



COUPLED DIPOLE APPROXIMATION

Applications in plasmonics & beyond

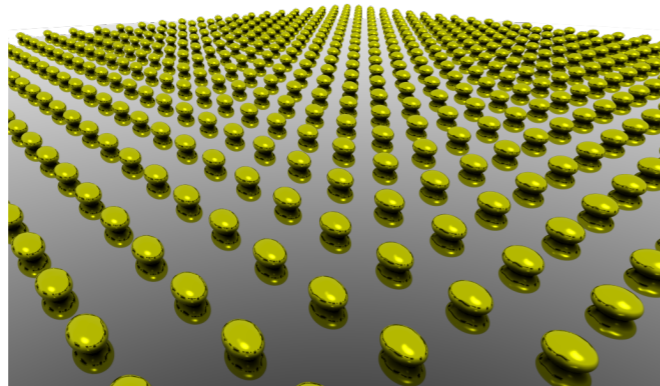
BAPTISTE AUGUIÉ

ERIC LE RU



COUPLED DIPOLES IN NANO-OPTICS: SELECTED TOPICS

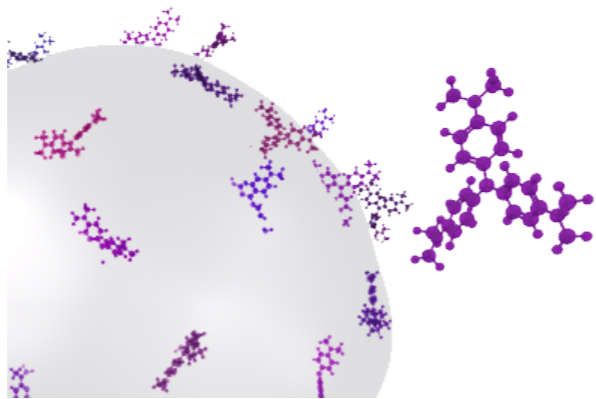
PARTICLE ARRAYS



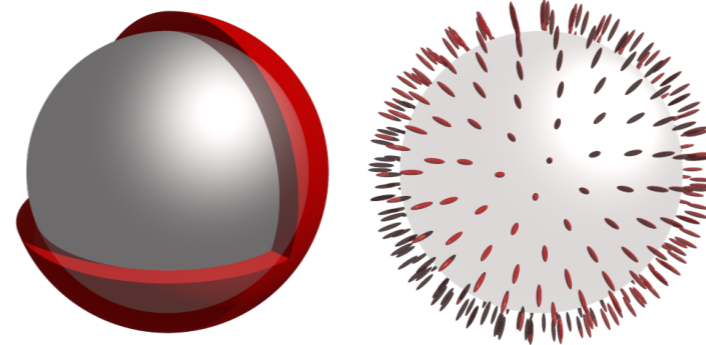
CHIRAL NANO-STRUCTURE



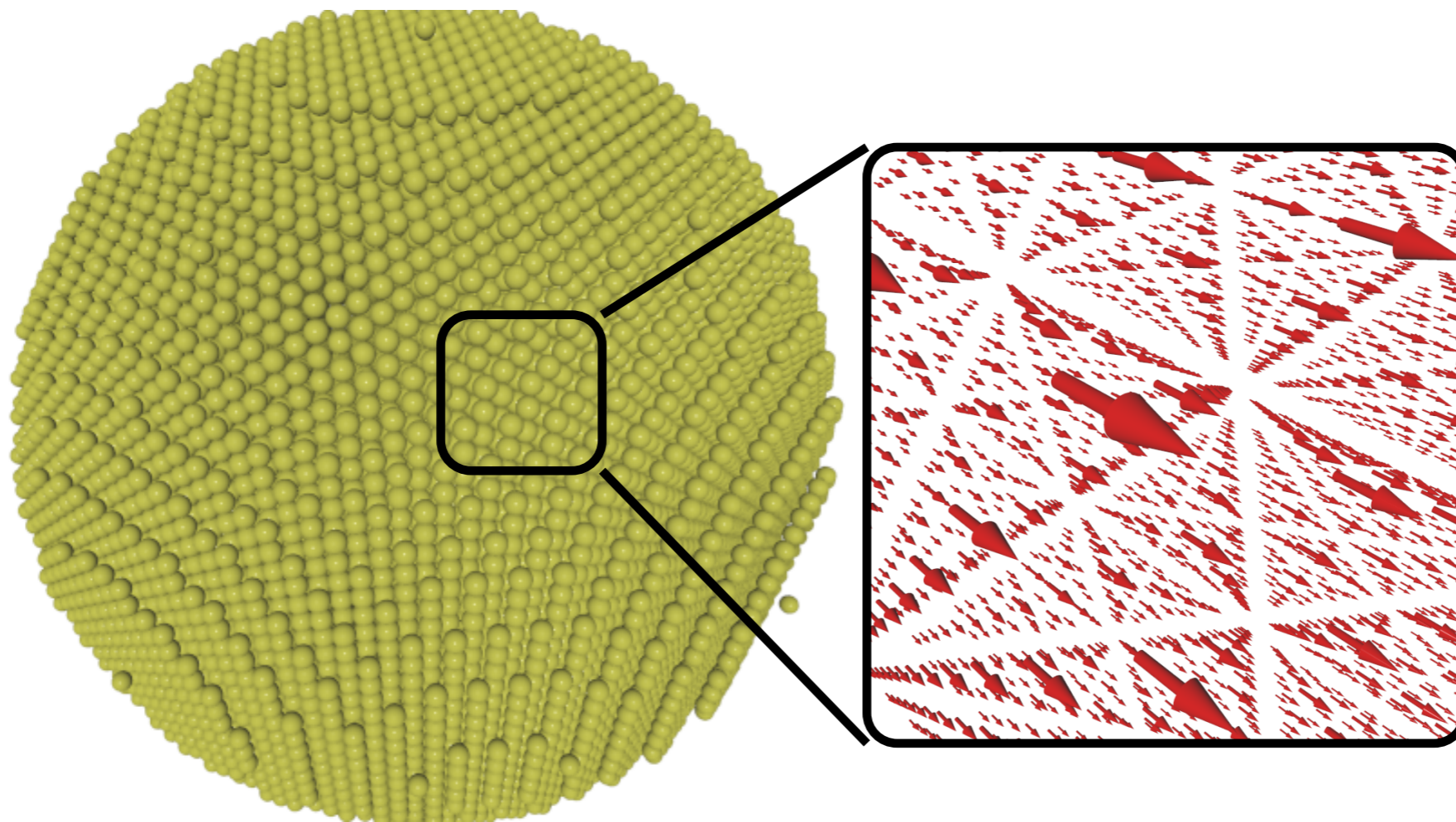
MOLECULES ON COLLOIDS



SHELLS OF INTERACTING DYES



(RELATED TOPIC) DISCRETE DIPOLE APPROXIMATION



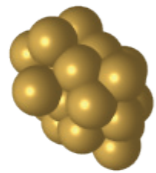
PERSONAL MUSINGS

- Why does DDA behave so poorly with metals?
- A link between DDA and the *Ewald-Oseen* extinction theorem?

COUPLED DIPOLE APPROXIMATION

(a)

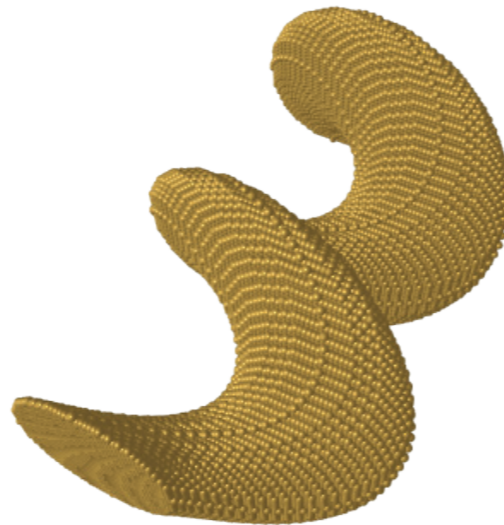
Au_{28}



~1nm

atomic cluster

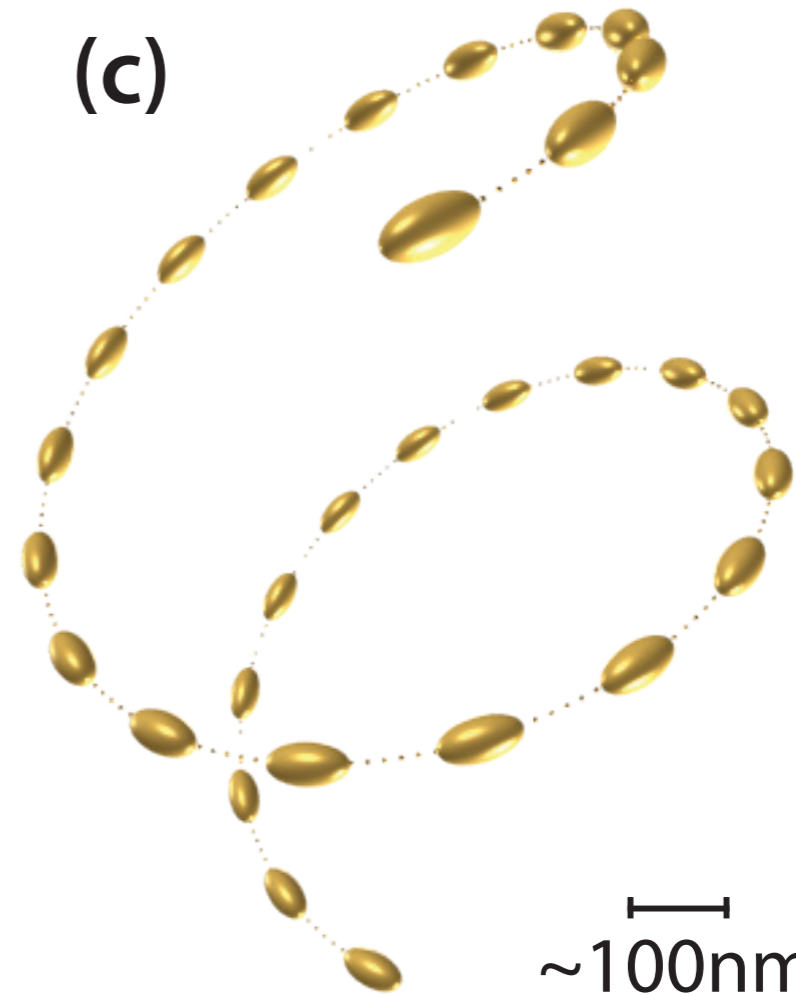
(b)



~10nm

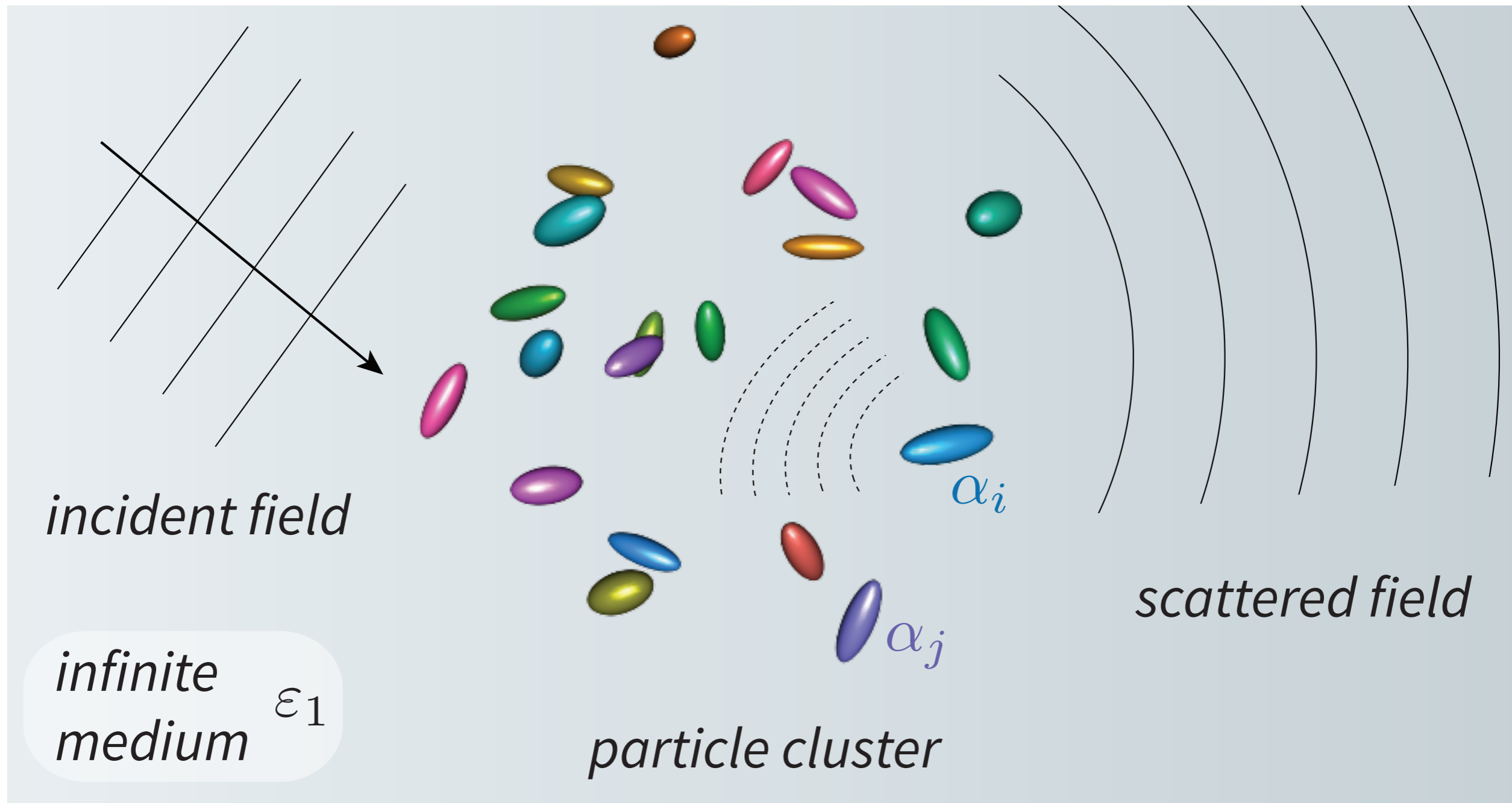
nanoparticle

(c)



