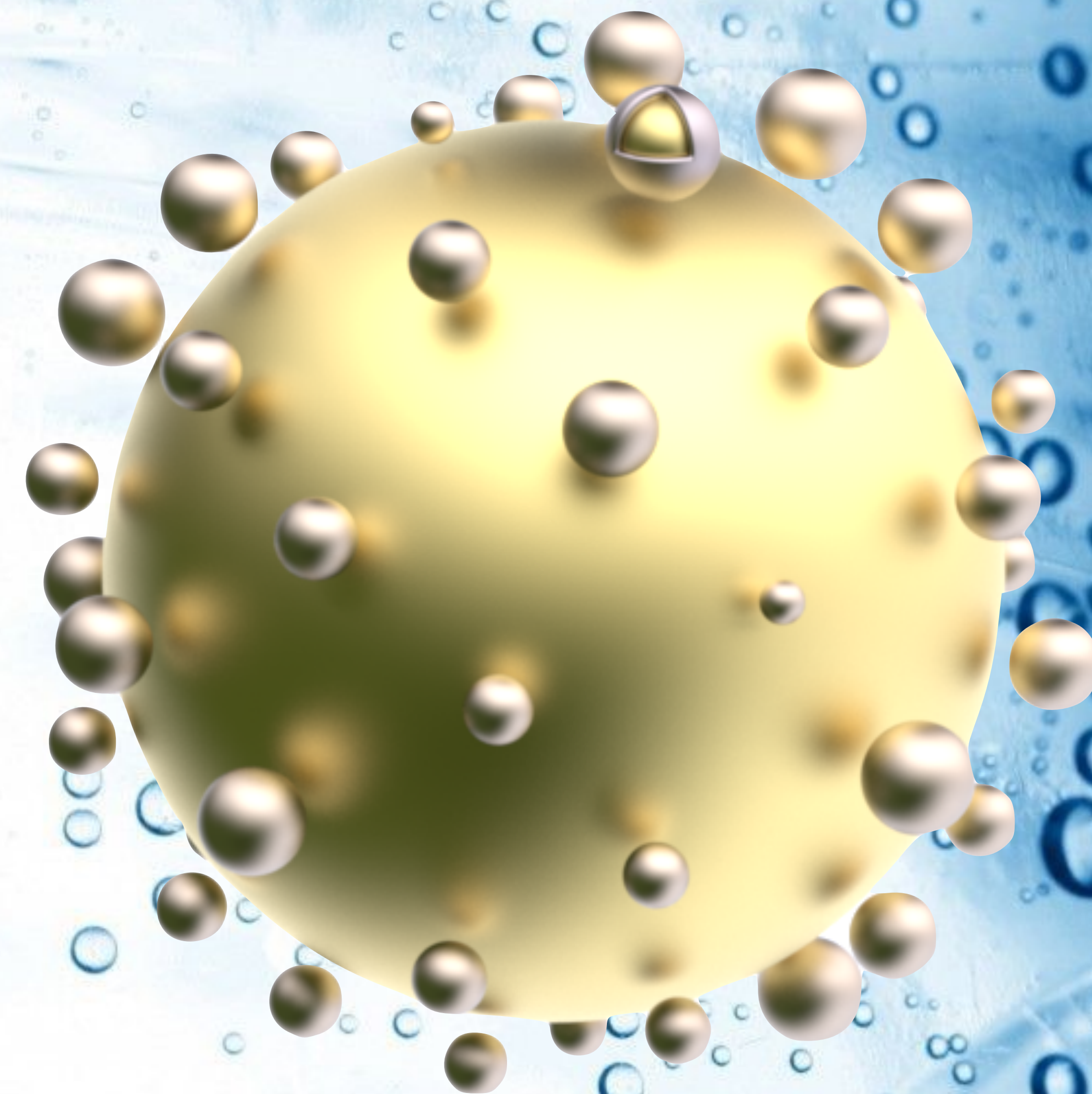

MODELLING LIGHT ABSORPTION IN HYBRID CORE-SATELLITE METAL NANOSTRUCTURES

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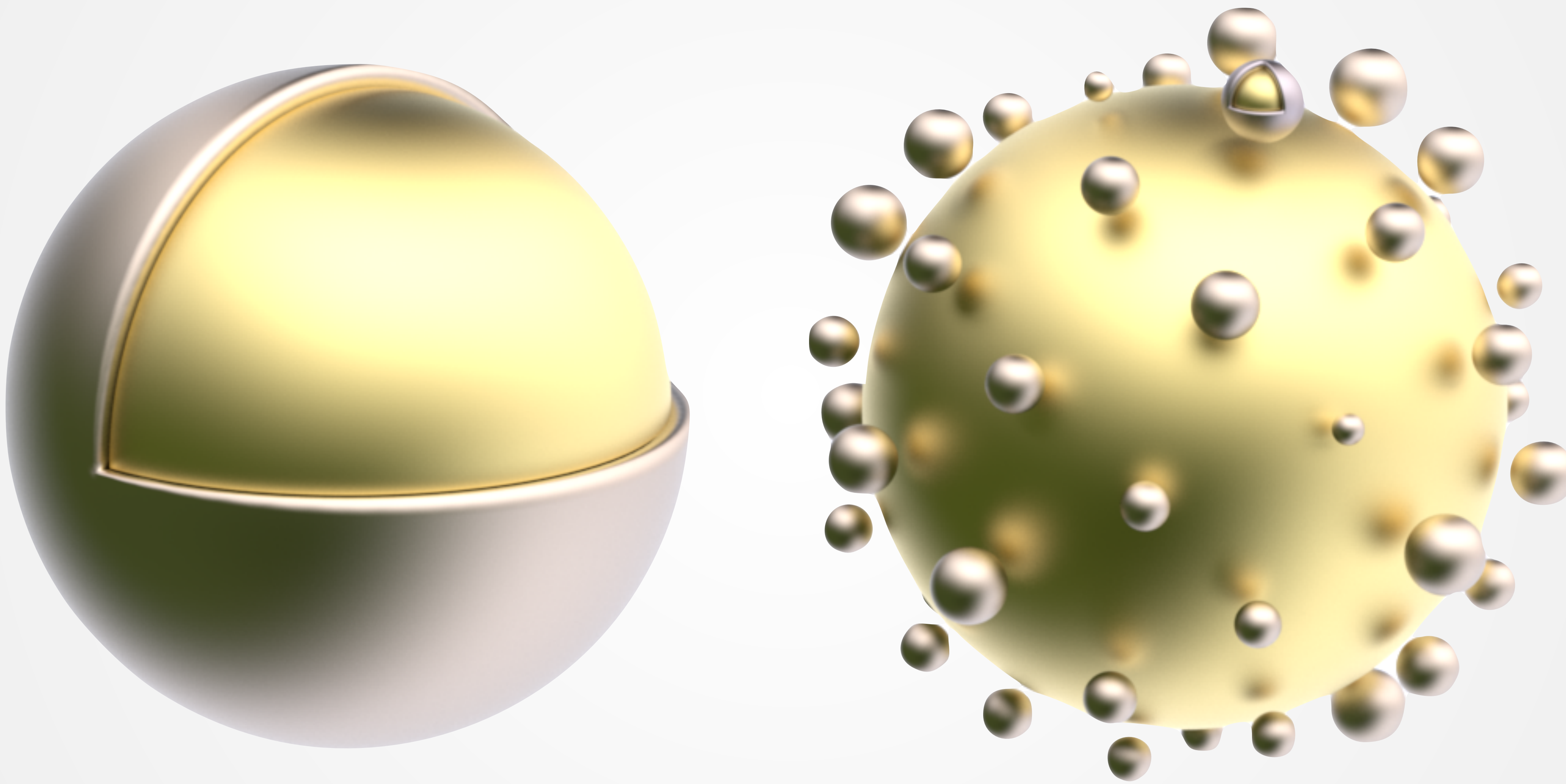
[2] Centro de Investigaciones Biomédicas, Universidade de Vigo, Spain

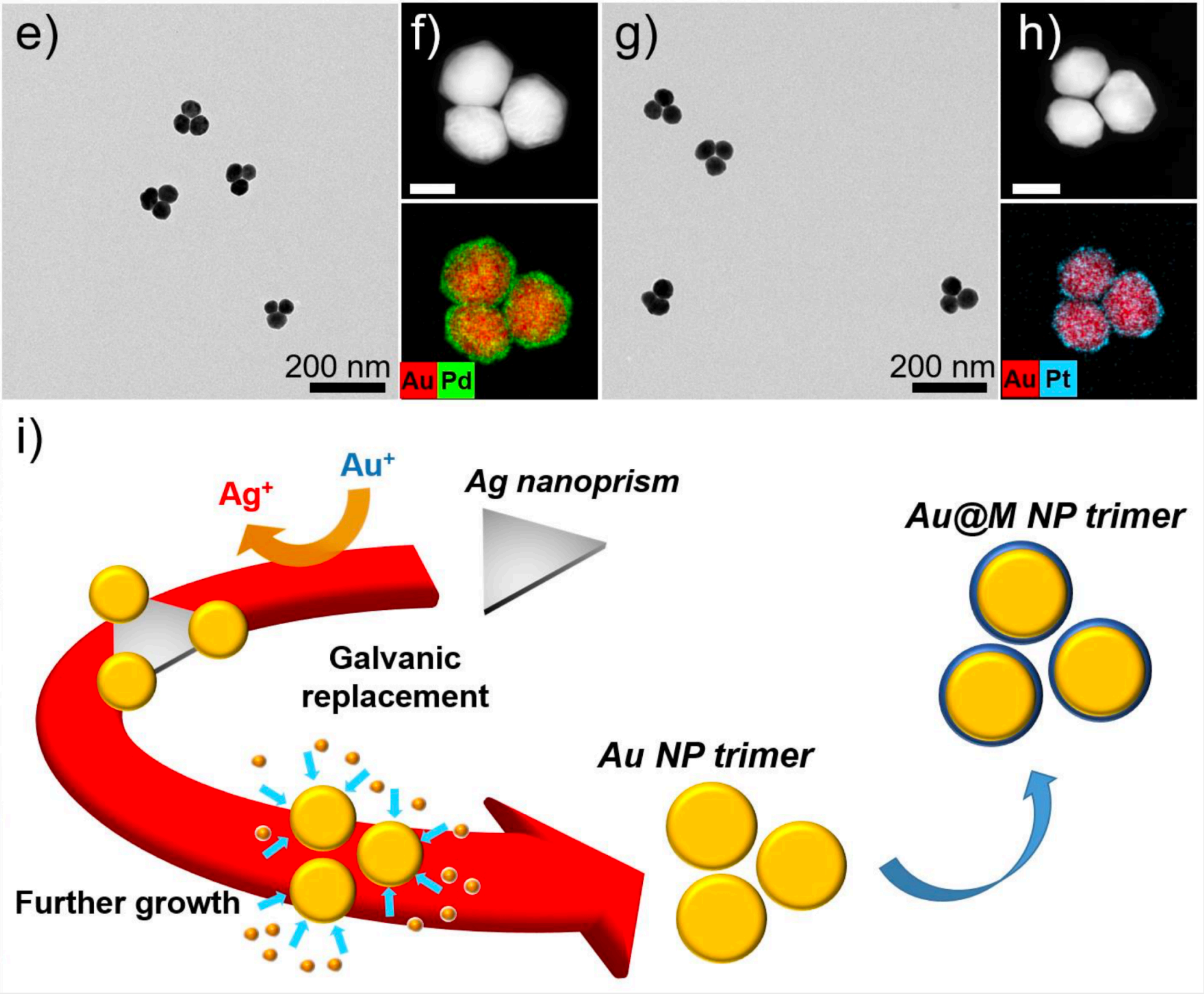
[3] School of Chemical & Physical Sciences, Victoria University of Wellington, Aotearoa NZ

