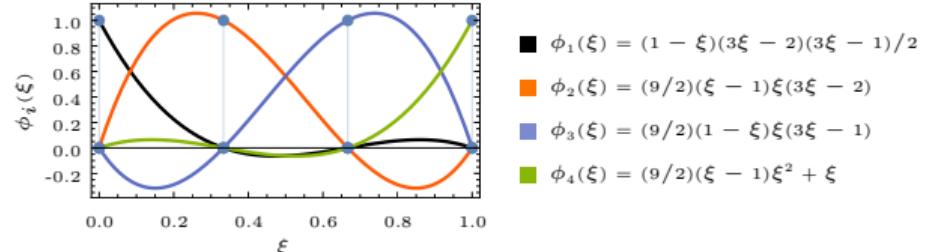
Elementos finitos^{1,2}

Sistema real, de referencia y ejemplos

$$\frac{\partial}{\partial r_i} = \frac{\partial \xi_i}{\partial r_j} \frac{\partial}{\partial \xi_j} \quad d\Omega_k \rightarrow \det[J] d\Omega_k$$



$$\mathcal{F}_\ell^L[f(\xi)] = f(\xi_{\ell_k})$$



¹ G. Dhatt et al. *Finite element method*. Numerical methods series. ISTE ; Wiley, London : Hoboken, N.J, 2012

² C. A. J. Fletcher. *Computational Galerkin Methods*. Springer Berlin Heidelberg, Berlin, Heidelberg, 1984

Condición de radiación de Sommerfeld generalizada

Contribuciones eléctricas y magnéticas debido a cargas y corrientes externas e inducidas^{1,2}

Descomposición en contribuciones eléctricas y magnéticas:

$$\mathbf{E} = \mathbf{E}_e + \mathbf{E}_m \quad \text{y} \quad \mathbf{H} = \mathbf{H}_e + \mathbf{H}_m$$

$$\nabla \cdot (\epsilon \mathbf{E}_e) = \rho_{\text{ext}},$$

$$\nabla \cdot (\epsilon \mathbf{E}_m) = 0$$

$$\nabla \cdot (\mu \mathbf{H}_e) = 0$$

$$\nabla \cdot (\mu \mathbf{H}_m) = \rho_m$$

$$\nabla \times \mathbf{E}_e = i\omega \mu \mathbf{H}_e$$

$$\nabla \times \mathbf{E}_m = i\omega \mu \mathbf{H}_m + \mathbf{J}_m$$

$$\nabla \times \mathbf{H}_e = \mathbf{J}_{\text{ext}} - i\omega \epsilon \mathbf{E}_e$$

$$\nabla \times \mathbf{H}_m = -i\omega \epsilon \mathbf{E}_m$$

Imponiendo la norma de Lorenz se cumple que

$$\nabla \cdot \mathbf{A} = -i\omega \mu \epsilon \phi_e \quad \text{y} \quad \nabla \cdot \mathbf{F} = -i\omega \mu \epsilon \phi_m$$

por lo que

$$\mathbf{E} = -\frac{\nabla[\nabla \cdot \mathbf{A}]}{i\omega \epsilon \mu} + i\omega \mathbf{A} + \frac{1}{\epsilon} \nabla \times \mathbf{F} \quad \mathbf{H} = -\frac{\nabla[\nabla \cdot \mathbf{F}]}{i\omega \epsilon \mu} + i\omega \mathbf{F} + \frac{1}{\mu} \nabla \times \mathbf{A}$$

donde

$$\mathbf{A} = \frac{\mu}{4\pi} \int_{\Omega} \mathbf{J}_{\text{ext}} \frac{\exp[i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')]}{\|\mathbf{r} - \mathbf{r}'\|} d\Omega'$$

$$\mathbf{F} = \frac{\epsilon}{4\pi} \int_{\Omega} \mathbf{J}_m \frac{\exp[i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')]}{\|\mathbf{r} - \mathbf{r}'\|} d\Omega'$$

¹ J.-M. Jin. *Theory and Computation of Electromagnetic Fields*. Wiley & Sons, 2010

² A. Bondeson et al. *Computational electromagnetics*. Springer, New York, N.Y., 2005