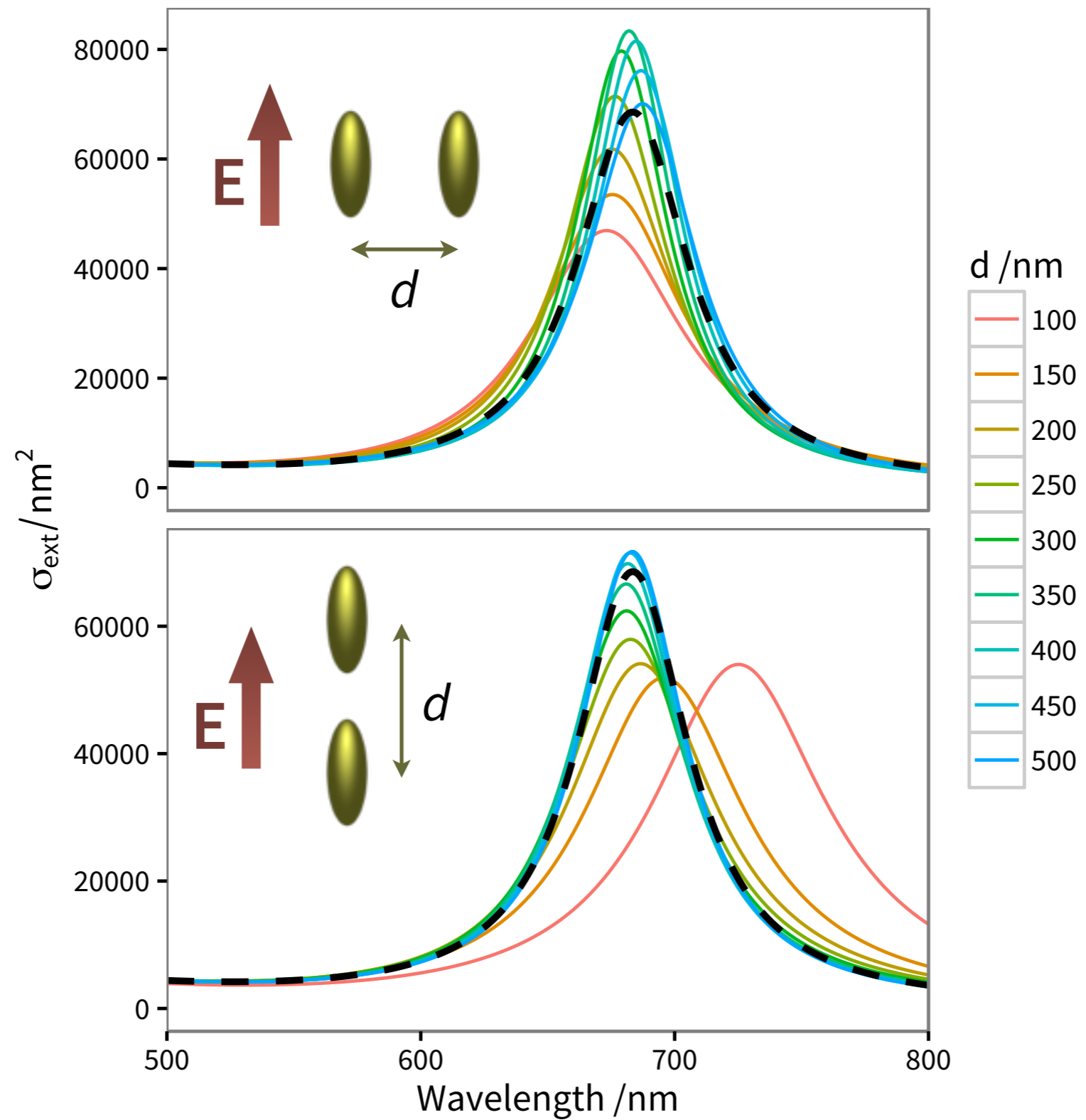
~100nm

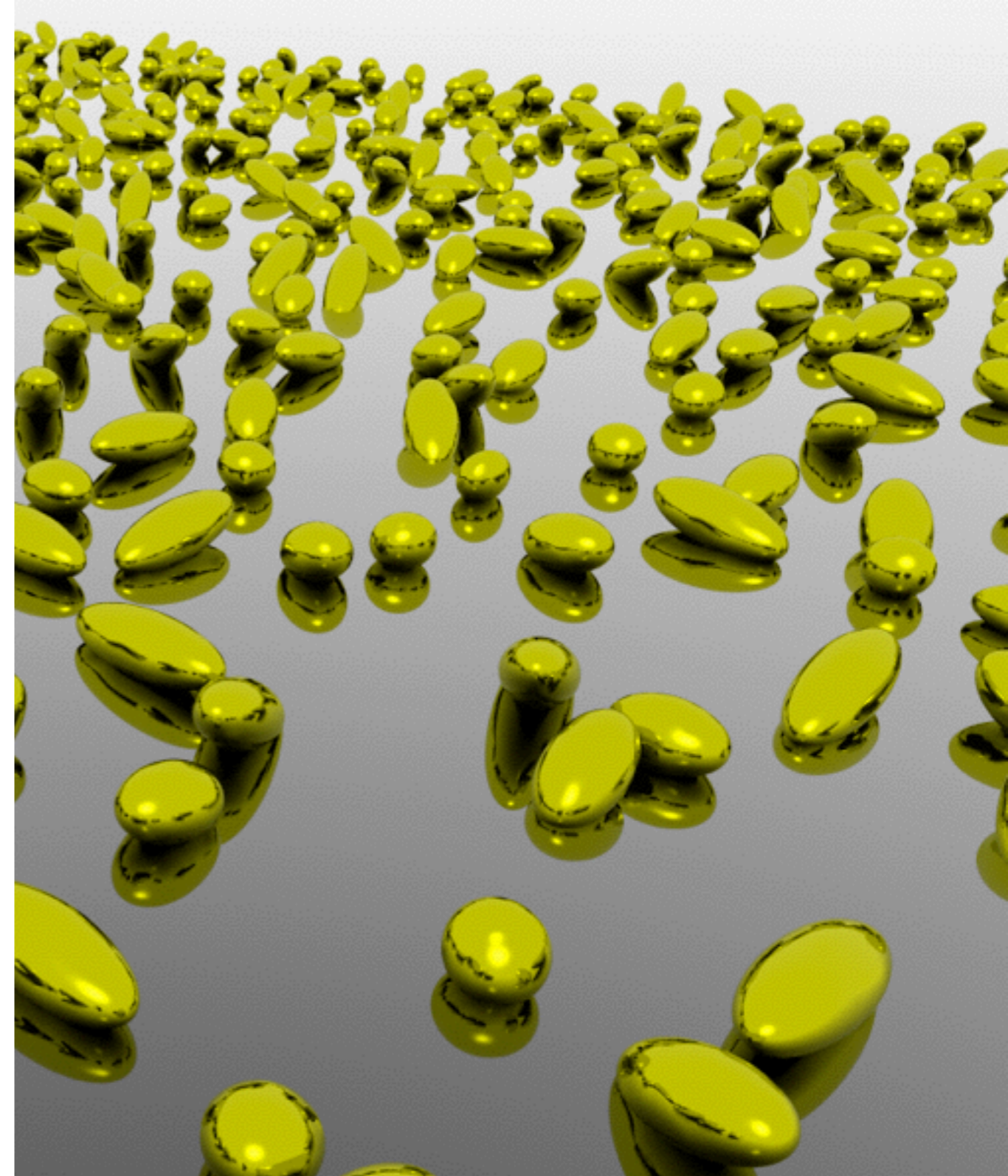
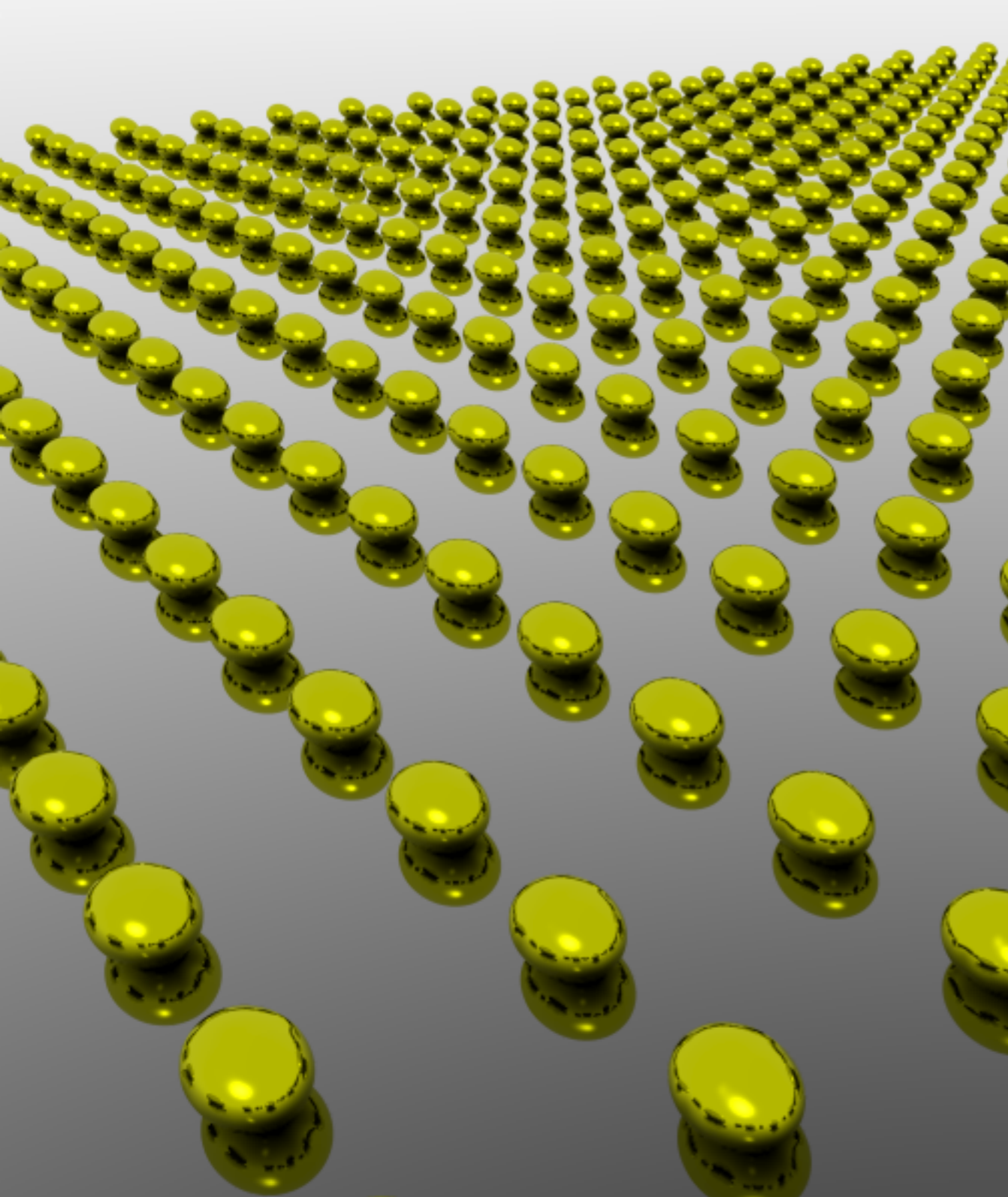
particle cluster



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

DIMER • PLASMON HYBRIDISATION





2D ARRAYS OF NANORODS
DIFFRACTIVE COUPLING

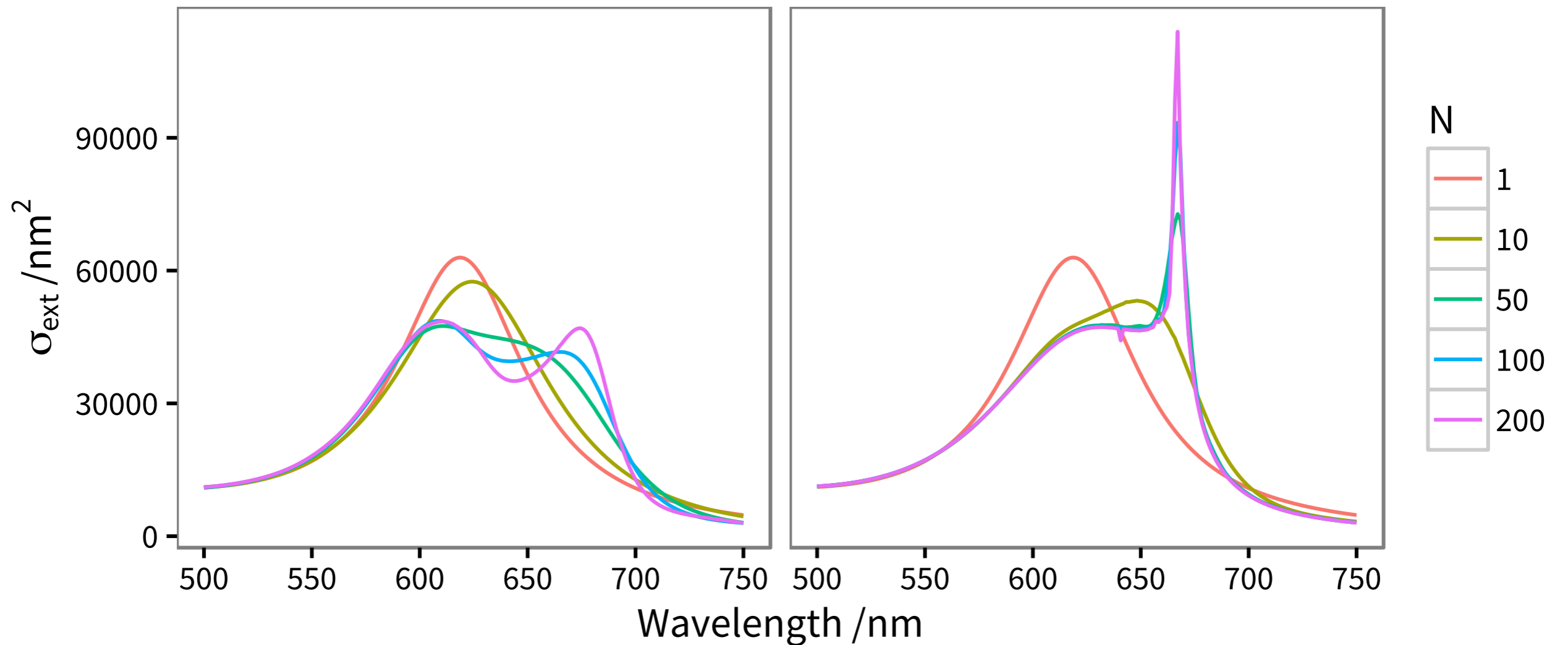
DIFFRACTIVE ARRAYS OF NANORODS

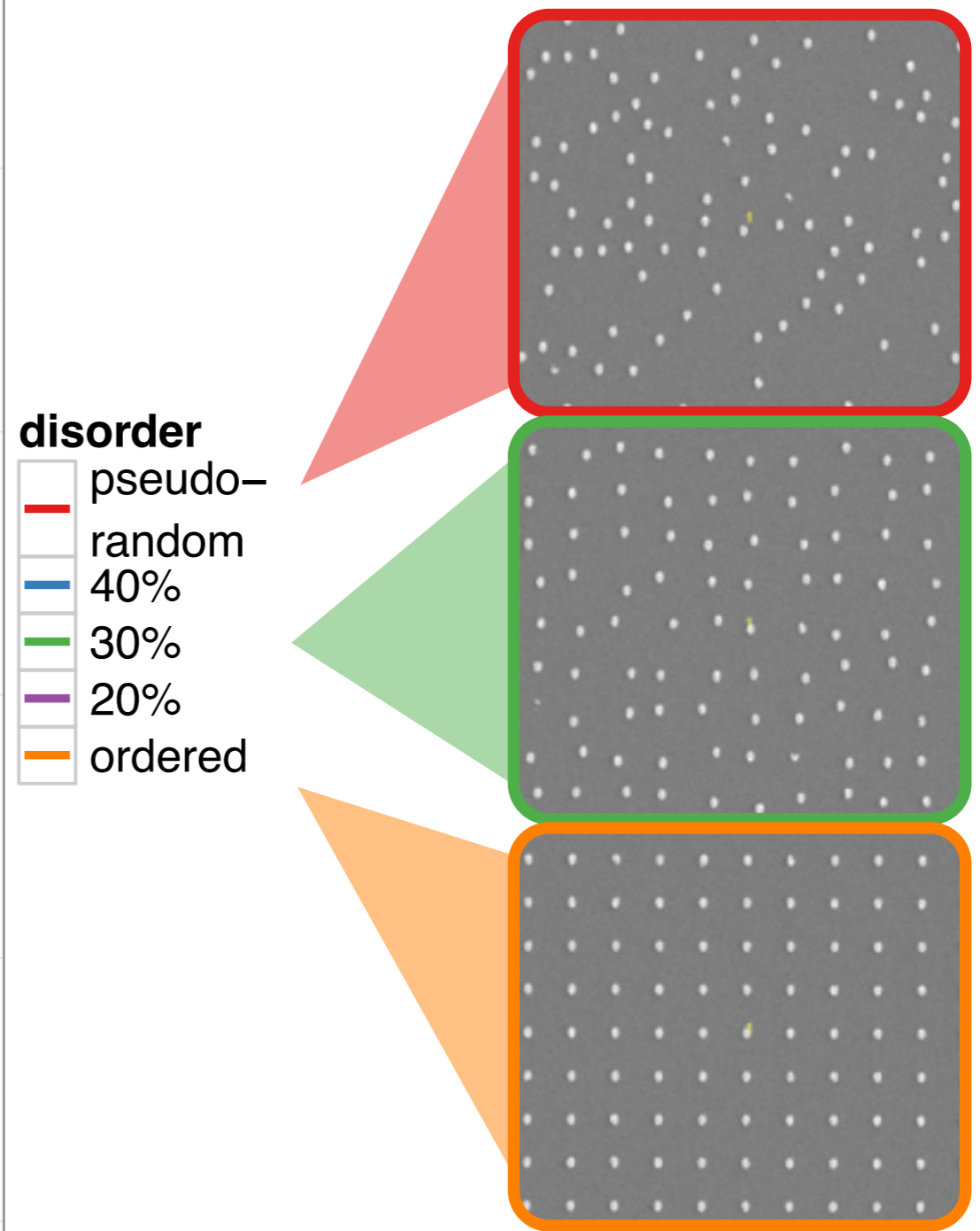
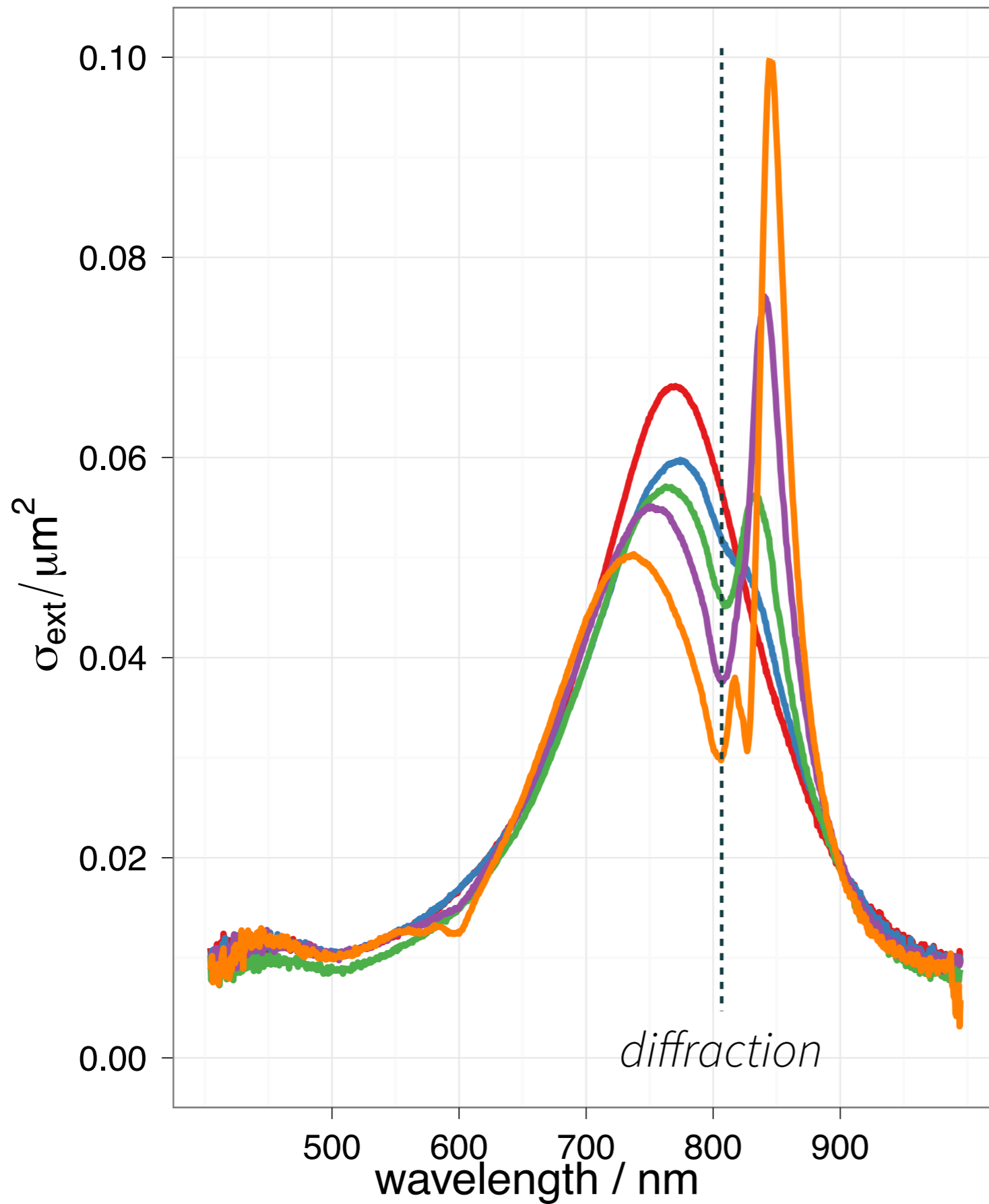