* baptiste.auguie@vuw.ac.nz – https://nano-optics.ac.nz

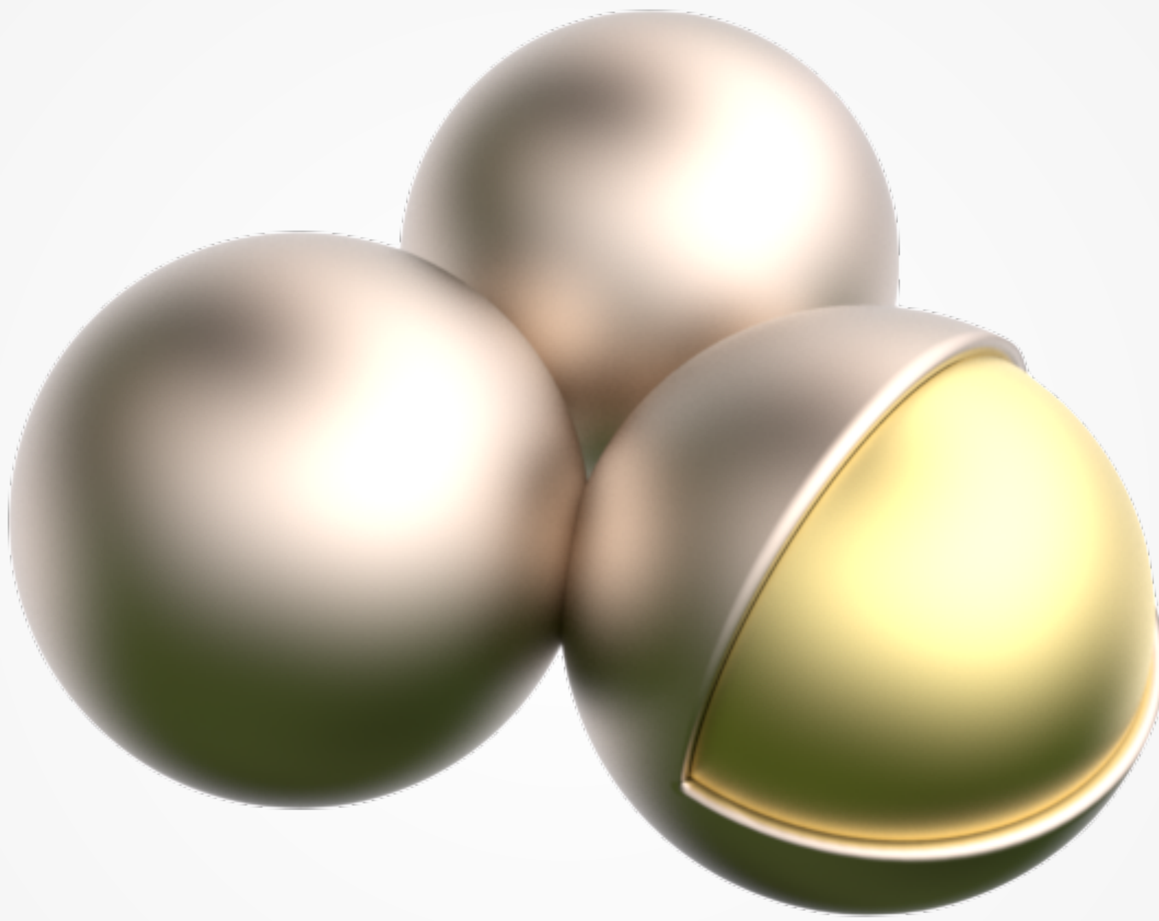
PLASMONIC ANTENNA + CATALYST HYBRIDS



- resonant antenna effect ⇒ strong absorption
- hot carriers (electrons/holes) ⇒ chemical reaction at catalyst surfaces


e)
200 nm
f)
Au Pd
g)
200 nm
h)
Au Pt
i)
Au+
Ag+
Ag nanoprism
Au@M NP trimer
Galvanic replacement
Au NP trimer
Further growth

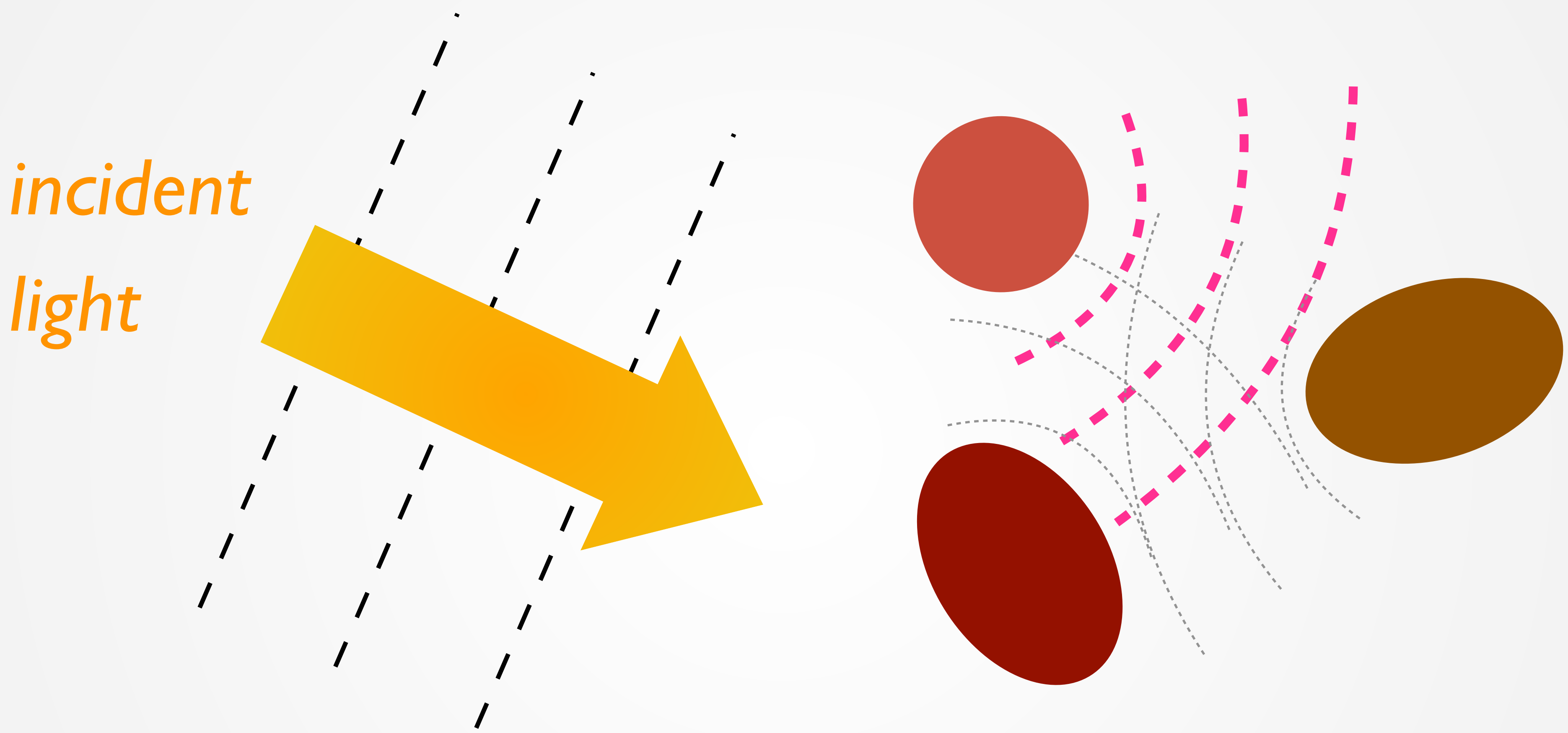
Au@Pd photocatalysts



S. Lee, H. Hwang, W. Lee, D. Schebarchov, Y. Wy, J. Grand, B. Auguié, D. Han Wi, E. Cortés and S. Woo Han. *ACS Energy Lett.* 5, 12, 3881–3890 (2020)

