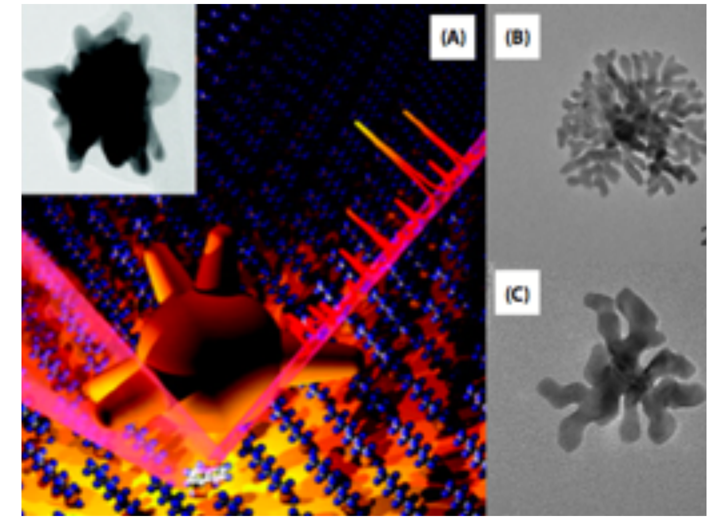
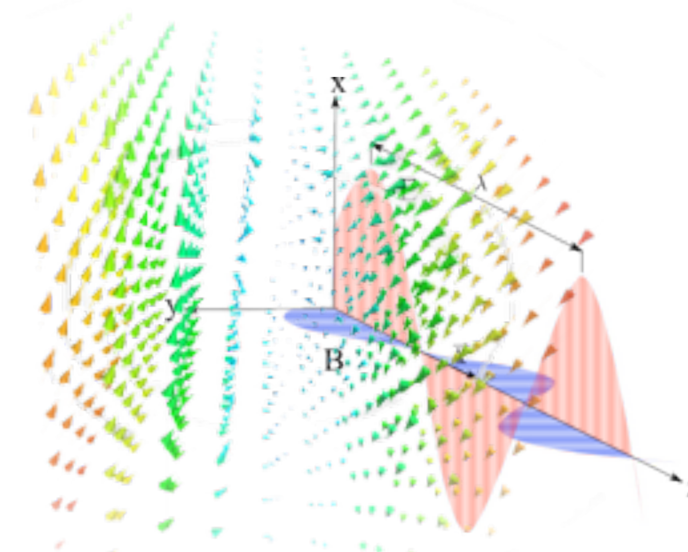
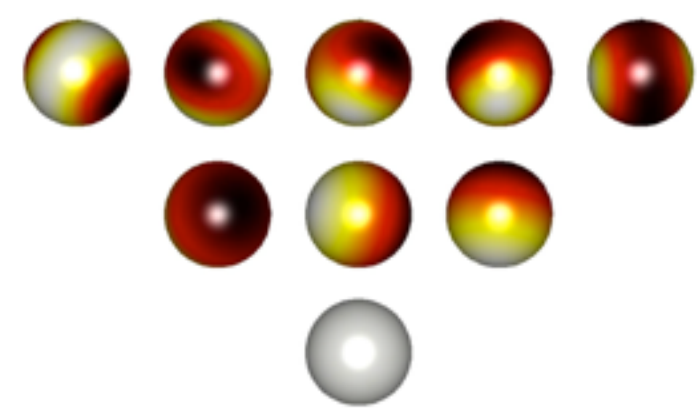
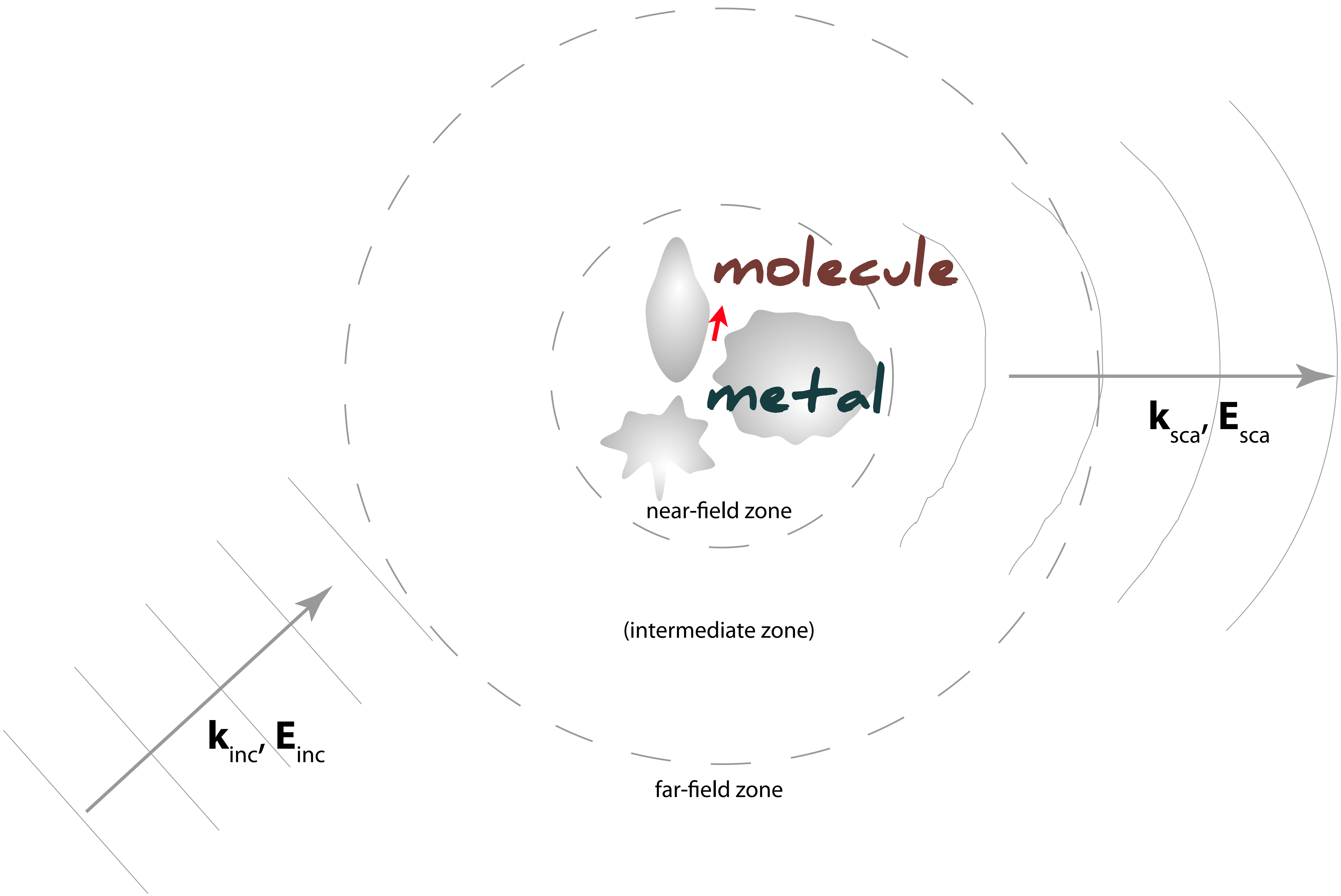





