Hybrid resonances in plasmonic nanoparticle gratings

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Skolkovo Institute of Science and Technology

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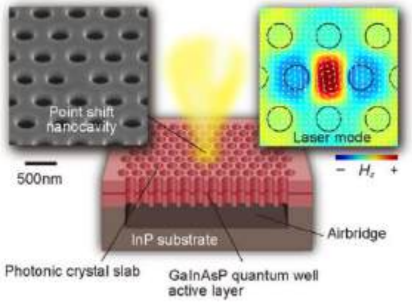
RSF | Russian Science Foundation

grant №22-12-00351

Clover

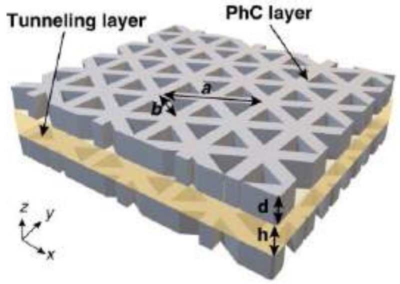
Resonances in nanophotonics

Photonic Crystal Defects



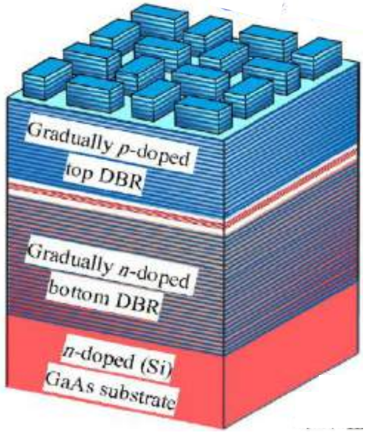
MRS Commun **5**, 4, 555 (2015)

Photonic Crystal Slabs



Light Sci Appl **10**, 157 (2021)

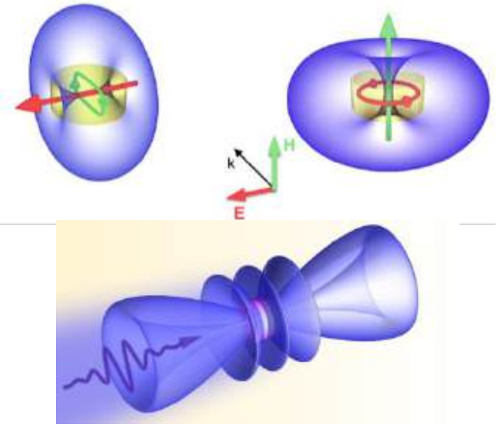
Fabry-Perot resonators



Phys Rev Applied **17**, L021001

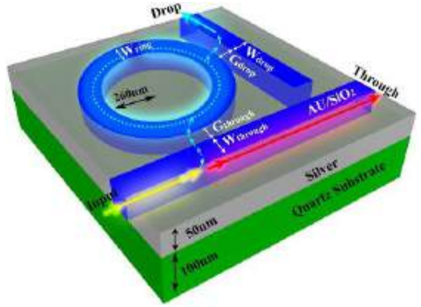
Dielectric Resonators

Mie resonances



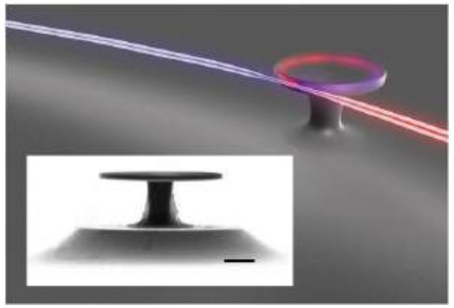
ACS Photonics **4**, 2638 (2017)

Ring resonators



Sci Rep **14**, 5787 (2024)

Whispering Galleries



Nat Commun **5**, 3109 (2014)

Resonances in nanophotonics

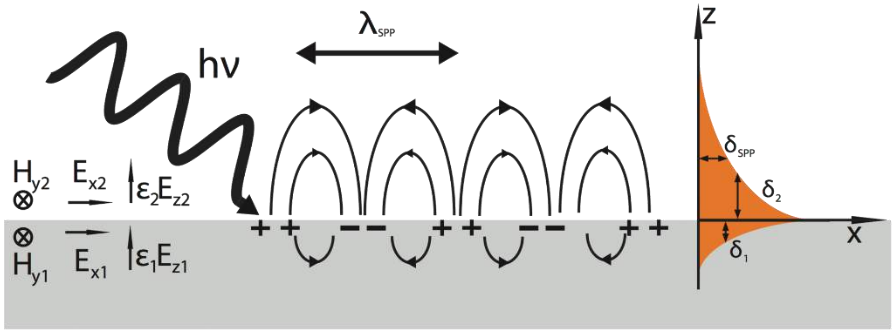
Dielectric Resonators

- Transparent, non-dissipating materials
- High quality factor (up to 10^{10})
- Delocalized fields

Resonances in nanophotonics

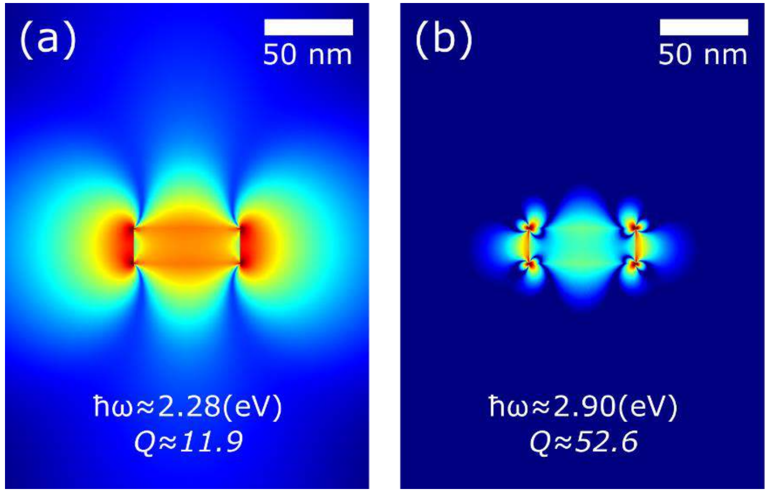
Plasmonic Resonators

Surface Plasmon Resonance



wikipedia.org

Localized Surface Plasmon Resonance



Resonances in nanophotonics

Plasmonic Resonators

- Intrinsic Joule heating
- Low quality factor ($10^1 - 10^2$)
- Deep-subwavelength field localization

Resonances in nanophotonics

Dielectric Resonators

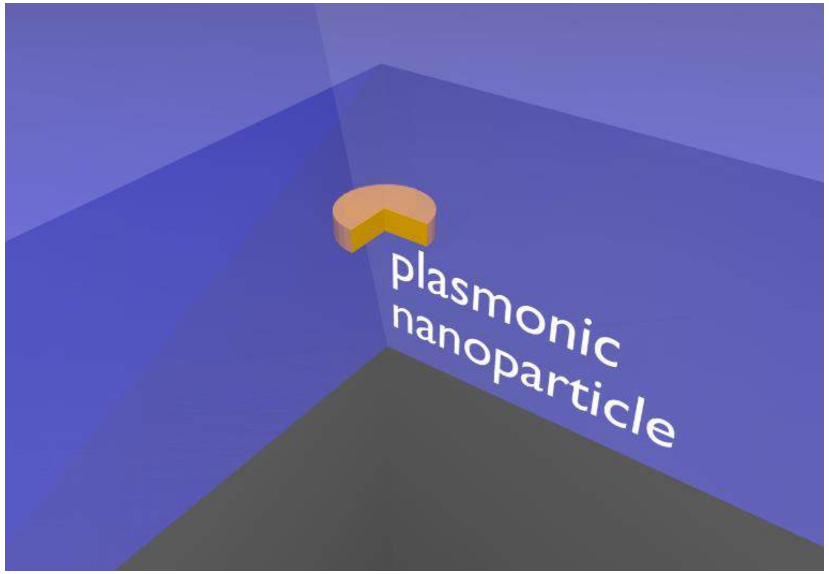
- Transparent, non-dissipating materials
- High quality factor (up to 10^{10})
- Delocalized fields

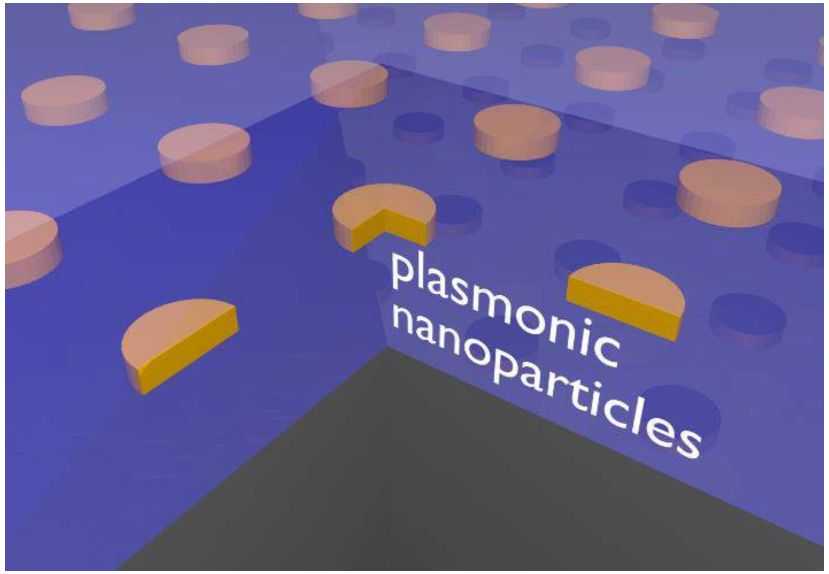
Plasmonic Resonators

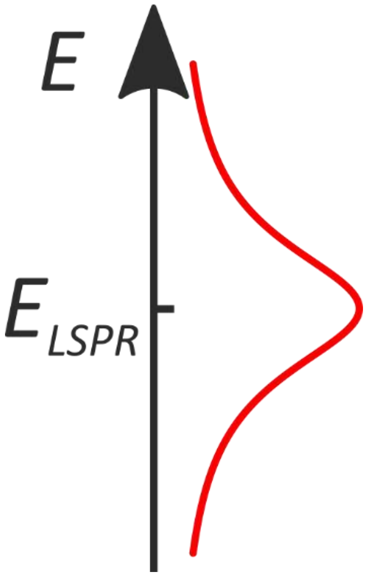
- Intrinsic Joule heating
- Low quality factor ($10^1 - 10^2$)
- Deep-subwavelength field localization

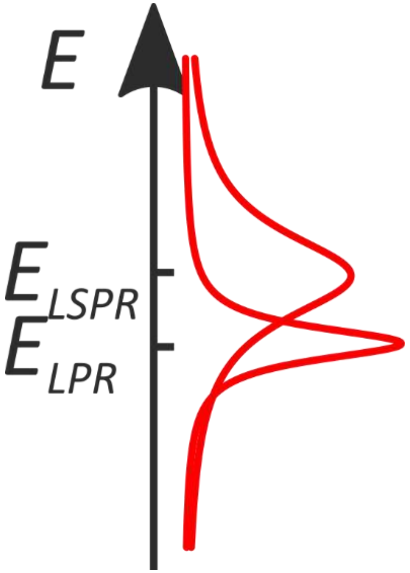
Is it possible to combine both advantages?

Hybrid resonances







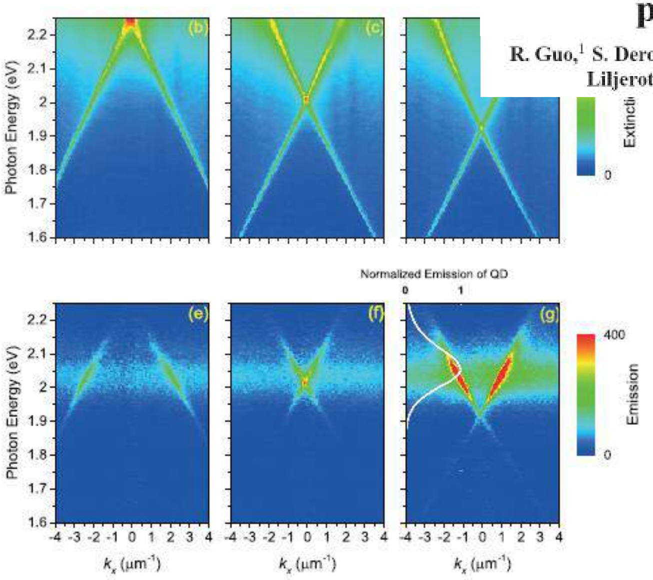


Collective mode!