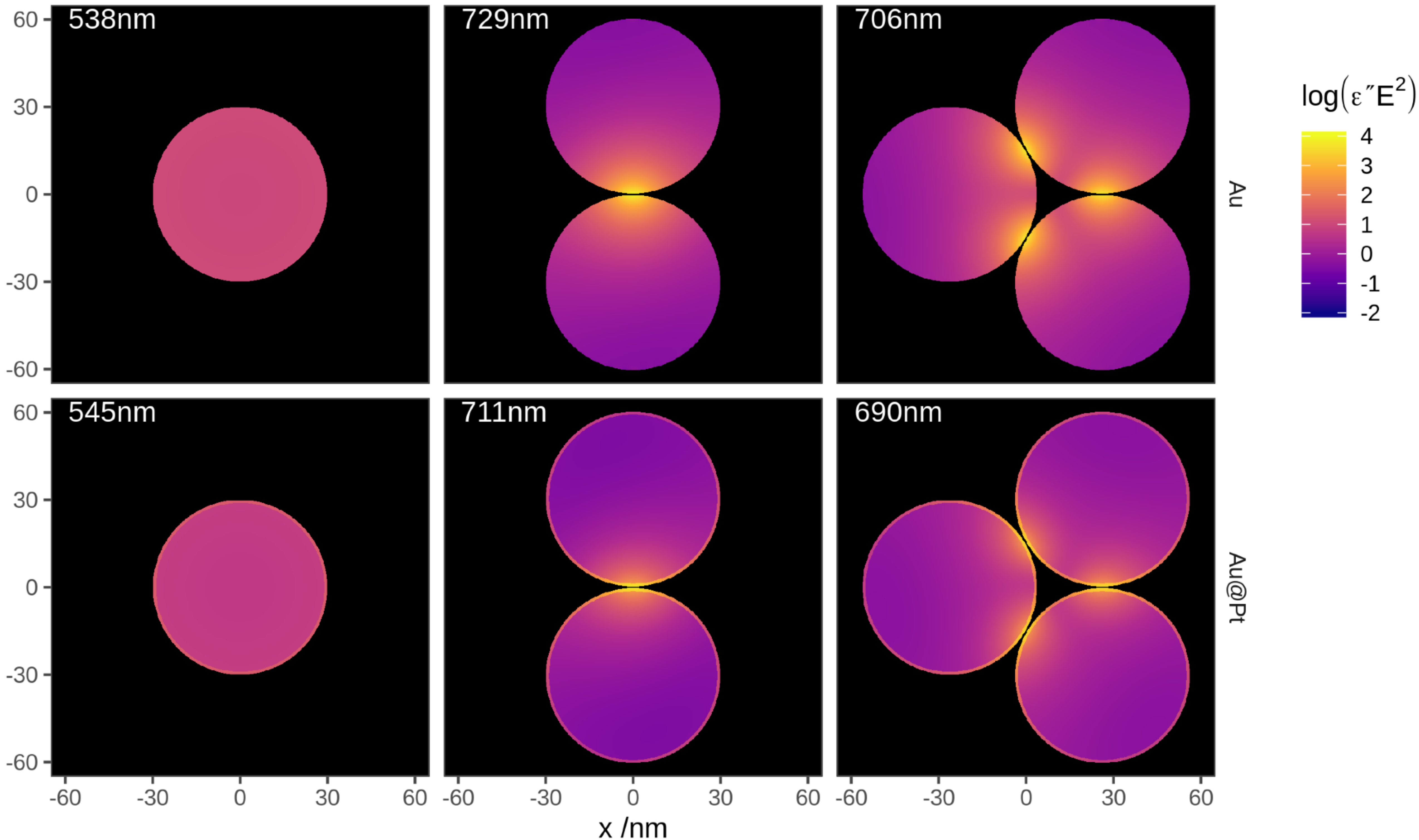

T.E.R.M.S.
(SUPERPOSITION T-MATRIX)
nano-optics.ac.nz/terms
10 nm

SUPERPOSITION T-MATRIX METHOD

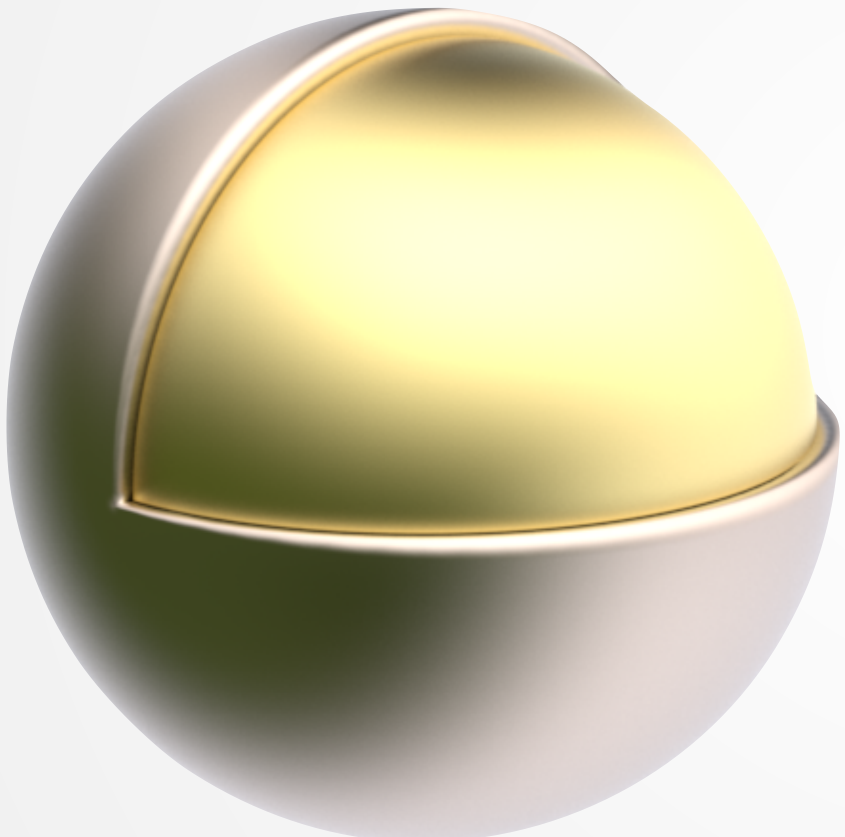


- expand fields in **spherical waves** (multipoles)
- exciting field = incident + scattered
- linear system for N particles

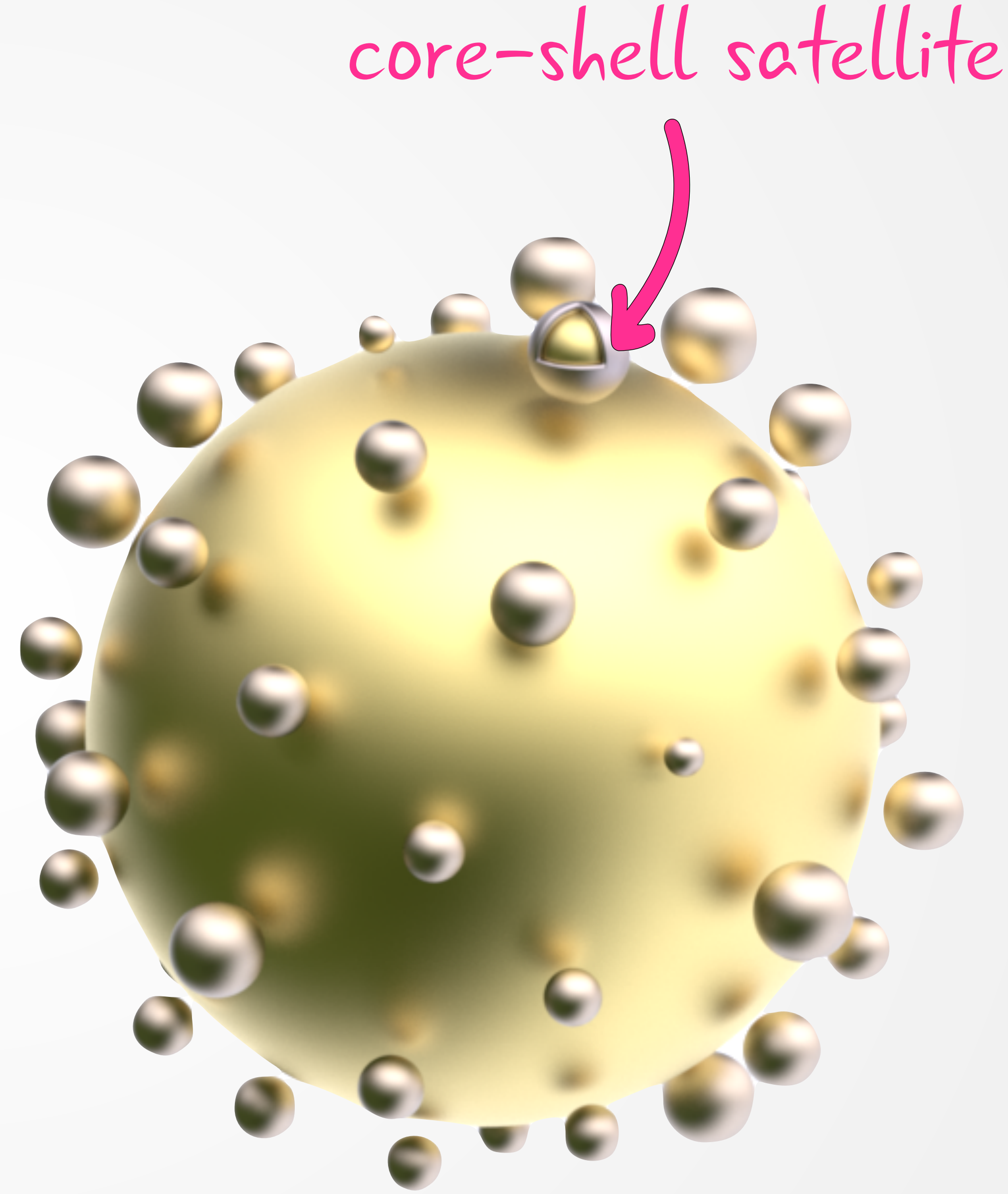
Local absorption in Au@Pt nano-trimers



NEW QUESTION: HOW TO COMBINE Au & Pd?