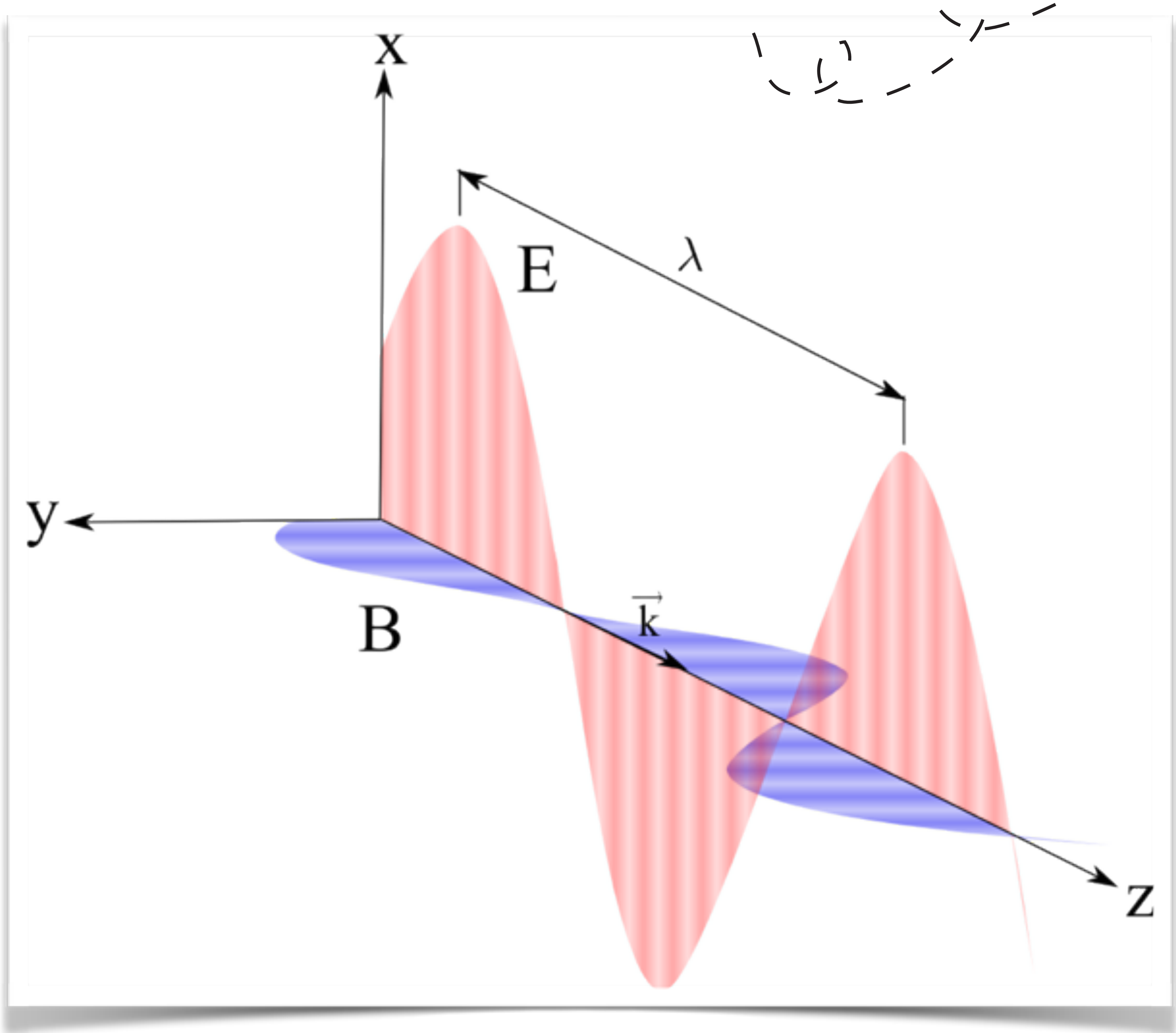


Modelling the scattering of light

Near field, far-field, and reciprocity



A plane wave



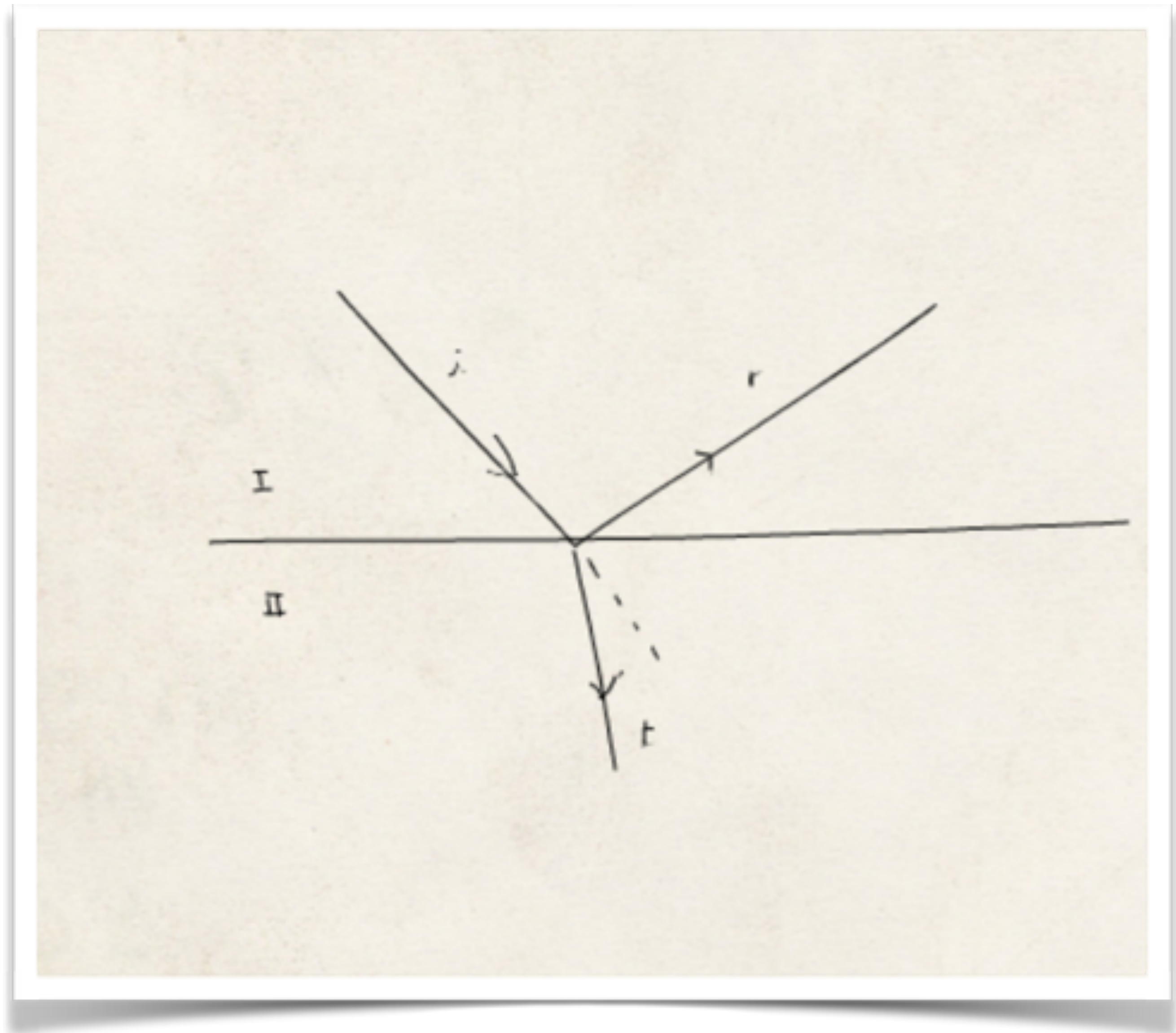
Why is it so hard? – a *conspiracy* theory

- Example: geometrical optics

- **Ewald-Oseen extinction theorem**

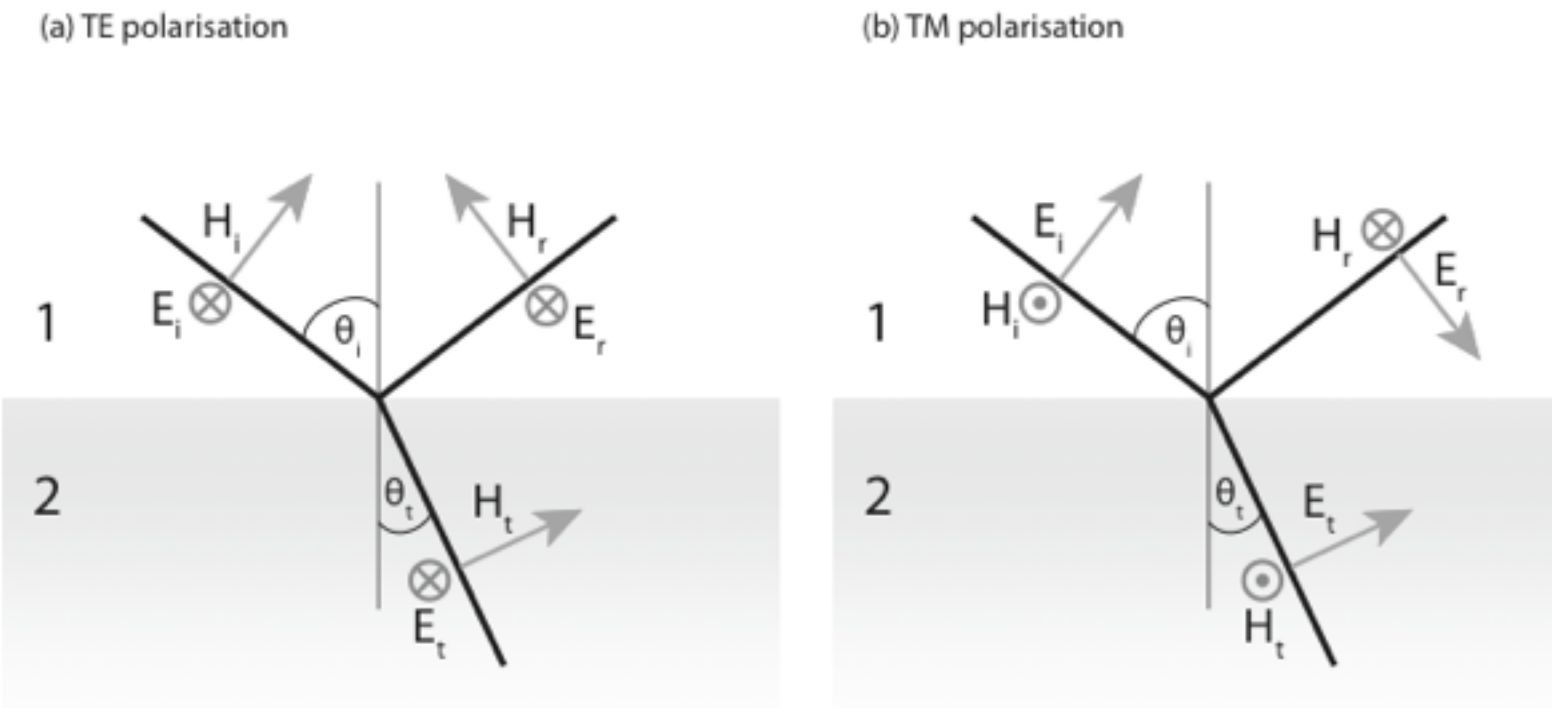
  All atoms conspire to
  - extinguish the incident ray
  - create a reflected wave
  - create a refracted wave

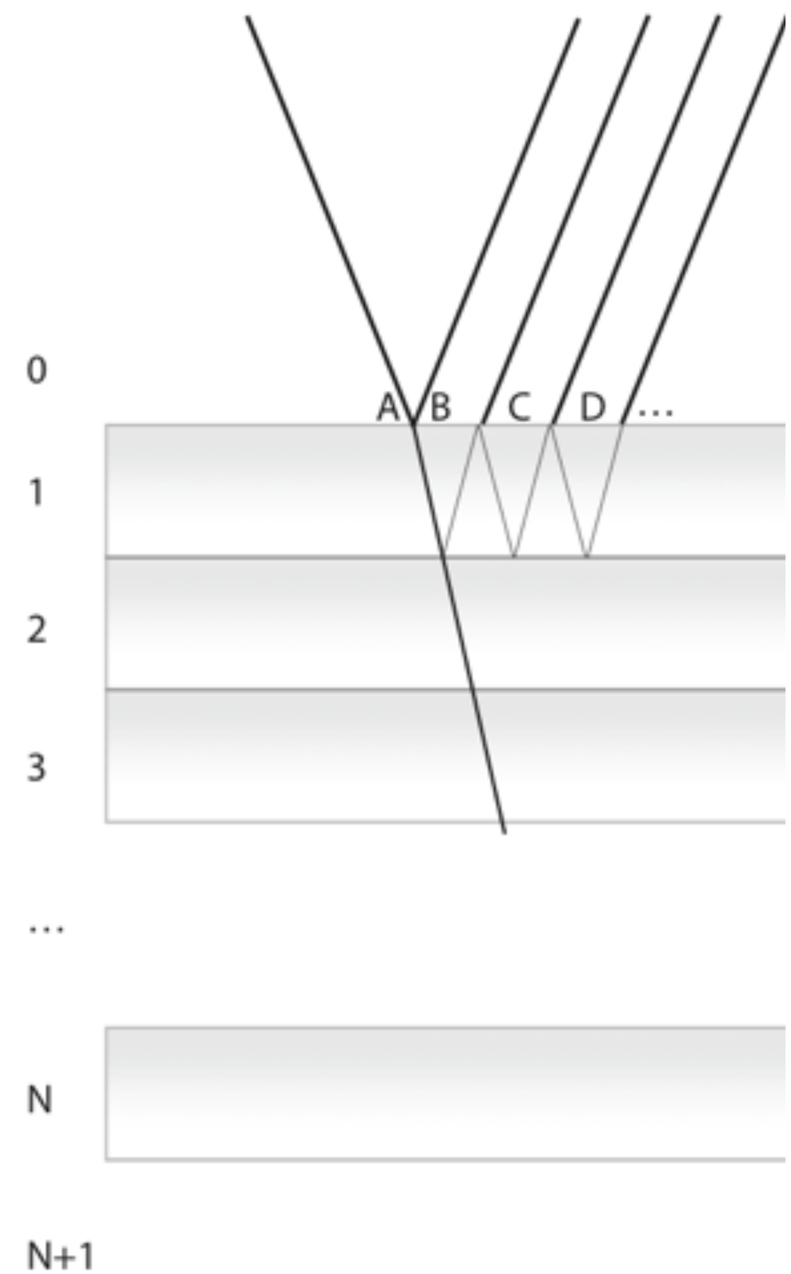
- Now, consider a curved particle with *arbitrary shape*