array



chain

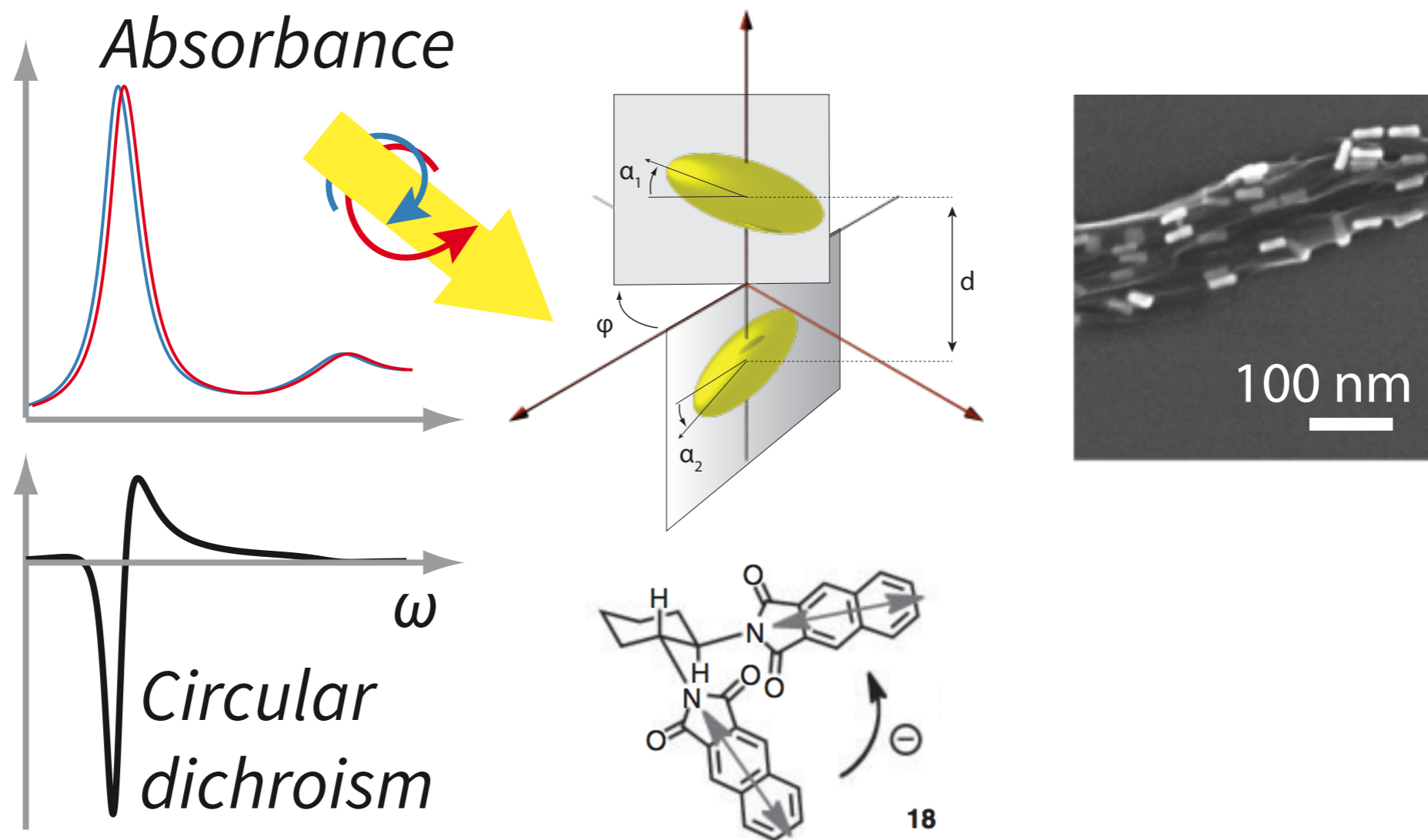


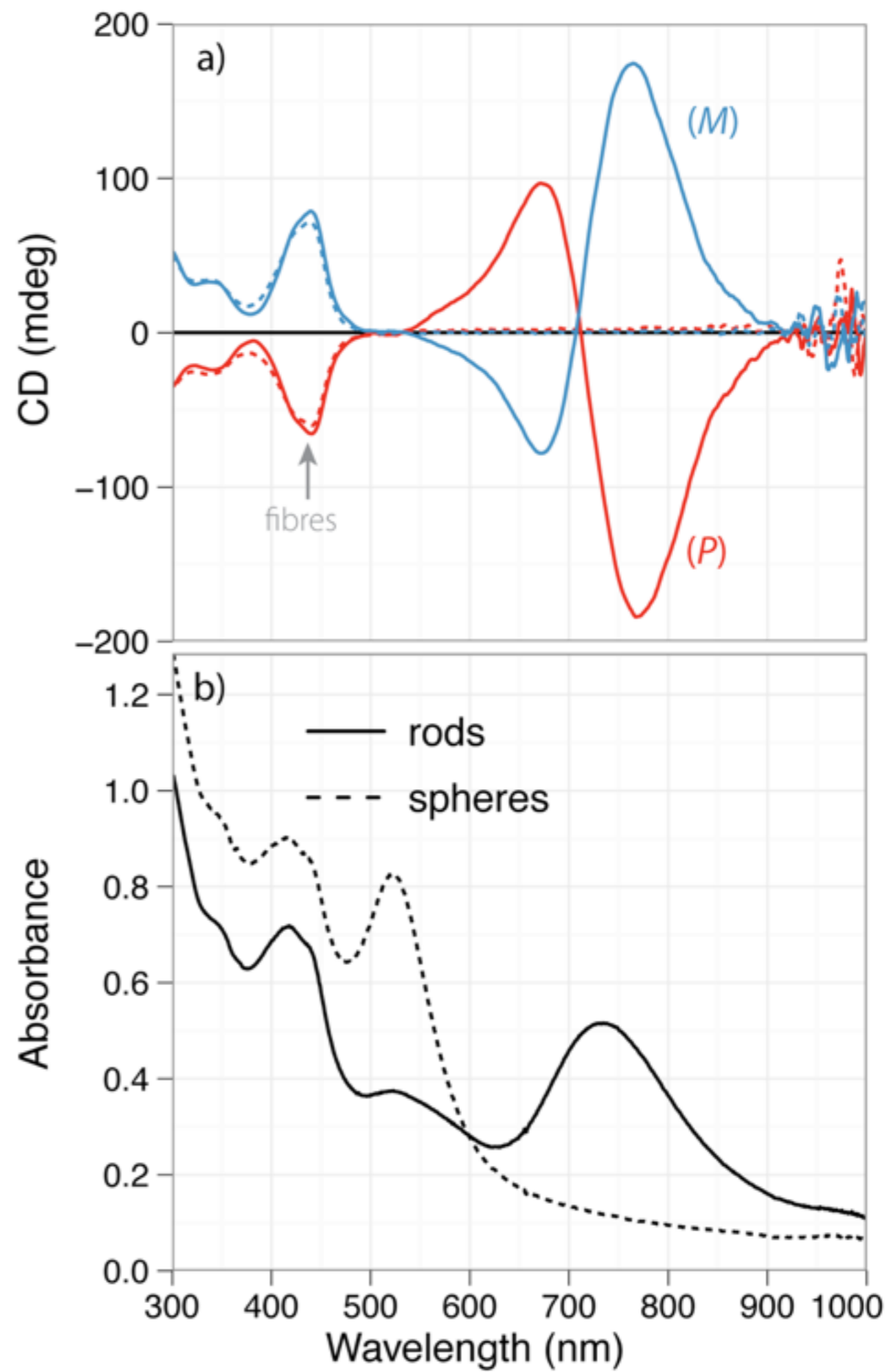
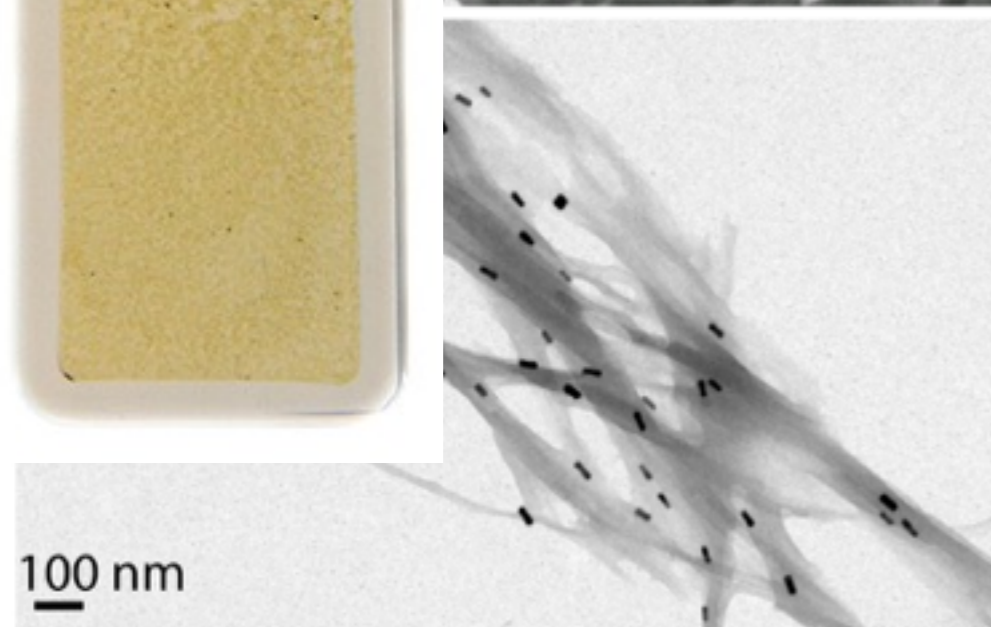
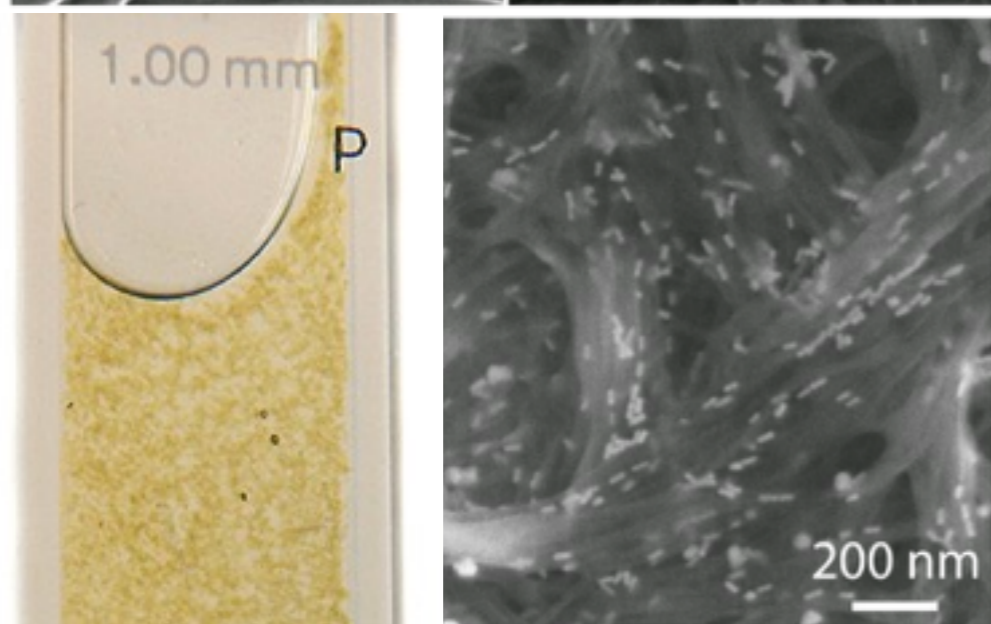
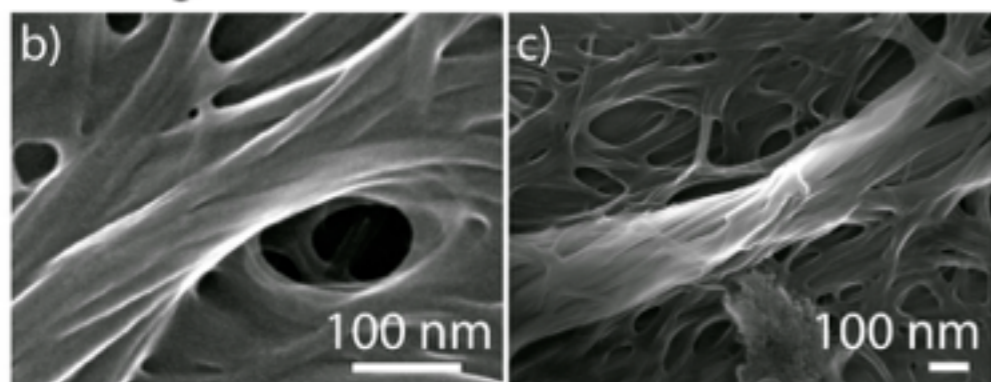
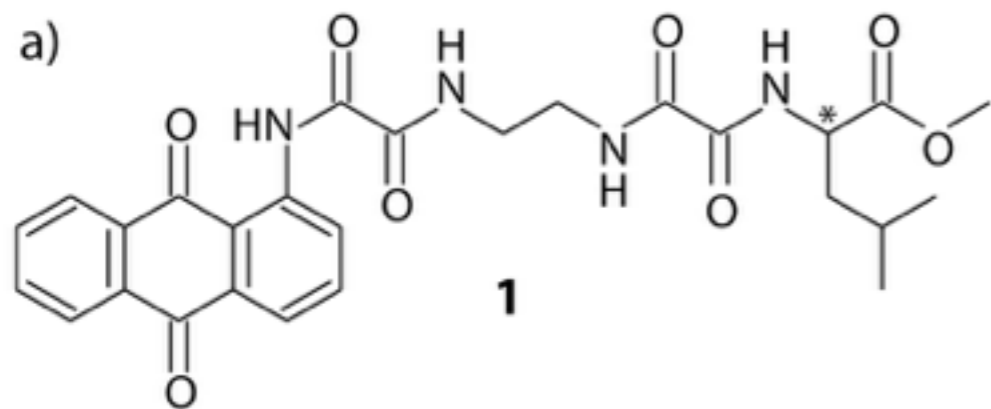




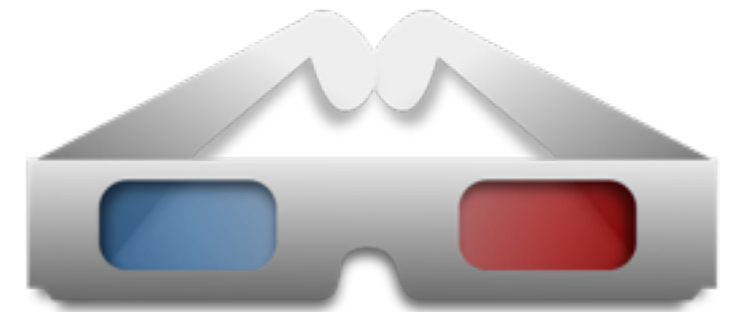
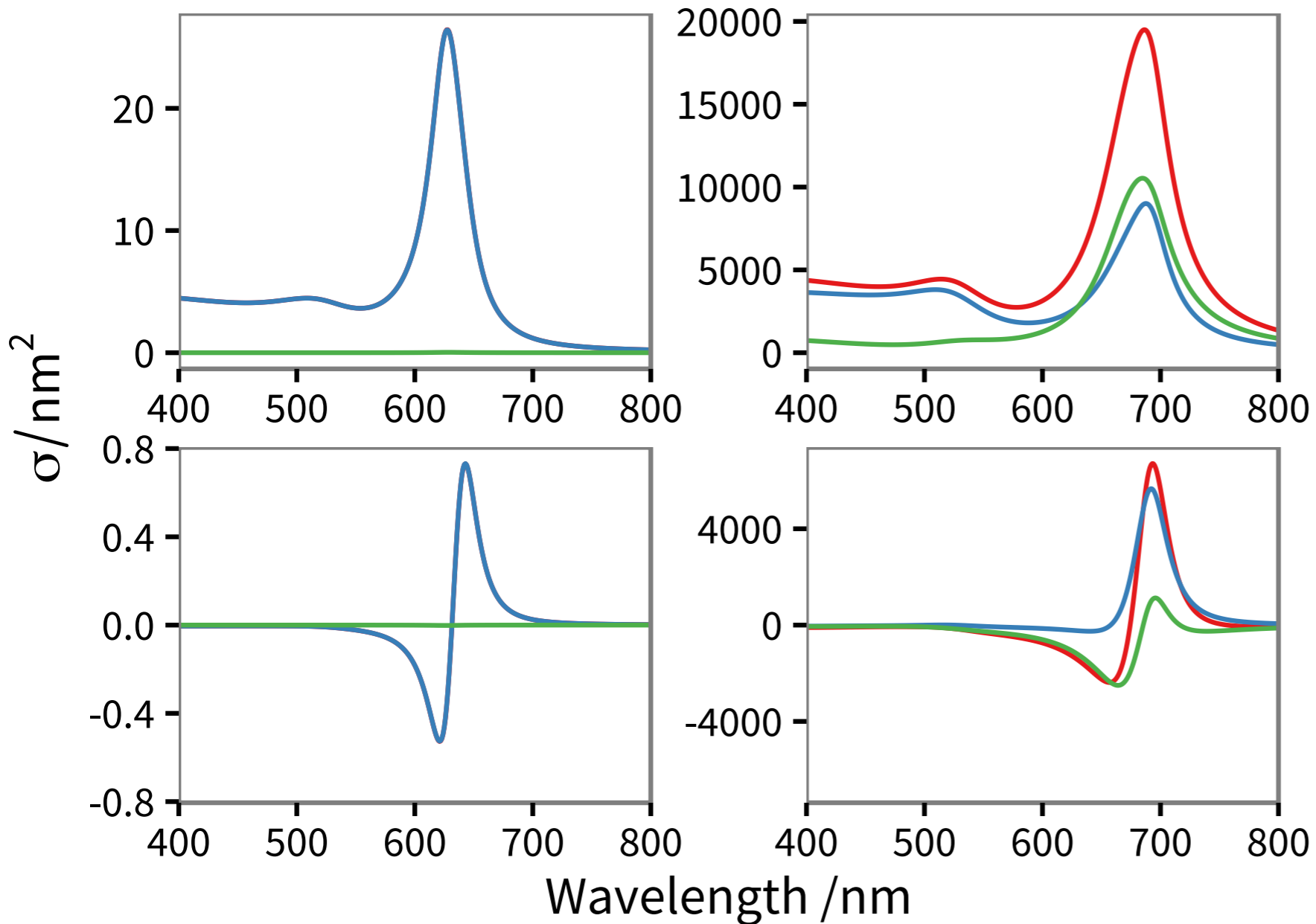
3D CHIRAL STRUCTURES
OPTICAL ACTIVITY