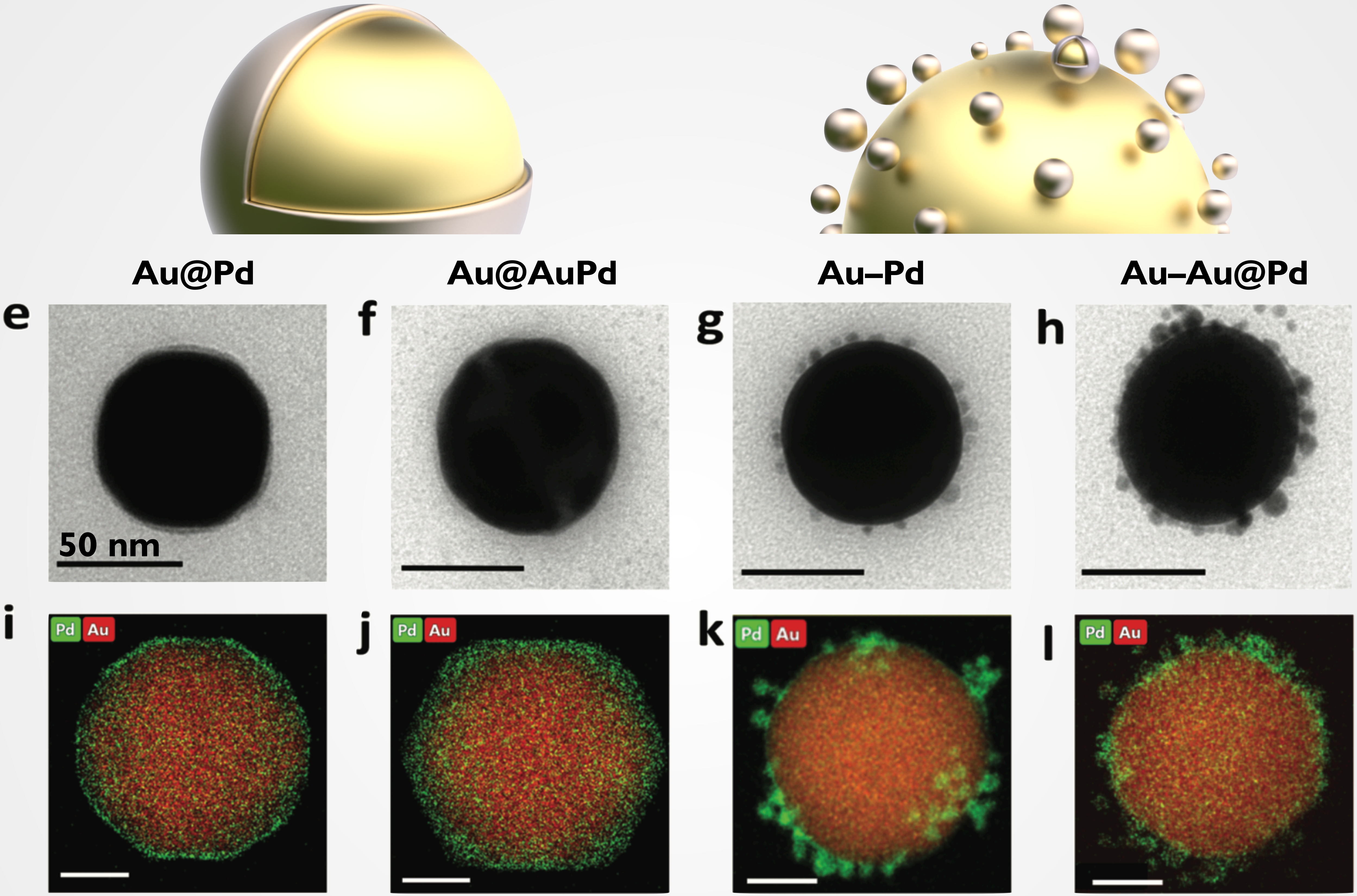


Antenna-Shell



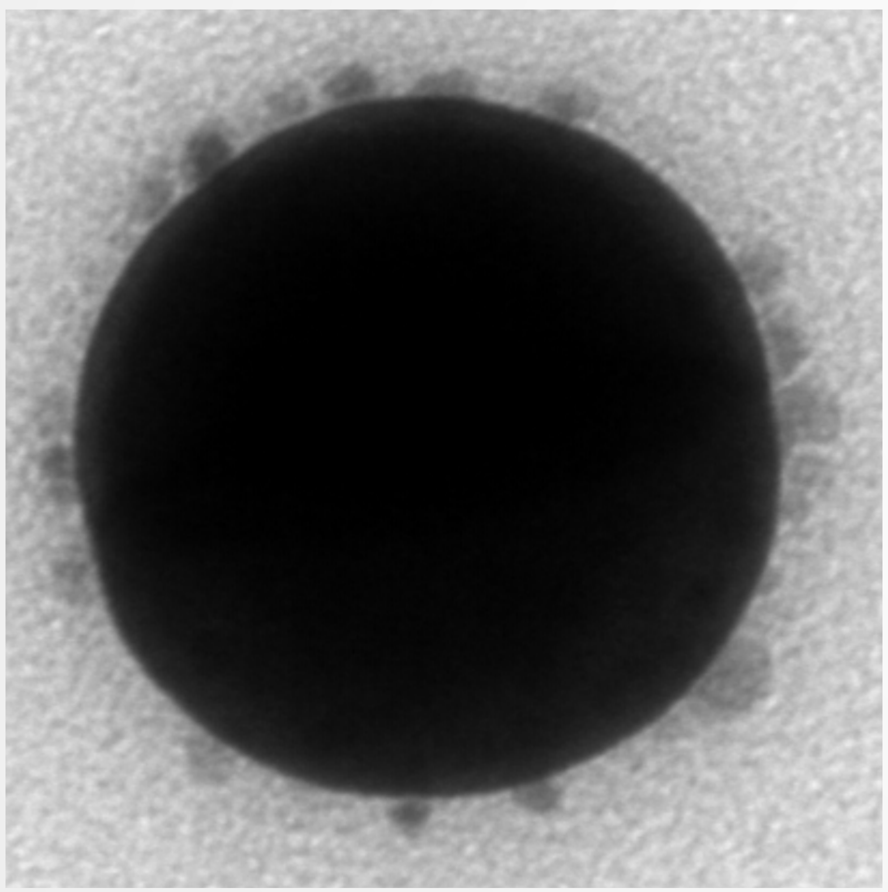
Antenna-Satellites cluster

SUB-QUESTION: **HOW DO WE MODEL *THAT* ↑ ?**

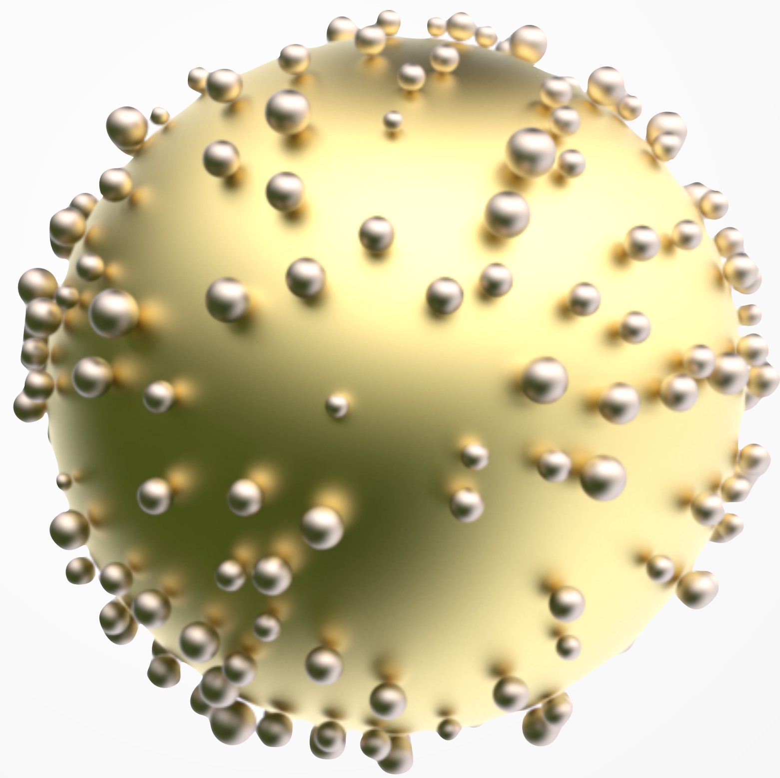


M. Herran, A. Sousa-Castillo, C. Fan, S. Lee, Wei Xie, M. Döblinger, B. Auguié and E. Cortés · *Adv. Func. Mat.* 32, 2203418 (2022)

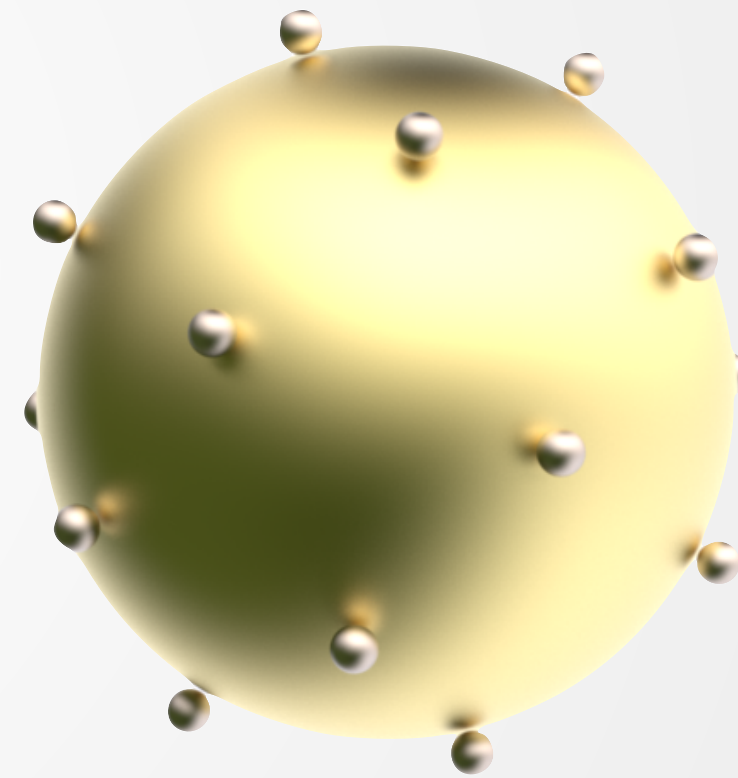
modelling Au–Pd core-satellite structures



TEM

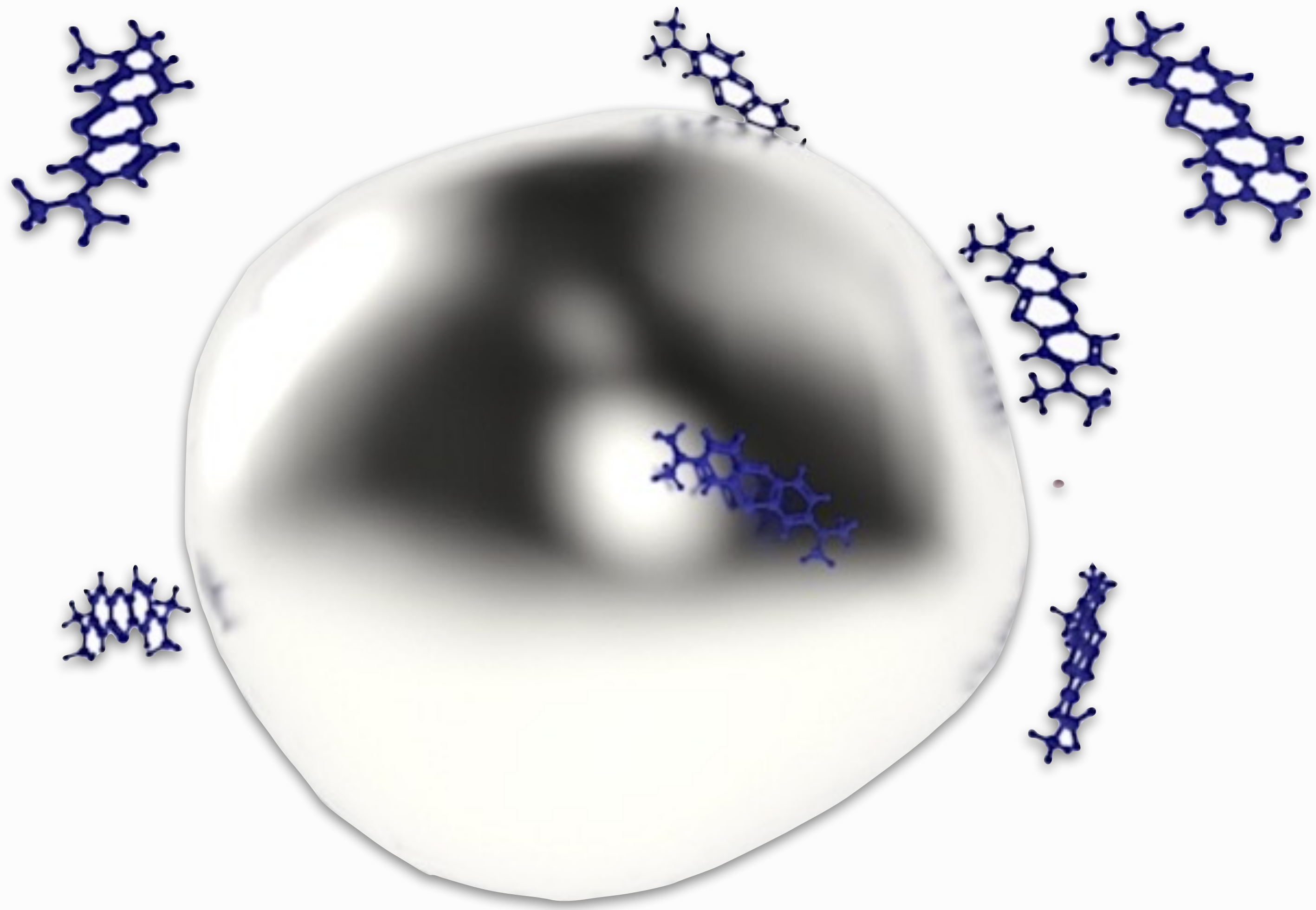


"model"