Pattanayak and Wolf, Opt. Com. 6 (1972)

Example: multilayers





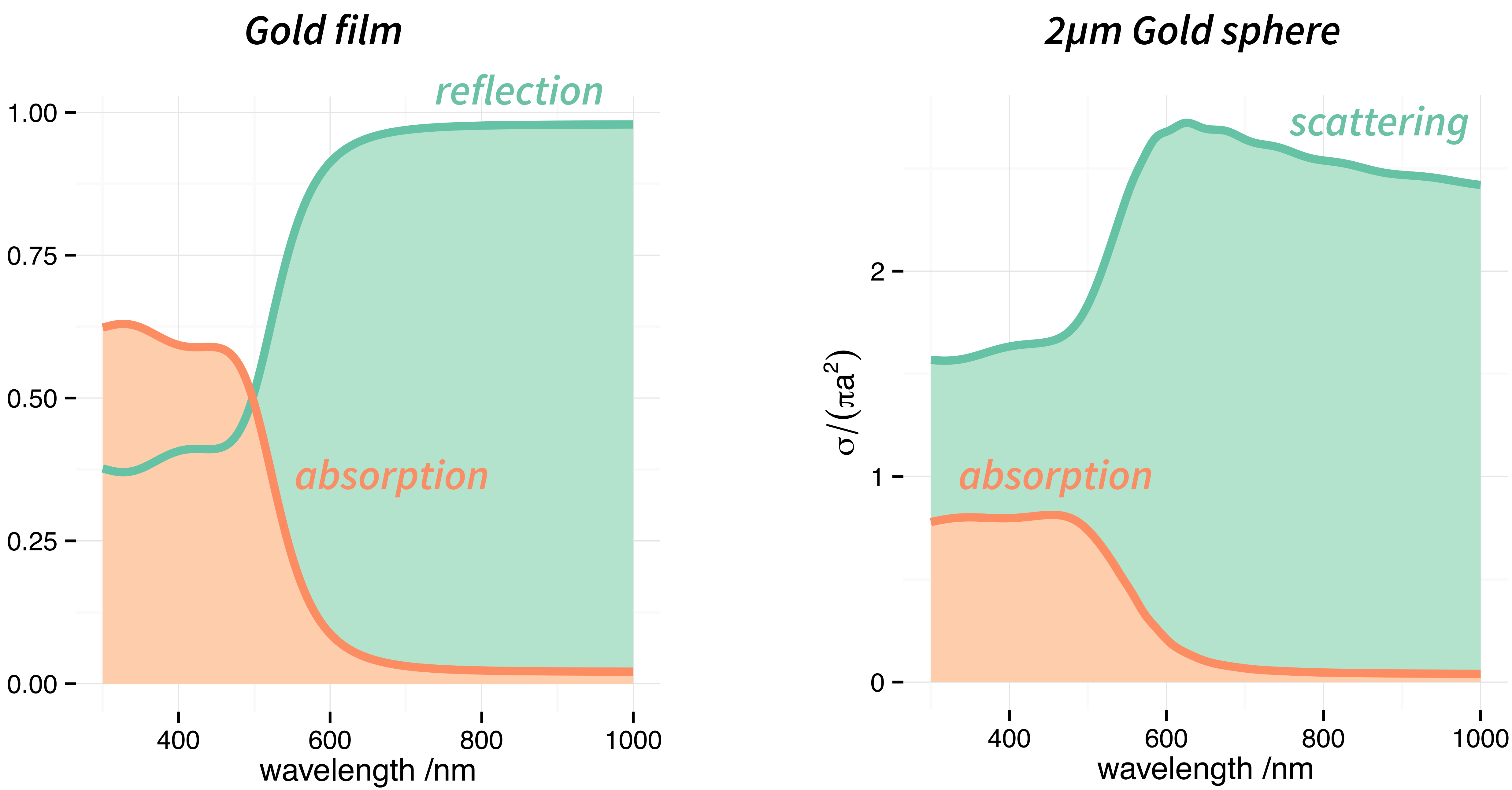
$$r_{\text{slab}} A = B + C + D + \dots$$
$$= \left[r_{01} + t_{10} t_{01} r_{12} \sum_{j=0}^{\infty} r_{12}^{j} r_{10}^{j} \exp(2jik_{z1}d) \right] A$$

$$r_{\text{slab}} = \frac{r_{01} + r_{12}\exp(2ik_{z1}d)}{1 + r_{01} r_{12} \exp(2ik_{z1}d)}$$

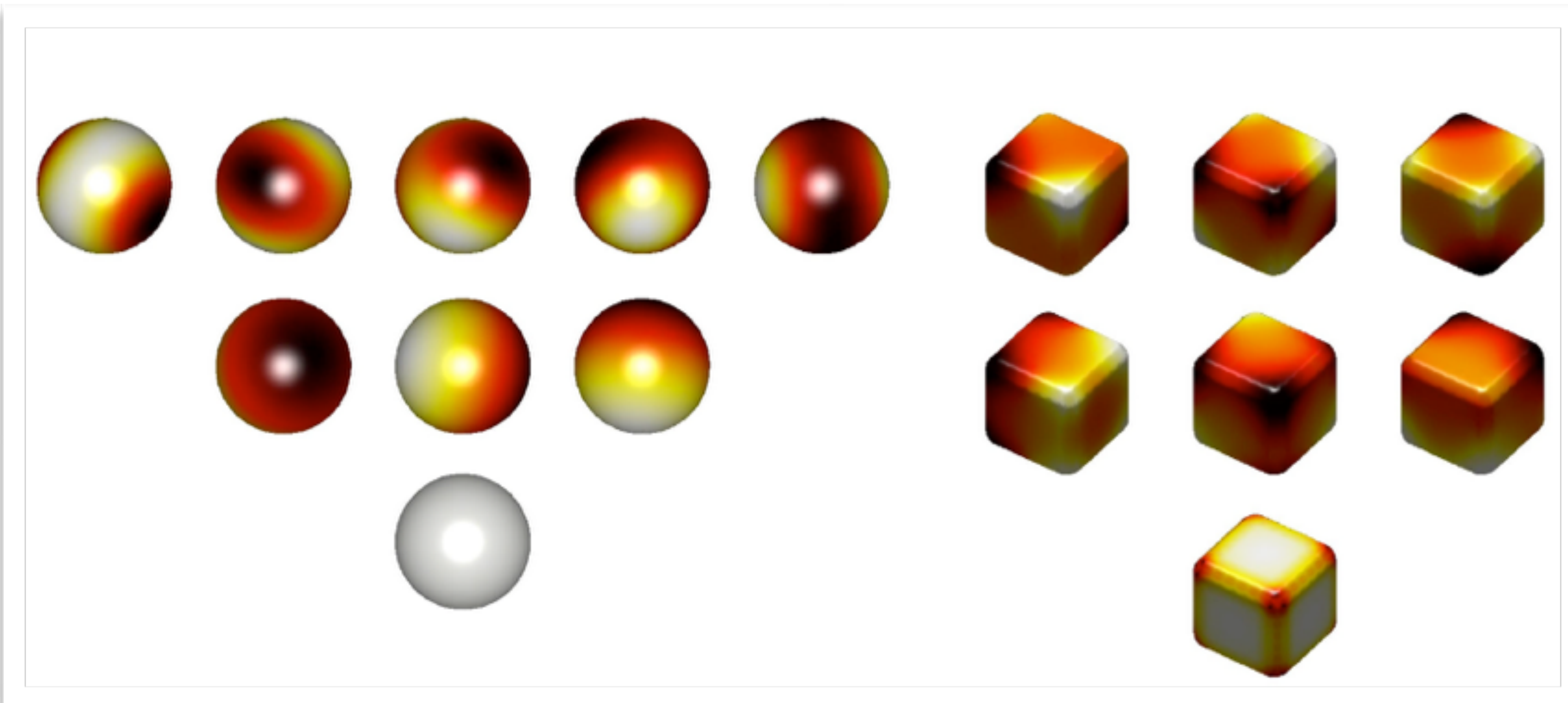
Things *we* ignore

- anisotropic, magnetic, chiral, non-local, charged particles
- lossy incident medium
- transient response
- non-linear response, gain
- inhomogeneous particles, deformations, ...
- people telling us to attempt the above