CIRCULAR DICHROISM – FINGERS CROSSED

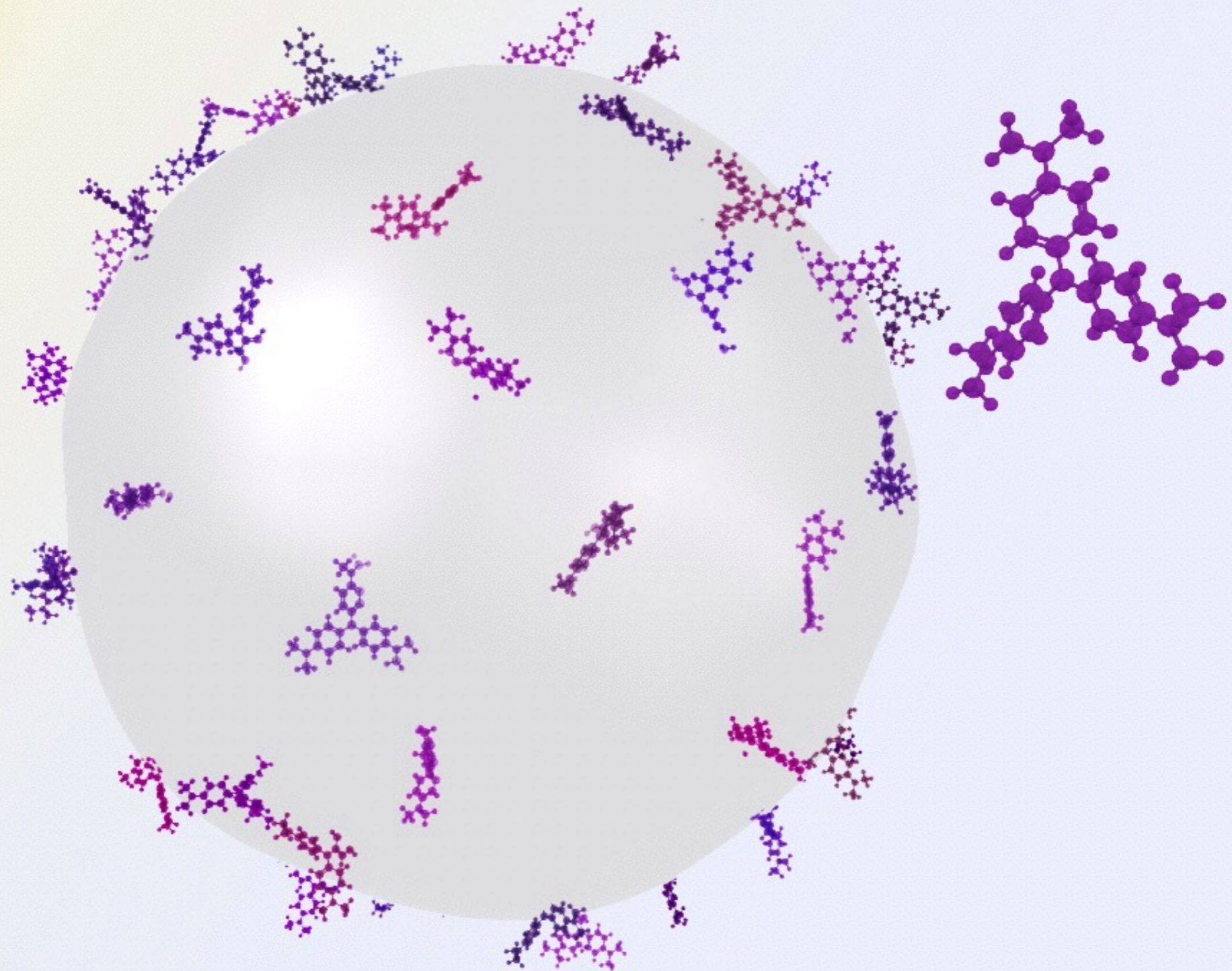




FINGERS CROSSED: A CHIRAL PLASMONIC DIMER



NEW
3D
*chiroptical effects
at the nanoscale!*

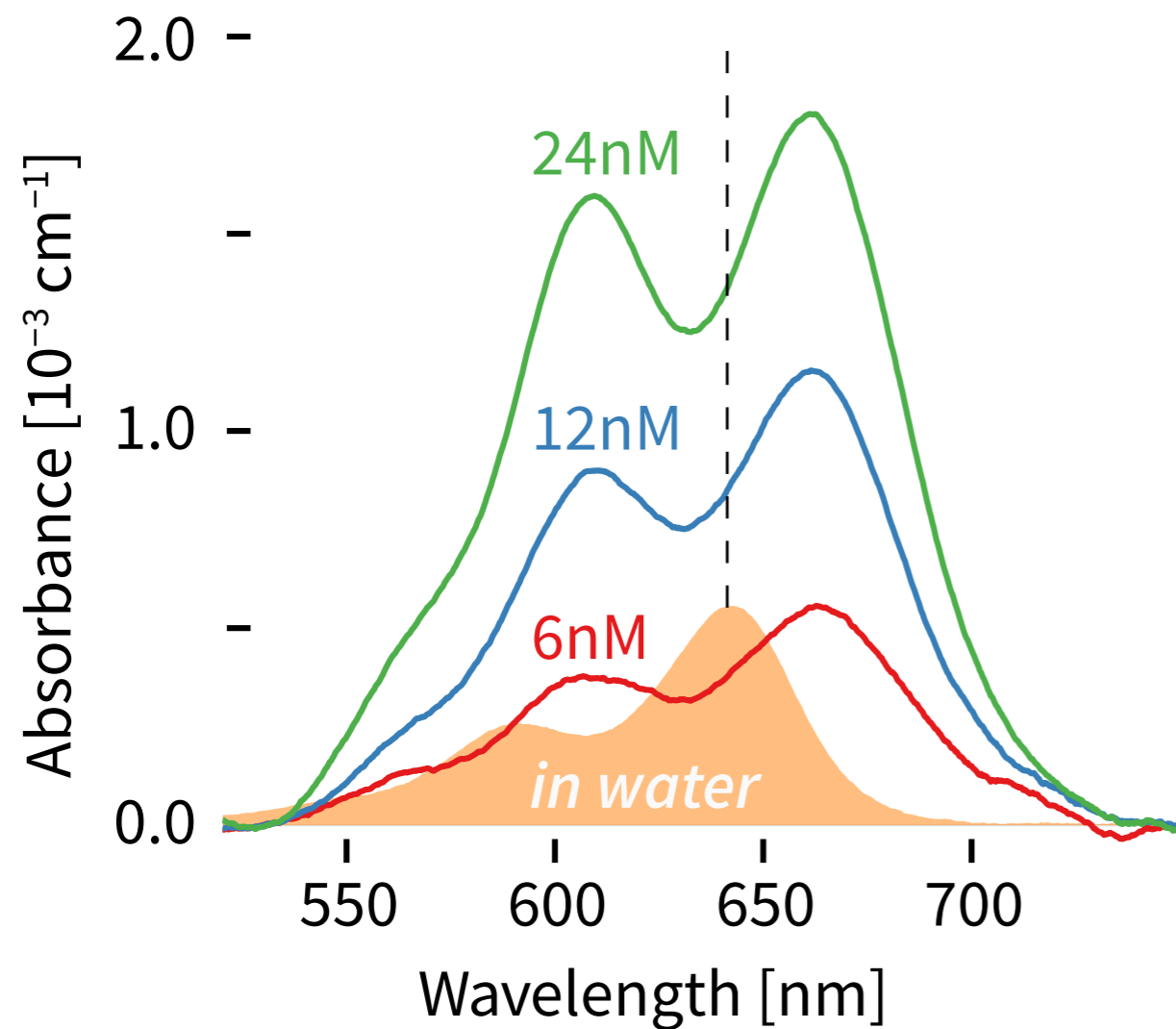


MODIFIED MOLECULAR ABSORBANCE ON METAL COLLOIDS

B. Darby, B. Augu  , M. Meyer, O. Pentoja, E. Le Ru • *Nature Photonics* 10.1 (2016)

CONCENTRATION DEPENDENCE – SHELL MODELS

EXPERIMENTS

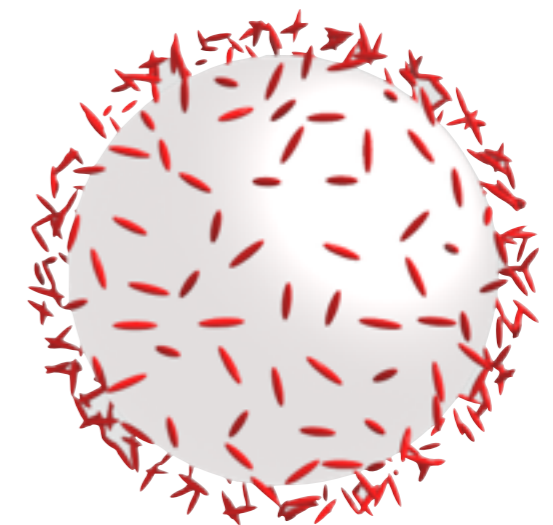


THEORY

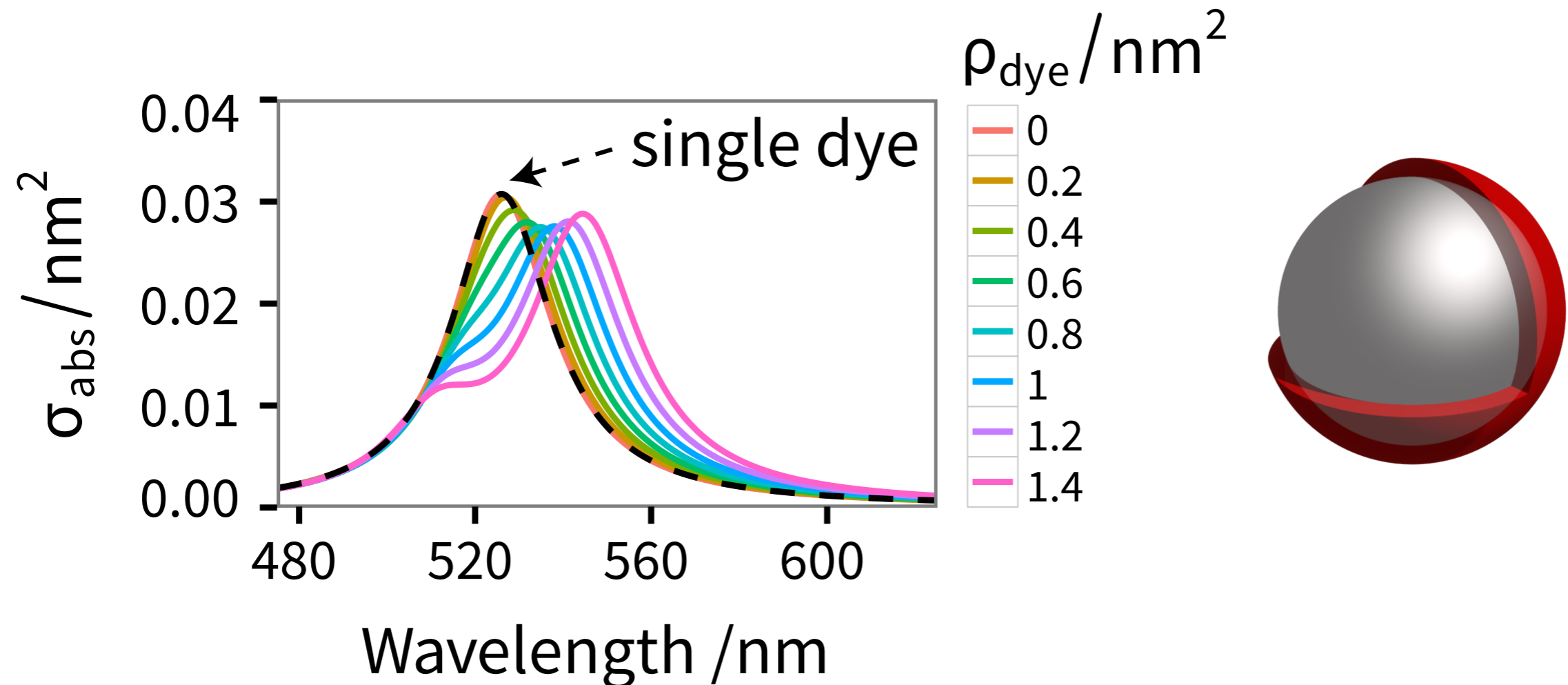
continous shell
(Mie theory)



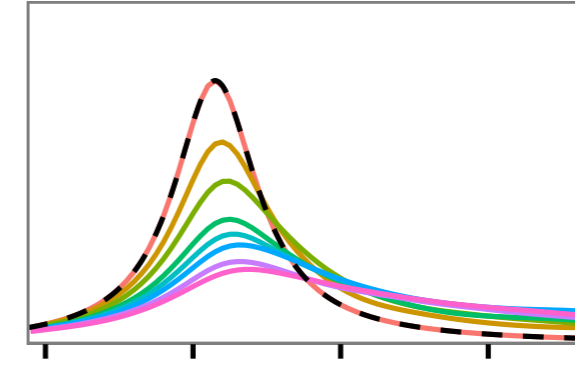
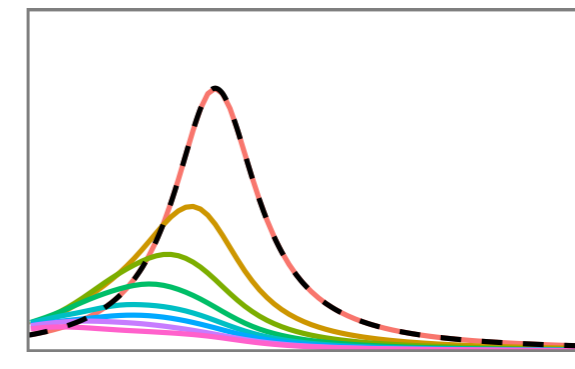
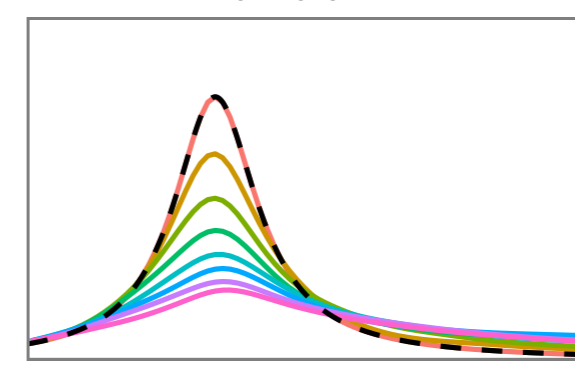
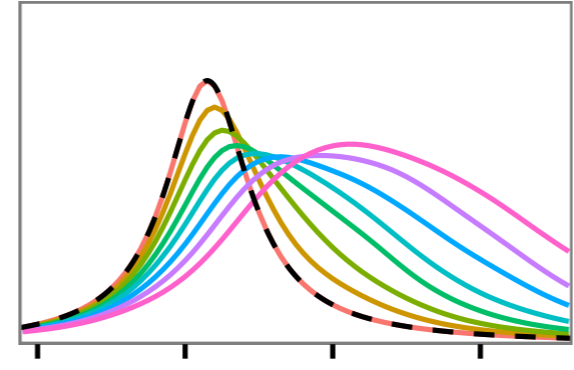
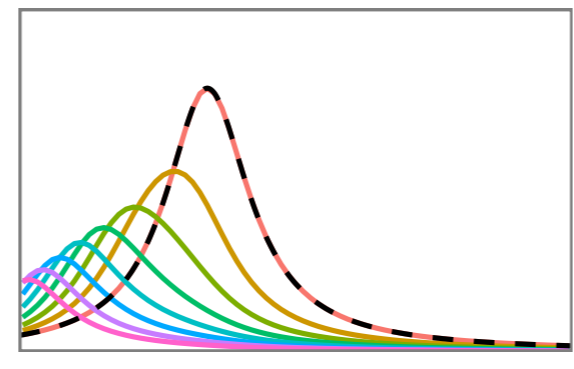
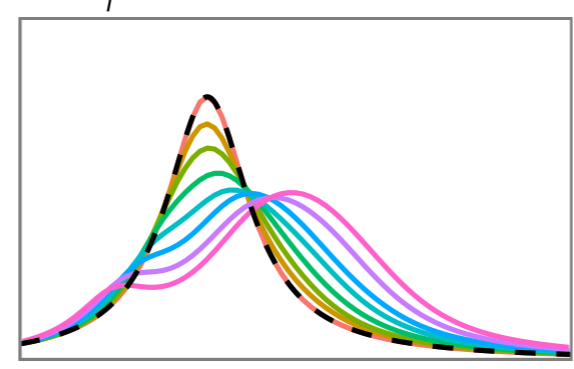
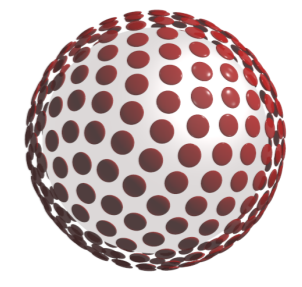
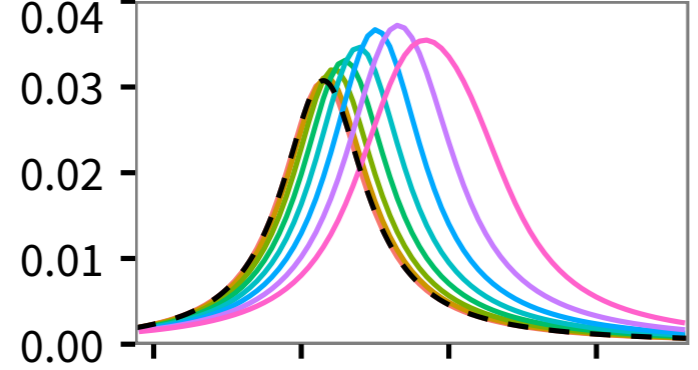
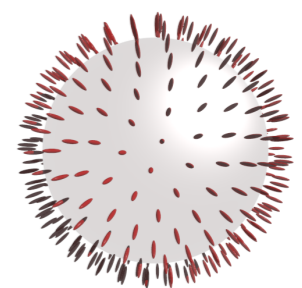
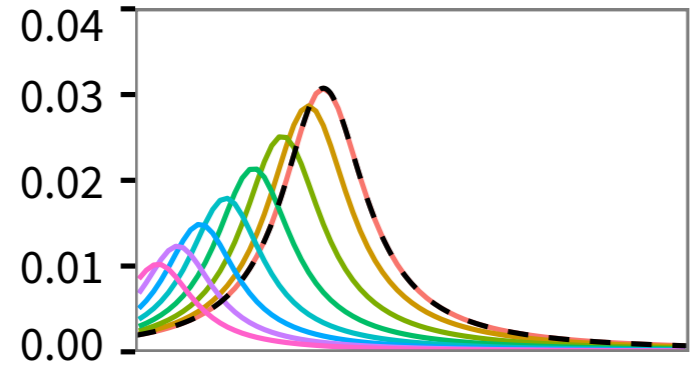
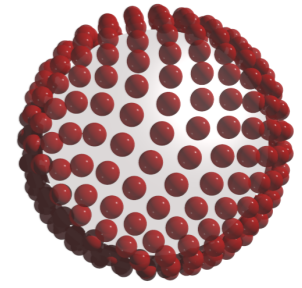
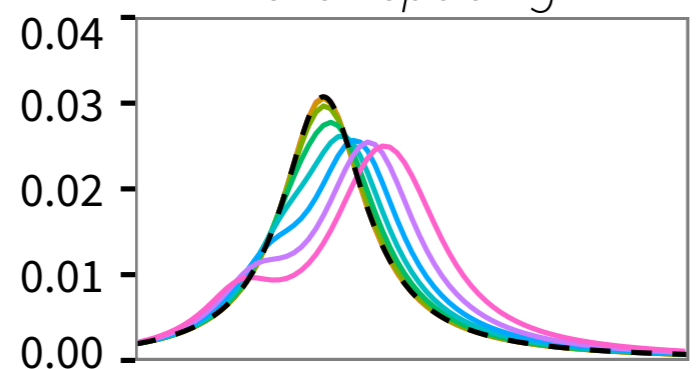
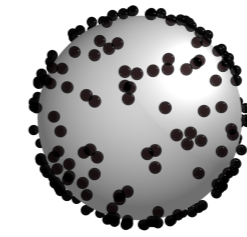
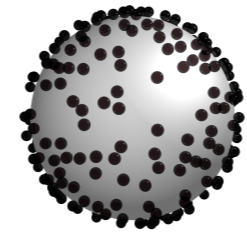
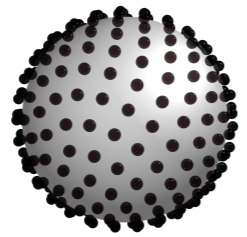
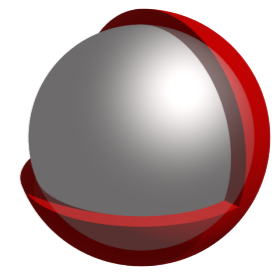
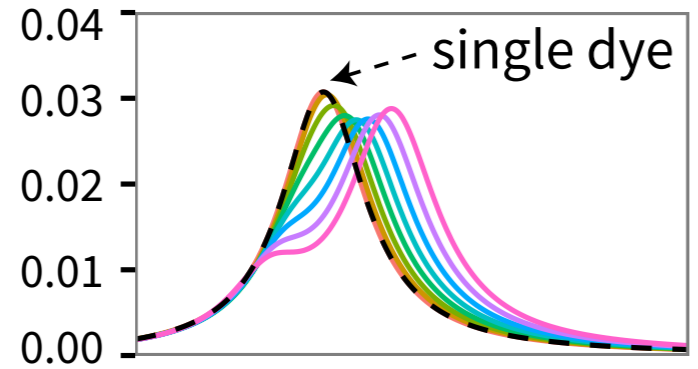
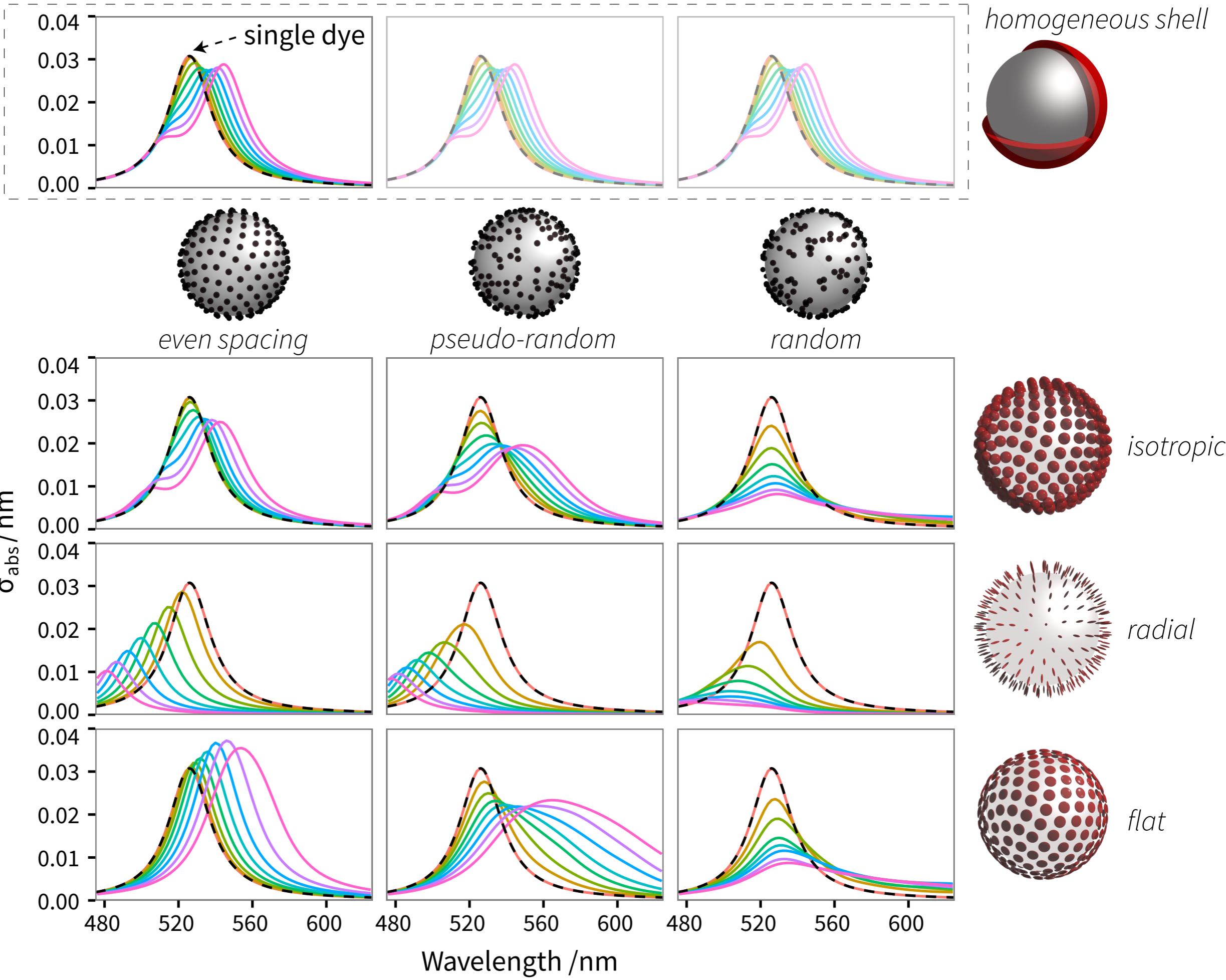
dipoles
&
Mie theory