N=20

MOLECULES NEAR A NANOPARTICLE: COUPLED-DIPOLE MODEL



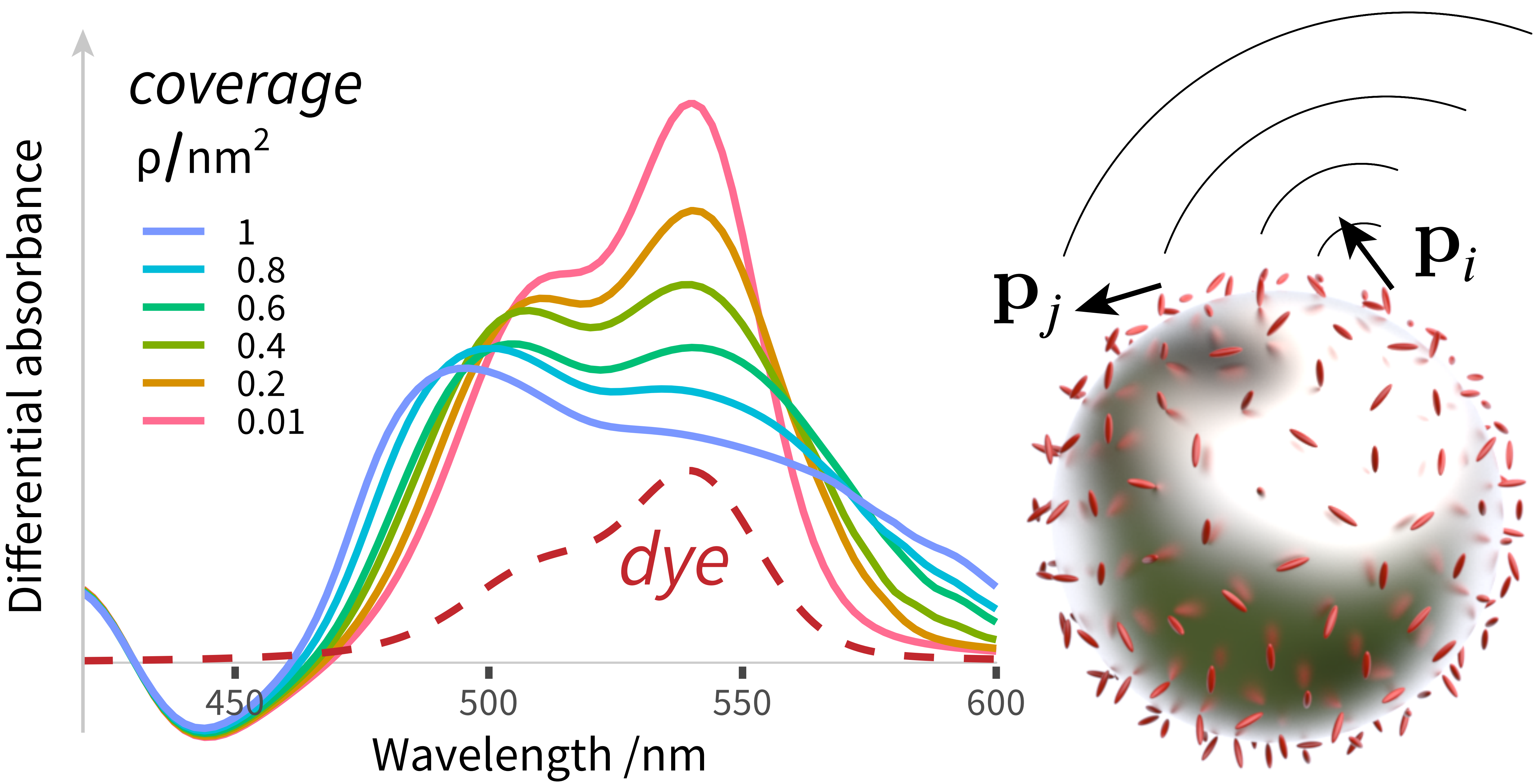
B. Auguié, B. Darby and E. Le Ru · *Nanoscale* 11, 12177-12187 (2019)

C. Tang, B. Auguié and E. Le Ru · *Phys. Rev. B* 103, 085436 (2021)

· *Phys. Rev. A* 104, 033502 (2021)

· *J. Phys. Chem. C*, 126, 24 (2022)

COUPLED DIPOLES AROUND A NANOSPHERE

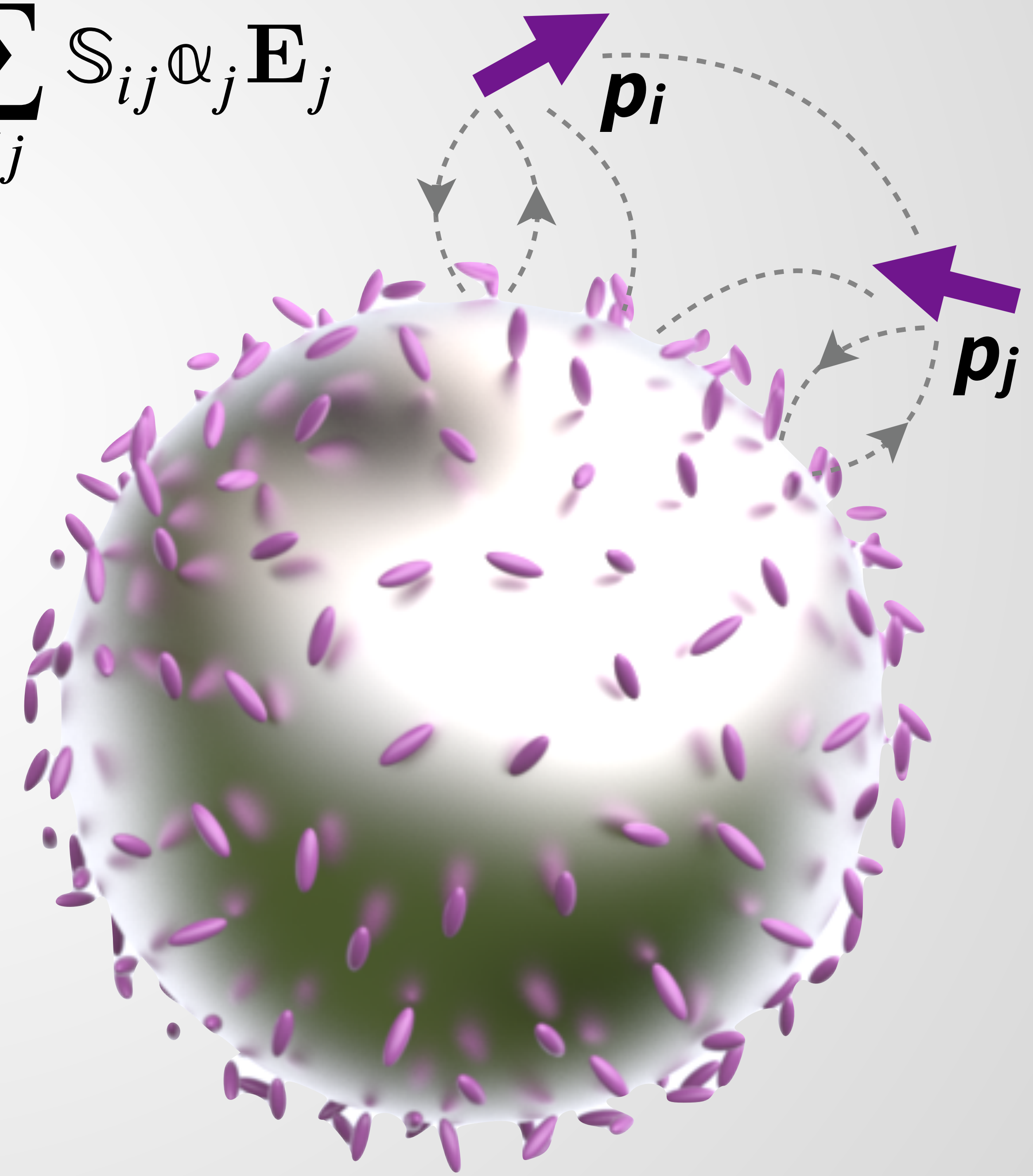


MODIFIED COUPLED-DIPOLE EQUATIONS

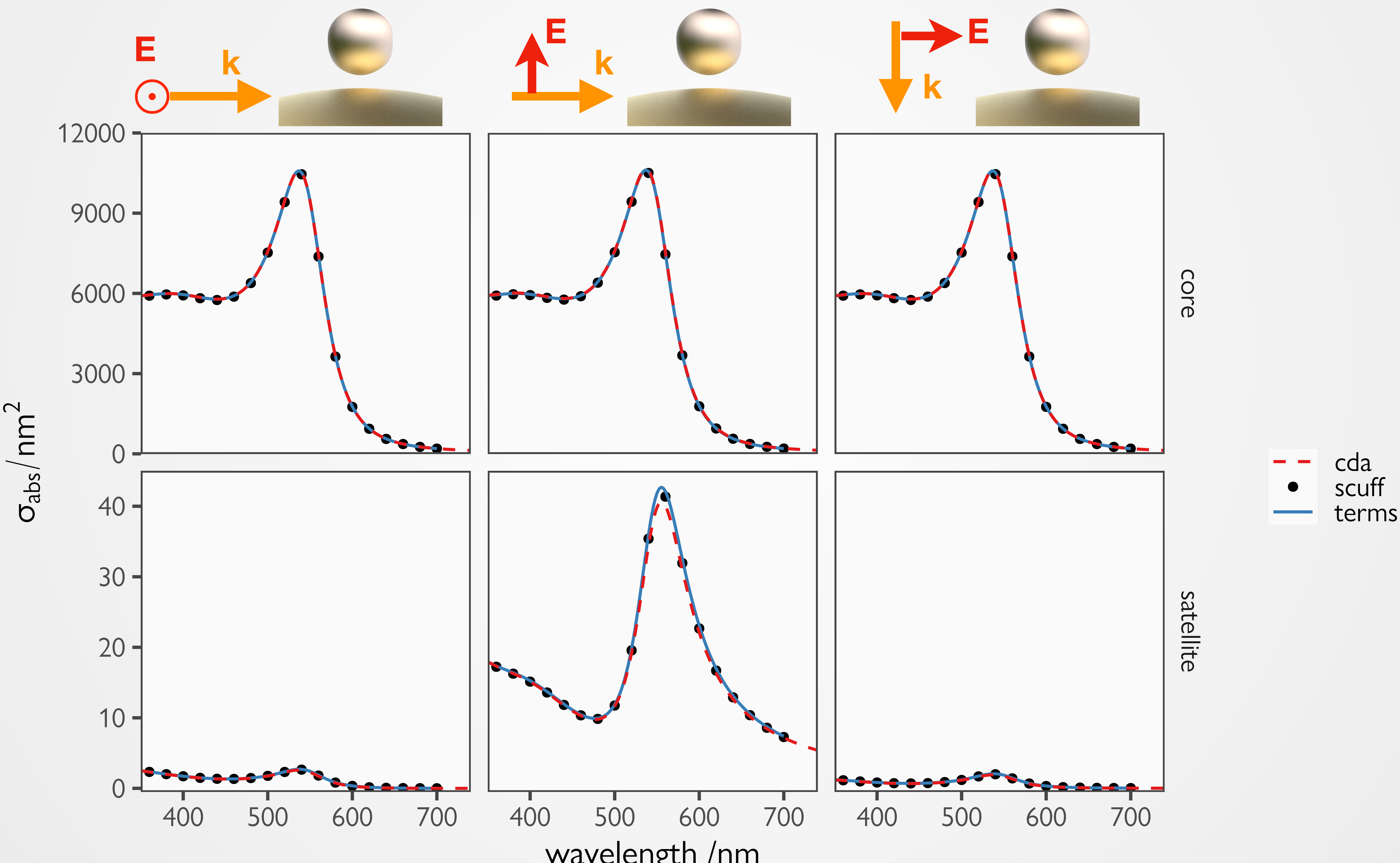
$$\mathbf{E}_i = \mathbf{E}_i^{\mathsf{INC}} + \mathbf{E}_i^{\mathsf{SPH}} + \sum_{j\neq i} \mathbb{G}_{ij}\alpha_j\mathbf{E}_j + \sum_{\forall j} \mathbb{S}_{ij}\alpha_j\mathbf{E}_j$$