Metals, from bulk to nanoparticles

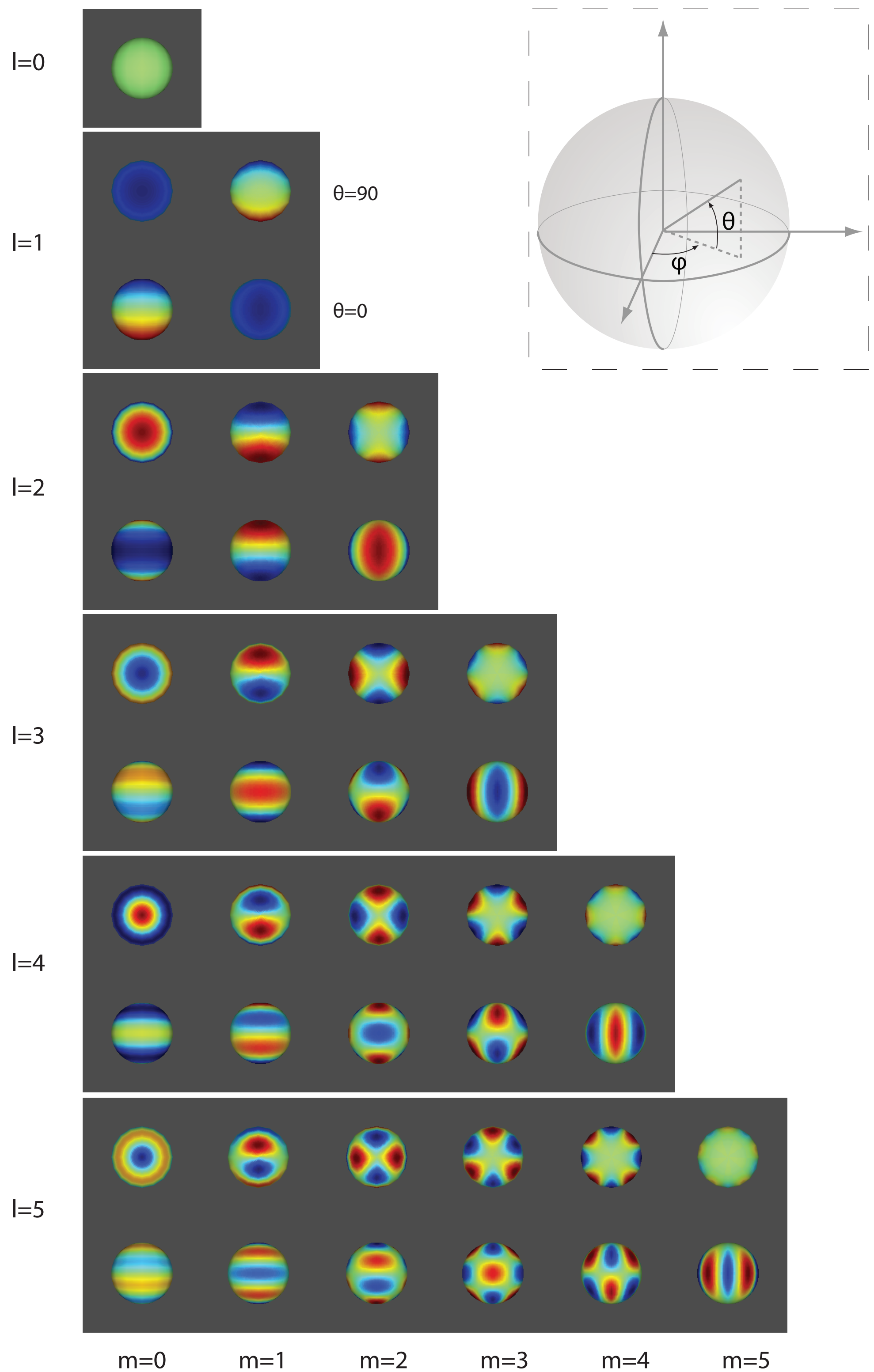


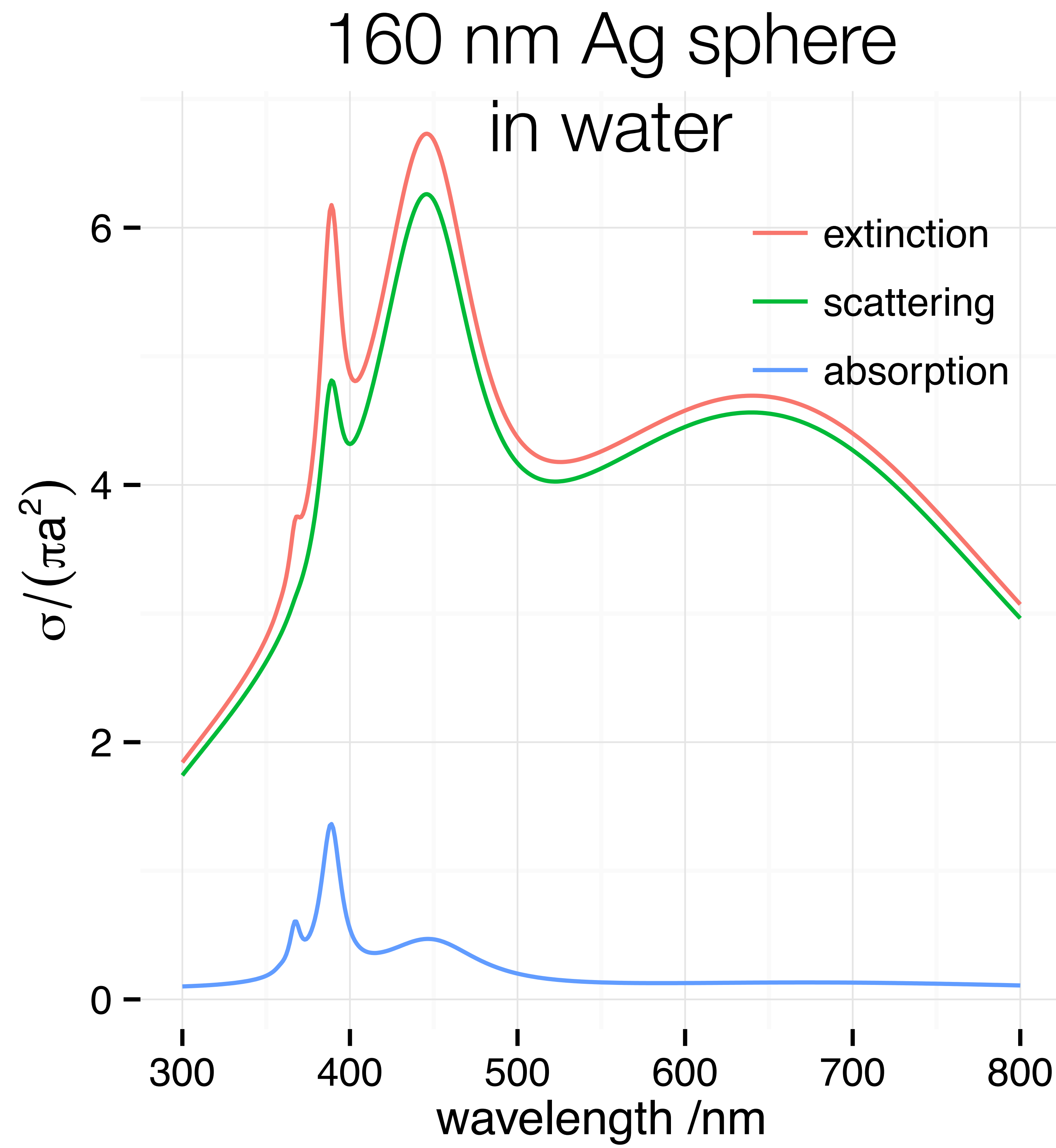
Localised surface-plasmons: nanoparticles



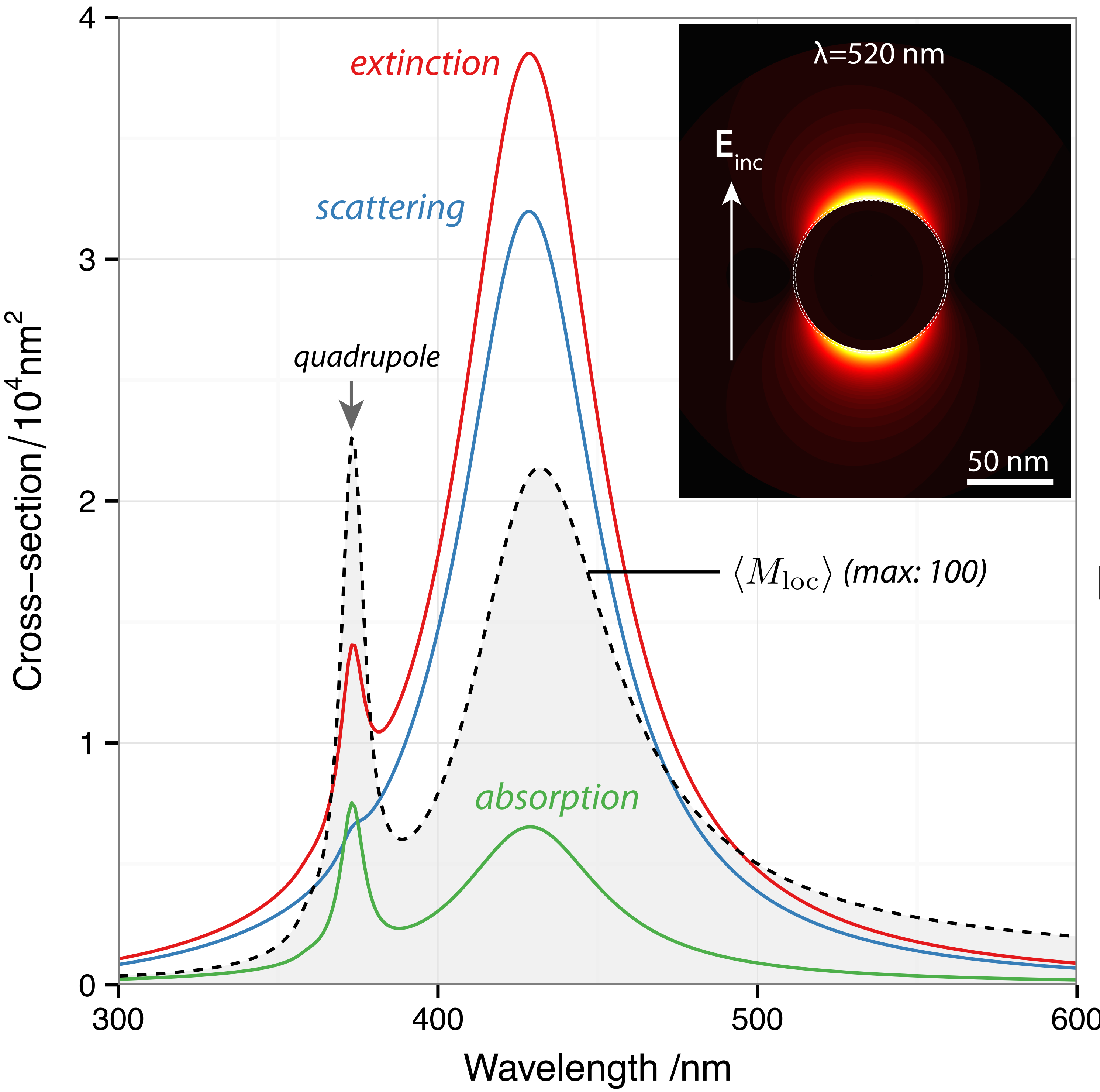
collective oscillations of the conduction electrons constrained by the particle geometry