EFFECTIVE-MEDIUM SHELL MODEL



- Concentration dependence: peak splitting, red-shift
- Cannot capture orientation effects and inhomogeneities



480 520 560 600 480 520 560 600 480 520 560 600

Wavelength / nm

THANKS

molecular absorbance Eric Le Ru & Raman lab
diffractive 2D arrays Bill Barnes
plasmonic chirality Luis Liz-Marzán's group

THANK YOU!

BAPTISTE AUGUIÉ

PhD in physics
French nationality • NZ residency
Born in 1982

LOCATION	Wellington, New Zealand
MOBILE	+64 (8) 224518532
EMAIL	baptiste.augue@gmail.com
SKYPE	baptiste.augue
WEBSITE	http://baptiste.github.io

WORK EXPERIENCE

I have worked passionately in cutting-edge physics research for 10 years, in England, Spain, New Zealand, and Argentina. This multi-faceted experience has led to 28 peer-reviewed publications (9-index: 14) in several high-impact journals (Nature Photonics, Physical Review Letters, Angewandte Chemie), cumulating 1300 citations.

2015 – 2016 **Research and teaching Fellow** VICTORIA UNIVERSITY OF WELLINGTON

- Lectured for the 3rd year physics curriculum (30 students, 1.5 trimesters)
- Contributed to a challenging study of absorption in turbid media published in *Nature Photonics*
- Co-wrote open-source programs and user guides for electromagnetic simulations

2013 – 2015 **Research Fellow** CENTRO ATÓMICO BARLOCHE, ARGENTINA

- Proposed and demonstrated a novel optical sensor, after initiating a new collaboration

2011 – 2013 **Post-doctoral Fellow** VICTORIA UNIVERSITY OF WELLINGTON

- Developed a new technique enabling Raman spectroscopy of highly fluorescent dyes
- Combined SPR and SERS spectroscopy with an original microscopy setup

2010 – 2011 **Post-doctoral Fellow** UNIVERSITY OF VIGO, SPAIN

- Conducted pioneering research in chiral plasmonics

2009, 2010 **Invited visiting research Fellow** CSIC, MADRID, SPAIN

- Elucidated incompatible results on supported arrays of metal nanoparticles

2005 – 2009 **PhD in physics** EXETER UNIVERSITY, UK

- Thesis: *Optical properties of gold nanostructures* (Advisor: Prof William L. Barnes)
- First publication in the prestigious journal *Physical Review Letters*

CORE COMPETENCIES

Physics **Expert in nano-technology, optics and spectroscopy**

- Fabrication: e-beam lithography • clean-room • sample preparation
- Characterisation: dark-field & SPR microscopy • Raman, fluorescence & co spectroscopy
- Theory: light scattering, optics, electromagnetism, nano-technology

Programming **Broad experience with data analysis, numerical modelling & simulations**

- Data analysis and simulations using R, MATLAB, and C++
- Active github profile since 2008. Over 70 git repositories, including > 15 R packages
- R user since 2007; contributions acknowledged in numerous books and over 30 publications (notably for: `grid`, `knitr`, `ggplot2`, `Rcpp`)
- Expert advice and help via mailing lists, > 1000 answers read by 1M users, 30k reputation on Stack Overflow: stackoverflow.com/users/471893/baptiste

June 9, 2016 Baptiste Auguié • <http://baptiste.github.io> page 1/2

ACQUIRED SKILLS

Writing **Experienced science communicator**

- Wrote several grant applications, numerous cover letters and high-impact scientific articles
- Strong advocate of dynamic report generation, using modern literate programming tools (markdown, pandoc, l^aT_EX and R) for a more reproducible and efficient data analysis workflow

Presentation **Advanced knowledge of R graphics, great attention to detail**

- My co-authors have trusted me with the figures for over 15 articles
- Long-time user of Adobe Illustrator, Indesign, Photoshop
- For specific visuals I also use 3D ray-tracing (scripted), and custom-made low-level R graphics

Speaking **Good communicator**

- Fluent in French (native speaker), English (4 years in England, 3 in New Zealand), and Spanish (1 year in Spain, 2 in Argentina)
- Over 20 talks at international conferences and meetings (audiences of 10–100 field experts)
- Invited speaker at a 3-day workshop, and 4 other seminars (30–50 students and researchers)

Leadership **Valued and adaptable team worker**

- Co-supervised 10 PhD students and visitors, and organised/co-supervised research visits for 4 PhD students (up to 3 months)
- Lecturer for 3rd year physics (over 20 lectures, 25 students)
- Obtained a £4,820 research fund to foster exchanges between our group, the UK, and Argentina
- Organised a one-day national meeting on plasmonics in 2012, and chaired a session at the MacDiarmid flagship conference AMN7, host to 500 international participants
- Referee for several high-impact journals

EDUCATION

2004 – 2005 **Masters in physics** MONTRÉAL, CANADA | RENNES, FRANCE

- Exchange programme at the prestigious École Polytechnique, Montréal
- Thesis: *Ultralow chromatic dispersion measurement of optical fibers with a tunable fiber laser*

2000 – 2005 **Engineering degree in physics** NATIONAL INSTITUTE OF APPLIED SCIENCES, RENNES, FRANCE

- Core topics: physics, technology, material science

— 2000 **Baccalauréat scientifique, with highest honors (mention très bien)** SEGRÉ, FRANCE

PERSONAL INTERESTS

 I am passionately curious about the world's diversity, and keen to connect with other cultures. I enjoy travelling, foreign literature (Murakami, Cortázar, Salter, Kundera) and cinema (Miyazaki, Iñárritu, Kusturica)

 My professional interest in graphics and presentation is intertwined with personal hobbies including typography, calligraphy and photography. I coded and designed my personal website: baptiste.github.io/photography

 During most holidays you will find me travelling, taking photos and exploring new areas. The rest of the year I enjoy regular running; in 2013 I completed Wellington's "Around the bays" half-marathon in under 2 hours

June 9, 2016 Baptiste Auguié • <http://baptiste.github.io> page 2/2

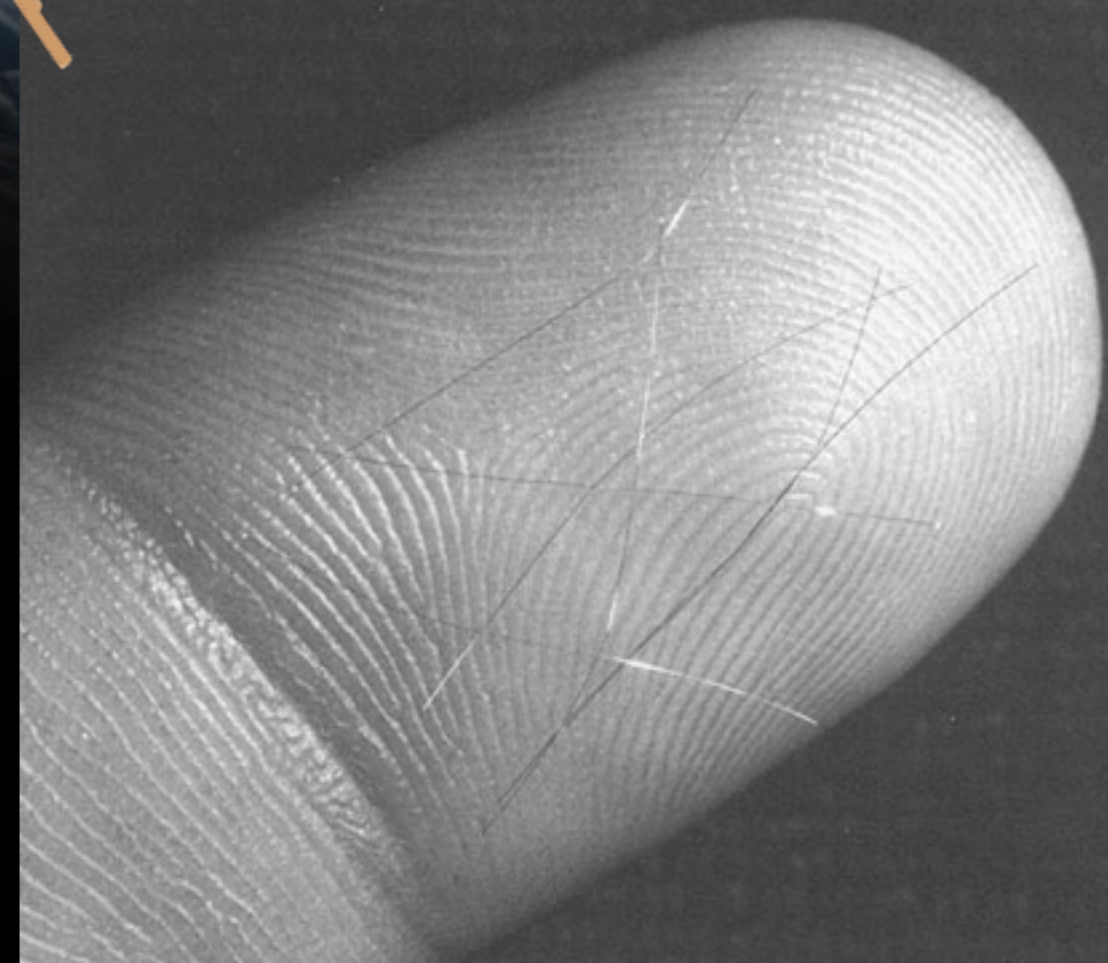
JOBS?

SUPPLEMENTARY INFORMATION

Project *West Ford* (1961–1963)

- 500 million copper needles
- Nature 192 (1961); Science 134, (1961)
Adv. Space Res. 35, (2005) ...
- Ignited some debate (astronomers...)

“At various times, apprehension has been expressed concerning several possible deleterious effects which might result from such a dipole belt”





★ **Eric Le Ru**

Today at 3:23 PM



To: baptiste.auguie

Re: DWC symposium

STOP TALKING ABOUT THE WEST FORD EXPERIMENT

Eric

On 23/06/2016, at 3:18 PM, Baptiste Auguie <baptiste.auguie@gmail.com> wrote:

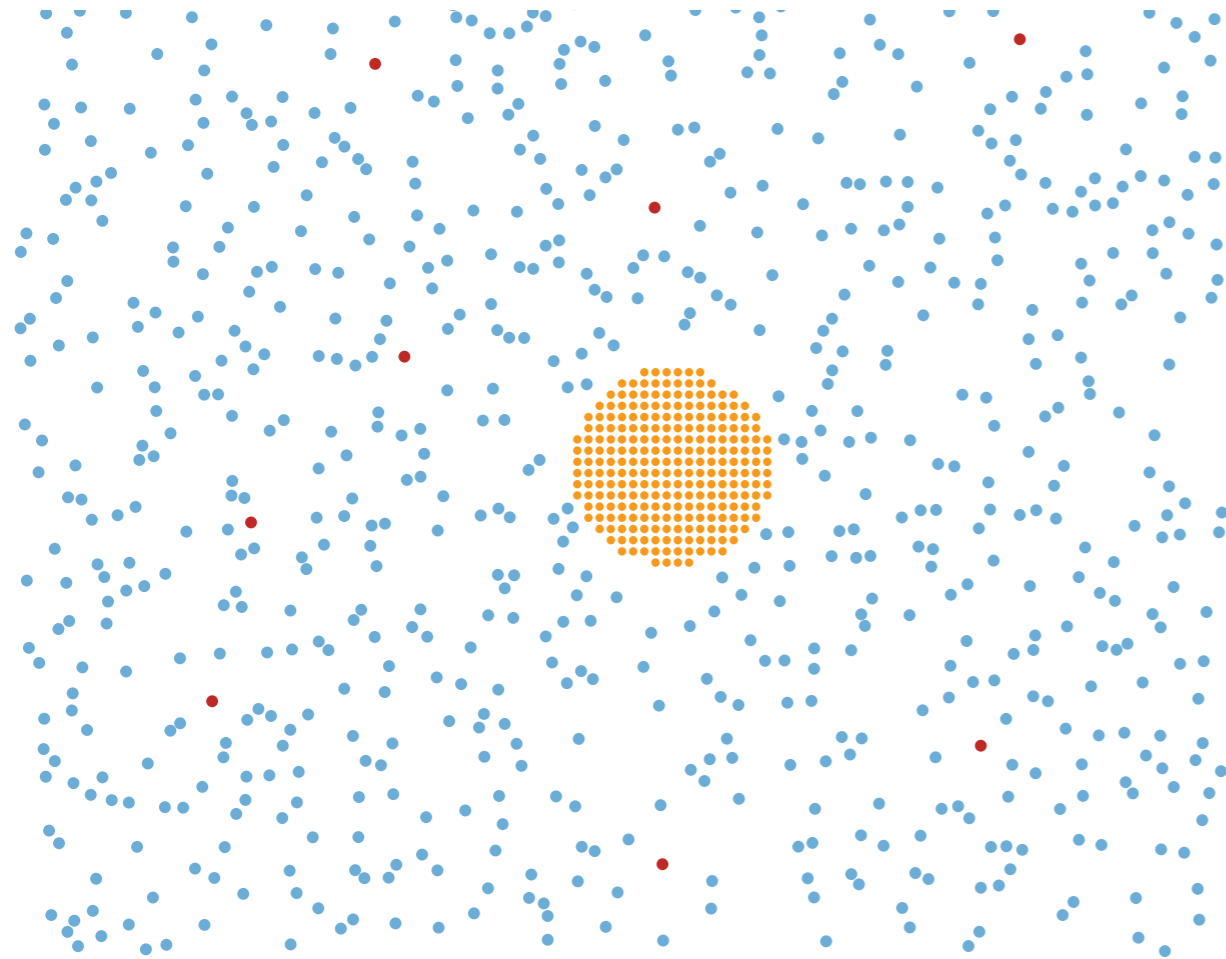
Hi Eric,

Attached are the slides for my presentation next week, let me know what you think.