$$\mathbb{A}\mathbf{E} = \mathbf{E}^{\mathsf{INC}} + \mathbf{E}^{\mathsf{SPH}}$$

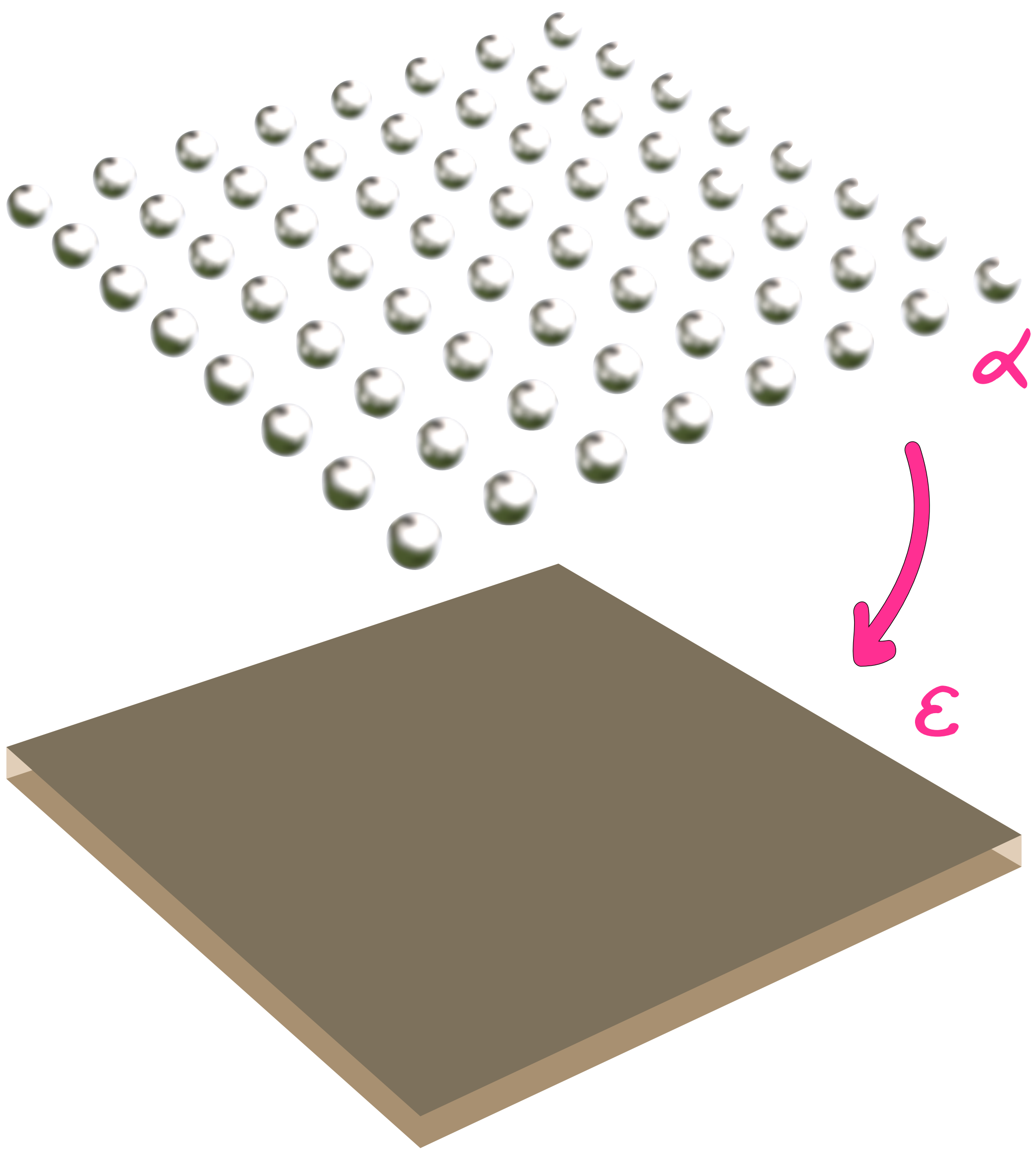
- Sphere-mediated coupling $\boldsymbol{S}_{\mathrm{ij}}$
- Self-reaction (“image” dipole) $\boldsymbol{S}_{\mathrm{ii}}$
- Additional excitation from sphere-scattered field $\boldsymbol{E}^{SPH}$



VALIDATION: FIXED INCIDENCE, SINGLE SATELLITE



MODEL #4: ANISOTROPIC EFFECTIVE MEDIUM



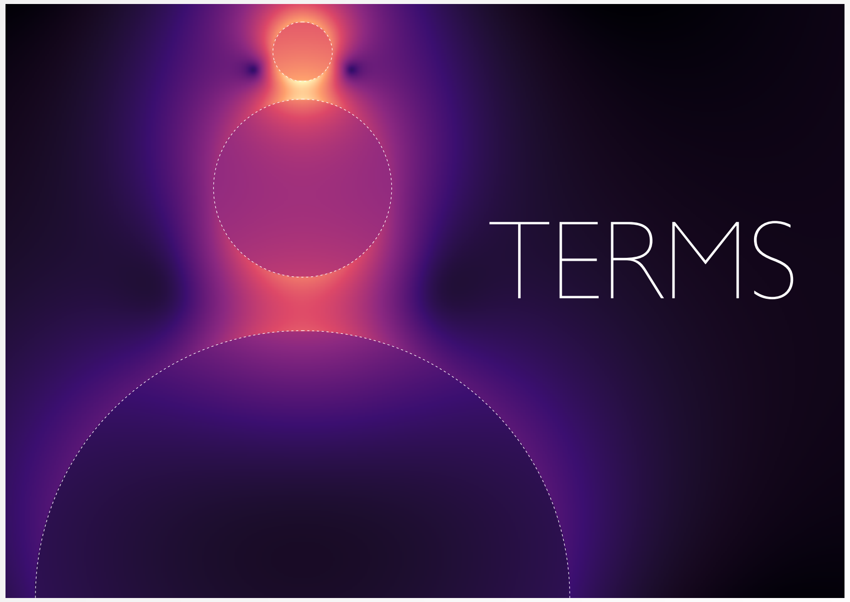
$$\alpha = a^3 \frac{\varepsilon - \varepsilon_m}{\varepsilon + 2\varepsilon_m} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\varepsilon_{xy} = \varepsilon_m + \frac{L_m^2 \frac{c_d \alpha}{\varepsilon_0}}{1 - \frac{\alpha}{8\pi\varepsilon_0} \frac{L_m^2}{\varepsilon_m} \rho^{3/2} (\xi_0 - \beta_m \xi_I)}$$

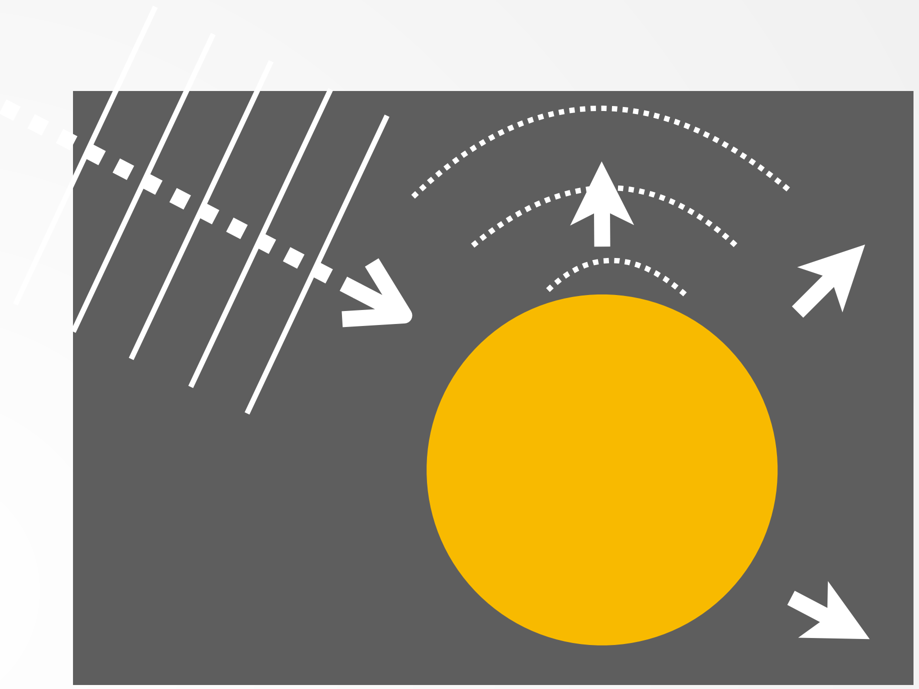
$$\frac{1}{\varepsilon_z} = \frac{1}{\varepsilon_m} - \frac{\frac{L_m^2}{\varepsilon_m^2} \frac{c_d \alpha}{\varepsilon_0}}{1 + \frac{\alpha}{4\pi\varepsilon_0} \frac{L_m^2}{\varepsilon_m} \rho^{3/2} (\xi_0 + \beta_m \xi_I)}$$

C. Tang, B. Auguié and E. Le Ru · *Phys. Rev. B* 103, 085436 (2021)
· *Phys. Rev. A* 104, 033502 (2021)
· *J. Phys. Chem. C*, 126, 24 (2022)