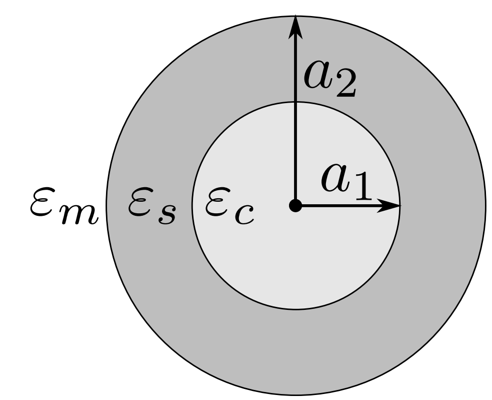
Spherical harmonics, Mie theory





Mie theory





$$\mathbf{E}_{\text{Inc}} = E_0 \sum_{l,m} a_{lm}\mathbf{M}^{(1)}_{lm}(k\mathbf{r}) + b_{lm}\mathbf{N}^{(1)}_{lm}(k\mathbf{r})$$

$$\mathbf{E}_{\text{Sca}} = E_0 \sum_{l,m} c_{lm}\mathbf{M}^{(3)}_{lm}(k\mathbf{r}) + d_{lm}\mathbf{N}^{(3)}_{lm}(k\mathbf{r})$$

$$c_l = \frac{s\psi_l(x)\psi_l'(sx) - \psi_l(sx)\psi_l'(x)}{\psi_l(sx)\xi_l'(x) - s\psi_l'(sx)\xi_l'(x)}a_l$$

$$d_l = \frac{\psi_l(x)\psi_l'(sx) - s\psi_l(sx)\psi_l'(x)}{s\psi_l(sx)\xi_l'(x) - \psi_l'(sx)\xi_l'(x)}b_l$$

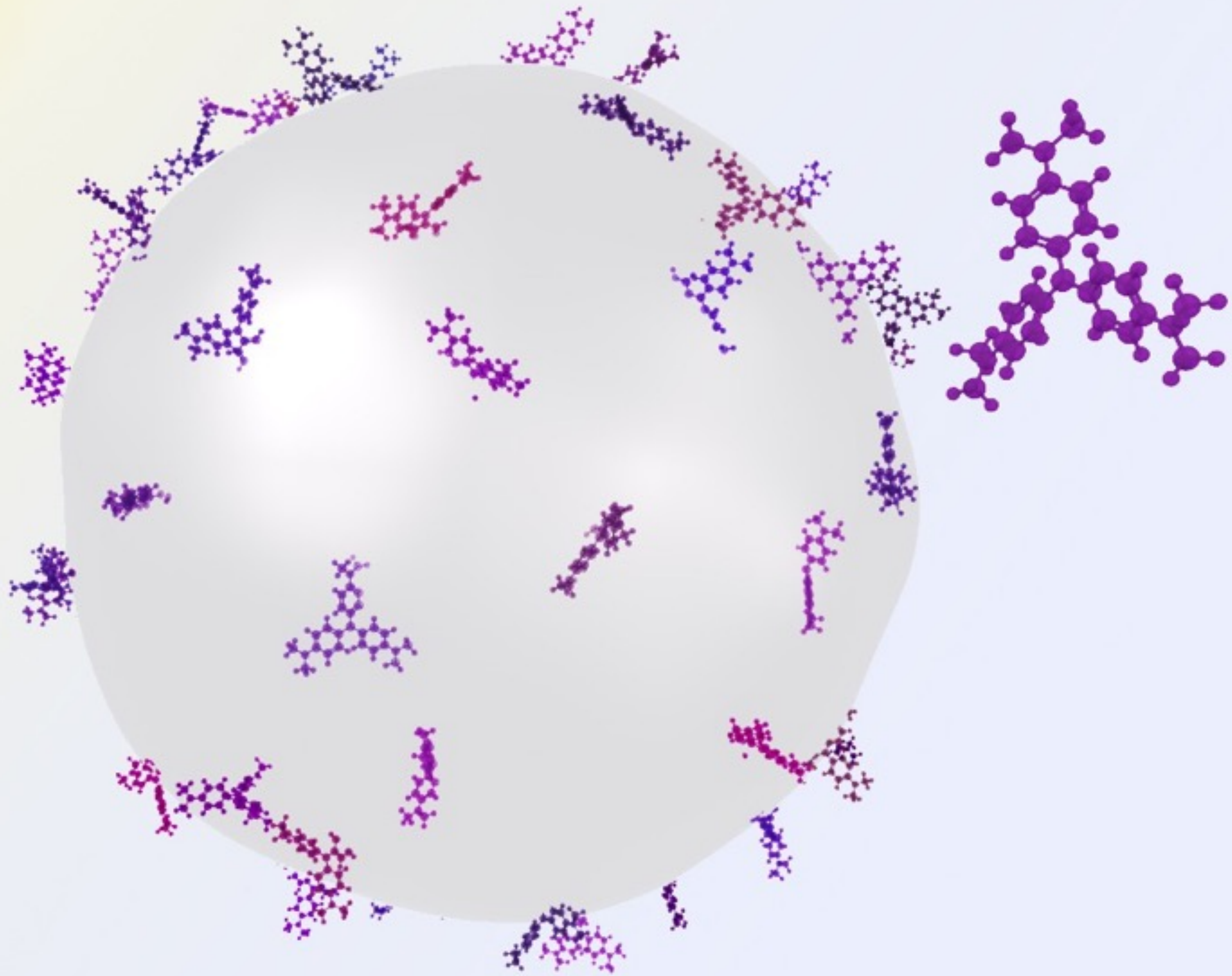
From there...

- Finite differences (time domain)
- Finite elements
- Boundary elements
- **T-matrix**
- Mie theory
- Periodic structures, ...
- Approximations, ...