Condición de radiación de Sommerfeld generalizada¹

Comportamiento en el régimen de campo lejano

En el régimen de campo lejano²:

$$\mathbf{A} = \frac{\mu \exp(ikr)}{4\pi r} \mathbf{N},$$

$$\text{con } \mathbf{N} = \int_{\Omega} \mathbf{J}_{\text{ext}} \exp(-i\mathbf{k} \cdot \mathbf{r}') d\Omega'$$

$$\mathbf{F} = \frac{\varepsilon \exp(ikr)}{4\pi r} \mathbf{L},$$

$$\text{con } \mathbf{L} = \int_{\Omega} \mathbf{J}_{\text{m}} \exp(-i\mathbf{k} \cdot \mathbf{r}') d\Omega'$$

por lo que los campos electromagnéticos se escriben como²

$$\left. \begin{array}{lcl} \lim_{r \rightarrow \infty} \mathbf{E} & = & -ik \frac{\exp(ikr)}{4\pi r} \left[\hat{\mathbf{e}}_r \times \mathbf{L} - \sqrt{\frac{\mu}{\varepsilon}} (\mathbf{N} - (\hat{\mathbf{e}}_r \cdot \mathbf{N}) \hat{\mathbf{e}}_r) \right] \\ \lim_{r \rightarrow \infty} \mathbf{H} & = & ik \frac{\exp(ikr)}{4\pi r} \left[\sqrt{\frac{\varepsilon}{\mu}} (\mathbf{L} - (\hat{\mathbf{e}}_r \cdot \mathbf{L}) \hat{\mathbf{e}}_r + \hat{\mathbf{e}}_r \times \mathbf{N}) \right] \end{array} \right\} \Rightarrow \lim_{r \rightarrow \infty} \left(\hat{\mathbf{e}}_r \times \mathbf{E} - \sqrt{\frac{\mu}{\varepsilon}} \mathbf{H} \right) = \mathbf{0}$$

Empleando la ley de Faraday-Lenz:

Condición de radiación de Sommerfeld³

$$\lim_{r \rightarrow \infty} r(\nabla \times \mathbf{E} - ik\hat{\mathbf{e}}_r \times \mathbf{E}) = \mathbf{0}$$

¹ J.-M. Jin. *Theory and Computation of Electromagnetic Fields*. Wiley & Sons, 2010

² J. D. Jackson. *Classical electrodynamics*. Wiley, New York, 3.^a edición, 1999

³ S. Silver. *Microwave Antenna Theory and Design*. The Institution of Engineering y Technology, 1984. 640 páginas

Perfect Matching Layer^{1,2} (PML)

Propiedades geométricas de Ω_{PML} , dominio que rodea a Ω

- Elongaciones geométricas³ y aproximación de campo lejano considerada como válida

$$\nabla_s \equiv \left(\frac{\hat{\mathbf{e}}_x}{s_x} \frac{\partial}{\partial x} + \frac{\hat{\mathbf{e}}_y}{s_y} \frac{\partial}{\partial y} + \frac{\hat{\mathbf{e}}_z}{s_z} \frac{\partial}{\partial z} \right) \rightarrow \mathbf{k} = \frac{k_x}{s_x} \hat{\mathbf{e}}_x + \frac{k_y}{s_y} \hat{\mathbf{e}}_y + \frac{k_z}{s_z} \hat{\mathbf{e}}_z$$

- Factores de deformación complejos: $s_{x_i} = s_{x_i}(x_i)$; en Ω , $s_{x_i} = 1$

$$\nabla_s \cdot \mathbf{v} = \frac{1}{s_x s_y s_z} \nabla \cdot [\text{diag}(s_y s_z, s_x s_z, s_x s_y) \mathbf{v}]$$

$$\nabla_s \times \mathbf{v} = \text{diag}\left(\frac{1}{s_y s_z}, \frac{1}{s_x s_z}, \frac{1}{s_x s_y}\right) \nabla \times [\text{diag}(s_x, s_y, s_z) \mathbf{v}]$$