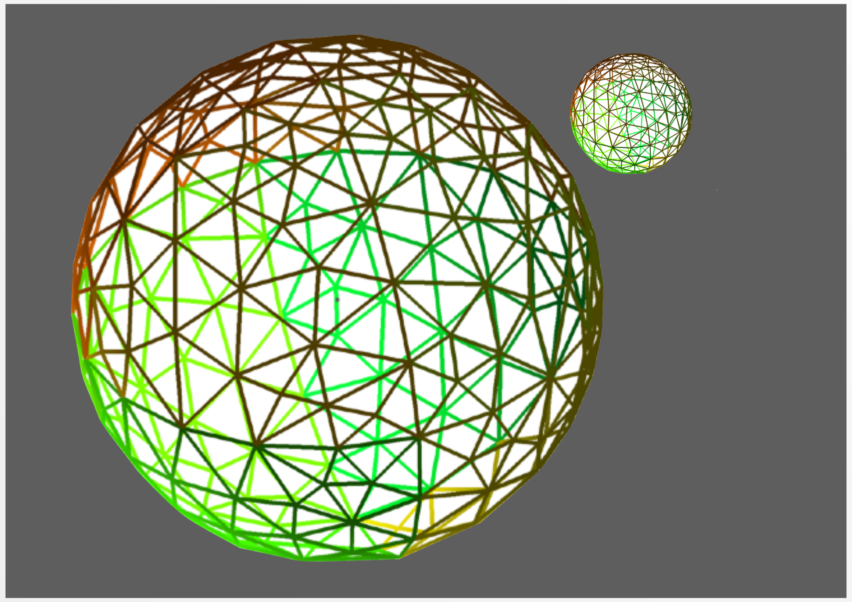
COMPARISON OF SIMULATION METHODS



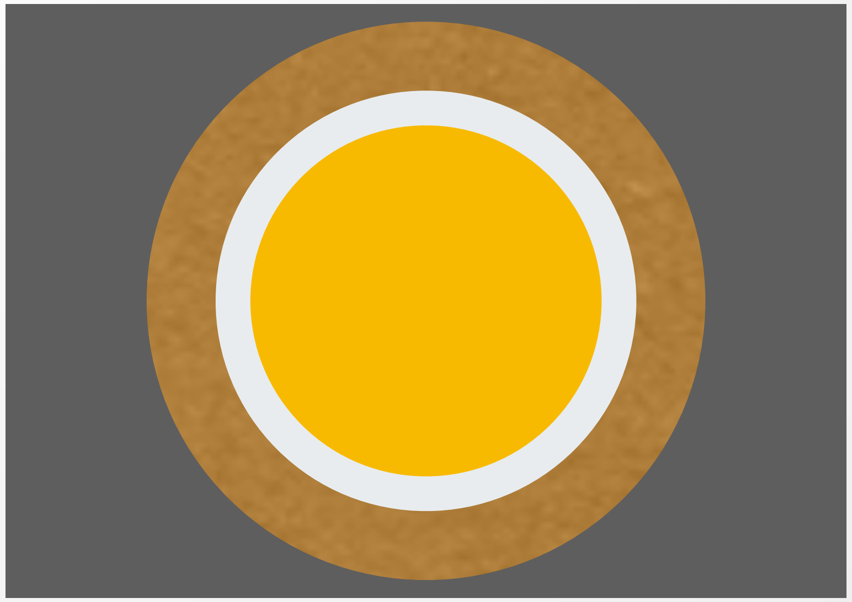
Superposition T-matrix



Generalised coupled-dipole

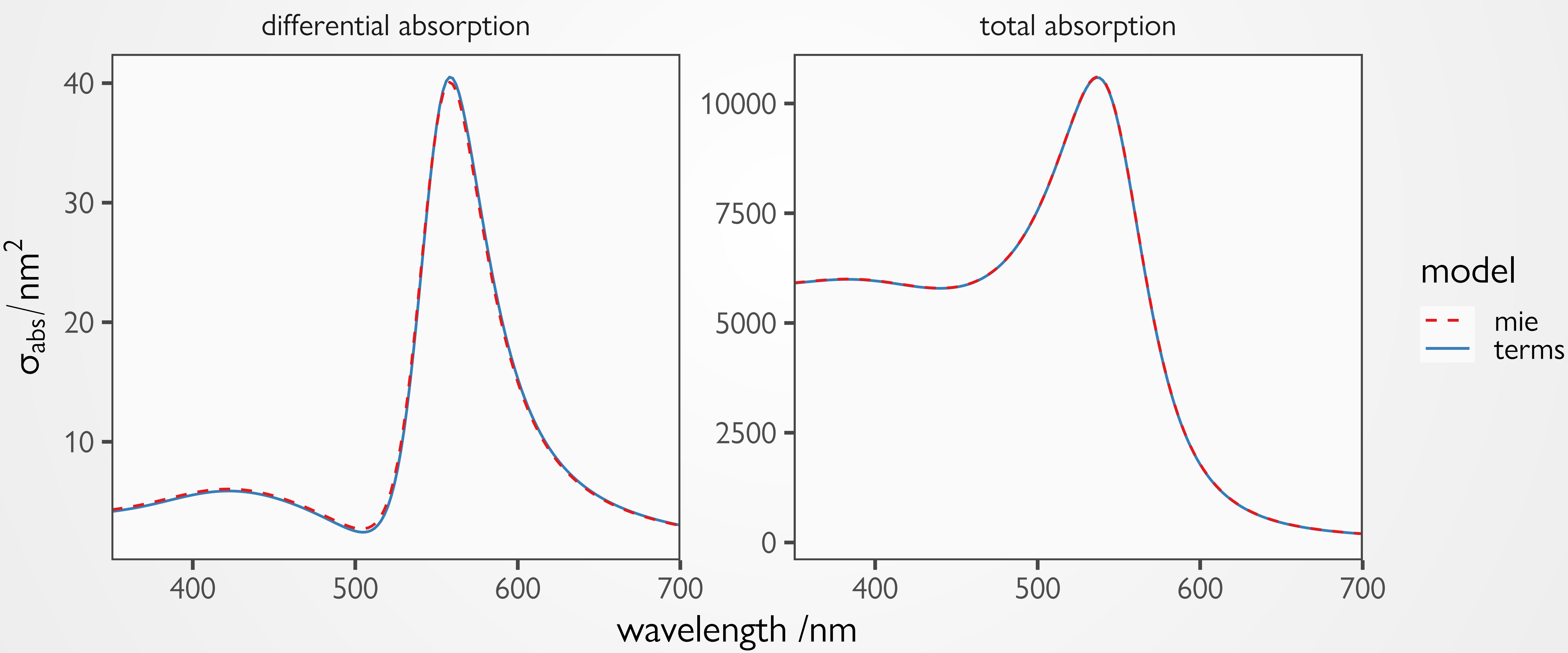


Boundary element method

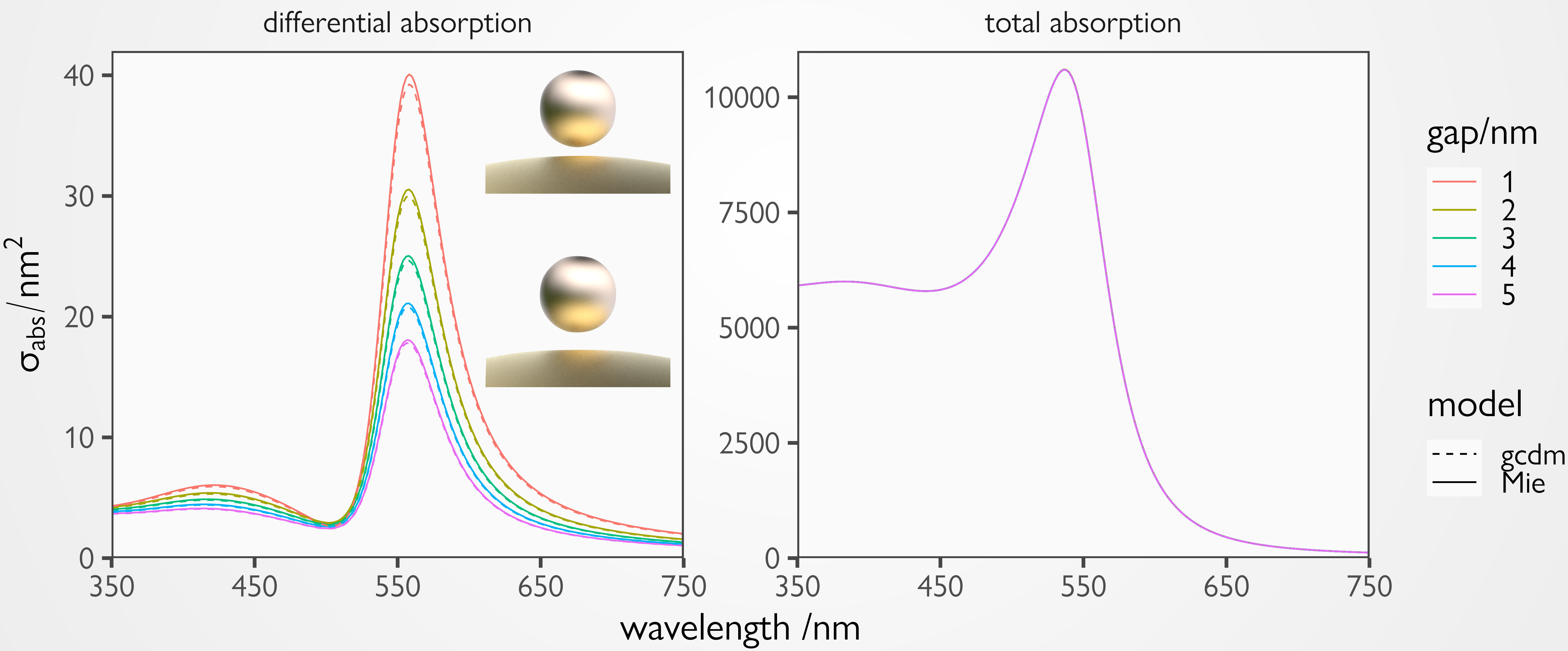


Effective medium + Mie

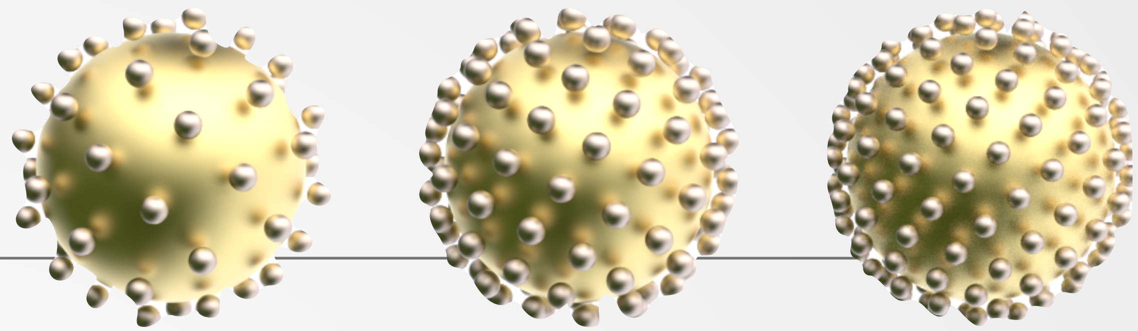
comparison: anisotropic Mie vs TERMS (benchmark)