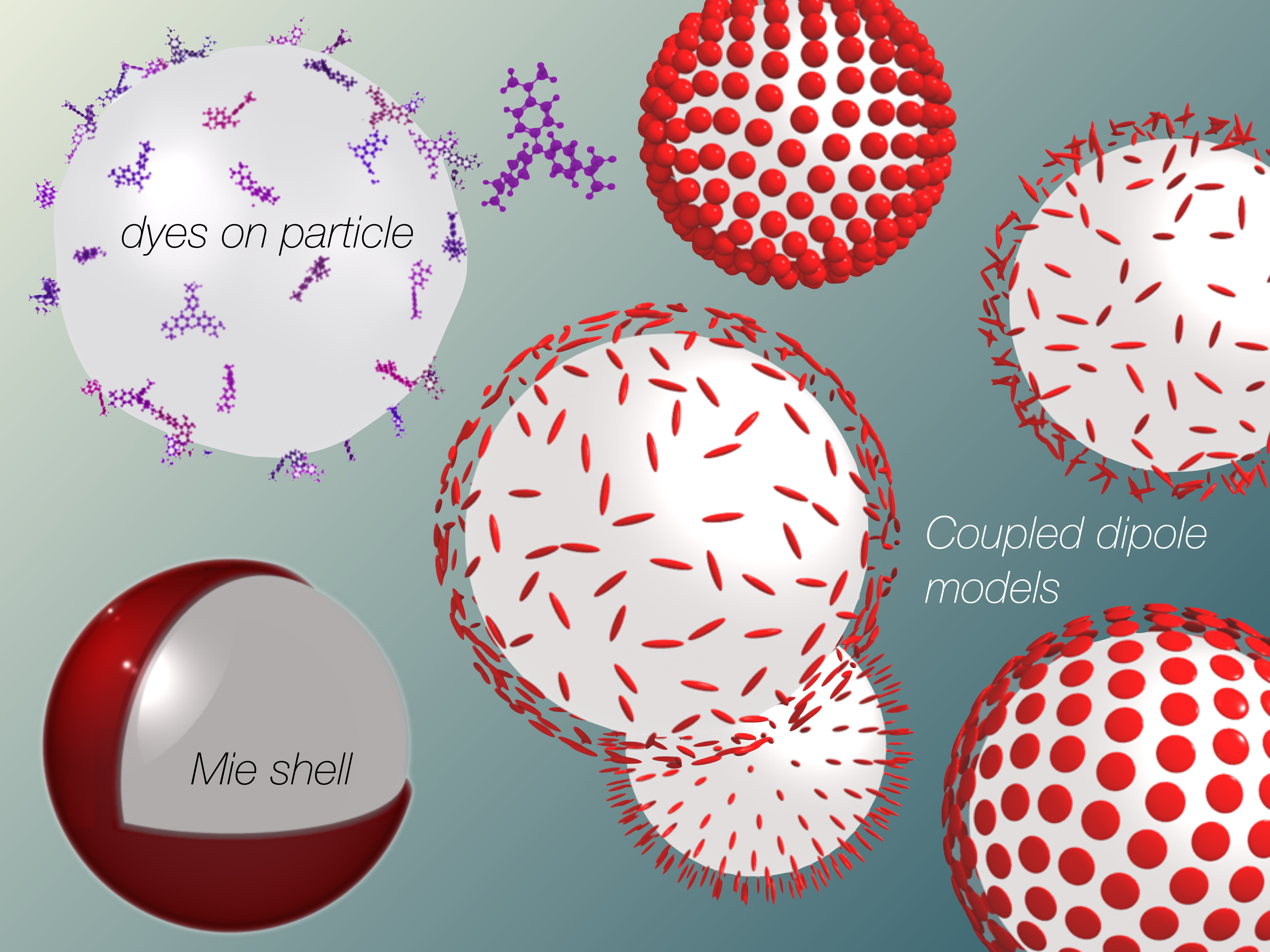
Numerical

Analytical

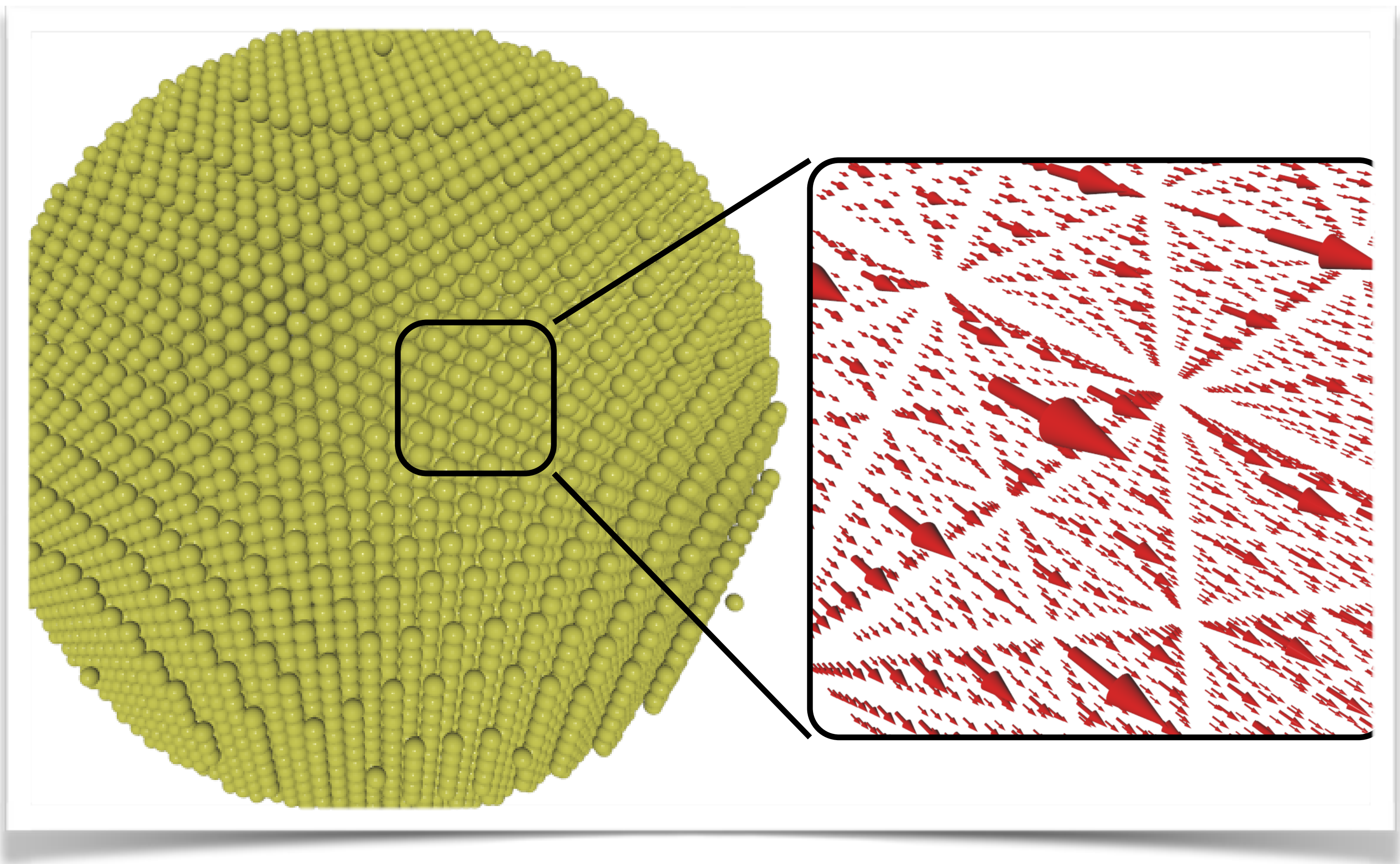
M. Mishchenko, *Scattering, Absorption, and Emission of Light by Small Particles,* Cambridge (2002)
M. Kahnert, *Numerical methods in electromagnetic scattering theory*, JQSRT **79** (2003)



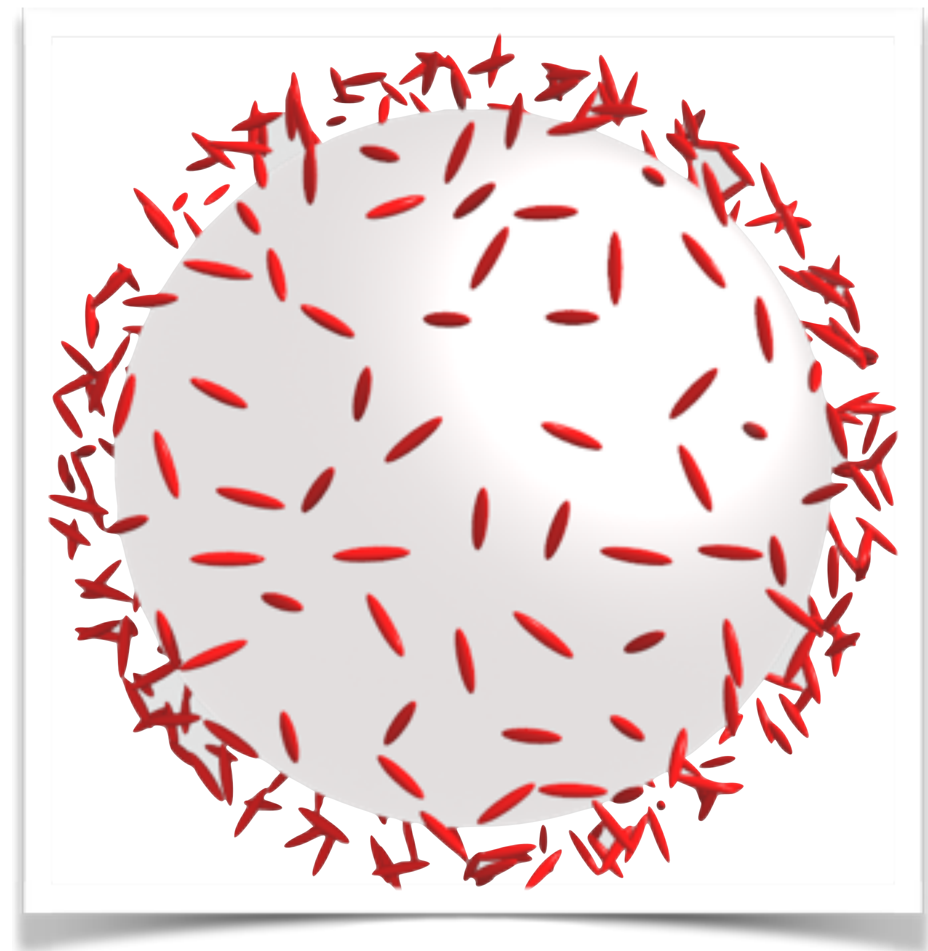
Dipole-dipole coupling & plasmonics


dyes on particle
Coupled dipole
models
Mie shell

Terminology



Discrete-Dipole Approx.



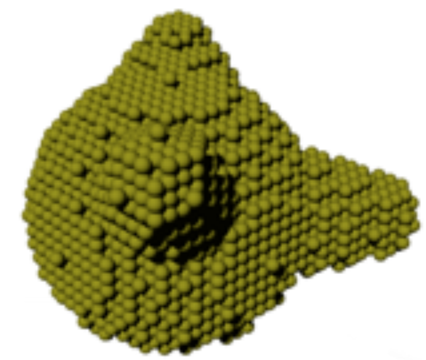
Coupled-Dipole Approx.

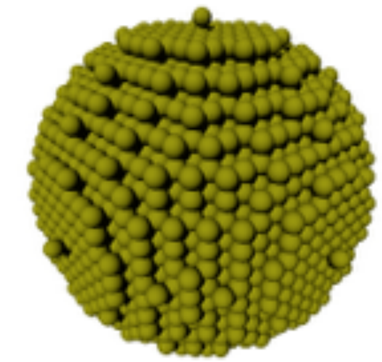
(and a sphere)