Applications

Controlling quantum dot emission by plasmonic nanoarrays

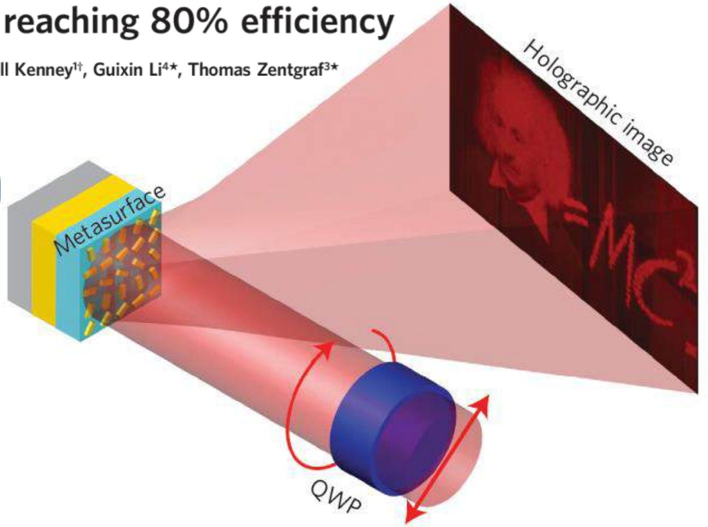
R. Guo,[1] S. Derom,[1] A. I. Väkeväinen,[1] R. J. A. van Dijk-Moes,[2] P. Liljeroth,[3] D. Vanmaekelbergh,[2] and P. Törmä[1,*]



nature nanotechnology LETTERS
PUBLISHED ONLINE: 23 FEBRUARY 2015 | DOI: 10.1038/NNANO.2015.2

Metasurface holograms reaching 80% efficiency

Guoxing Zheng[1,2†], Holger Mühlenbernd[3†], Mitchell Kenney[1†], Guixin Li[4*], Thomas Zentgraf[3*] and Shuang Zhang[1*]



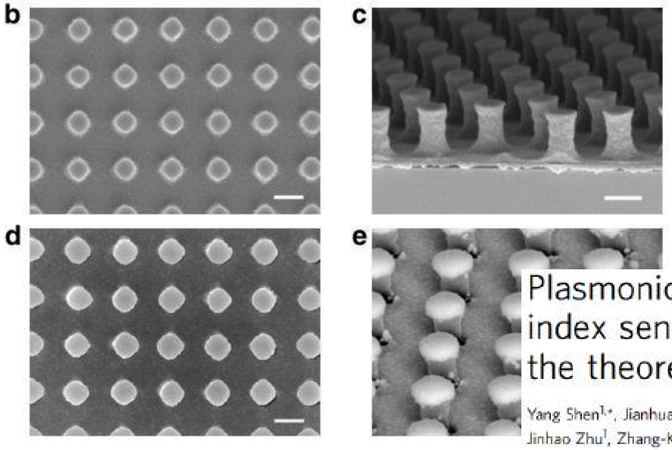
Emission control

Holography

Plasmonic lattices

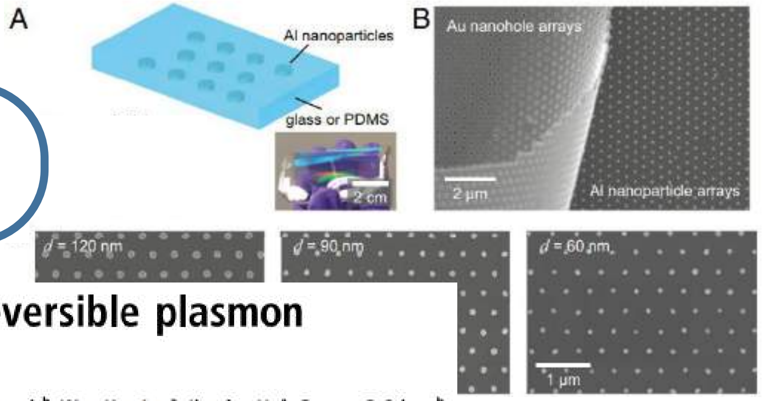
Sensing

Tunable metasurfaces



Plasmonic gold mushroom arrays with refractive index sensing figures of merit approaching the theoretical limit

Yang Shen[1,*], Jianhua Zhou[2,*], Tianran Liu[1], Yuting Tao[3], Ruibin Jiang[3], Mingxuan Liu[1], Guohui Xiao[1], Jinhao Zhu[1], Zhang-Kai Zhou[1], Xuehua Wang[1], Chongjun Jin[1] & Jianfang Wang[3]



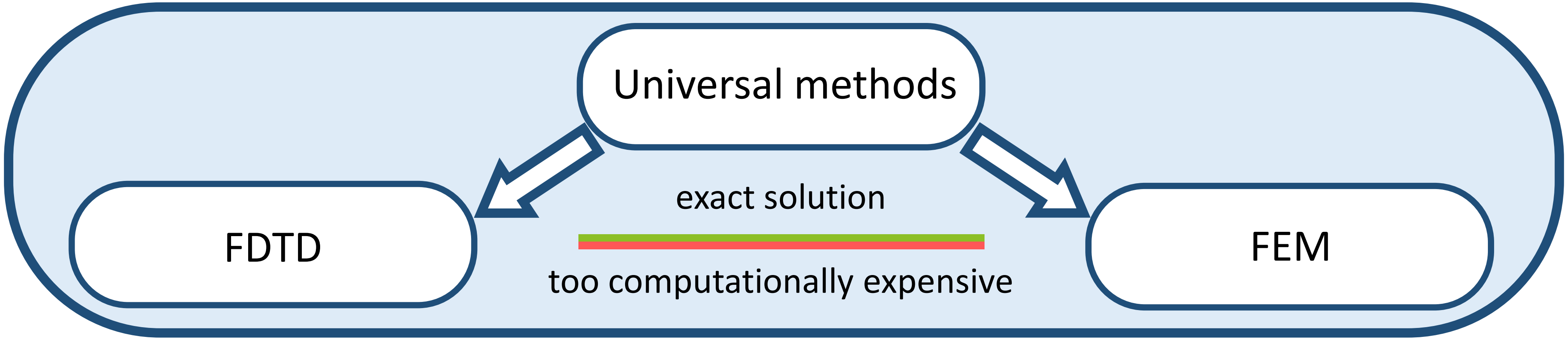
Programmable and reversible plasmon mode engineering

Ankun Yang[a], Alexander J. Hryn[a], Marc R. Bourgeois[b], Won-Kyu Lee[a], Jingtian Hu[a], George C. Schatz[b], and Teri W. Odom[a,b,1]

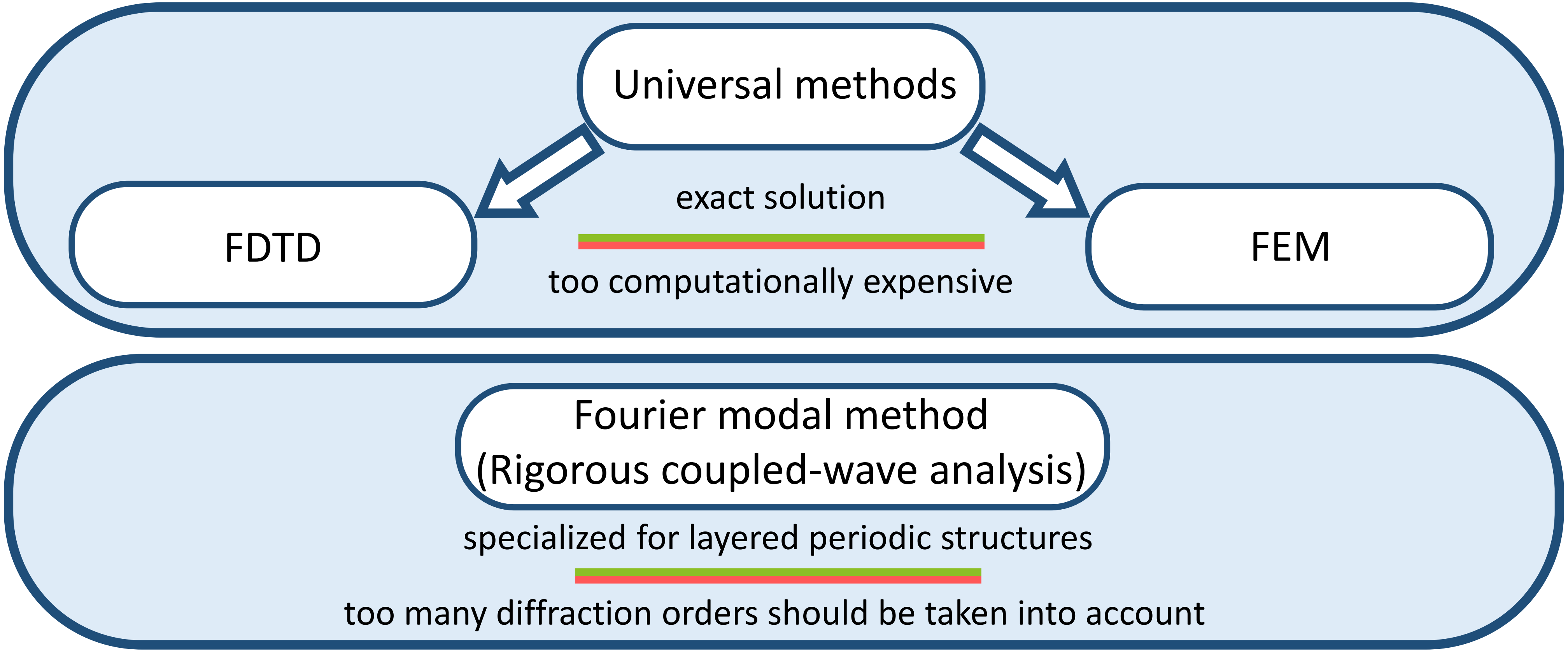
Outline

- How do plasmonic lattices work?
  - Interaction via waveguide modes and Rayleigh anomalies
- How to describe plasmonic lattices accurately?
  - Hybrid computational approach: dipole approximation and Fourier modal method
  - Dipole approximation validity
  - Polarizability calculation
  - Lattice sum calculation
- Applications
  - Stack of plasmonic lattices
  - Grating for routing circularly polarized light
- Conclusions

Theoretical approaches



Theoretical approaches



Theoretical approaches

Universal methods

FDTD

FEM

exact solution

too computationally expensive

Fourier modal method
(Rigorous coupled-wave analysis)

specialized for layered periodic structures

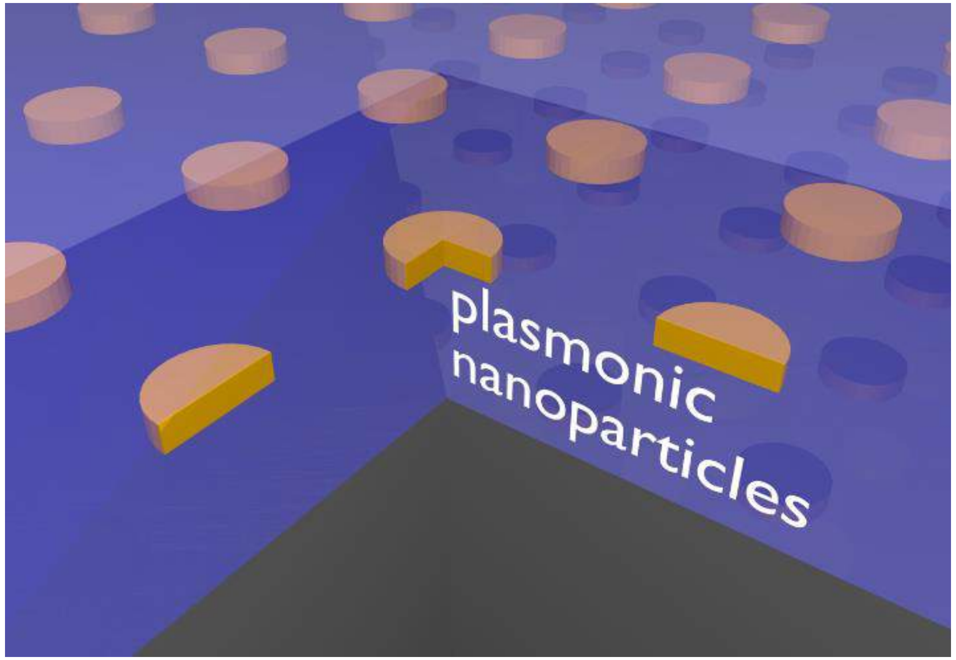
too many diffraction orders should be taken into account

Discrete dipole approximation

fast and efficient

hardly applicable for layered structures

Effective polarizability



$$\mathbf{P}_i = \hat{\alpha}\mathbf{E}_i^{\mathrm{bg}}$$

$$\mathbf{E}_i^{\mathrm{bg}} = \mathbf{E}_i^0 + \sum_{j\neq i} \hat{G}(\mathbf{r}_i, \mathbf{r}_j)\mathbf{P}_j$$

We apply Bloch theorem and solve the system of equations.