- Relación de dispersión de una onda plana:

$$\mathbf{k} \cdot \mathbf{k} = k^2 = \mu \epsilon \omega^2 = \left(\frac{k_x}{s_x}\right)^2 + \left(\frac{k_y}{s_y}\right)^2 + \left(\frac{k_z}{s_z}\right)^2$$

$$k_x = k s_x \sin \theta \cos \varphi \quad k_y = k s_y \sin \theta \sin \varphi \quad k_z = k s_z \cos \theta$$

¹ C. A. J. Fletcher. *Computational Galerkin Methods*. Springer Berlin Heidelberg, Berlin, Heidelberg, 1984

² J.-M. Jin. *Theory and Computation of Electromagnetic Fields*. Wiley & Sons, 2010

³ M. Bergot et al. *Journal of Computational and Applied Mathematics*, **234**(6):1937-1944, 2010

Perfect Matching Layer (PML)

Condiciones para nulas reflexiones

- ▶ Coeficientes de amplitud de reflexión¹:

$$r_s = \frac{k_z^{(\text{PML})} s_z^{(\text{PML})} \mu_{\text{PML}} - k_z^{(\Omega)} s_z^{(\Omega)} \mu_\Omega}{k_z^{(\text{PML})} s_z^{(\text{PML})} \mu_{\text{PML}} + k_z^{(\Omega)} s_z^{(\Omega)} \mu_\Omega} \quad r_p = \frac{k_z^{(\text{PML})} s_z^{(\text{PML})} \varepsilon_{\text{PML}} - k_z^{(\Omega)} s_z^{(\Omega)} \varepsilon_\Omega}{k_z^{(\text{PML})} s_z^{(\text{PML})} \varepsilon_{\text{PML}} + k_z^{(\Omega)} s_z^{(\Omega)} \varepsilon_\Omega}$$

- ▶ Condiciones de empalme de fase (componentes paralelas a la interfaz entre Ω y Ω_{PML})

$$\begin{aligned} k^{(\text{PML})} s_x^{(\text{PML})} \sin \theta_{\text{PML}} \cos \varphi_{\text{PML}} &= k^{(\Omega)} s_x^{(\Omega)} \sin \theta_\Omega \cos \varphi_\Omega \\ k^{(\text{PML})} s_y^{(\text{PML})} \sin \theta_{\text{PML}} \sin \varphi_{\text{PML}} &= k^{(\Omega)} s_y^{(\Omega)} \sin \theta_\Omega \sin \varphi_\Omega \end{aligned}$$

Condiciones para una PML²

$$\left. \begin{array}{l} \varepsilon_\Omega = \varepsilon_{\text{PML}}, \quad \mu_\Omega = \mu_{\text{PML}} \\ s_x^{(\Omega)} = s_x^{(\text{PML})}, \quad s_y^{(\Omega)} = s_y^{(\text{PML})} \end{array} \right\} \implies r_s = r_p = 0.$$

Adicionalmente $\text{Im}[s_z^{(\text{PML})}] < 0$ para que sea un material absorbente.

¹ J. D. Jackson. *Classical electrodynamics*. Wiley, New York, 3.^a edición, 1999

² J.-M. Jin. *Theory and Computation of Electromagnetic Fields*. Wiley & Sons, 2010

Perfect Matching Layer (PML)

Campos electromagnéticos¹

- Relación entre los campos en Ω y Ω_{PML}

$$\begin{aligned}\mathbf{E}^{(\Omega)} = \text{diag}(s_x, s_y, s_z) \mathbf{E}^{(\text{PML})} &\iff \mathbf{E}^{(\text{PML})} = \text{diag}\left(\frac{1}{s_x}, \frac{1}{s_y}, \frac{1}{s_z}\right) \mathbf{E}^{(\Omega)} \\ \mathbf{H}^{(\Omega)} = \text{diag}(s_x, s_y, s_z) \mathbf{H}^{(\text{PML})} &\iff \mathbf{H}^{(\text{PML})} = \text{diag}\left(\frac{1}{s_x}, \frac{1}{s_y}, \frac{1}{s_z}\right) \mathbf{H}^{(\Omega)}\end{aligned}$$