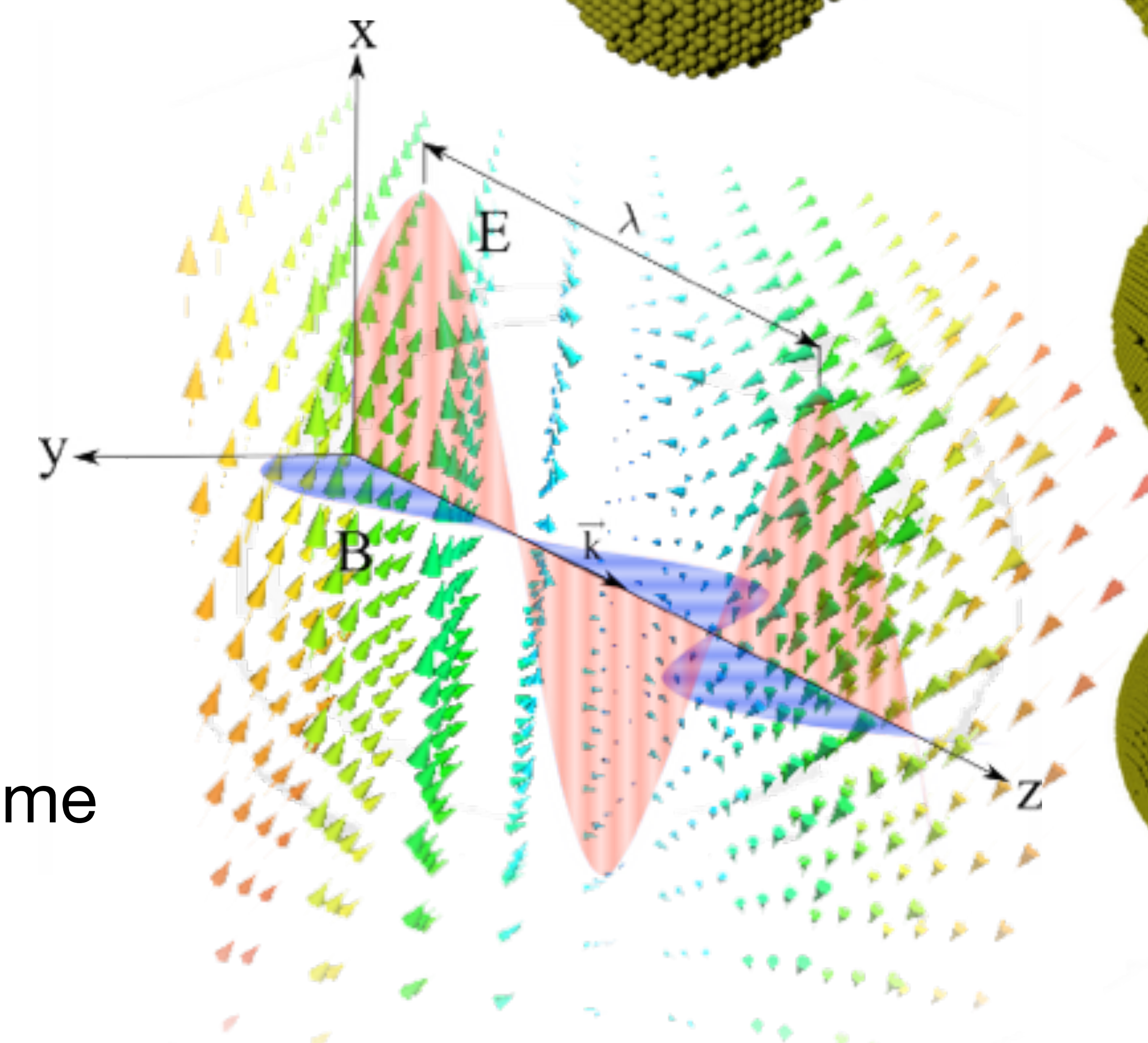
The Discrete-Dipole Approximation

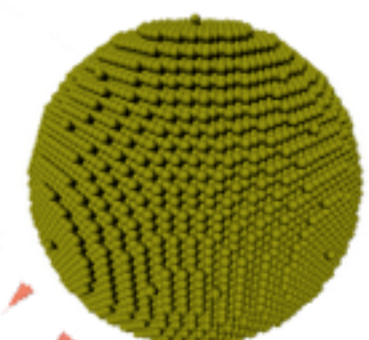
… as a phenomenological approach to scattering

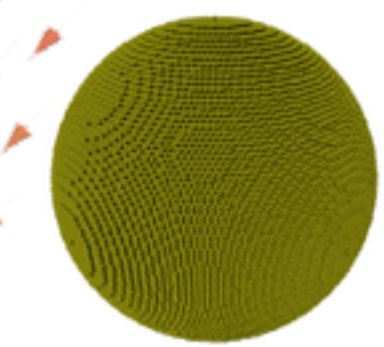
- Microscopic Maxwell equations (in a vacuum)
- Point dipoles
- Retardation (phase)
- $a \ll \lambda$: Rayleigh regime
  $a \sim \lambda$: resonance (Mie) regime



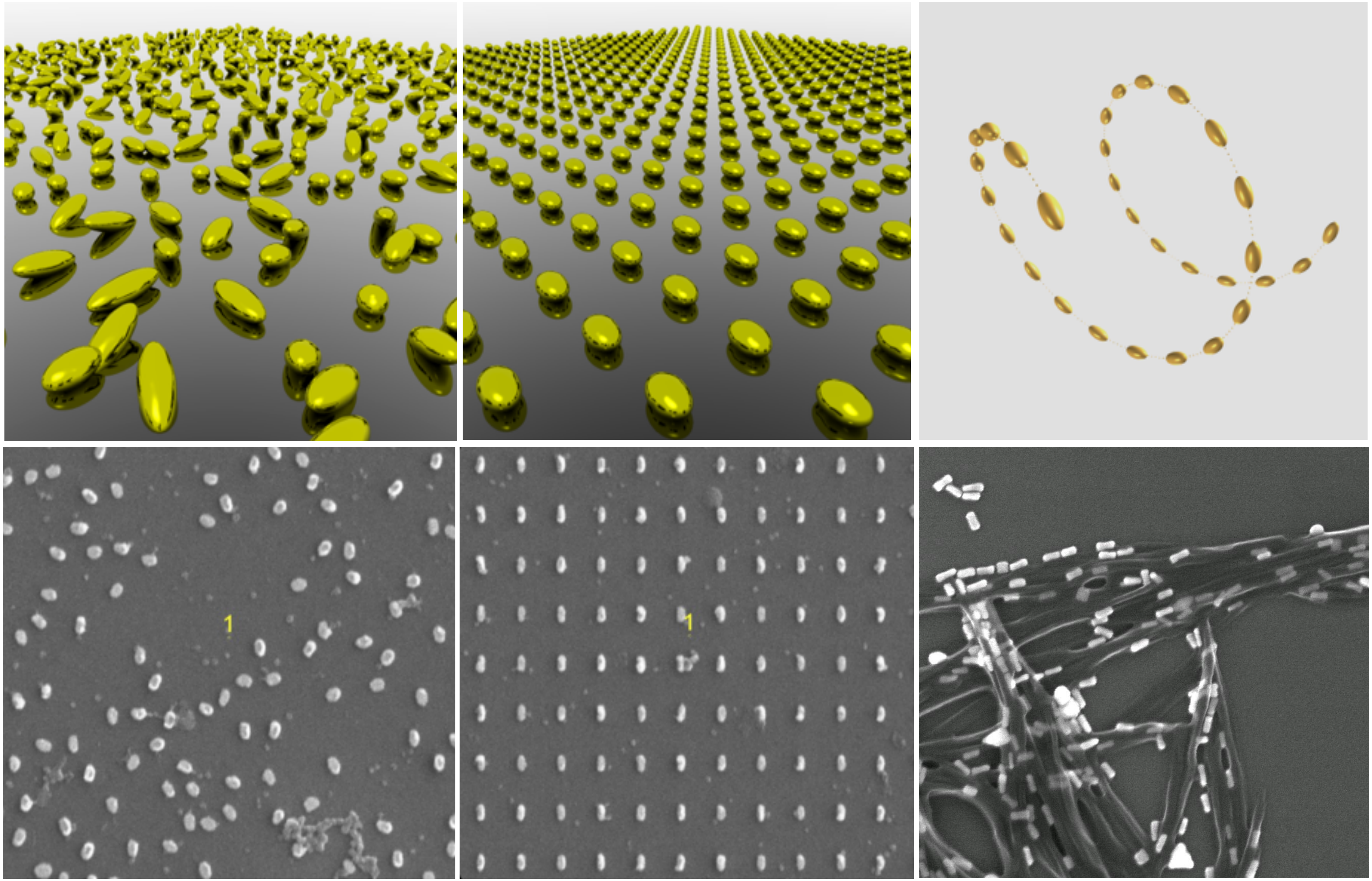








Other plasmonic applications

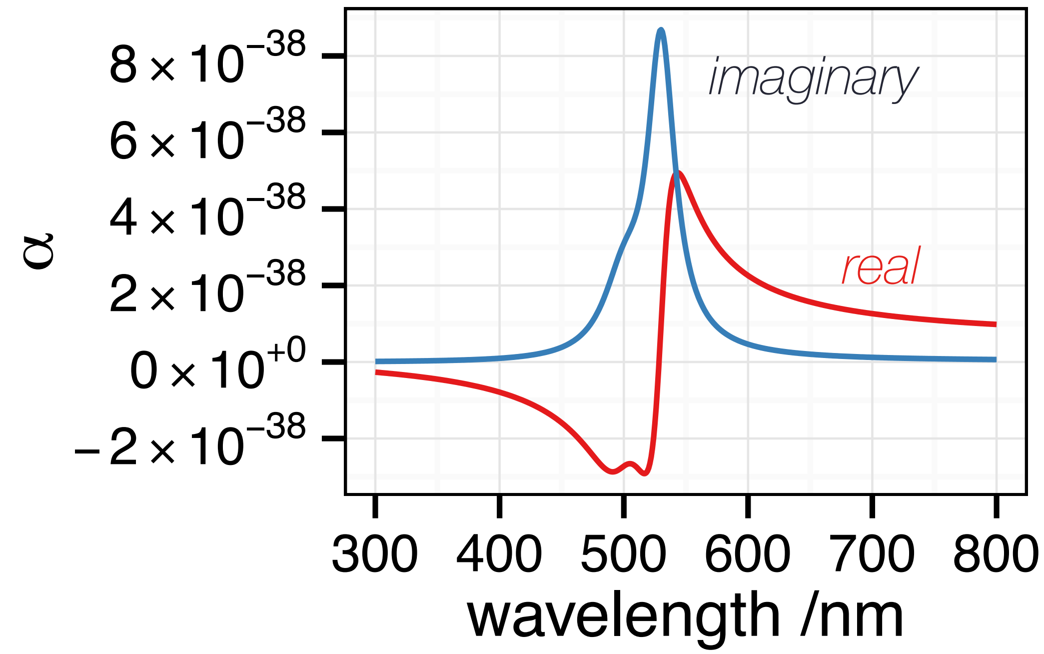


Shell model: effective medium

Bare dye in water

$$\sigma_{\text{abs}}(\omega) = \frac{(\epsilon_M + 2)^2}{9\sqrt{\epsilon_M}} \frac{\omega}{\varepsilon_0 c} \text{Im}\left[\alpha_D(\omega)\right]$$

$$\alpha(\lambda) = \alpha_{\text{static}} + \sum_{n=0,1} \frac{\alpha_n \lambda_n}{\mu_n} \left[\frac{1}{1 - \frac{\lambda_n^2}{\lambda} - i\frac{\lambda_n^2}{\lambda \mu_n}} - 1 \right]$$