$$\mathbf{P}_i = \hat{\alpha}^{\mathrm{eff}}\mathbf{E}_i^0 \qquad \hat{\alpha}^{\mathrm{eff}} = \hat{\alpha}(\hat{I} - \hat{C}(\mathbf{k}_{\|})\hat{\alpha})^{-1}$$

$$\hat{C}(\mathbf{k}_{\|}) = \sum_{j\neq i} \hat{G}(\mathbf{r}_i, \mathbf{r}_j) e^{-i\mathbf{k}_{\|}(\mathbf{r}_i - \mathbf{r}_j)}$$

And obtain generalized **effective polarizability** tensor

Hybrid resonances

$$\hat{\alpha}^{\text{eff}} = \hat{\alpha}\left(\hat{I} - \hat{C}(\mathbf{k}_{\parallel})\hat{\alpha}\right)^{-1}$$

Localized resonance of individual nanoparticle

$$\mathrm{Re}\hat{\alpha}^{-1}(\omega) = 0$$

Hybrid lattice resonance

$$\mathrm{Re}\hat{\alpha}^{-1}(\omega) = \mathrm{Re}\hat{C}(\omega, \mathbf{k}_{\parallel})$$

Hybrid resonances

$$\hat{\alpha}^{\mathrm{eff}} = \hat{\alpha}\left(\hat{I} - \hat{C}(\mathbf{k}_{\parallel})\hat{\alpha}\right)^{-1}$$

Localized resonance of individual nanoparticle

$$\mathrm{Re}\hat{\alpha}^{-1}(\omega) = 0$$

Hybrid lattice resonance

$$\mathrm{Re}\hat{\alpha}^{-1}(\omega) = \mathrm{Re}\hat{C}(\omega, \mathbf{k}_{\parallel})$$

Particles are small

⇩

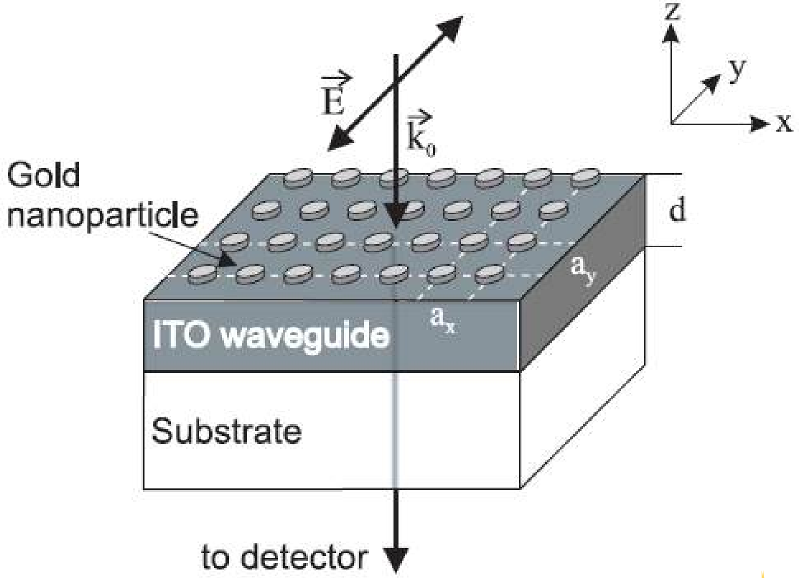
$\hat{\alpha}$ is small

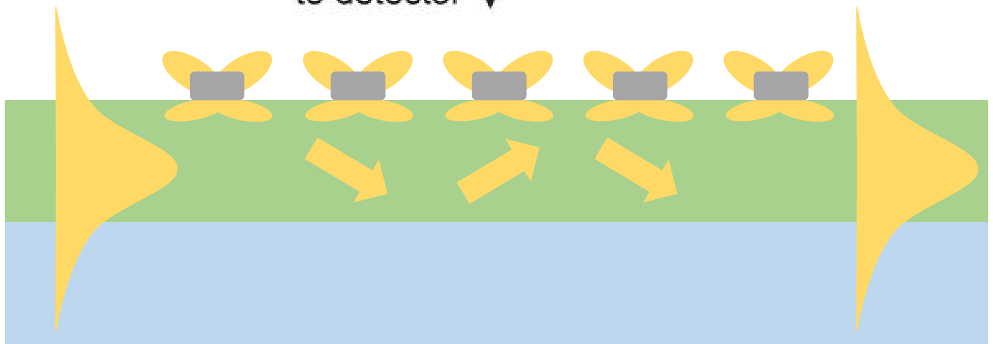
⇩

$\hat{C}$ should be large!

Plasmonic lattices

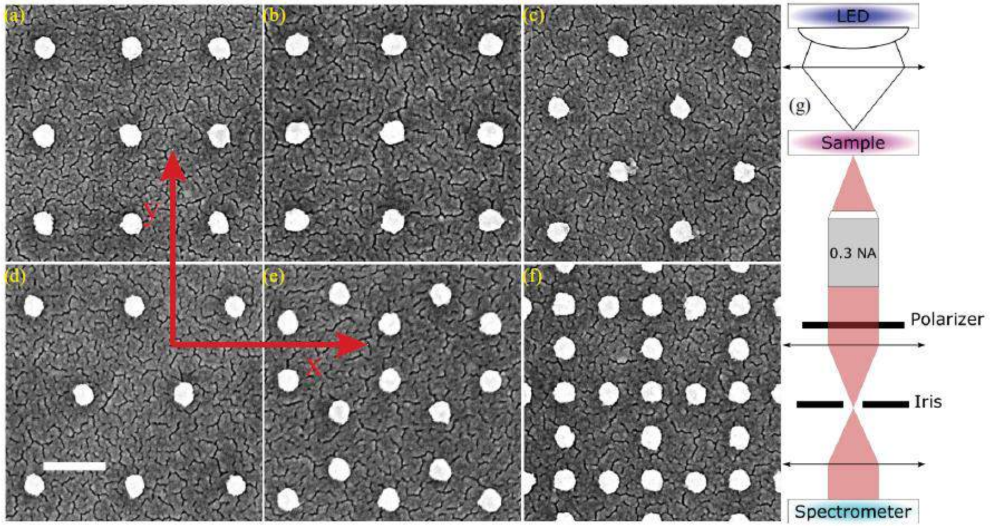
Interaction via waveguide modes

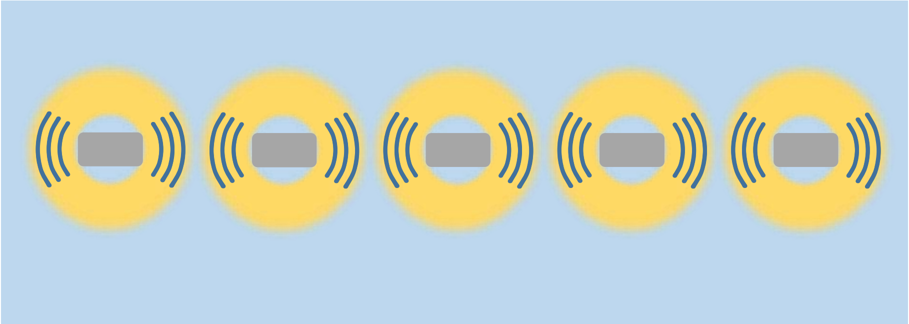




Linden, S., Kuhl, J., & Giessen, H. (2001), *Physical review letters*, *86*(20), 4688.

Direct interaction via far-field





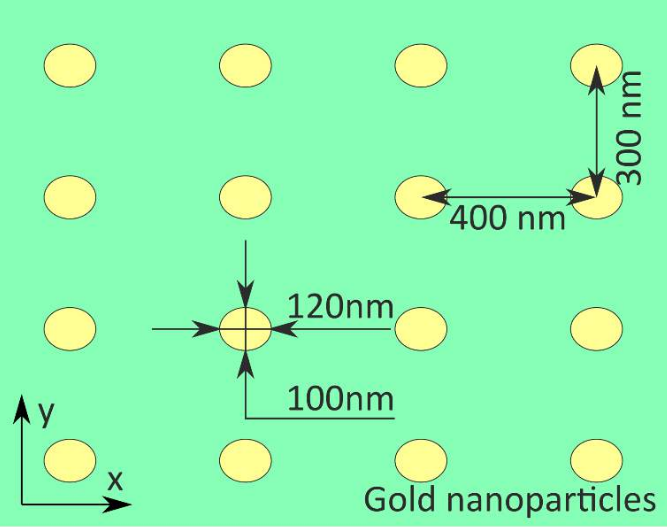
Guo, R., Hakala, T. K., & Törmä, P. (2017), *Physical Review B*, *95*(15), 155423.

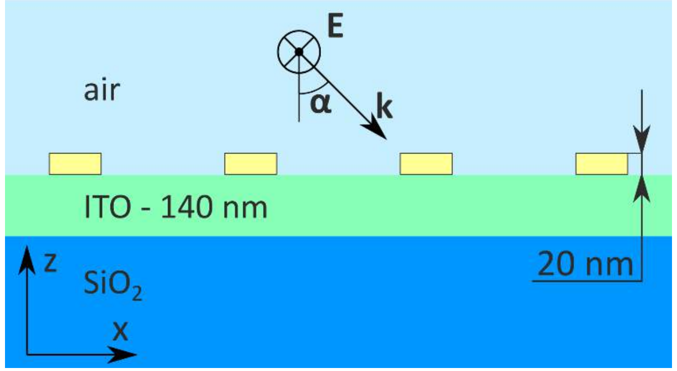
Plasmonic lattice on a waveguide

S. Linden, J. Kuhl and H. Giessen

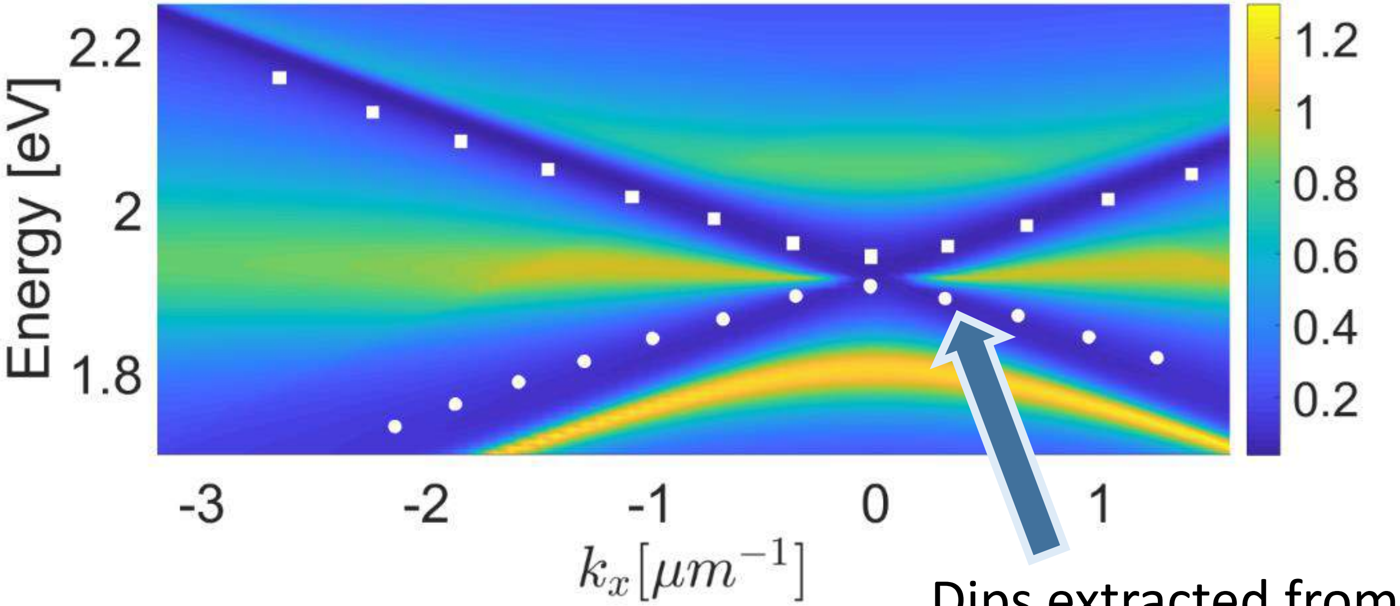
Controlling the Interaction between Light and Gold Nanoparticles: Selective Suppression of Extinction

PHYSICAL REVIEW LETTERS **86**, 4688 (2001)