- Transformación de las ecuaciones de Maxwell

$$\begin{aligned}\nabla_s \cdot (\varepsilon \mathbf{E}^{(\text{PML})}) &= 0 \implies \nabla \cdot [(\varepsilon \mathbb{A}) \mathbf{E}^{(\Omega)}] = 0 \\ \nabla_s \cdot (\mu \mathbf{H}^{(\text{PML})}) &= 0 \implies \nabla \cdot [(\mu \mathbb{A}) \mathbf{H}^{(\Omega)}] = 0 \\ \nabla_s \times \mathbf{E}^{(\text{PML})} &= i\omega \mu \mathbf{H}^{(\text{PML})} \implies \nabla \times (\mathbf{E}^{(\Omega)}) = i\omega (\mu \mathbb{A}) \mathbf{H}^{(\Omega)} \\ \nabla_s \times (\mu \mathbf{H}^{(\text{PML})}) &= -i\omega \varepsilon \mathbf{E}^{(\text{PML})} \implies \nabla \times [(\mu \mathbb{A}) \mathbf{E}^{(\Omega)}] = -i\omega (\varepsilon \mathbb{A}) \mathbf{E}^{(\Omega)}\end{aligned}$$

- Matriz de transformación:

$$\mathbb{A} = \text{diag}\left(\frac{s_y s_z}{s_x}, \frac{s_x s_z}{s_y}, \frac{s_x s_y}{s_z}\right)$$

¹ J.-M. Jin. *Theory and Computation of Electromagnetic Fields*. Wiley & Sons, 2010

Función dieléctrica: corrección por tamaño¹

Contribución intrabanda

- Modelo de Drude:

$$\frac{\varepsilon_{\text{Drude}}(\omega)}{\varepsilon_0} = 1 - \frac{\omega_p^2}{\omega(\omega + i\gamma)}$$

- Constantes de amortiguamiento para partículas esféricas:

$$\gamma_a^{\text{NP}} = \gamma^{\text{Bulk}} + A \frac{v_F}{a} \quad \gamma^{\text{Bulk}} = \frac{v_F}{L}$$

- Corrección: Ajuste y término con efectos de borde

$$\frac{\varepsilon_{\text{Size}}(\omega)}{\varepsilon_0} = \frac{\varepsilon_{\text{Exp}}(\omega)}{\varepsilon_0} + \left(-\frac{\varepsilon_{\text{Drude}}(\omega)}{\varepsilon_0} \Big|_{\gamma=\gamma^{\text{Bulk}}} + \frac{\varepsilon_{\text{Drude}}(\omega)}{\varepsilon_0} \Big|_{\gamma=\gamma_a^{\text{NP}}} \right).$$