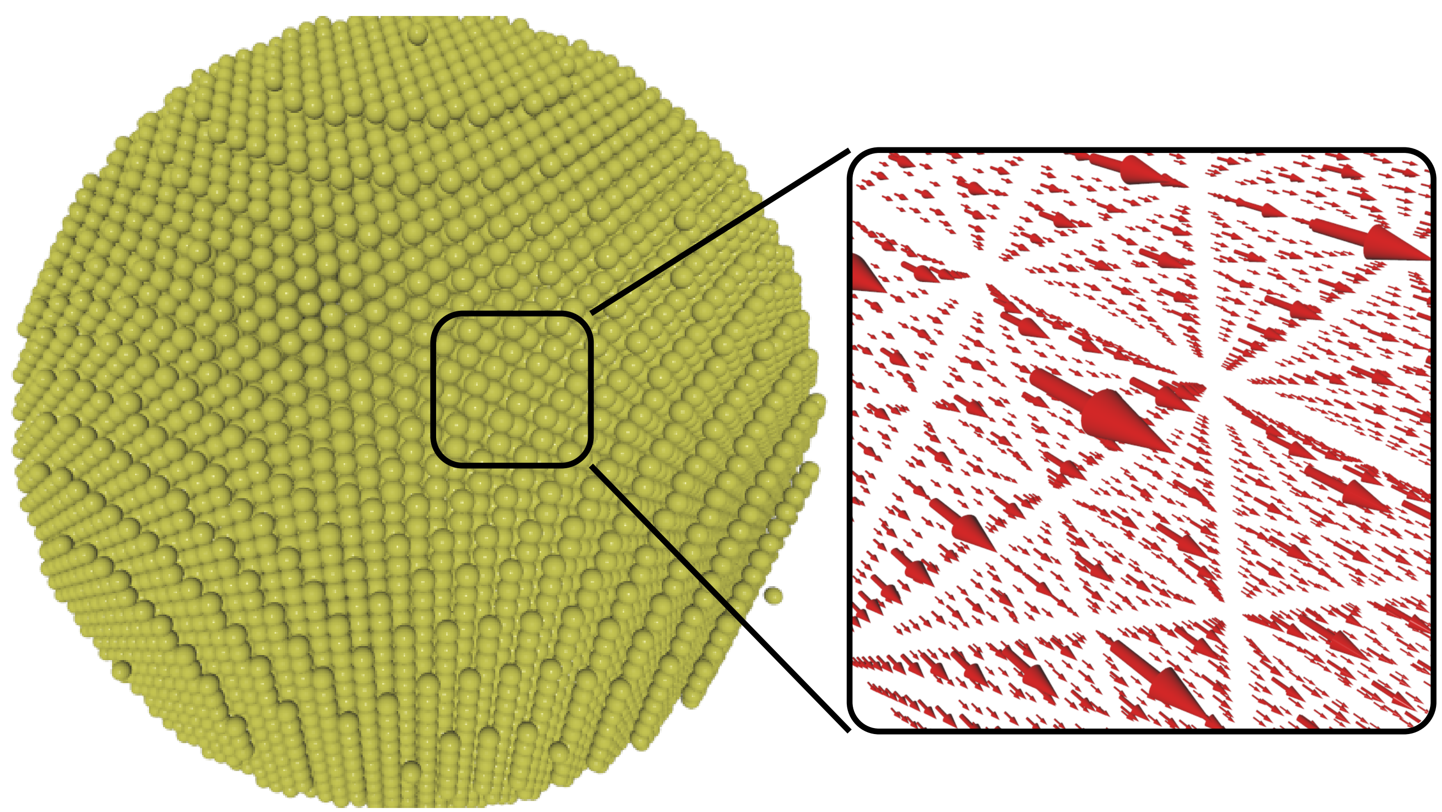


Clausius-Mossotti relation

$$\varepsilon_{\text{dye}} = \frac{1 + \frac{2}{3}(\tilde{\alpha}_M + \tilde{\alpha}_D)}{1 - \frac{1}{3}(\tilde{\alpha}_M + \tilde{\alpha}_D)}$$

concentration-dependence:

$$\tilde{\alpha}_D(\omega) = c_D \frac{\alpha_D}{\varepsilon_0}$$



Coupled-dipole equations

$$\mathbf{E}^{i} = \mathbf{E}^{\mathrm{inc}} + \sum_{j\neq i} \mathbb{G}_{ij}\mathbf{P}^{\mathrm{j}} \qquad \mathbf{P}^{\mathrm{j}} = \alpha_j \mathbf{E}^{\mathrm{j}}$$

$$\mathbb{G}_{ij} = -\frac{e^{(ikr_{ij})}}{r_{ij}} \left\{ k^2(\widehat{\mathbf{r}} \otimes \widehat{\mathbf{r}} - \mathbb{I}) + \frac{ikr_{ij} - 1}{r_{ij}^2}(3\widehat{\mathbf{r}} \otimes \widehat{\mathbf{r}} - \mathbb{I}) \right\}$$

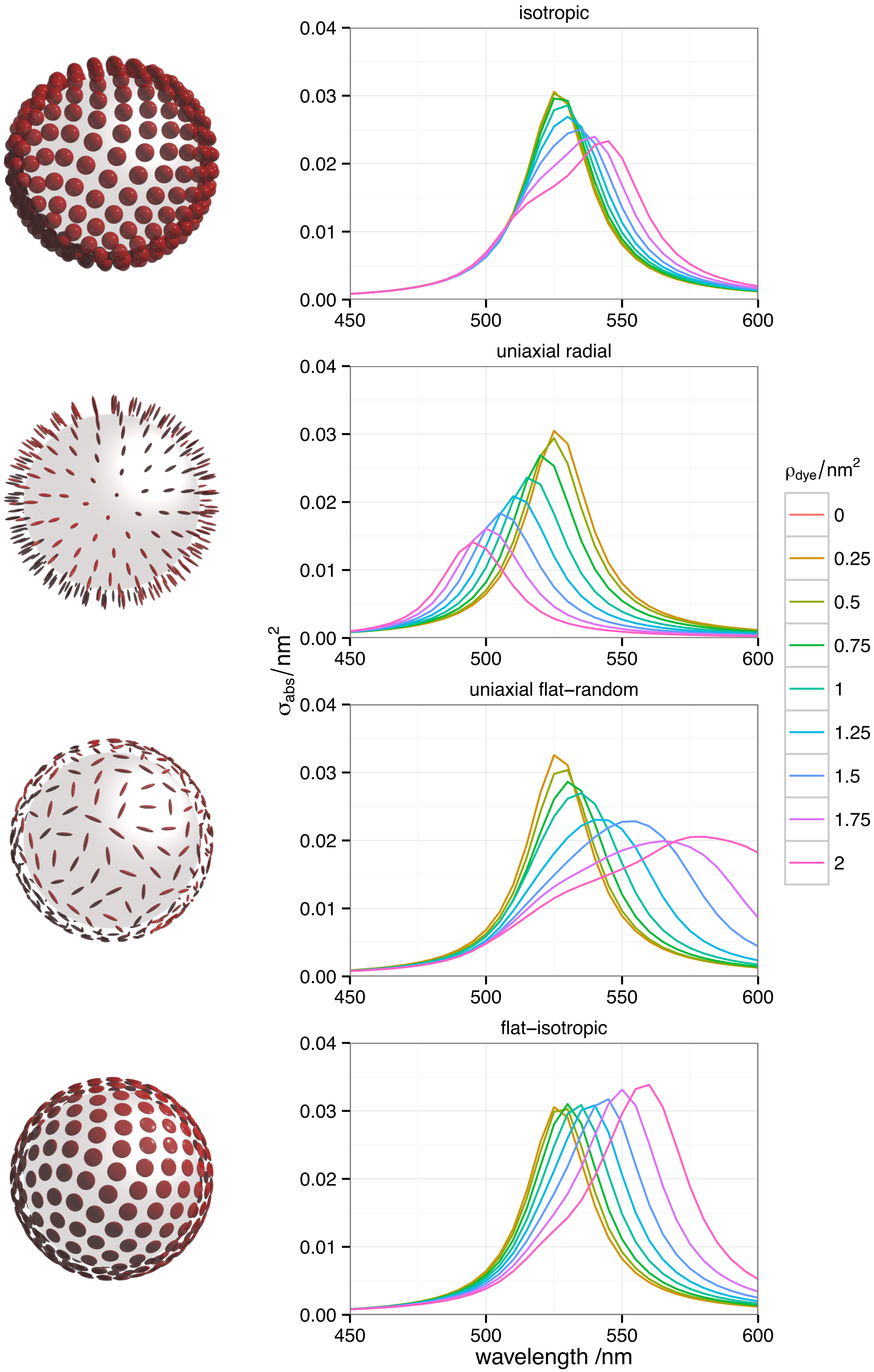
Linear system

$$\mathbb{A}\mathbf{E} = \mathbf{E}^{\mathrm{inc}}$$

Cross-sections

$$\sigma_{\mathrm{ext}} = 4\pi k \Im({\mathbf{E}_{\mathrm{inc}}}^* \cdot \mathbf{P})$$

$$\sigma_{\mathrm{abs}} = 4\pi k \left[\Im(\mathbf{E}^* \cdot \mathbf{P}) - k^3 |\mathbf{P}|^2 \right]$$



Preliminary results

- Rich behaviour
- Orientation matters!
- No direct comparison with continuous model?

Including the sphere

$$\mathbf{E}^i = \mathbf{E}^i_{\text{inc}} + \mathbf{E}^i_{\text{sphere}} + \sum_{j\neq i} \mathbb{G}_{ij}\alpha_j \mathbf{E}^j + \sum_{\forall j} \mathbb{S}_{ij}\alpha_j \mathbf{E}^j$$

Linear system (3x3 example)

$$\left[\begin{pmatrix} \mathbb{I} & \mathbb{O} & \mathbb{O} \\ \mathbb{O} & \mathbb{I} & \mathbb{O} \\ \mathbb{O} & \mathbb{O} & \mathbb{I} \end{pmatrix} - \begin{pmatrix} \mathbb{O} & \mathbb{G}_{12}\alpha_2 & \mathbb{G}_{13}\alpha_3 \\ \mathbb{G}_{21}\alpha_1 & \mathbb{O} & \mathbb{G}_{23}\alpha_3 \\ \mathbb{G}_{31}\alpha_1 & \mathbb{G}_{32}\alpha_2 & \mathbb{O} \end{pmatrix} - \begin{pmatrix} \mathbb{S}_{11}\alpha_1 & \mathbb{S}_{12}\alpha_2 & \mathbb{S}_{13}\alpha_3 \\ \mathbb{S}_{21}\alpha_1 & \mathbb{S}_{22}\alpha_2 & \mathbb{S}_{23}\alpha_3 \\ \mathbb{S}_{31}\alpha_1 & \mathbb{S}_{32}\alpha_2 & \mathbb{S}_{33}\alpha_3 \end{pmatrix}\right] \begin{pmatrix} \mathbf{E}^1 \\ \mathbf{E}^2 \\ \mathbf{E}^3 \end{pmatrix} = \begin{pmatrix} \mathbf{E}^1_{\text{inc}} \\ \mathbf{E}^2_{\text{inc}} \\ \mathbf{E}^3_{\text{inc}} \end{pmatrix} + \begin{pmatrix} \mathbf{E}^1_{\text{sphere}} \\ \mathbf{E}^2_{\text{sphere}} \\ \mathbf{E}^3_{\text{sphere}} \end{pmatrix}$$

Steps:

- *Solve the Mie scattering problem for plane-wave (E_{sphere})*
- *Solve the Mie scattering problem for dipole source (S)*
- *Solve system*
- *Calculate cross-sections*