Extinction $-\ln(I_T/I_0)$



Dips extracted from experimental data

Calculation time

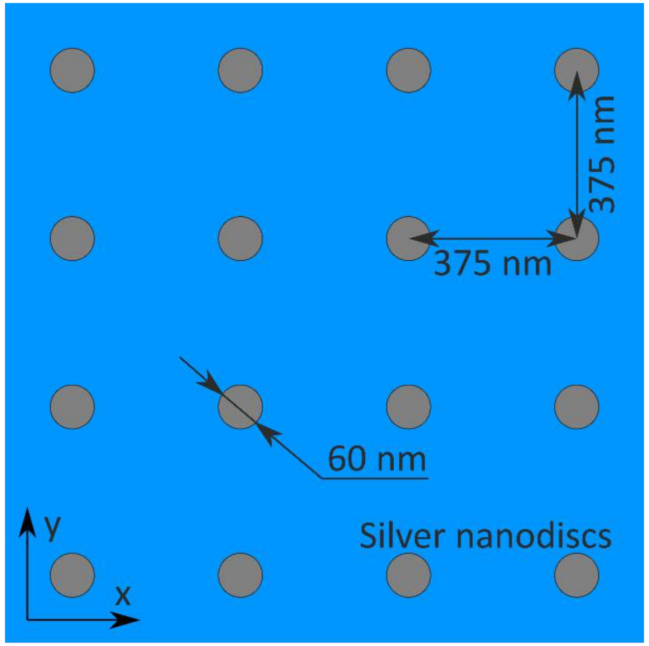
This work ≈ 5 minutes

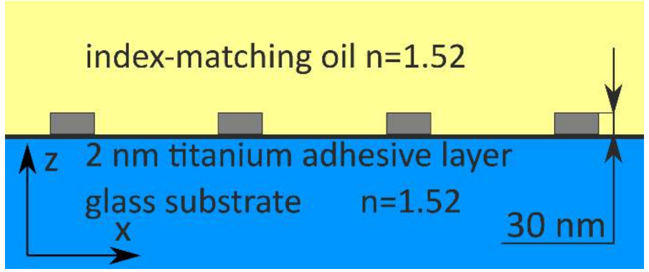
COMSOL: ~ 1 month

1 point ~ 1min   200x200 points ~ 40000 min

Plasmonic lattice in homogeneous medium

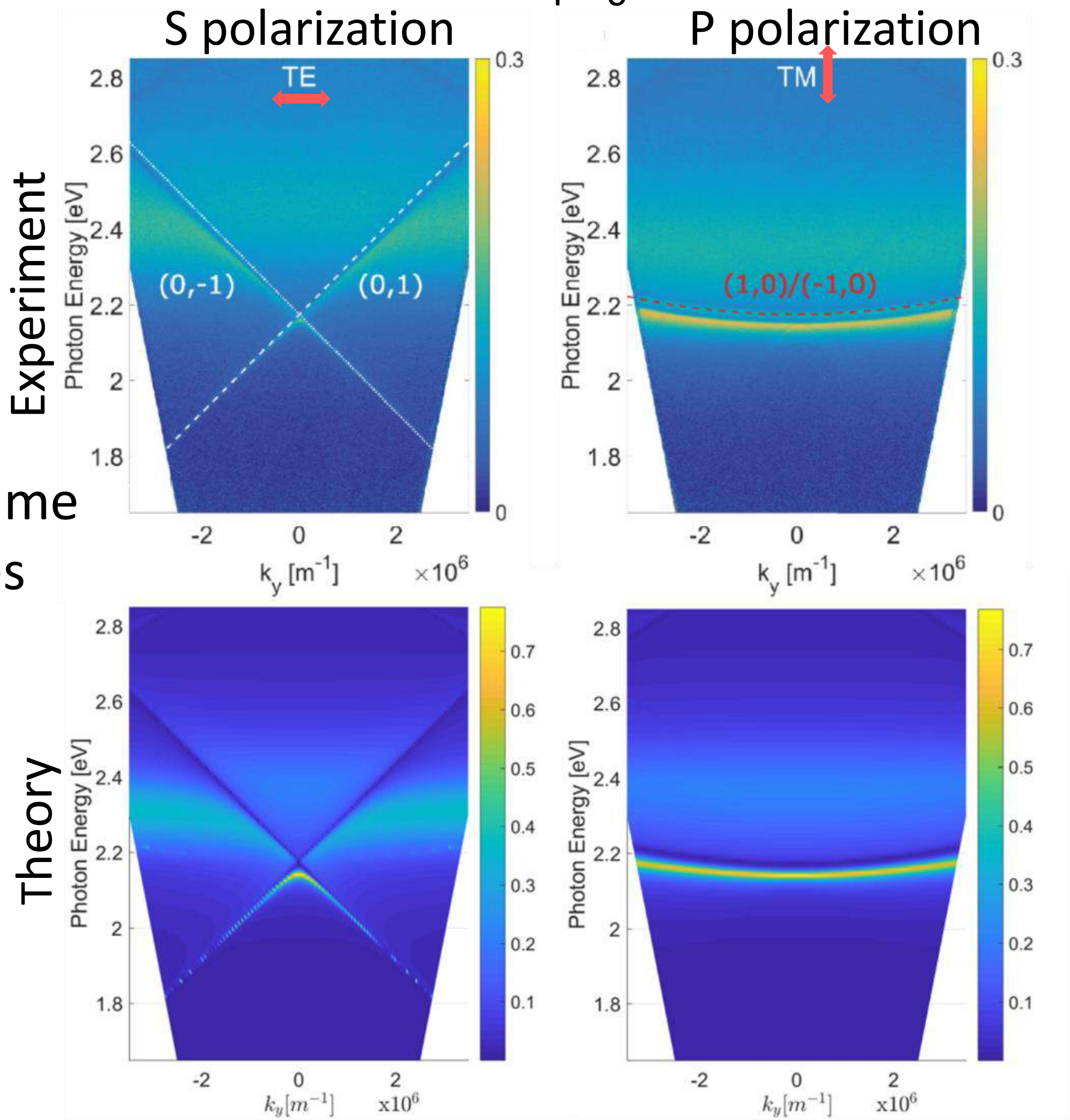
R. Guo, T. K. Hakala, and P. Törmä
Geometry dependence of surface lattice resonances in plasmonic nanoparticle arrays
PHYSICAL REVIEW B **95**, 155423 (2017)





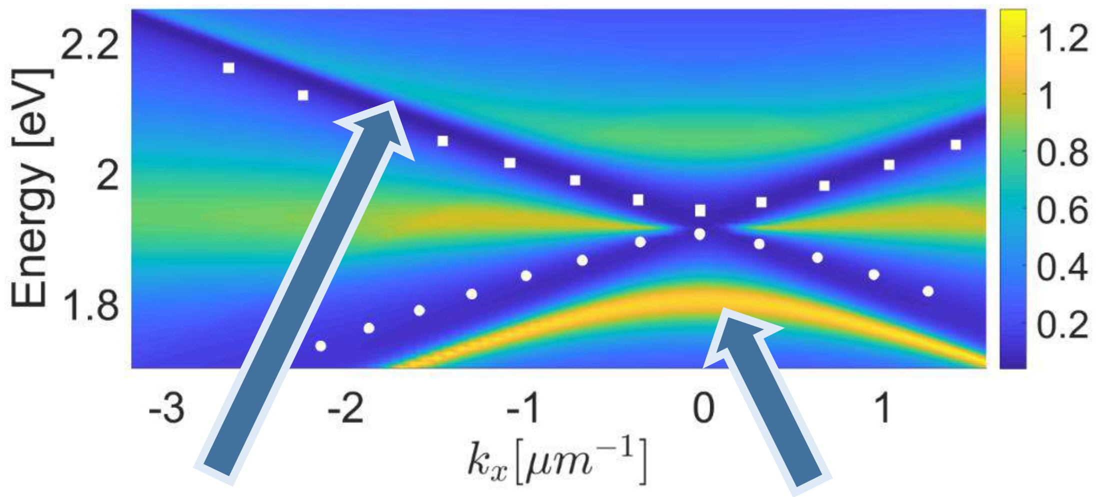
Calculation time ≈ 2 minutes

$1 - I_T/I_0$



Plasmonic lattices

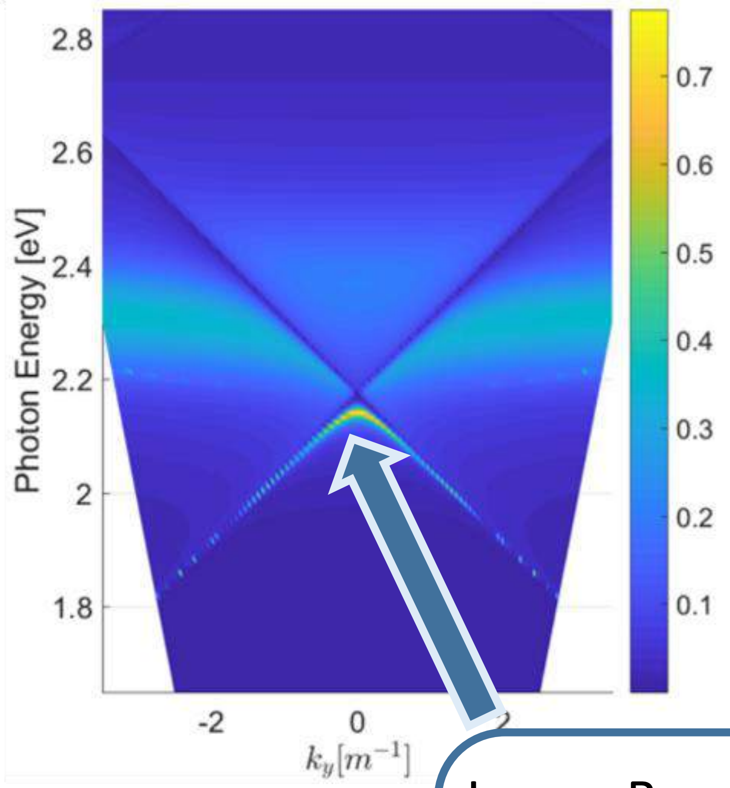
Interaction via waveguide modes



Upper Branch

Lower Branch

Direct interaction via far-field

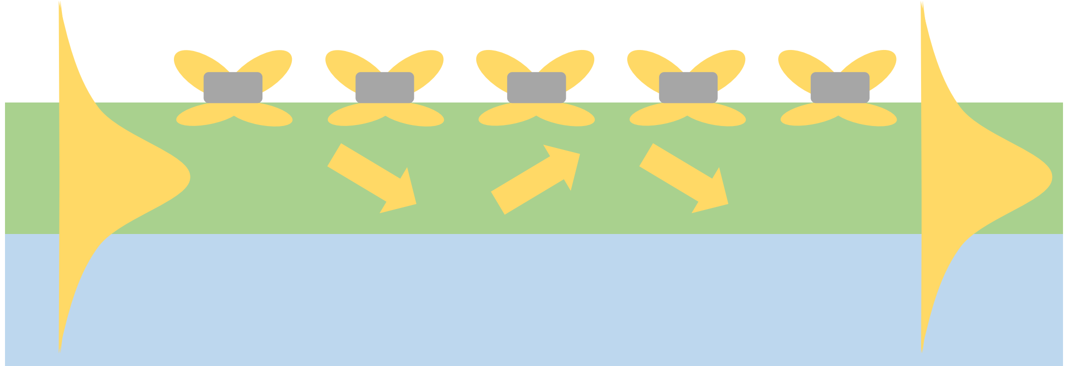


Lower Branch

Why there is such a difference?