- Determinación de parámetros mediante relaciones lineales

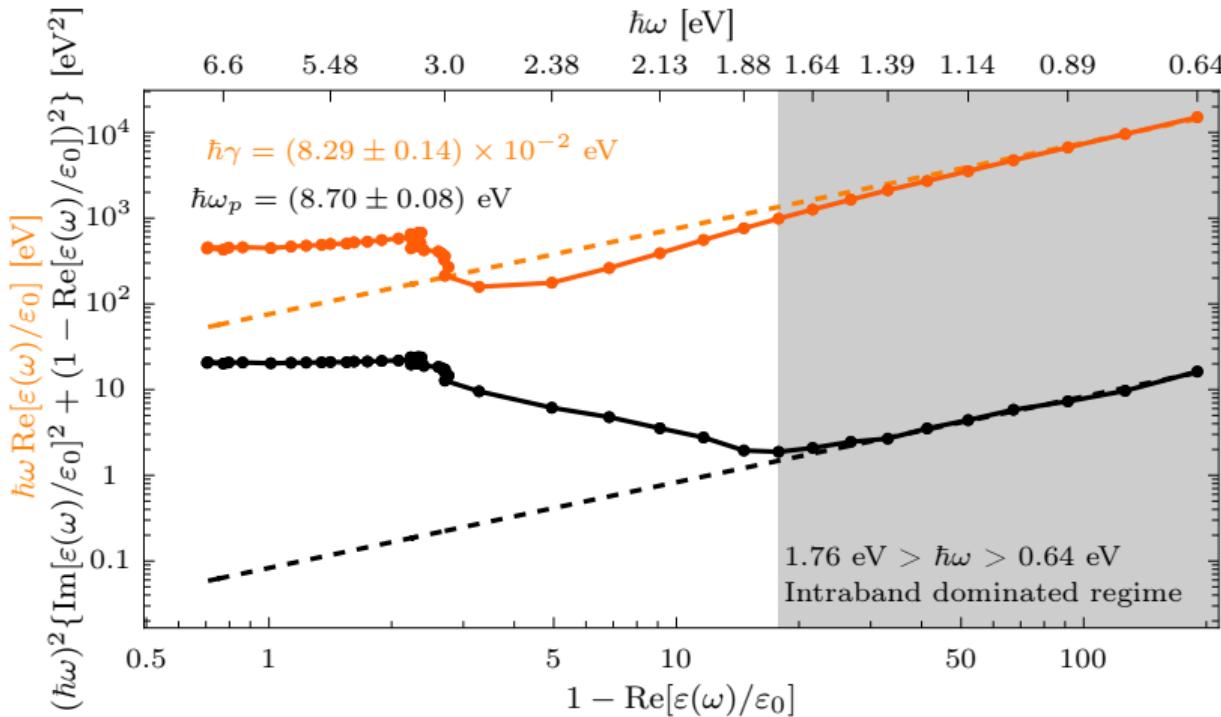
$$\omega \text{Im} \left[\frac{\varepsilon_{\text{Drude}}(\omega)}{\varepsilon_0} \right] = \gamma \left(1 - \text{Re} \left[\frac{\varepsilon_{\text{Drude}}(\omega)}{\varepsilon_0} \right] \right)$$

$$\omega^2 \left\{ \text{Im} \left[\frac{\varepsilon_{\text{Drude}}(\omega)}{\varepsilon_0} \right]^2 + \left(1 - \text{Re} \left[\frac{\varepsilon_{\text{Drude}}(\omega)}{\varepsilon_0} \right] \right)^2 \right\} = \omega_p^2 \left(1 - \text{Re} \left[\frac{\varepsilon_{\text{Drude}}(\omega)}{\varepsilon_0} \right] \right)$$

¹ L. J. Mendoza Herrera et al. *Journal of Applied Physics*, **116**(23):233105, 2014

Función dieléctrica: corrección por tamaño

Determinación de los parámetros de Drude¹ a partir de los datos experimentales del Au en bulto²