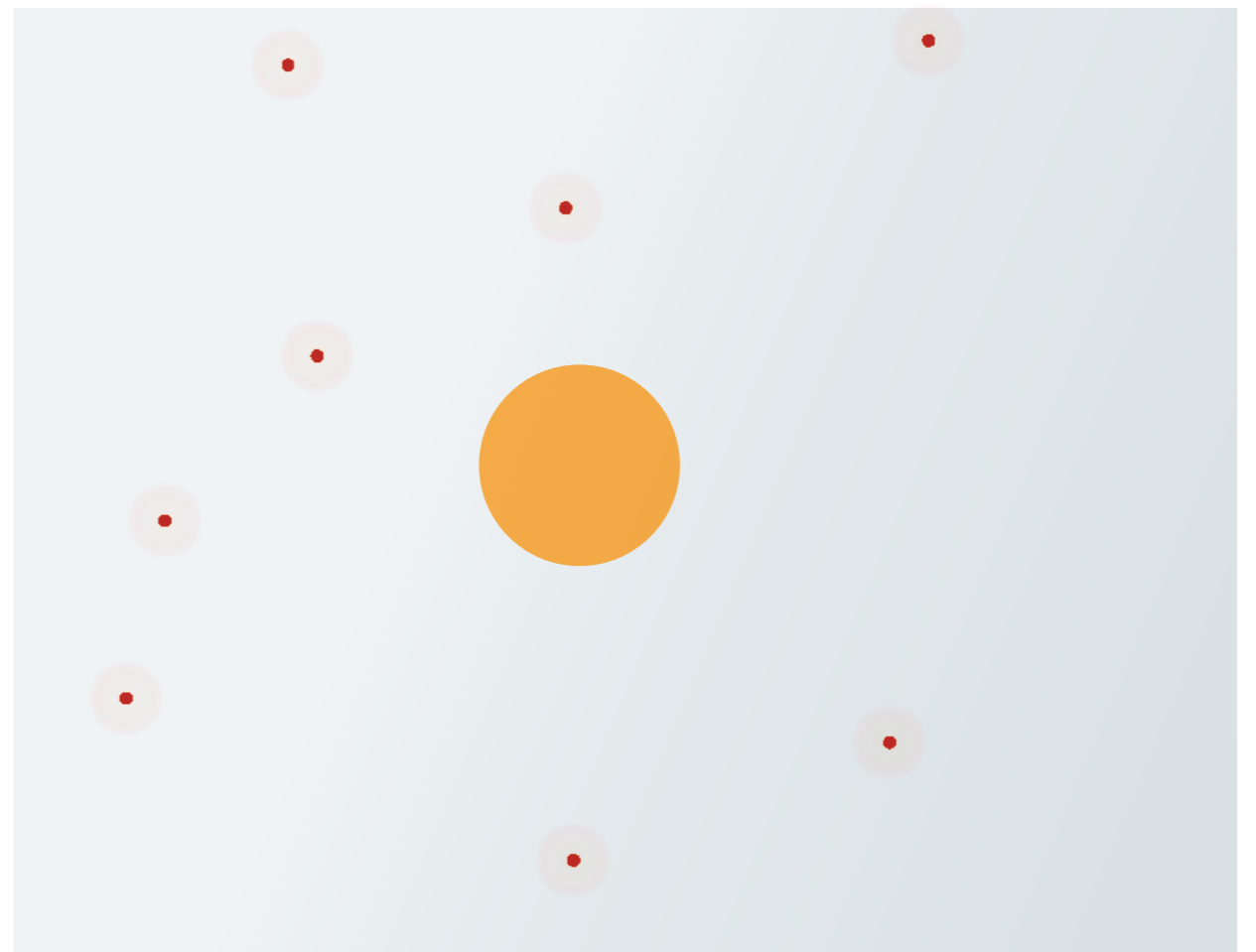
Cheers,

baptiste

MICROSCOPIC VIEWPOINT



discrete medium



homogeneous medium

$$\mathbf{E}_{\text{loc}} = \mathbf{E}_{\text{inc}} + \sum_{\text{dipoles} \setminus \text{itself}} \mathbf{E}_{\text{dip}} \quad \mathbf{p}_{\text{dip}} = \alpha \mathbf{E}_{\text{loc}}$$

$$\mathbf{E}^{\text{dipole}} = \frac{e^{i\omega r/c}}{4\pi\epsilon_0} \left\{ \frac{\omega^2}{c^2 r} \hat{\mathbf{r}} \times \mathbf{p} \times \hat{\mathbf{r}} + \left(\frac{1}{r^3} - \frac{i\omega}{cr^2} \right) [3(\hat{\mathbf{r}} \cdot \mathbf{p})\hat{\mathbf{r}} - \mathbf{p}] \right\}$$

$$\mathbf{A}\mathbf{P} = \mathbf{E}_{\text{inc}}$$

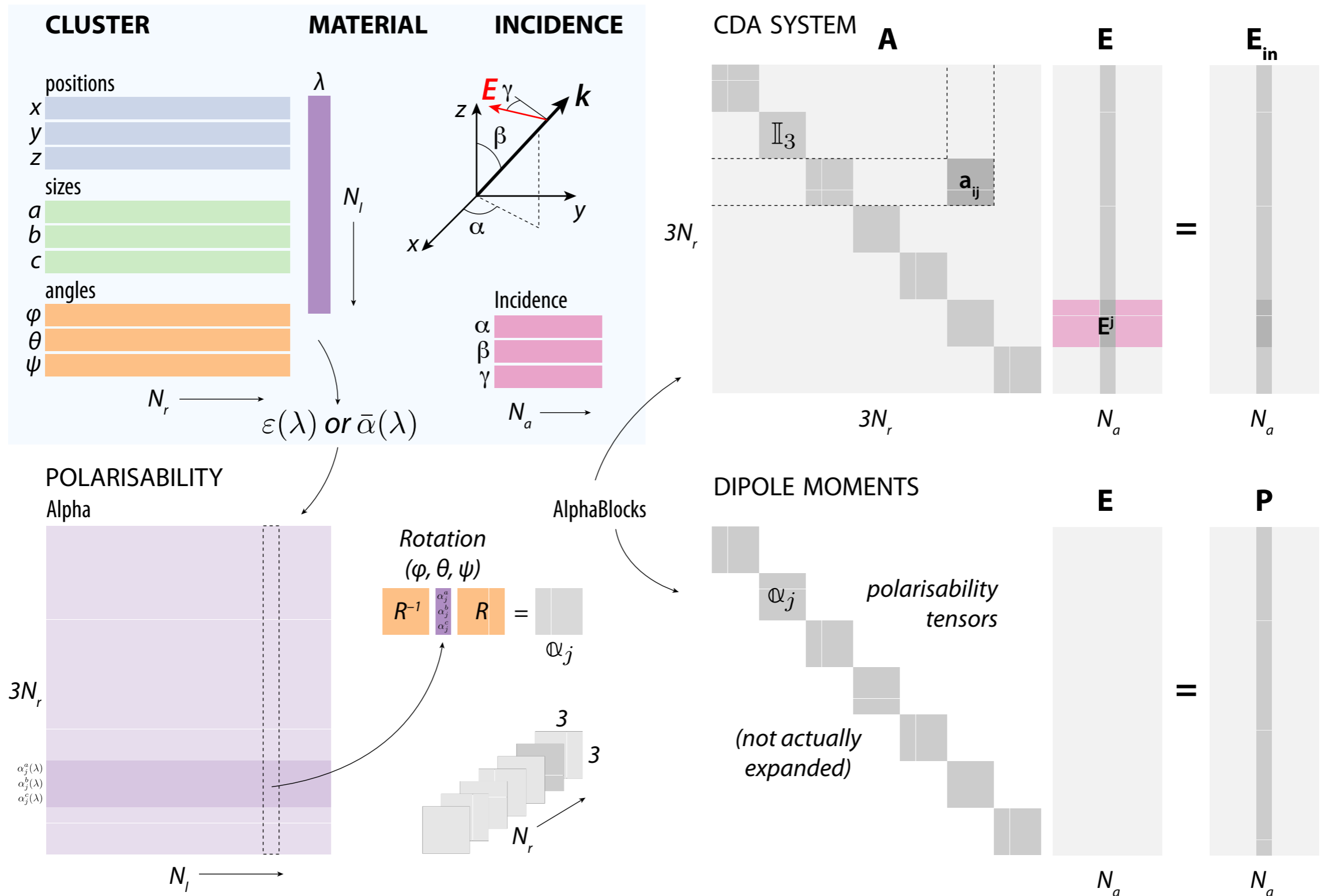
$$A_{ij} = \frac{e^{(ikr_{ij})}}{r_{ij}} \left\{ k^2 (\hat{\mathbf{r}}_{ij} \otimes \hat{\mathbf{r}}_{ij} - \mathbb{I}) + \frac{ikr_{ij} - 1}{r_{ij}^2} (3\mathbf{r}_{ij} \otimes \mathbf{r}_{ij} - \mathbb{I}) \right\}$$

$$\sigma_{\text{ext}} = \frac{4\pi k}{|\mathbf{E}_{\text{inc}}|^2} \Im(\mathbf{E}_{\text{inc}}^* \cdot \mathbf{P}) \quad \sigma_{\text{CD}} = \langle \sigma_L \rangle_{\Omega} - \langle \sigma_R \rangle_{\Omega}$$

$$\mathbf{E}_{\text{inc}} = \frac{\exp i(\omega t - k_x x)}{\sqrt{2}} \begin{pmatrix} 0 \\ i \\ 1 \end{pmatrix} \quad (\text{right-handed})$$

$$\mathbf{E}_{\text{inc}} = \frac{\exp i(\omega t - k_x x)}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ i \end{pmatrix} \quad (\text{left-handed})$$