Hybrid resonances

Interaction via waveguide modes



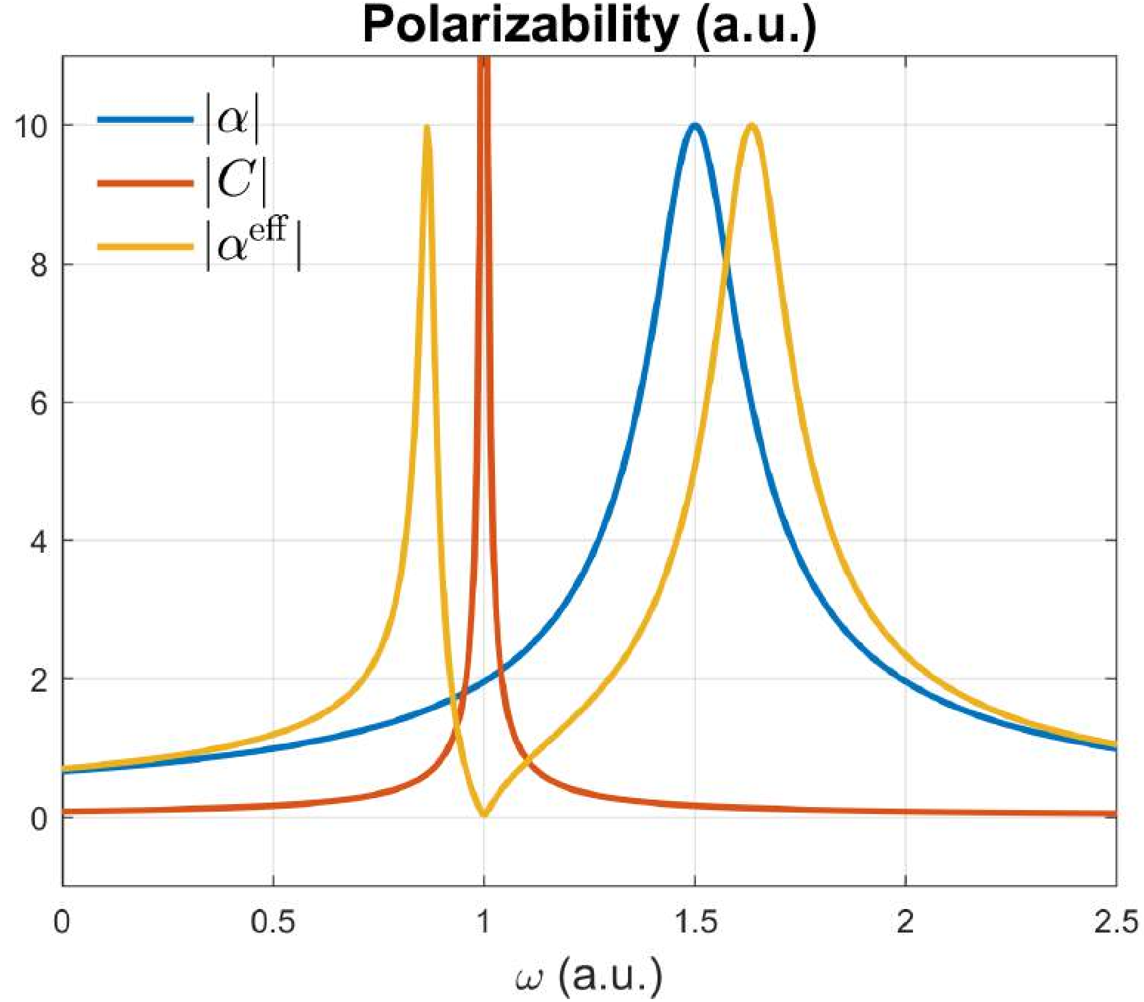
Let us consider a toy model:

$$\alpha \propto \frac{A}{\omega - \tilde{\omega}_{\mathrm{LSPR}}} \qquad C \propto \frac{B}{\omega - \tilde{\omega}_{\mathrm{WG}}}$$

$$\alpha^{\mathrm{eff}} \propto \frac{\omega - \tilde{\omega}_{\mathrm{WG}}}{(\omega - \tilde{\omega}_1)(\omega - \tilde{\omega}_2)}$$

Hybrid resonances

$$\alpha^{\text{eff}} \propto \frac{\omega - \widetilde{\omega}_{\text{WG}}}{(\omega - \widetilde{\omega}_1)(\omega - \widetilde{\omega}_2)}$$



Hybrid resonances

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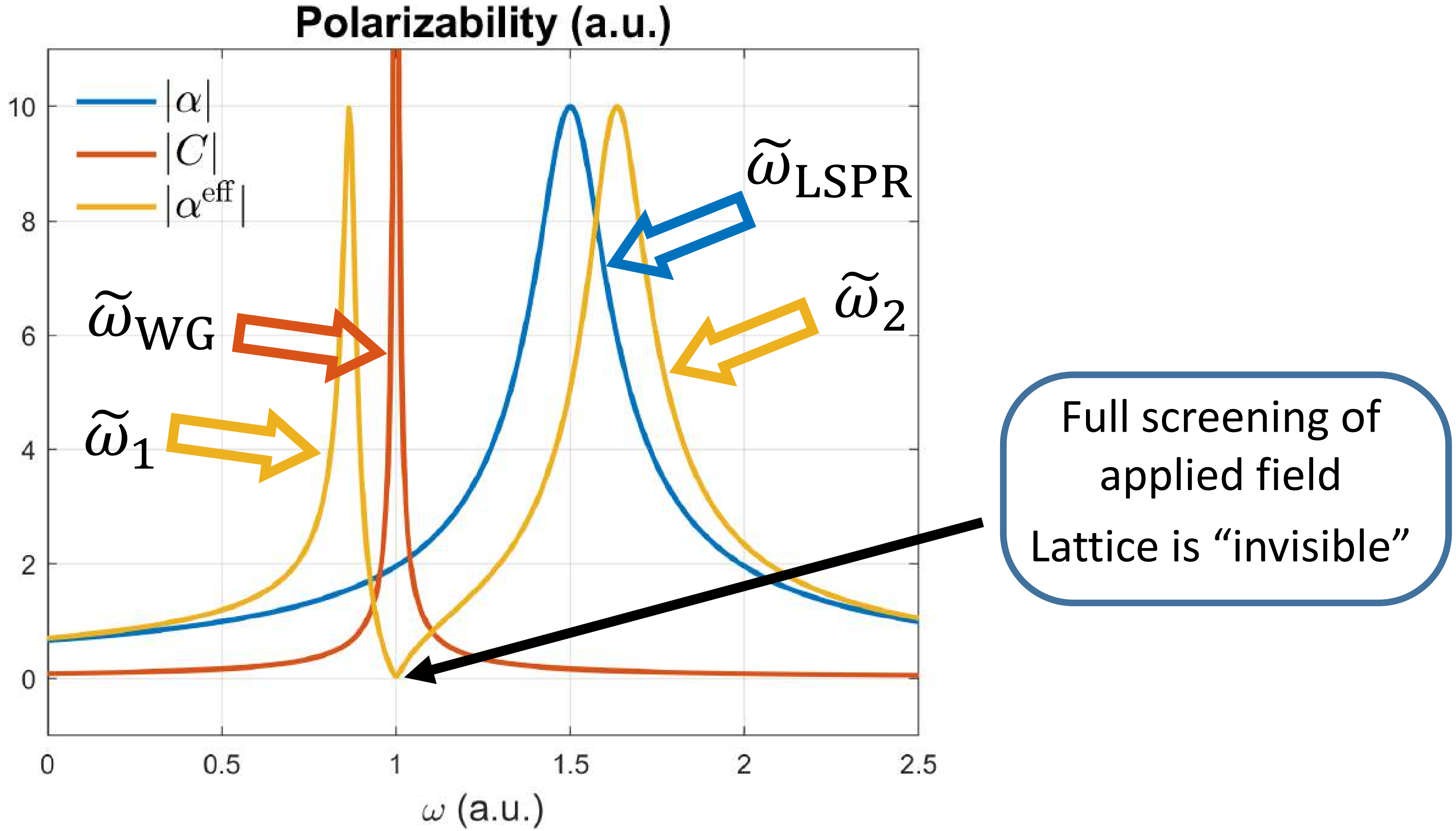

Hybrid resonances

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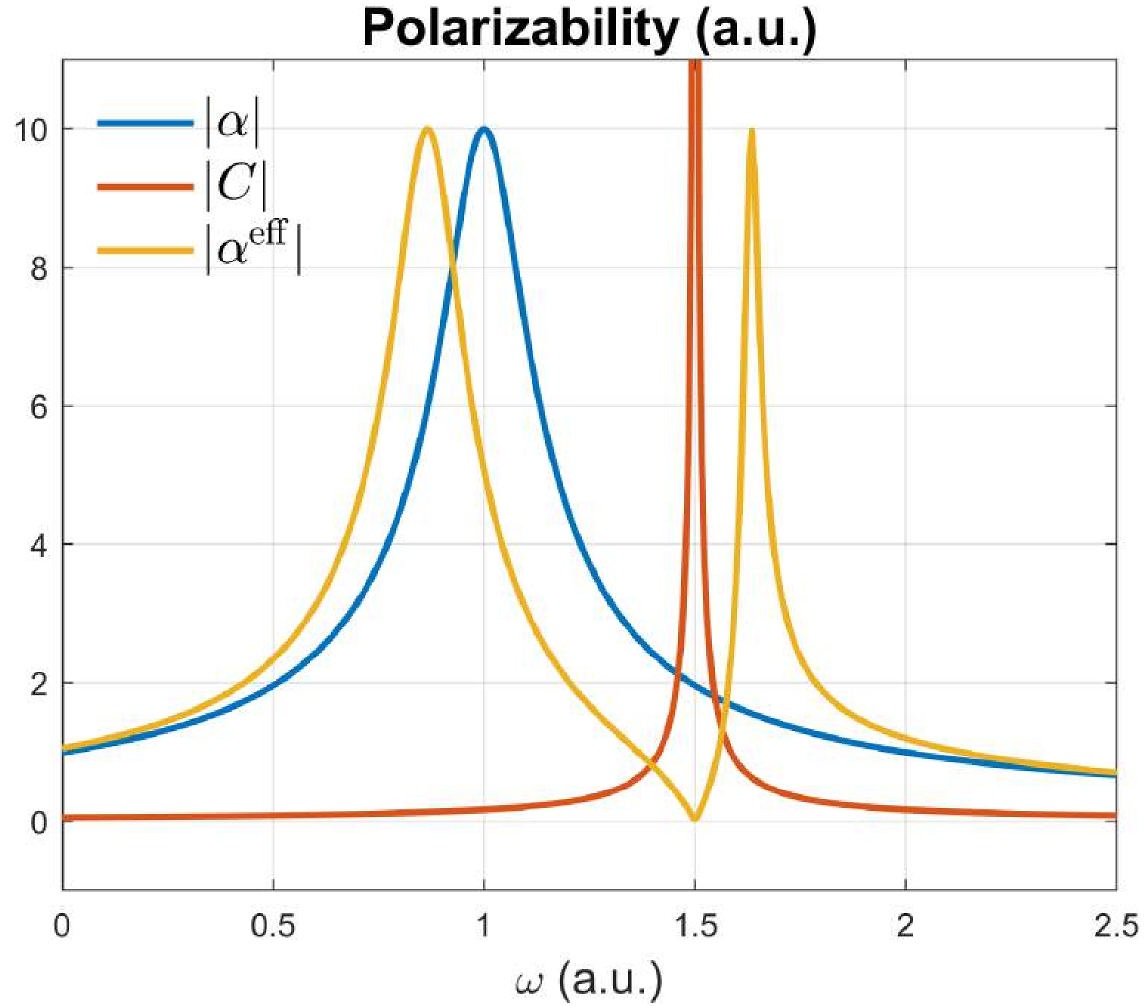

Hybrid resonances

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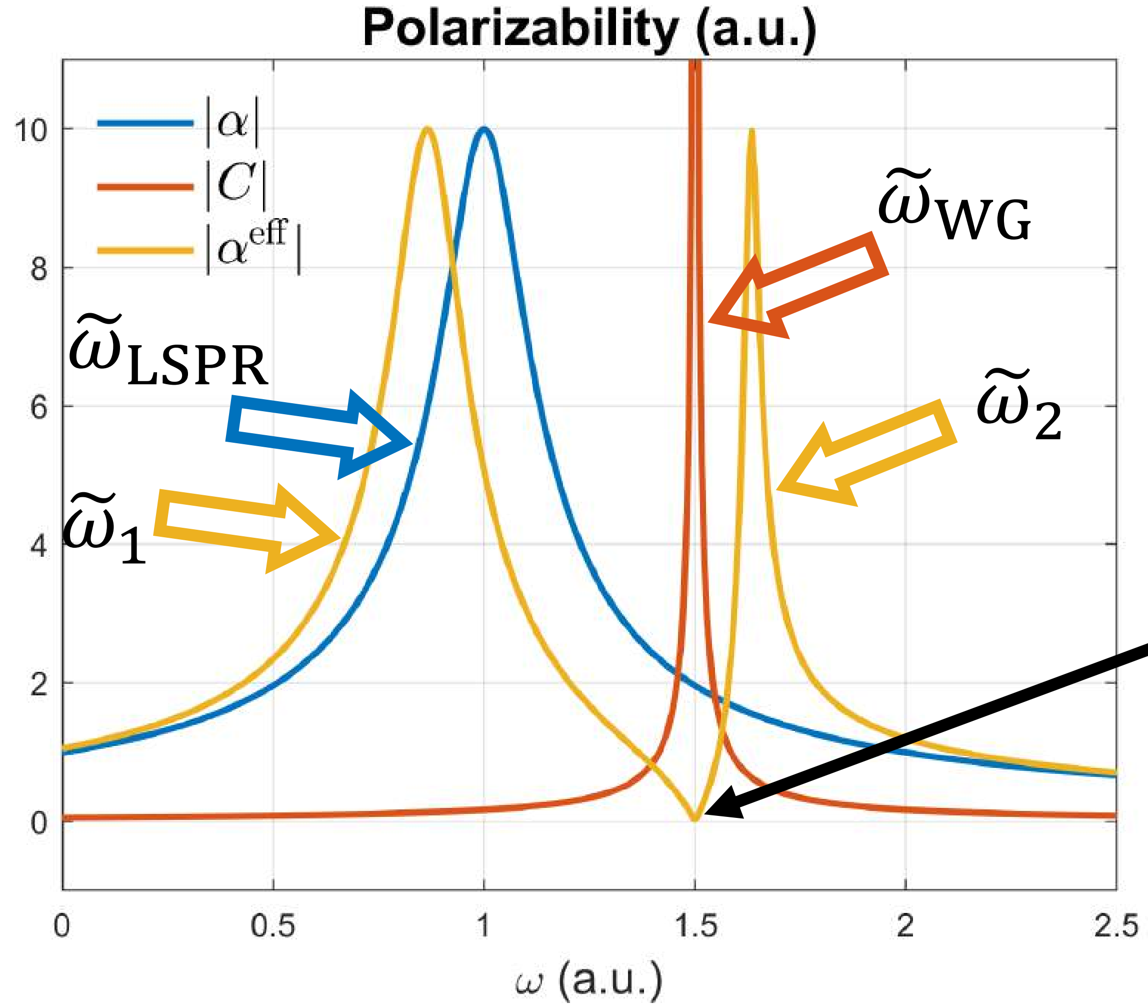