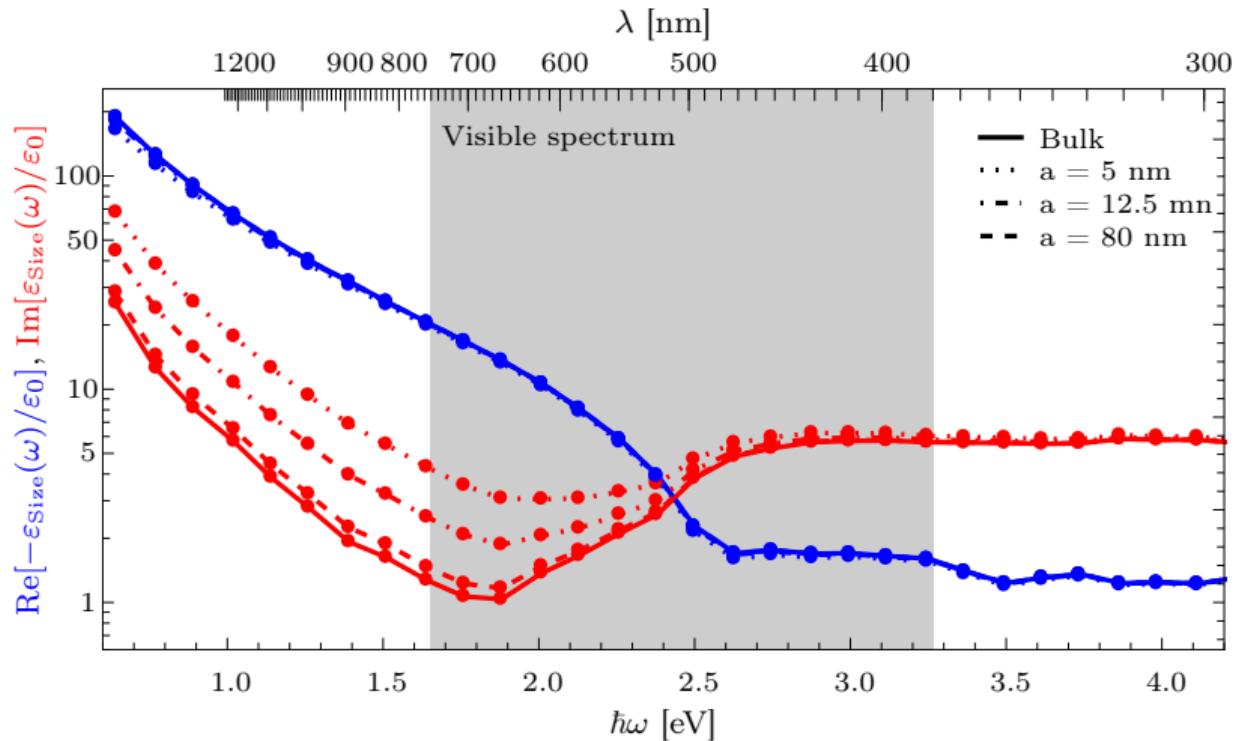


¹ L. J. Mendoza Herrera et al. *Journal of Applied Physics*, 116(23):233105, 2014