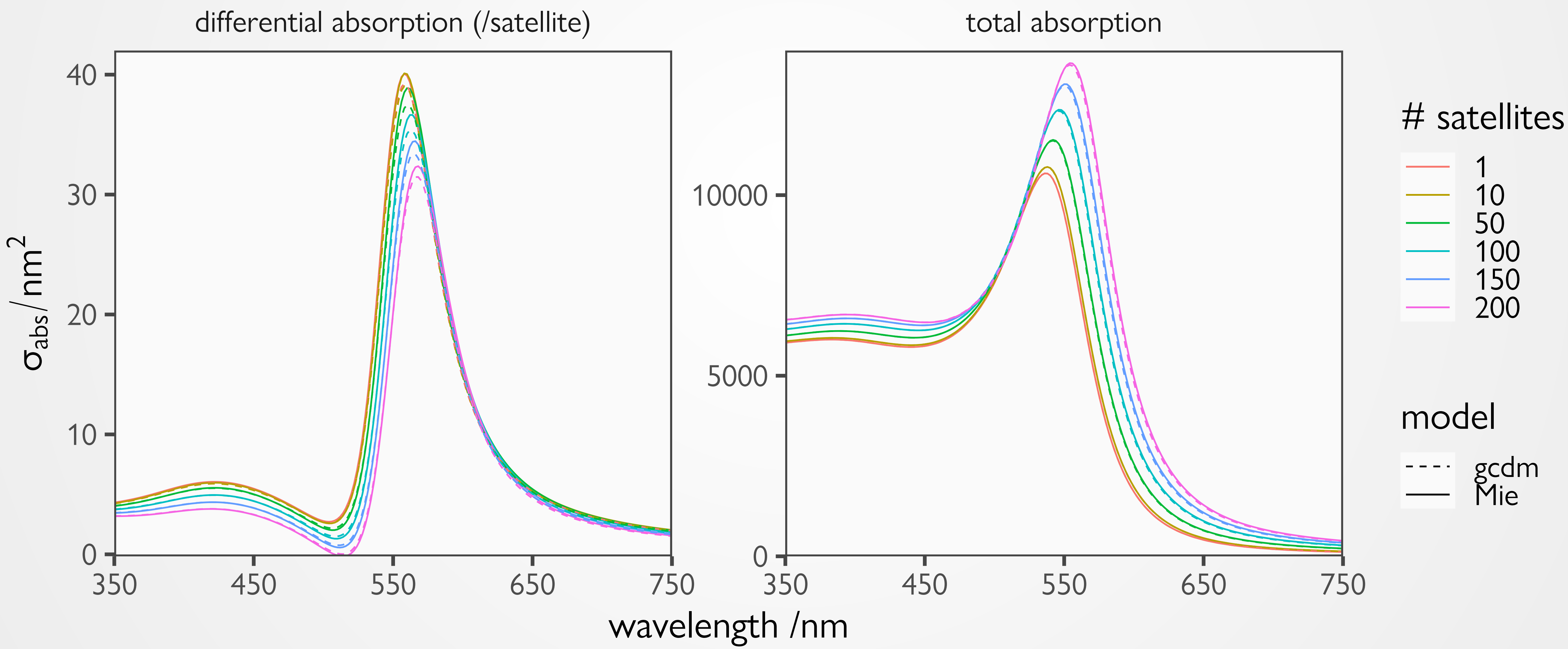


EFFECT OF GAP DISTANCE

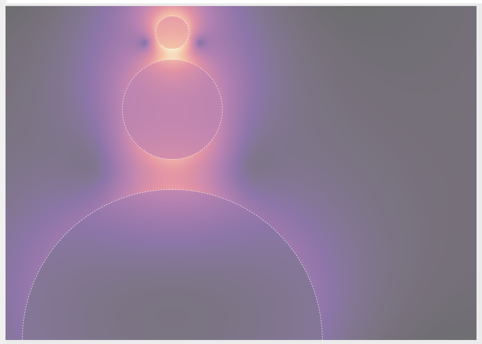
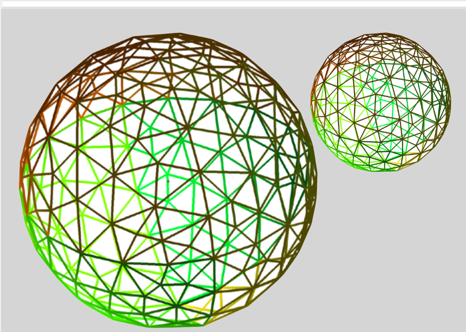
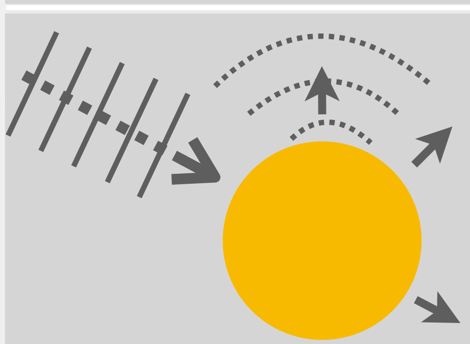
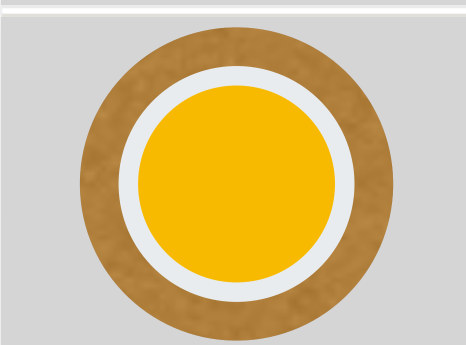


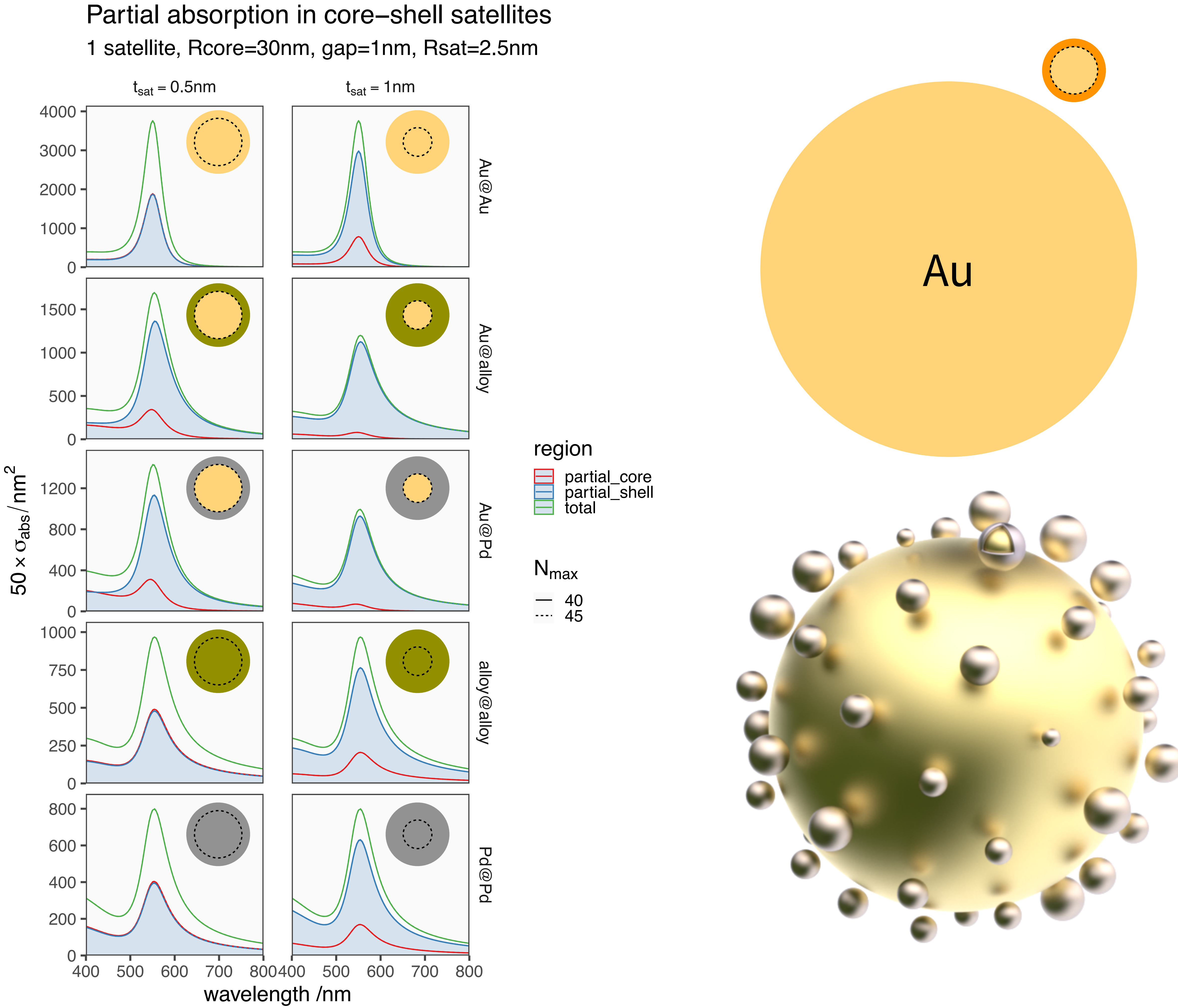
EFFECT OF SATELLITE CONCENTRATION





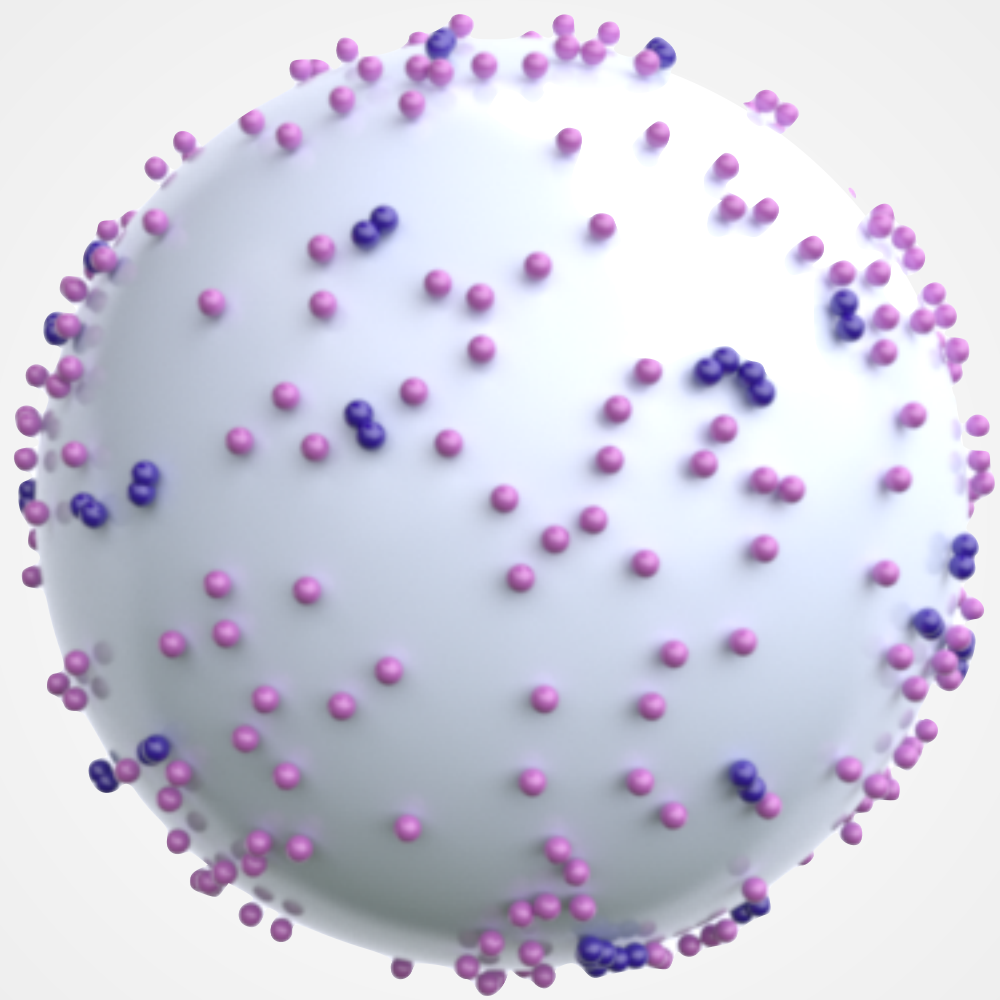
STRENGTHS AND WEAKNESSES 👍👌👎🤞

	METHOD	ACCURACY	TIME	SCALING	DETAILED INFO
	TERMS (T-matrix)	✔	✘	✘	✔
	SCUFF (surface int.)	✔	✘	≈	✔
	GCDM (coupled dip.)	✔	≈	≈	≈
	Mie	≈	✔	✔	✘



Partial absorption in core–shell satellites
1 satellite, Rcore=30nm, gap=1nm, Rsat=2.5nm
t_sat = 0.5nm
t_sat = 1nm
Au@Au
Au@alloy
Au@Pd
alloy@alloy
Pd@Pd
50 × σ_abs / nm²
wavelength /nm
400 500 600 700 800
region
partial_core
partial_shell
total
N_max
40
45
Au

INFERRING DIMERS FROM ABSORPTION SPECTRA



Interface-Dependent Selectivity in Plasmon-Driven Chemical Reactions – A. Stefancu, J. Gargiulo, G. Laufersky, B. Auguié, V. Chiş, E. Le Ru, M. Liu, N. Leopold and E. Cortés · *ACS Nano* just accepted (2023)