Full screening of applied field

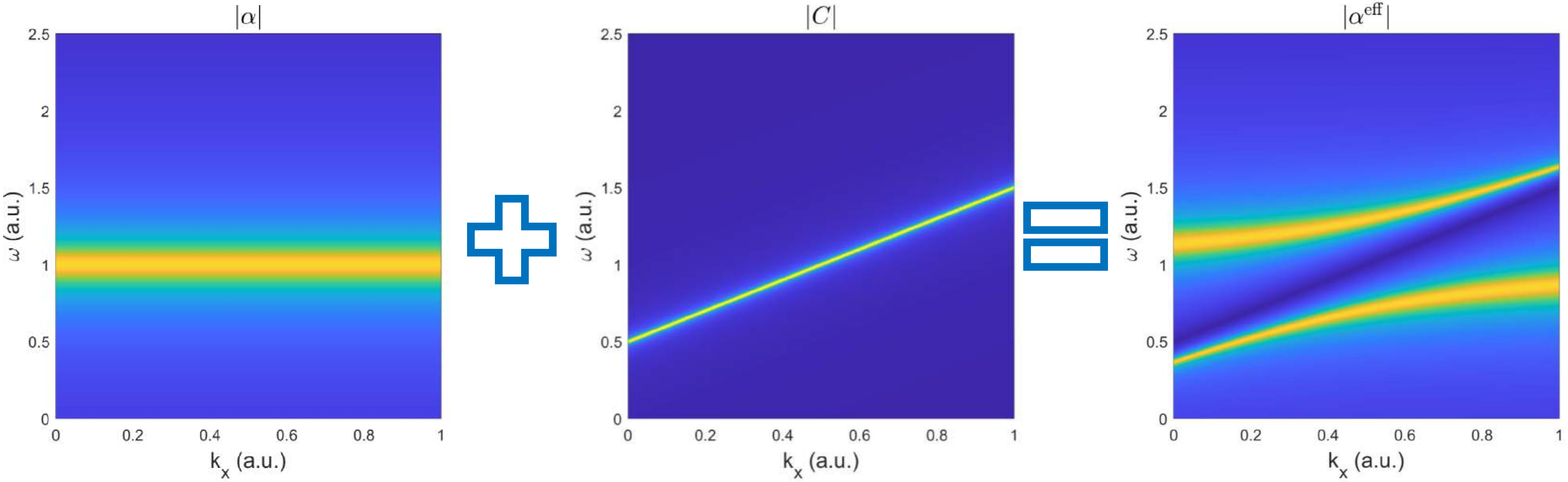
Lattice is "invisible"

Hybrid resonances

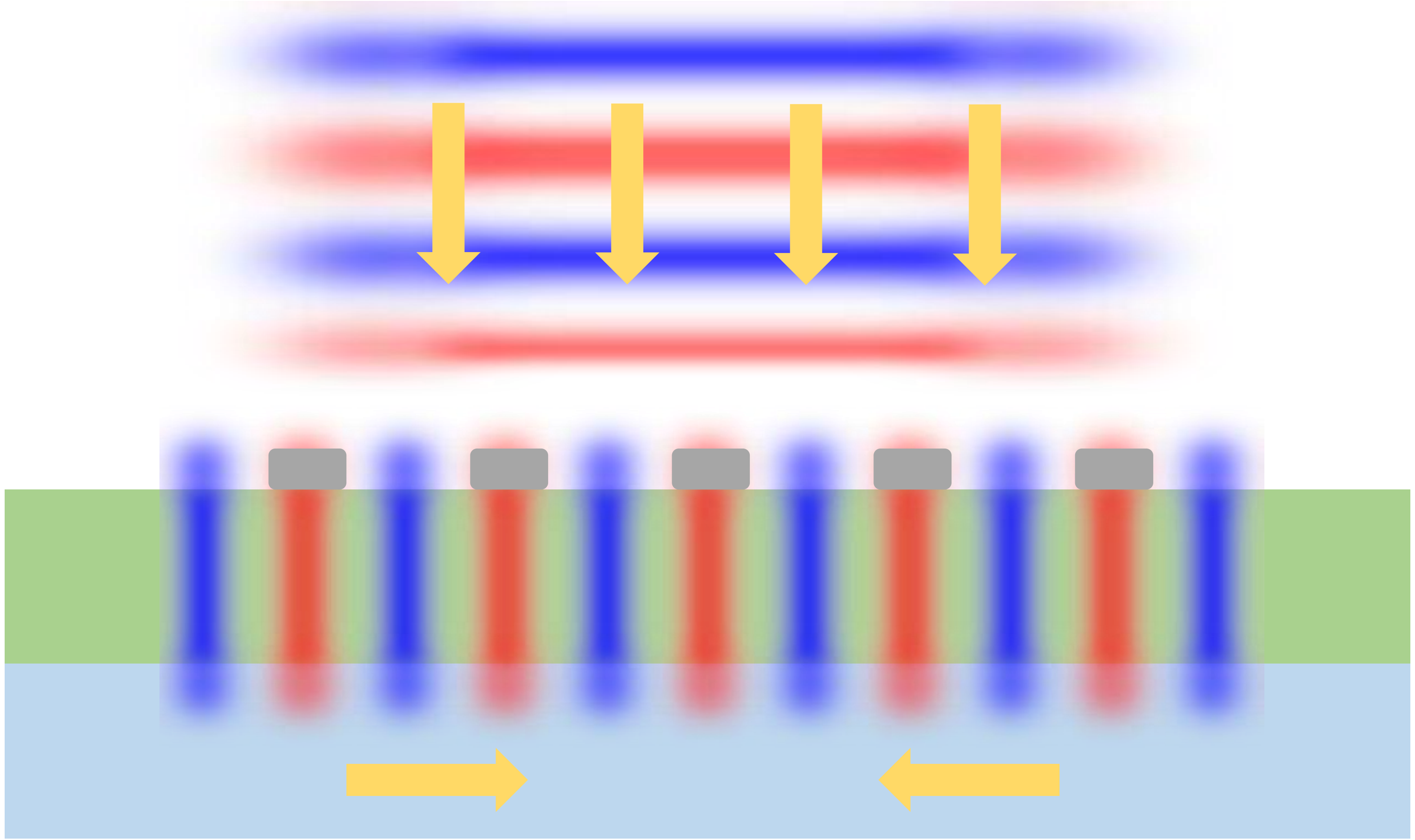
“Localized Surface Plasmon Resonance”

“Waveguide mode”

Classical Avoided Crossing



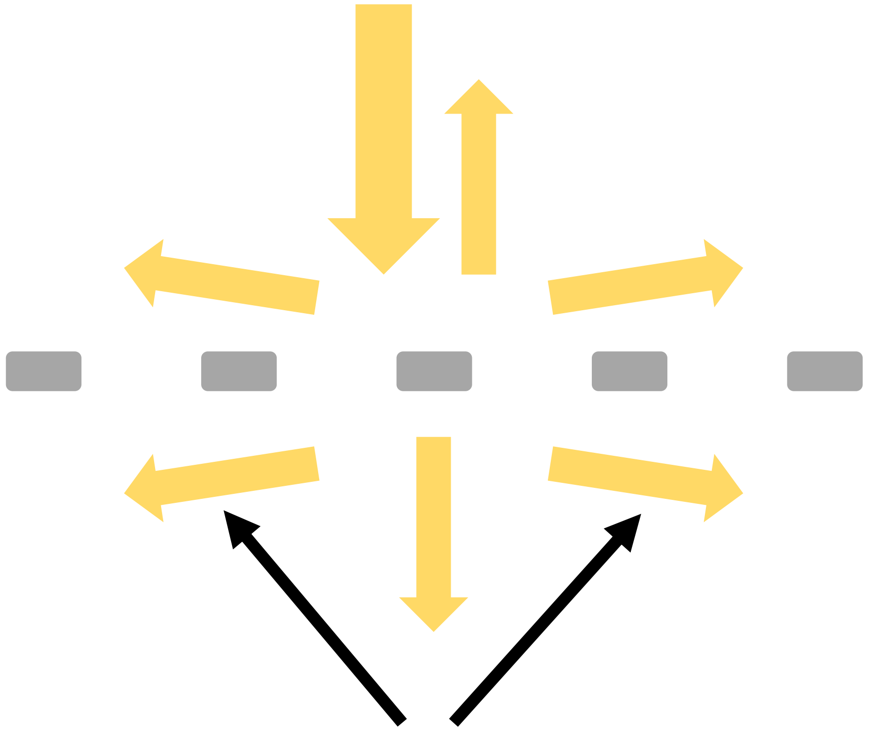
Hybrid resonances



Waveguide modes fully compensate incident field

Hybrid resonances

Direct interaction via far-field



Opening of new diffraction channels – Rayleigh Anomaly

Let us consider a toy model:

$$\alpha \propto \frac{A}{\omega - \tilde{\omega}_{\mathrm{LSPR}}}$$

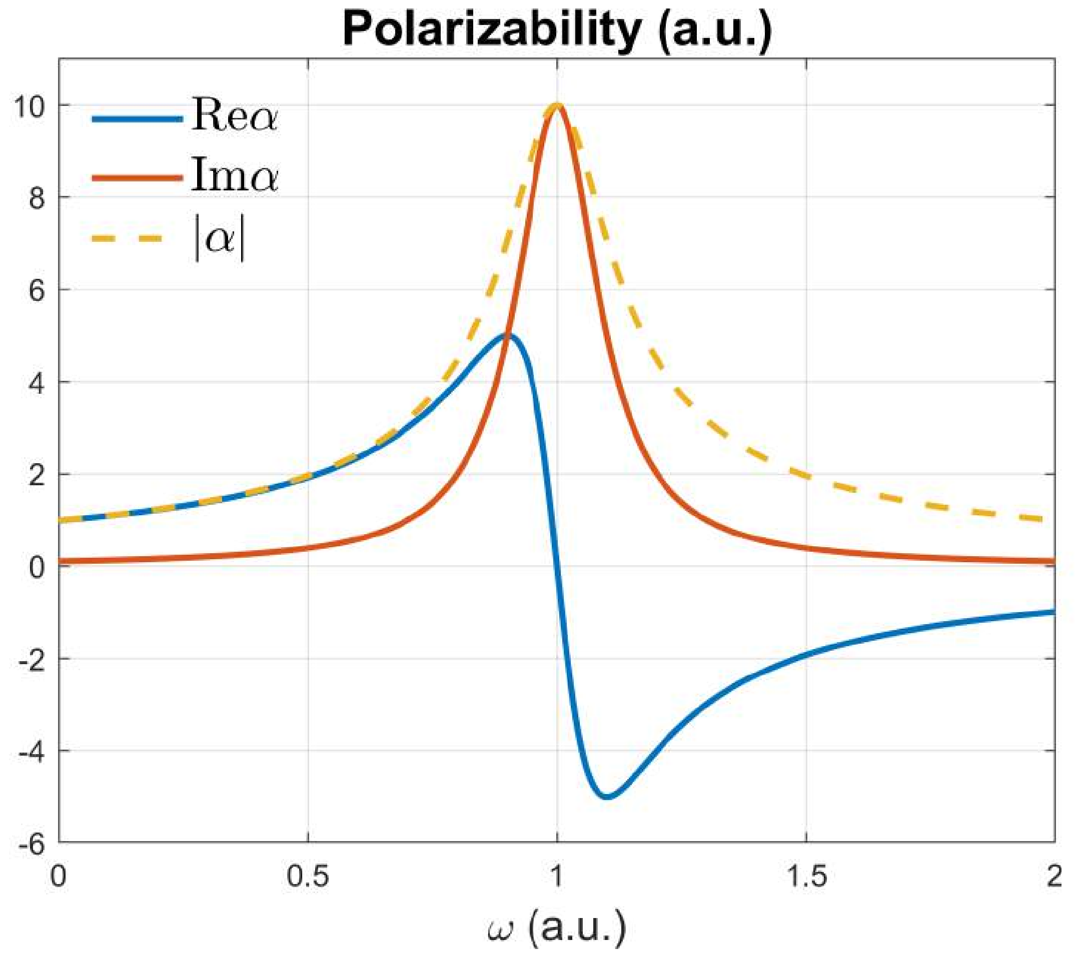
$$C \propto \frac{iB}{k_{z,n}} = \frac{iB}{\sqrt{\frac{\varepsilon\omega^2}{c^2} - (k_x + G_n)^2}} \propto \frac{iB}{\sqrt{\omega - \tilde{\omega}_n^{\mathrm{RA}}}}$$