² P. B. Johnson et al. *Physical Review B*, 6(12):4370-4379, 1972

Función dieléctrica: corrección por tamaño¹

Función dieléctrica del Au para bulto² y nanoesferas de radio a

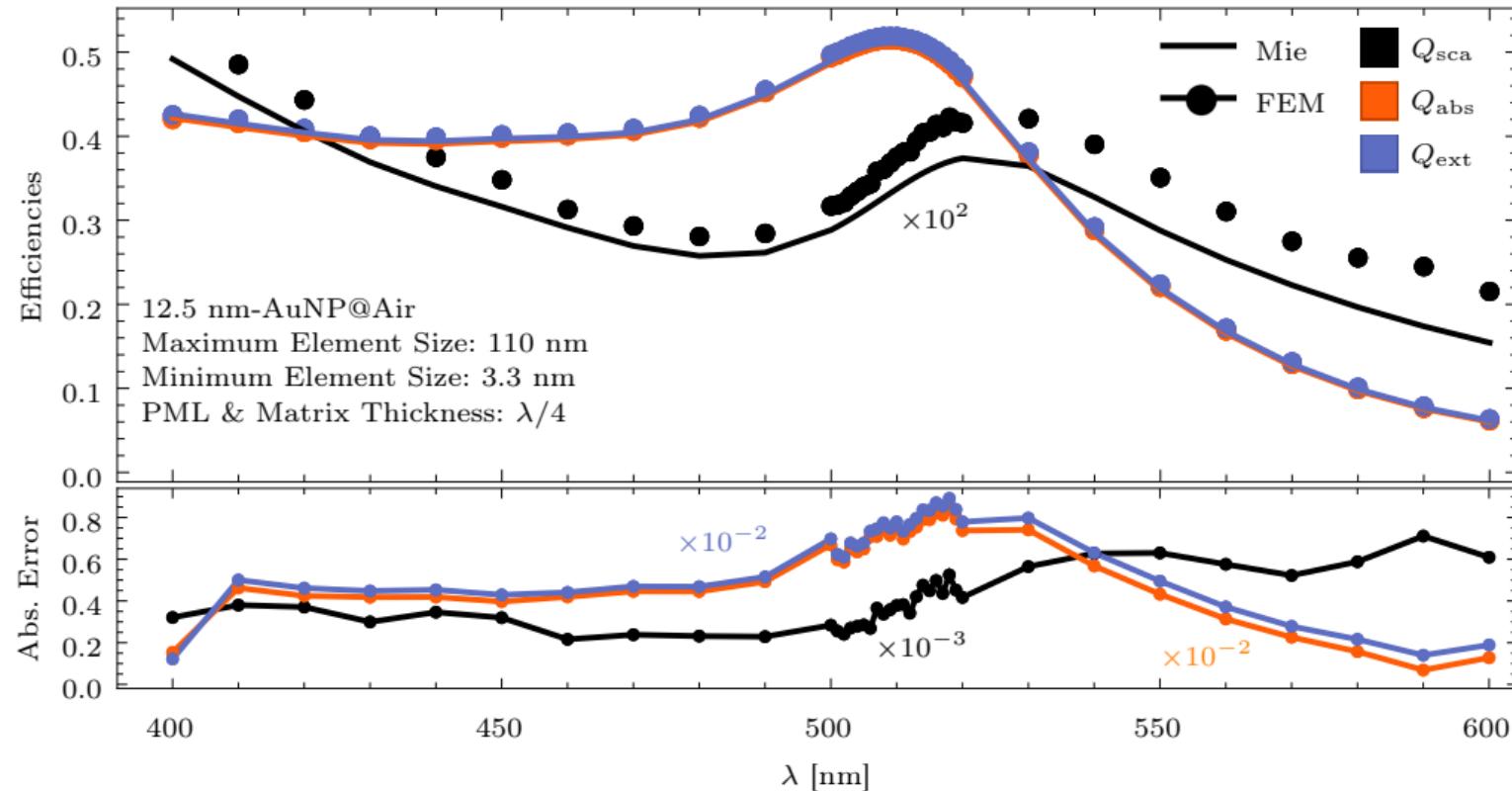


¹ L. J. Mendoza Herrera et al. *Journal of Applied Physics*, **116**(23):233105, 2014