MATRIX LAYOUT

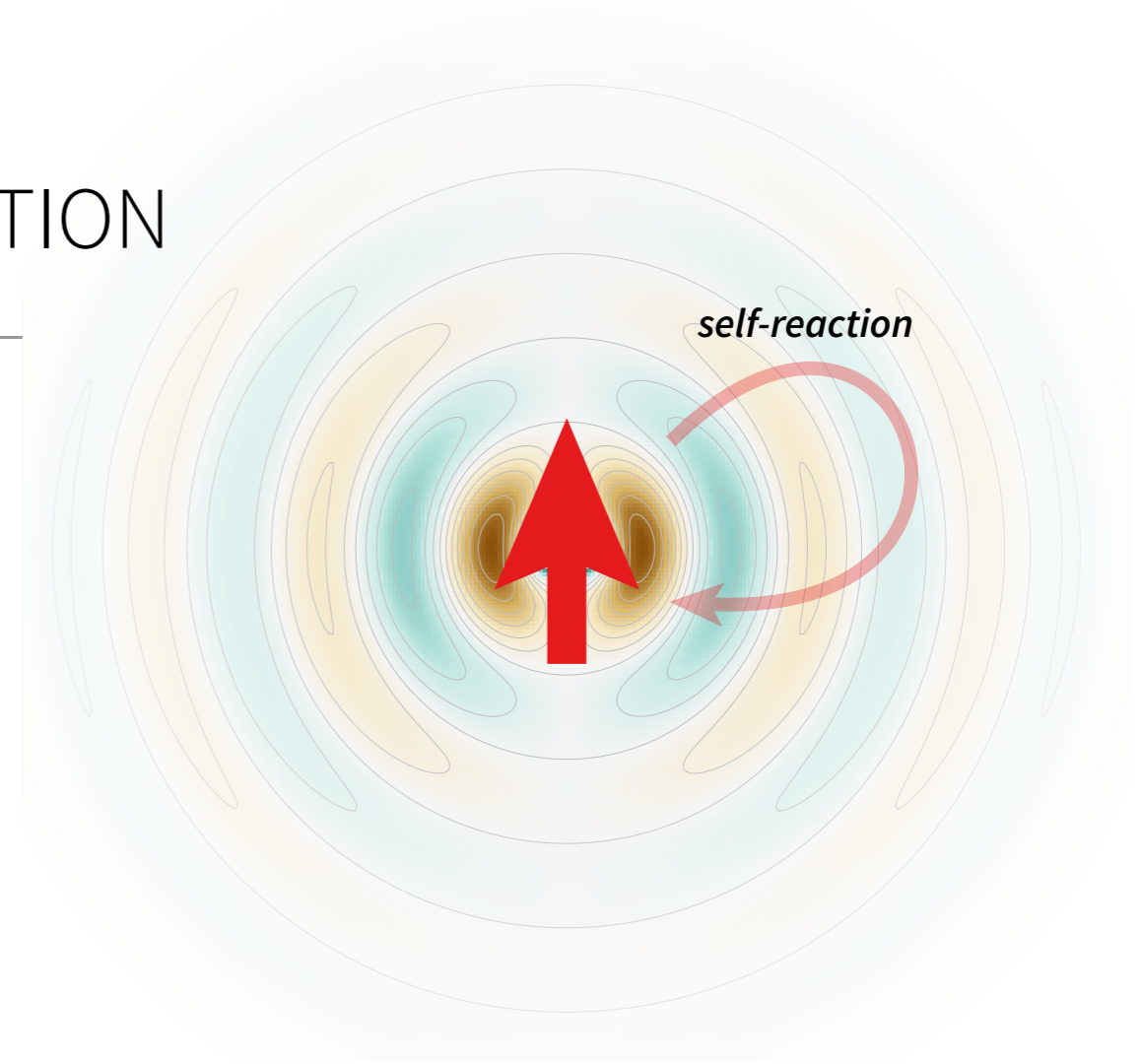


FUN WITH CONSTANTS AND PRE-FACTORS

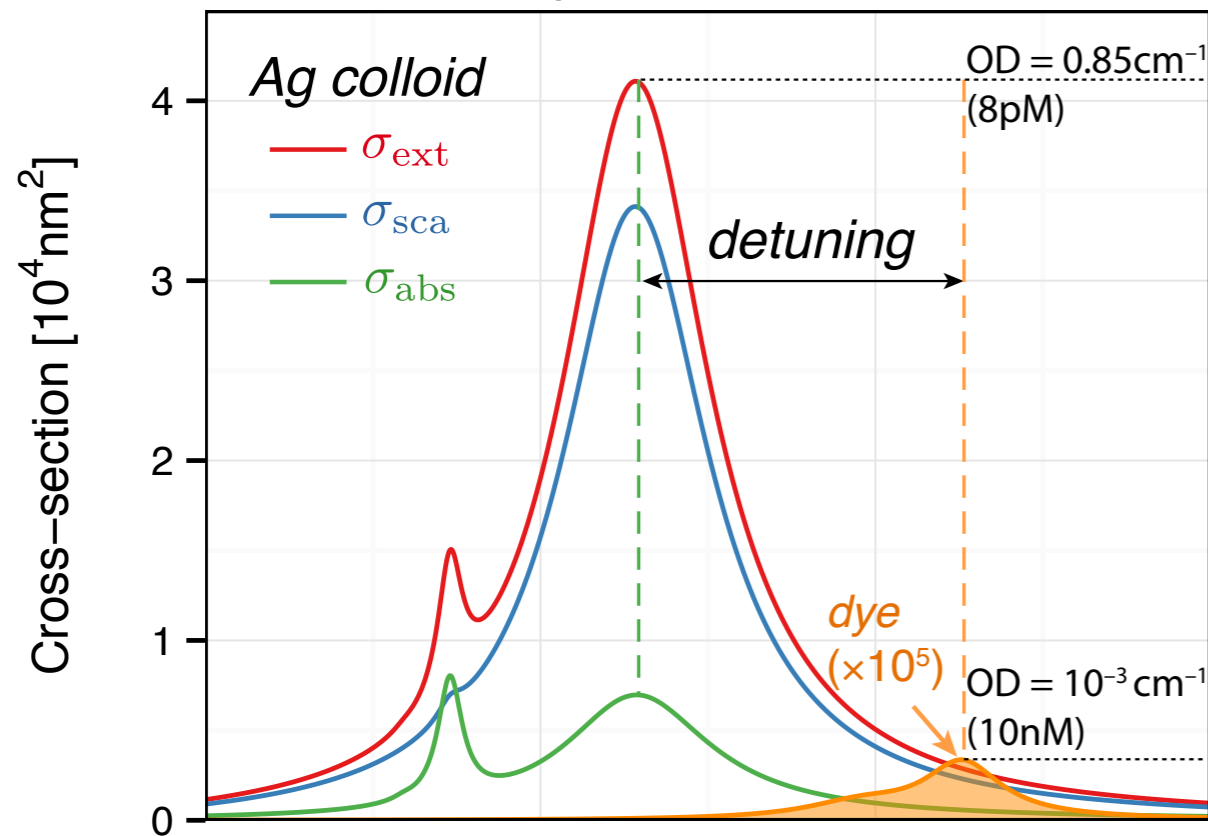
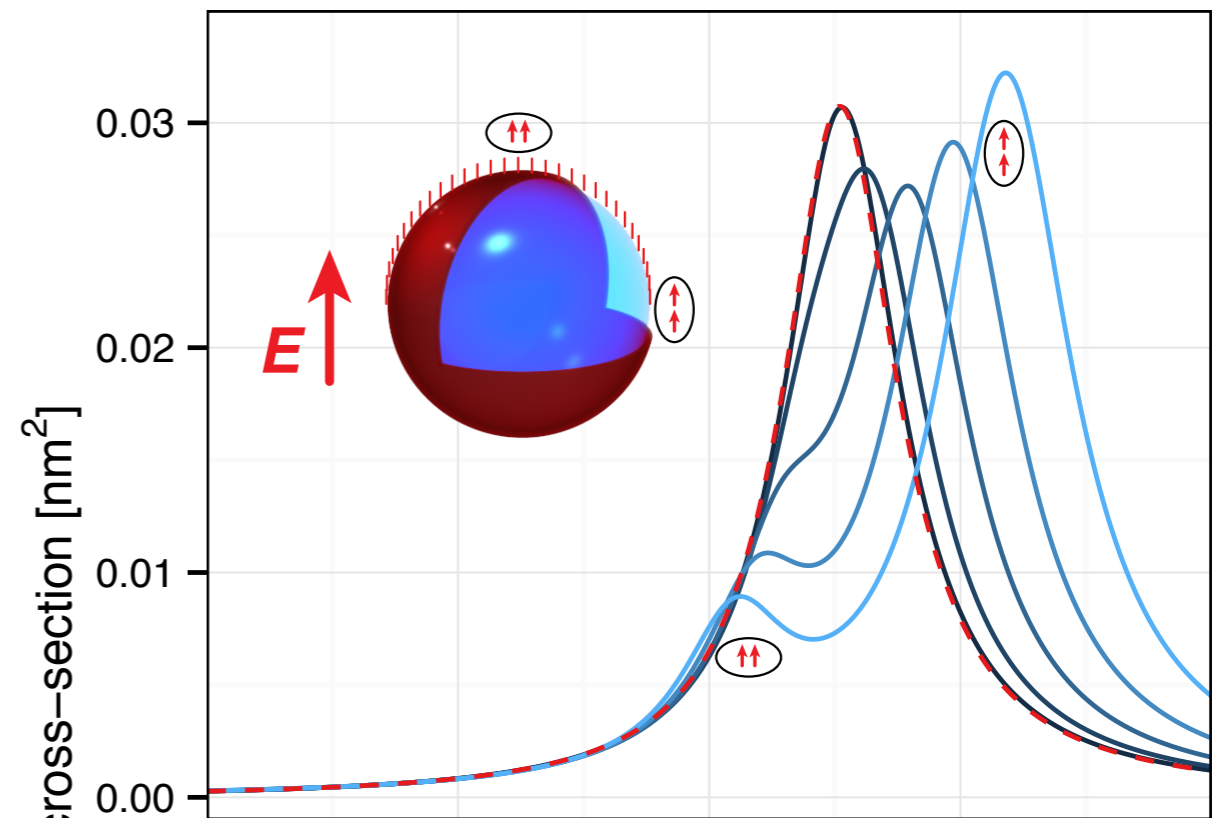
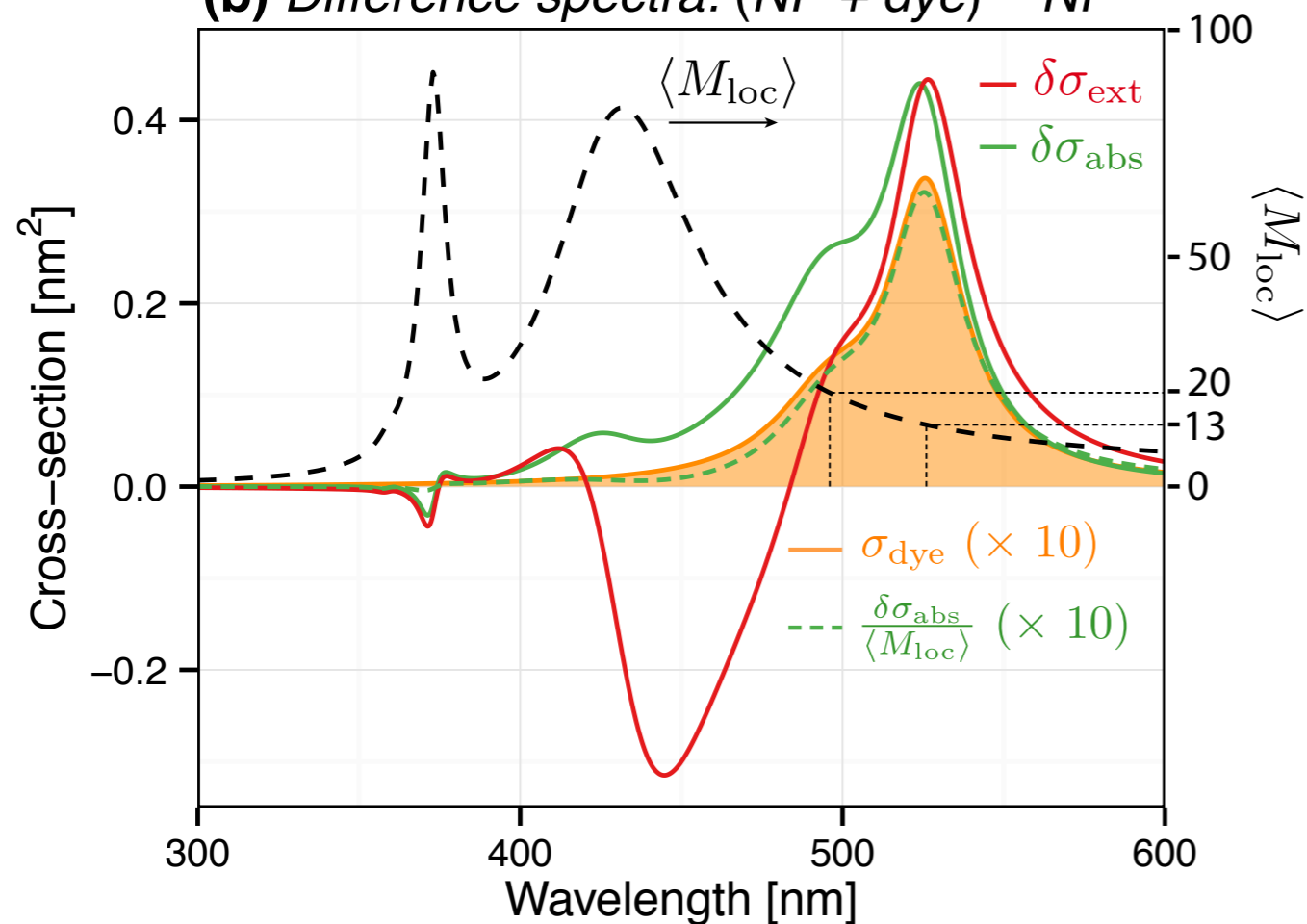
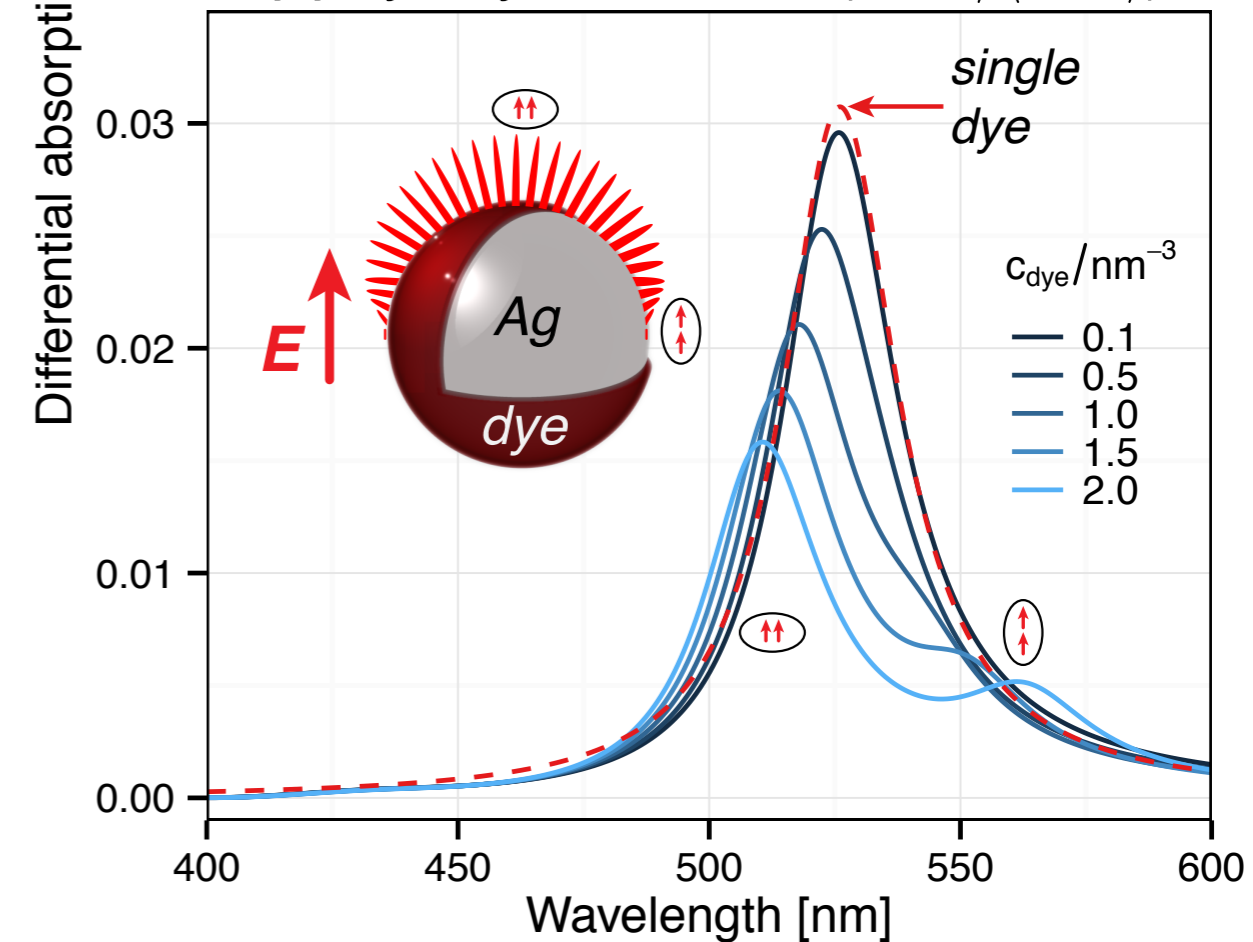
	Theory ($\kappa = 4\pi\epsilon_0\epsilon_1$ prefactor)	Equivalent formulation used in the code
polarisability	α	$\bar{\alpha} = \kappa^{-1}\alpha$
sphere (CM)	$\alpha_{\text{CM}} = \kappa a^3 \frac{\epsilon_1 - \epsilon_1}{\epsilon_1 + 2\epsilon_1}$	$\bar{\alpha}_{\text{CM}} = a^3 \frac{\epsilon_1 - \epsilon_1}{\epsilon_1 + 2\epsilon_1}$
dipole moment	$\mathbf{p} = \alpha \mathbf{E}$	$\bar{\mathbf{p}} = \kappa^{-1} \mathbf{p}$
Green's function	$\mathbb{G} = \kappa^{-1} \frac{e^{ik_1 r}}{r} \{\dots\}$	$\bar{\mathbb{G}} = \kappa \mathbb{G} = \frac{e^{ik_1 r}}{r} \{\dots\}$
cross-sections	$\sigma_{\text{ext}} = 4\pi k_1 \kappa^{-1} \Im(\mathbf{P} \cdot \mathbf{E}_{\text{inc}}^*)$ $\sigma_{\text{abs}} = 4\pi k_1 \kappa^{-1} \left[\Im(\mathbf{P} \cdot \mathbf{E}^*) - \frac{2}{3} k^3 \mathbf{P} ^2 \right]$ $\sigma_{\text{sca}} = \frac{\kappa^{-2} k_1^4}{4\pi} \iint_{\Omega} \left \sum_i (\mathbb{I} - \hat{\mathbf{n}} \otimes \hat{\mathbf{n}}) \mathbf{p}_i e^{-ik_1 \mathbf{r}_i \cdot \hat{\mathbf{n}}} \right ^2 d\Omega$	$\sigma_{\text{ext}} = 4\pi k_1 \Im(\bar{\mathbf{P}} \cdot \mathbf{E}_{\text{inc}}^*)$ $\sigma_{\text{abs}} = 4\pi k_1 \left[\Im(\bar{\mathbf{P}} \cdot \mathbf{E}^*) - \frac{2}{3} k^3 \bar{\mathbf{P}} ^2 \right]$ $\sigma_{\text{sca}} = \frac{k_1^4}{4\pi} \iint_{\Omega} \left \sum_i (\mathbb{I} - \hat{\mathbf{n}} \otimes \hat{\mathbf{n}}) \bar{\mathbf{p}}_i e^{-ik_1 \mathbf{r}_i \cdot \hat{\mathbf{n}}} \right ^2 d\Omega$

RADIATIVE CORRECTION & SELF-REACTION

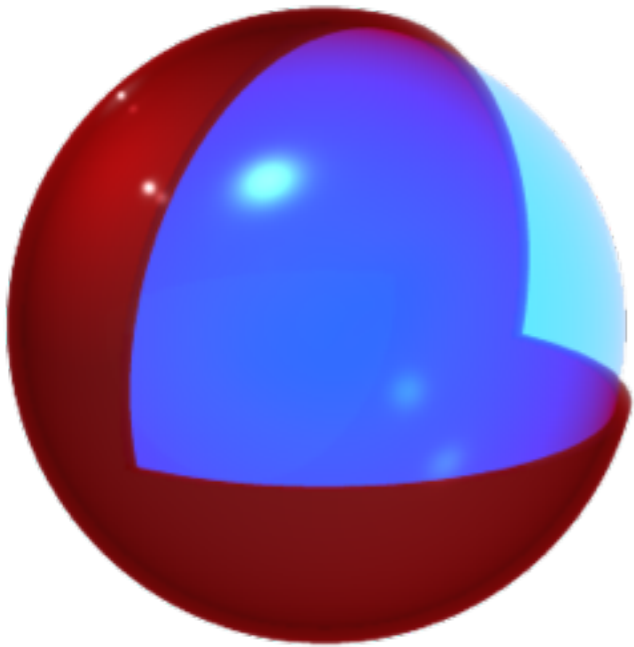
- Radiating dipole loses energy
- Conservation of energy requires a correction to the polarisability
- Introduced via G , or alpha



	Radiative correction	Self-reaction
total field	$\mathbf{E}^i = \mathbf{E}_{\text{inc}} + \sum_{j \neq i} \mathbb{G}_{ij} \alpha_j \mathbf{E}^j$	$\tilde{\mathbf{E}}^i = \mathbf{E}^i + \mathbf{E}^{\text{SR}} = \mathbf{E}^i + \mathbb{G}_{ii} \alpha_i \mathbf{E}^i$
dipole moment	$\mathbf{p} = \alpha \mathbf{E}$	$\mathbf{p} = \alpha^0 \tilde{\mathbf{E}} = \alpha^0 (\mathbf{E} + \mathbf{E}^{\text{SR}})$
polarisability	$\alpha = \frac{1}{\frac{1}{\alpha^0} - G} \text{ (RC)}$	$\alpha^0 \text{ (static)}$
absorption	$P_{\text{abs}} = \frac{\omega}{2} (\Im(\alpha) \mathbf{E} ^2 - \Im(G) \mathbf{P} ^2)$	$P_{\text{abs}} = \frac{\omega}{2} \Im(\alpha^0) \tilde{\mathbf{E}} ^2$

(a) Bare components**(c) Hollow dye shell ($\delta\sigma_{\text{abs}}$)****(b) Difference spectra: (NP + dye) - NP****(d) Dye layer on colloid ($\delta\sigma_{\text{abs}}/\langle M_{\text{loc}} \rangle$)**

MIE SHELL MODEL



$$\sigma_{\text{abs}}(\omega) = \frac{(\epsilon_M + 2)^2}{9\sqrt{\epsilon_M}} \frac{\omega}{\epsilon_0 c} \text{Im} [\alpha_D(\omega)]$$

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

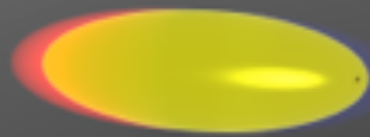


$$\epsilon_{\text{dye}} = \frac{1 + \frac{2}{3}(\tilde{\alpha}_M + \tilde{\alpha}_D)}{1 - \frac{1}{3}(\tilde{\alpha}_M + \tilde{\alpha}_D)}$$