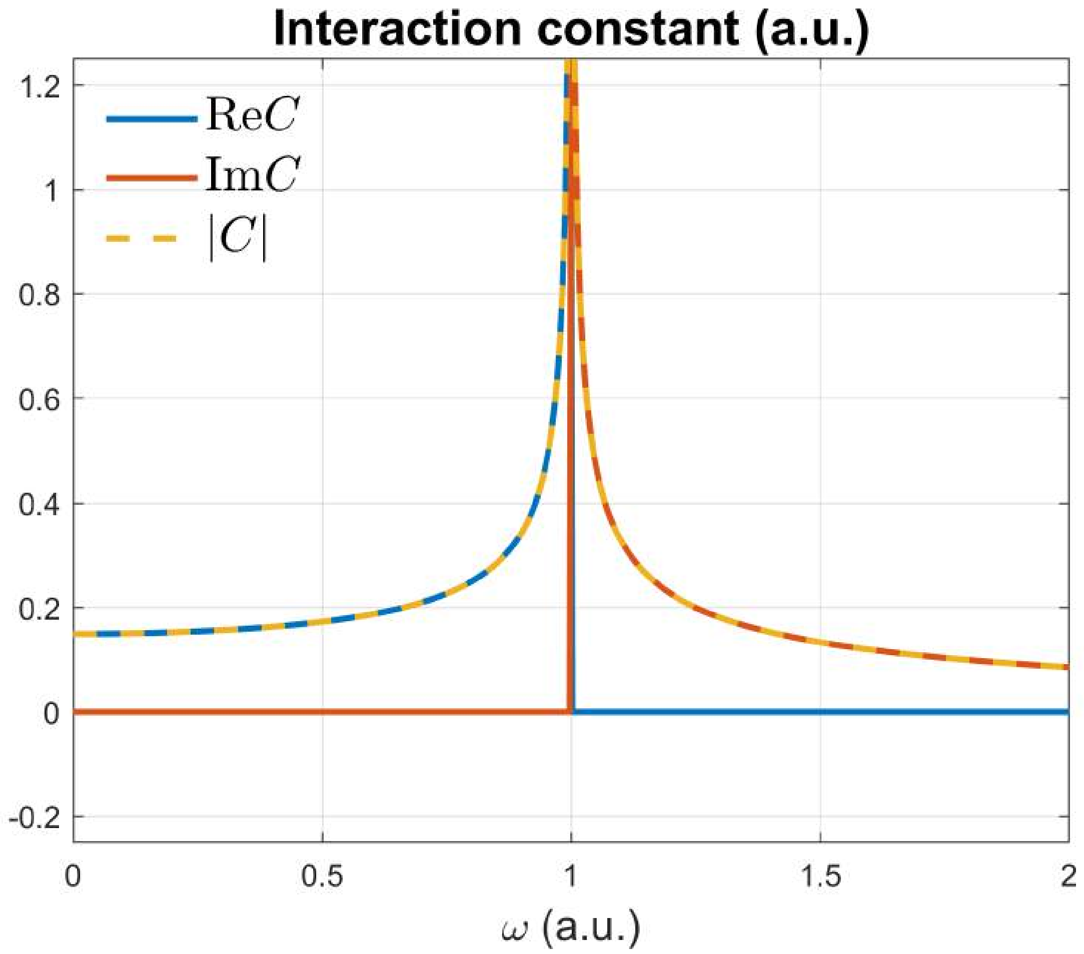
$$\alpha^{\mathrm{eff}} \propto \frac{\sqrt{\omega - \tilde{\omega}_n^{\mathrm{RA}}}}{(\omega - \tilde{\omega}_{\mathrm{LSPR}})\sqrt{\omega - \tilde{\omega}_n^{\mathrm{RA}}} - iAB}$$

Hybrid resonances

When resonant condition might be fulfilled?

$$\mathrm{Re}\hat{\alpha}^{-1}(\omega) = \mathrm{Re}\hat{C}(\omega, \mathbf{k}_{\parallel})$$





Hybrid resonances

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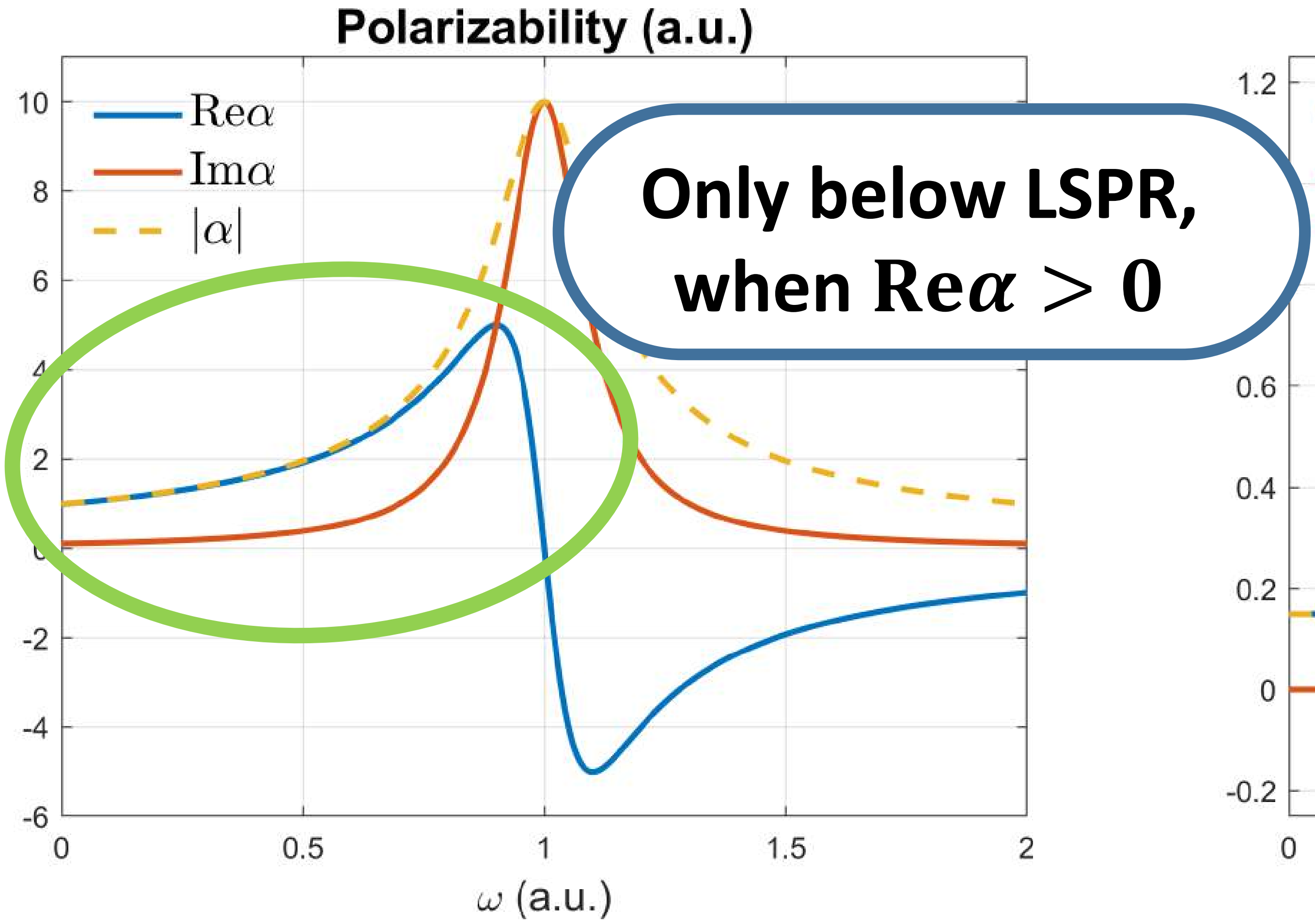
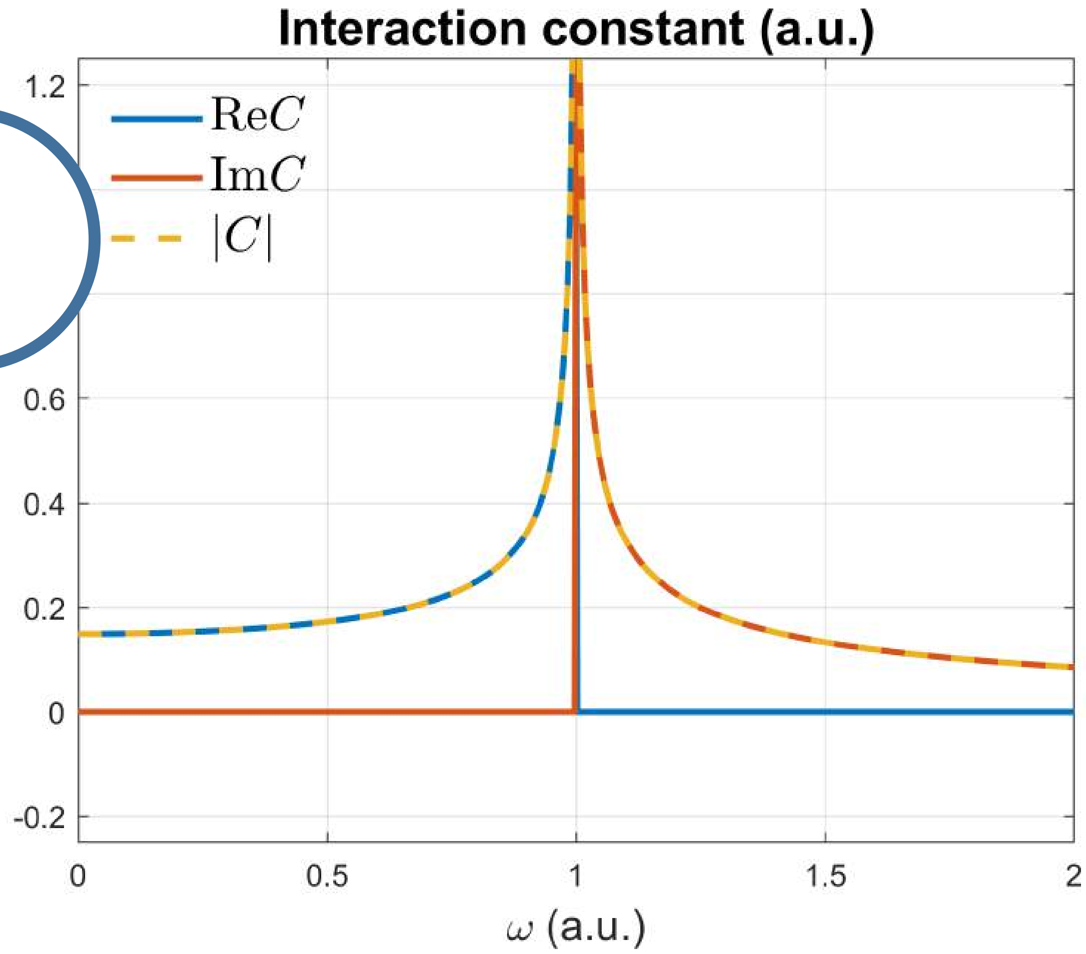
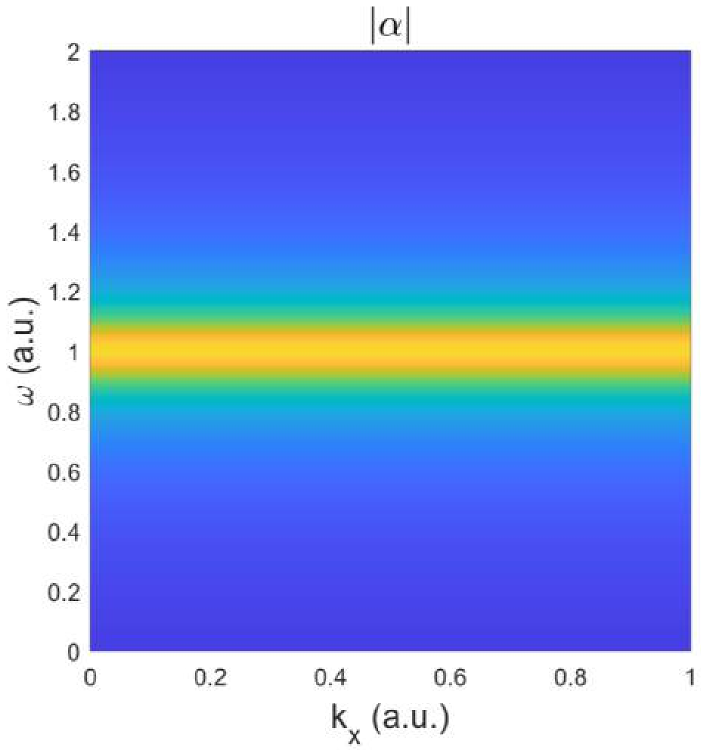
$$\mathrm{Re}\hat{\alpha}^{-1}(\omega) = \mathrm{Re}\hat{C}(\omega, \mathbf{k}_{\|})$$