² P. B. Johnson et al. *Physical Review B*, **6**(12):4370-4379, 1972

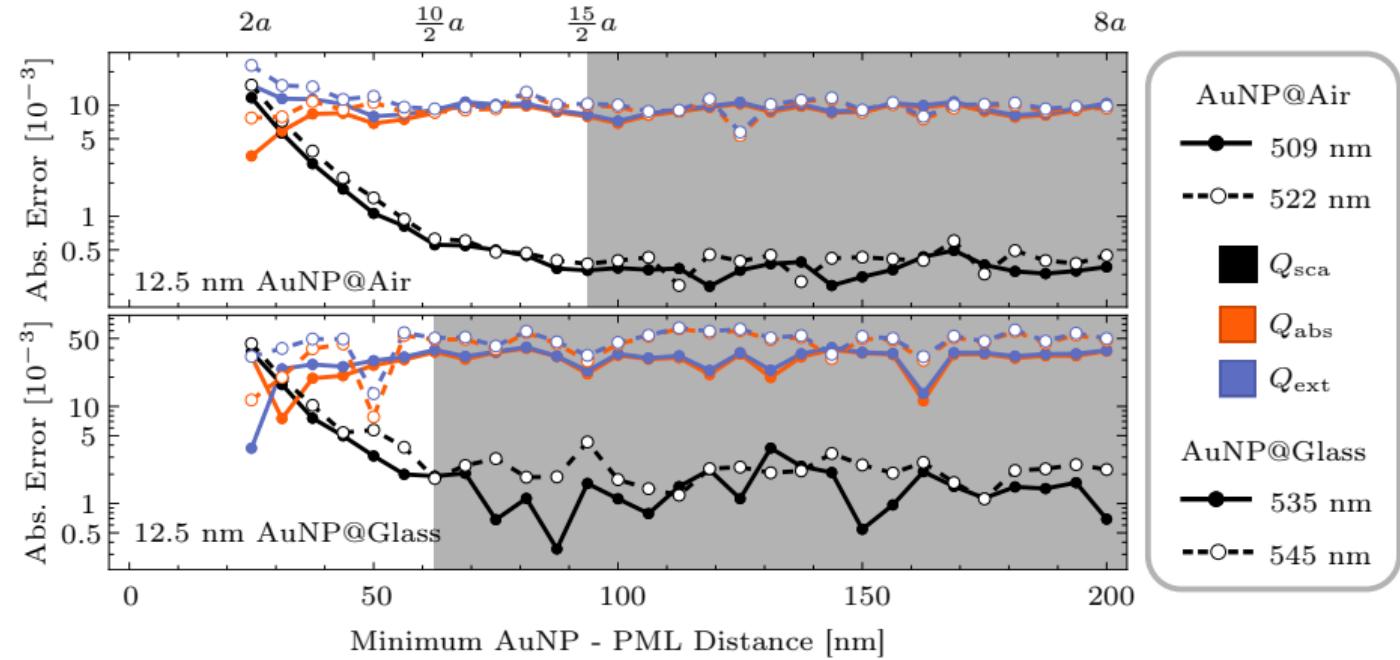
Análisis de convergencia

COMSOL vs Solución de Mie: Valores predeterminados



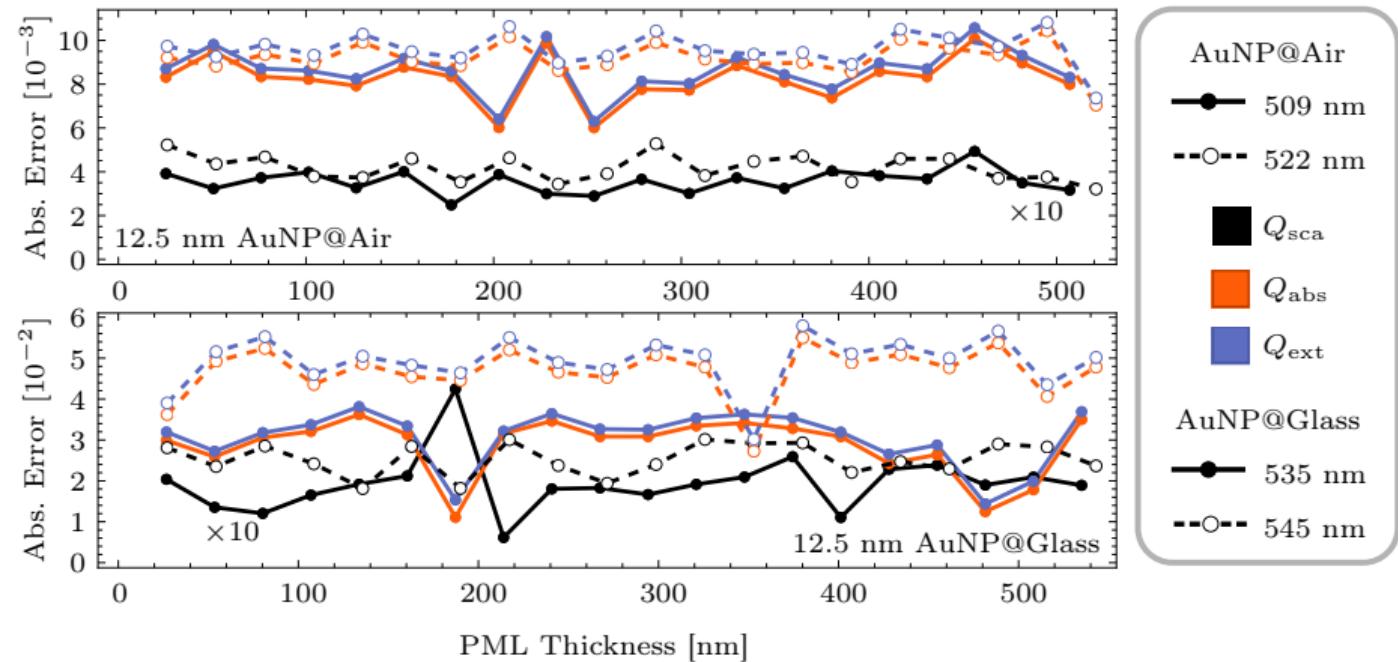
Análisis de convergencia

COMSOL vs Solución de Mie: Tamaño de la matrix



Análisis de convergencia

COMSOL vs Solución de Mie: Grosor del PML



Análisis de convergencia

COMSOL vs Solución de Mie: Mallado de la AuNP