$$\tilde{\alpha}_D(\omega) = c_D \frac{\alpha_D}{\epsilon_0}$$

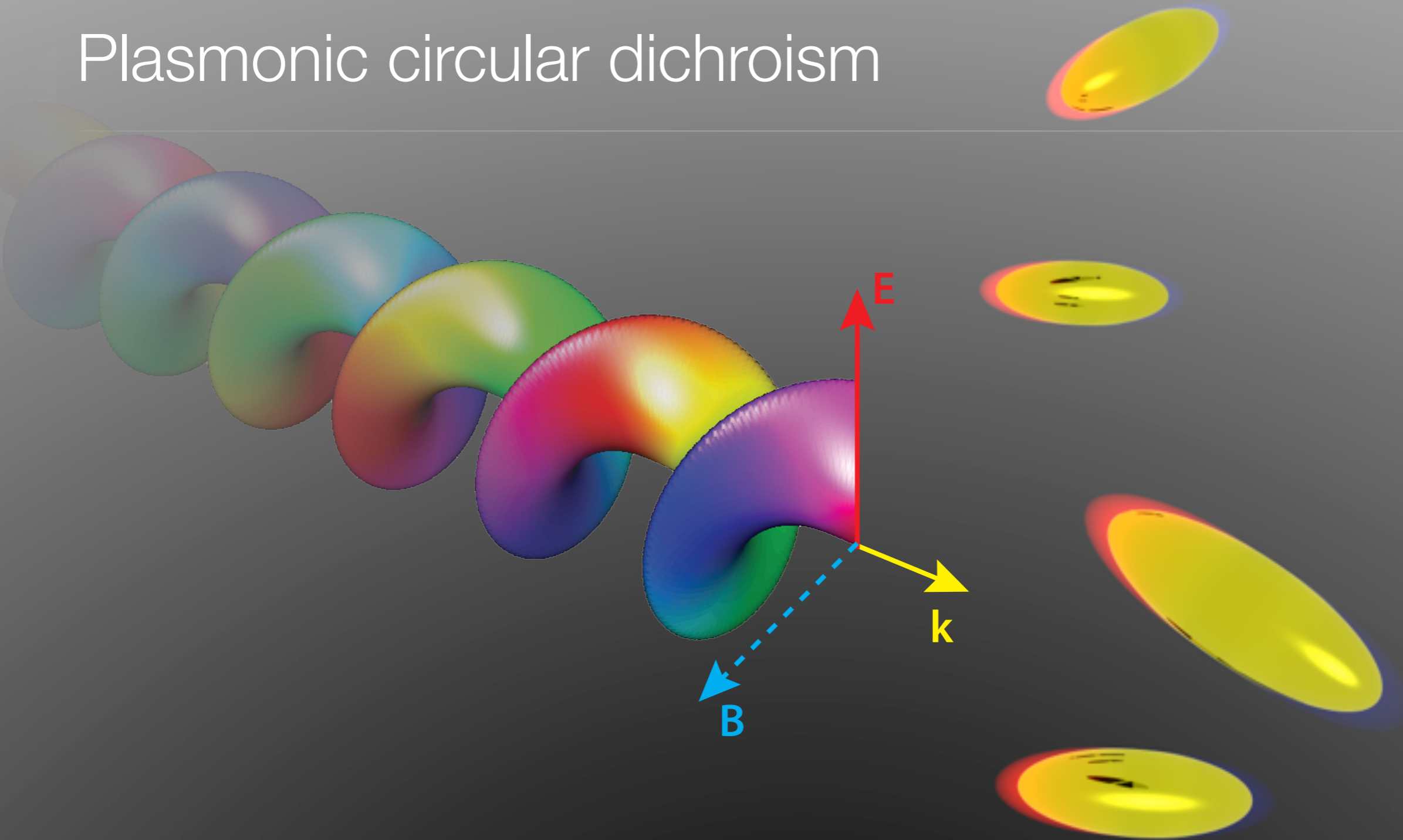
COUPLED-DIPOLE APPROXIMATION

$$a \ll \lambda$$

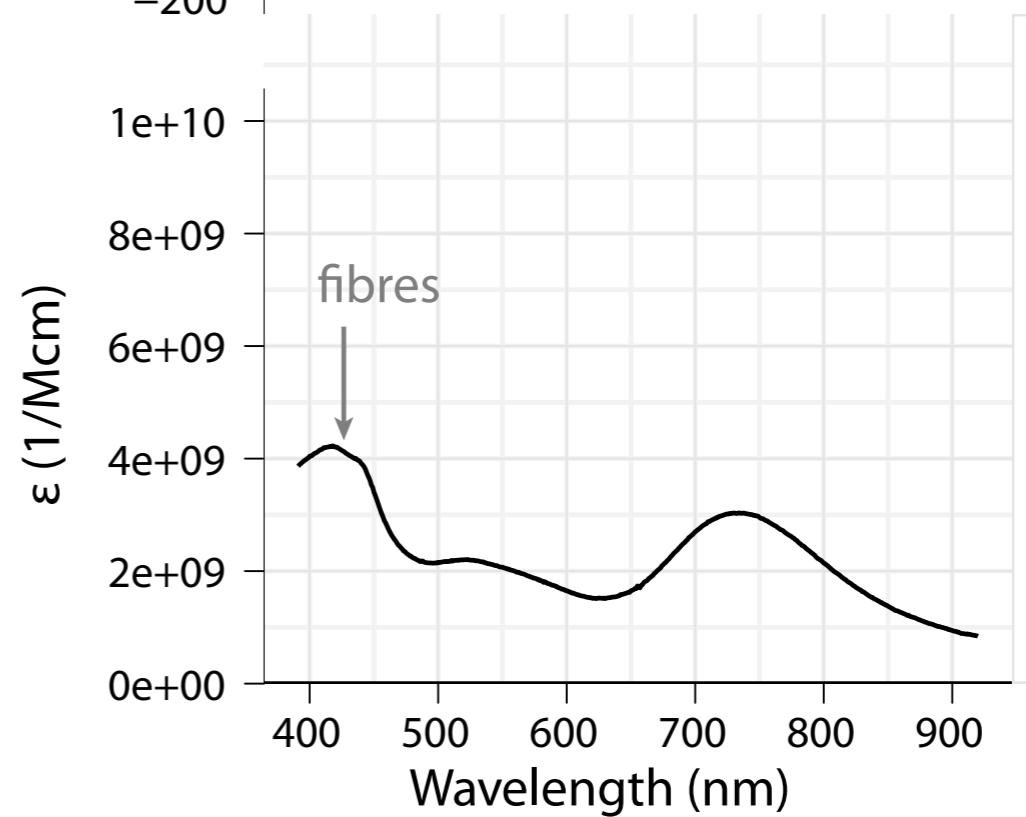
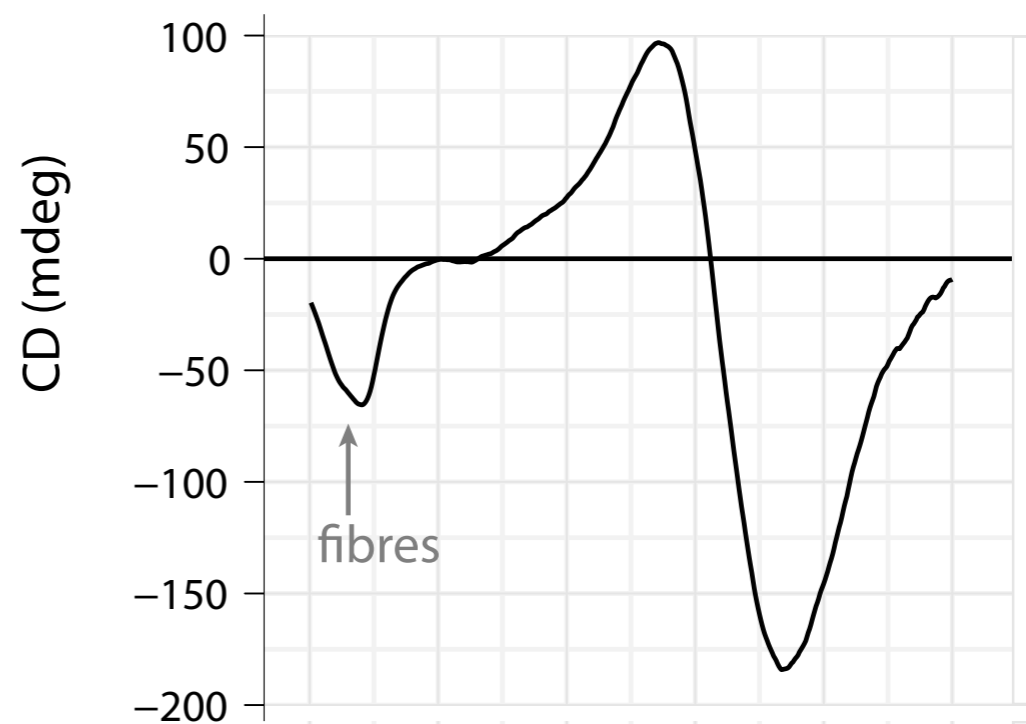
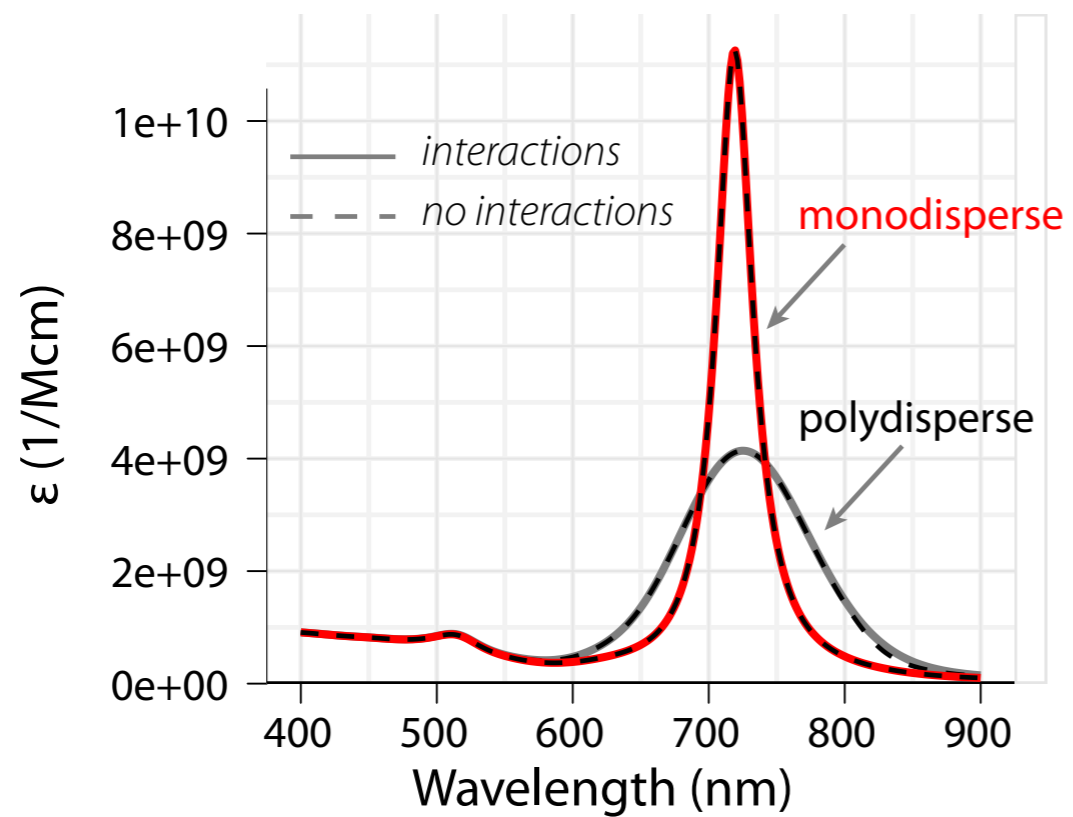
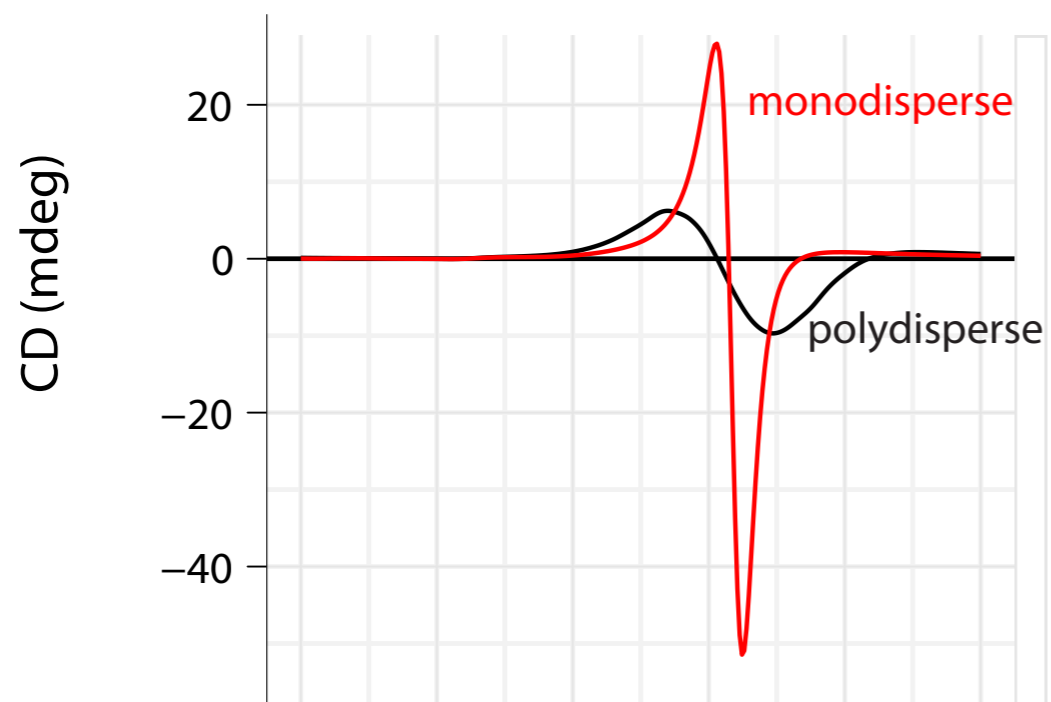


$$d \gg a$$

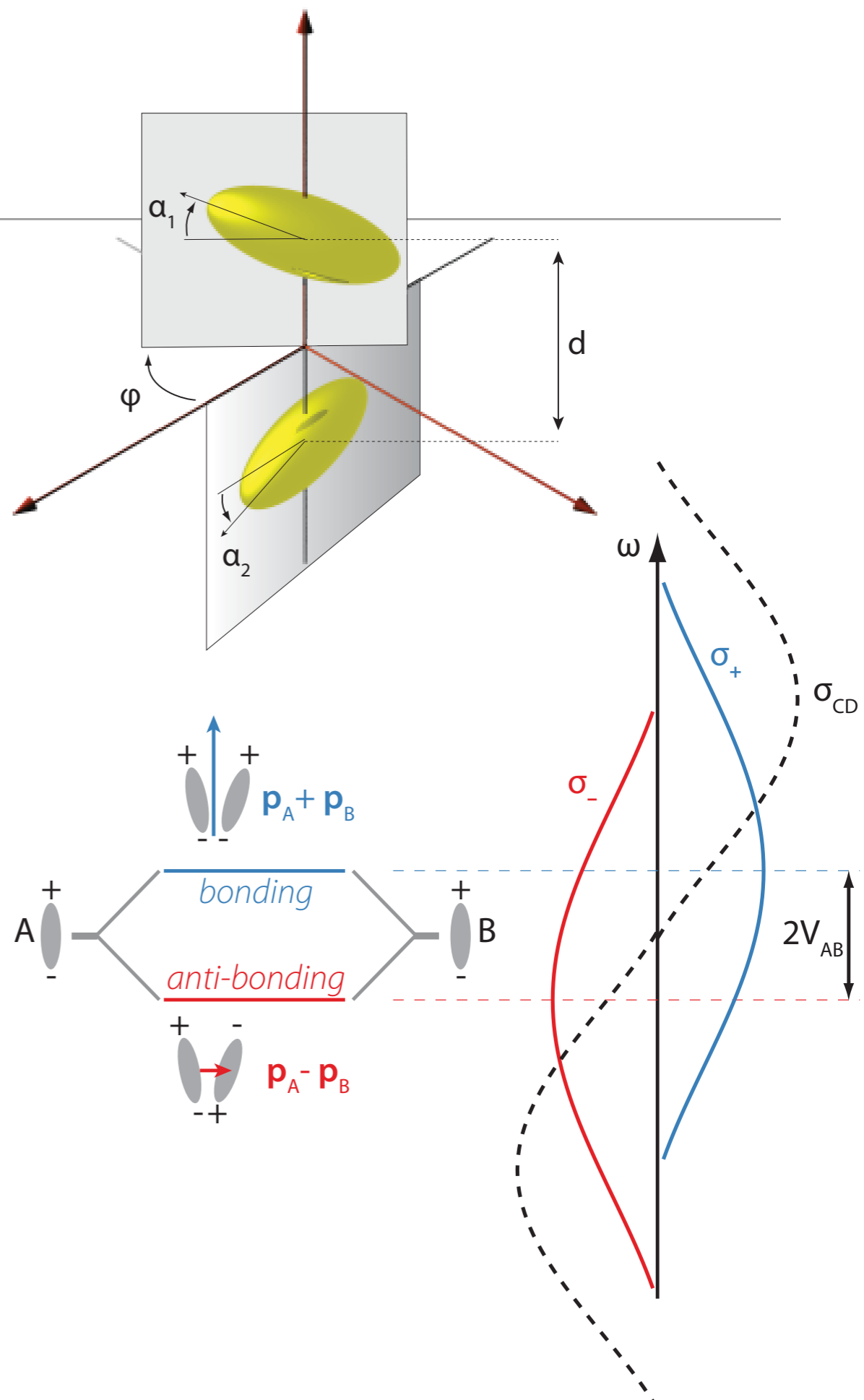
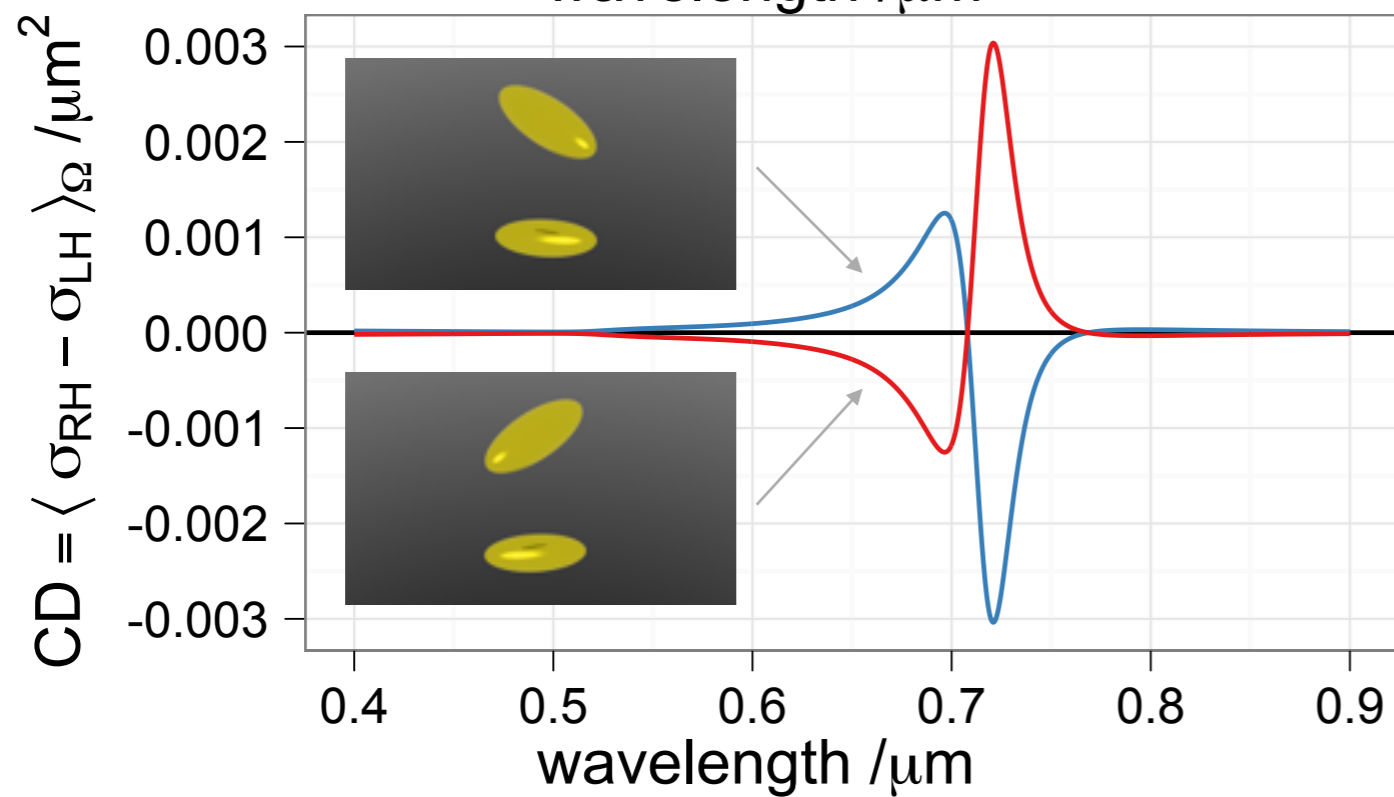
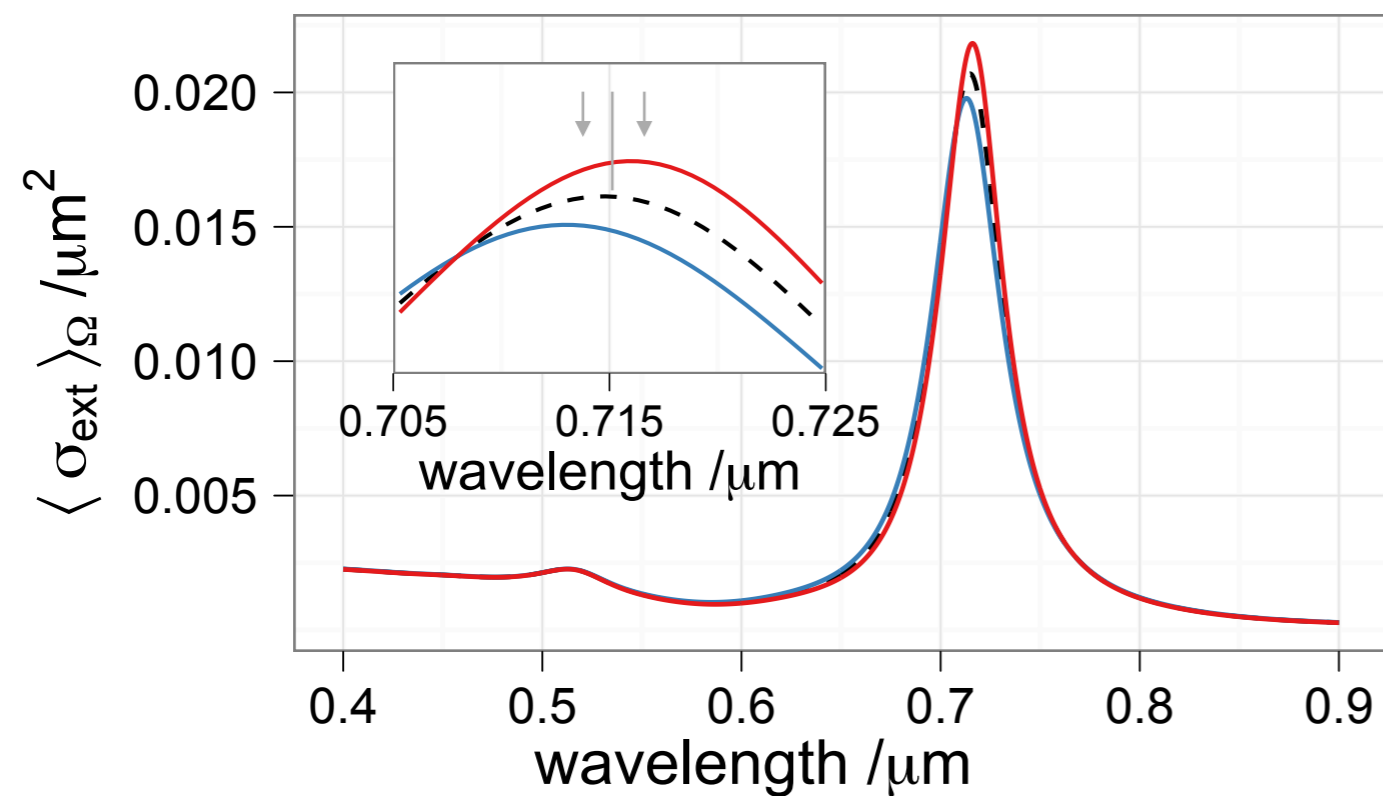
Plasmonic circular dichroism



chiral cluster
electromagnetic coupling



CHIRAL PLASMON HYBRIDISATION



HELIX OF NANORODS