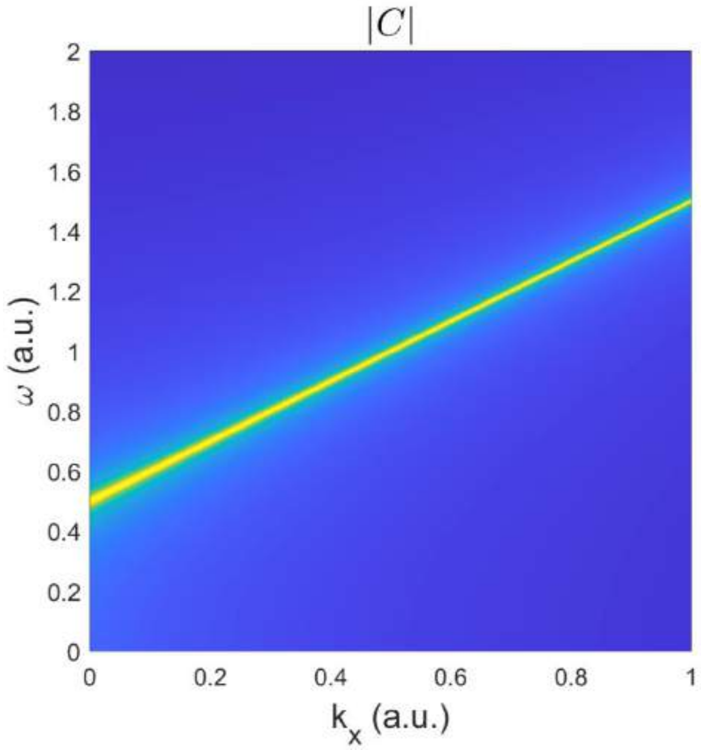
Hybrid resonances

“Localized Surface Plasmon Resonance”



+

“Rayleigh Anomaly”



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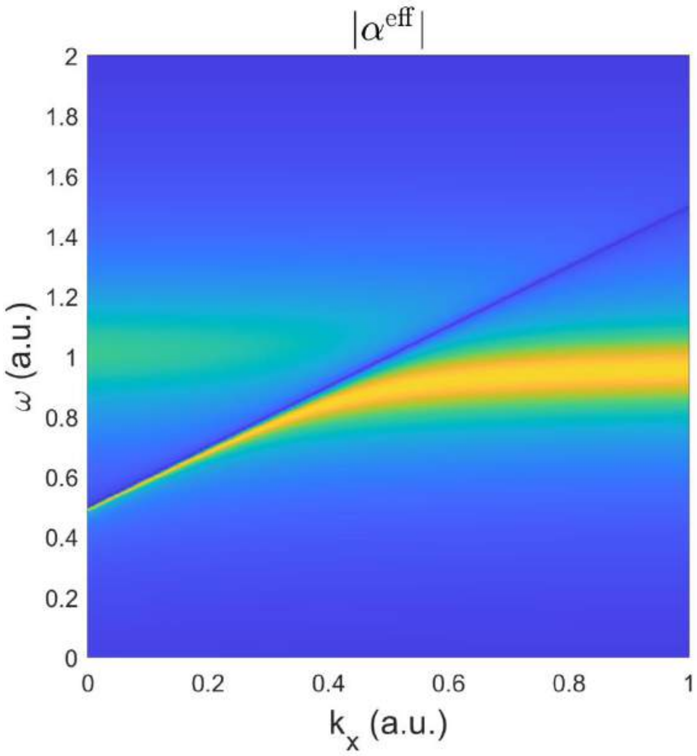
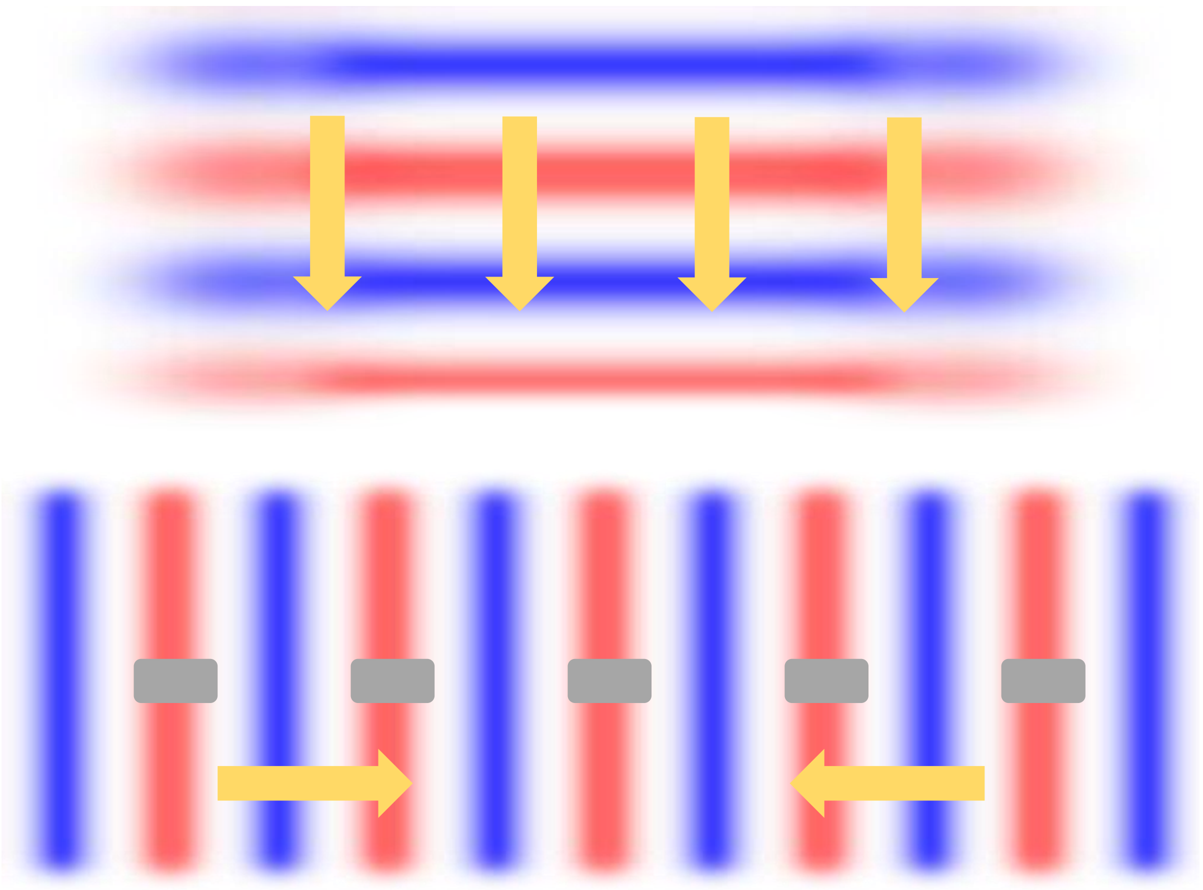
“One-sided” hybridization



Hybrid resonances

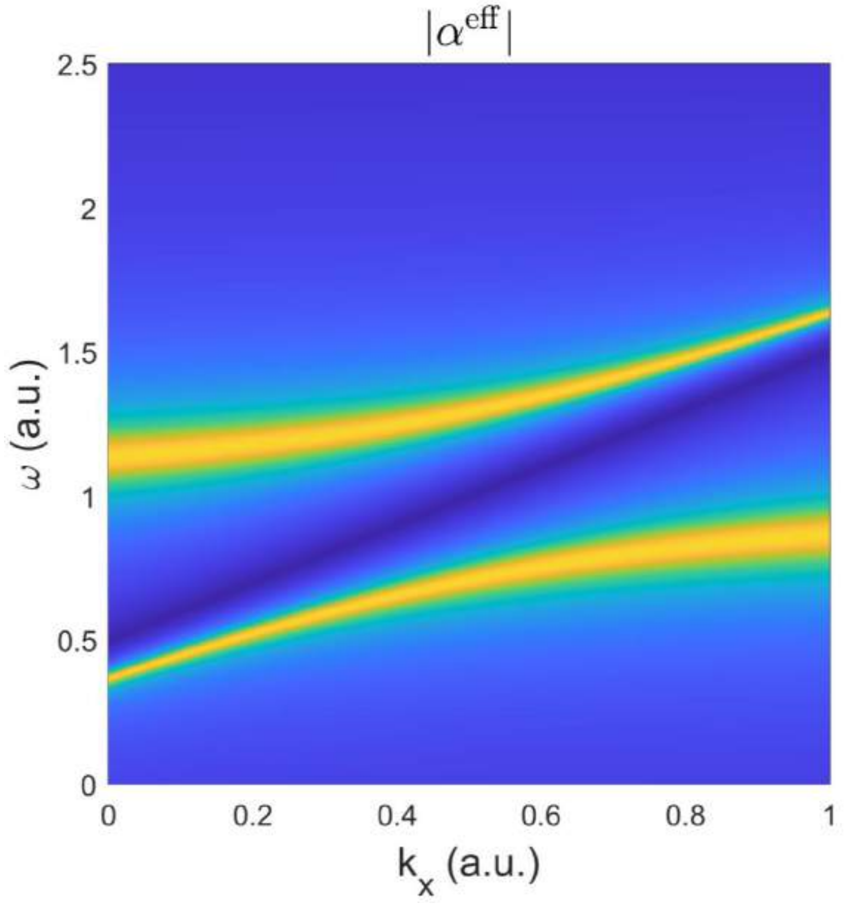


Field of ± 1 diffraction orders fully compensate incident field

Hybrid resonances

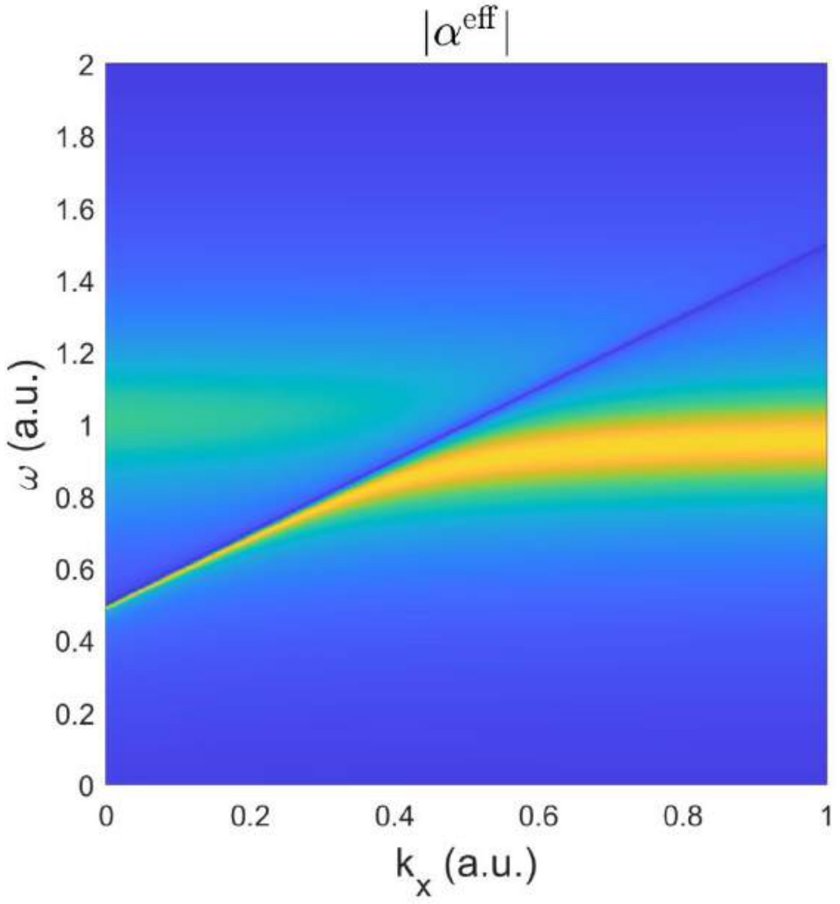
Interaction via waveguide modes

Classical Avoided Crossing



Direct interaction via far-field

"One-sided" hybridization



Theoretical approaches

Universal methods

FDTD

FEM

exact solution

too computationally expensive

Fourier modal method (Rigorous coupled-wave analysis)

specialized for layered periodic structures

too many diffraction orders should be taken into account

Discrete dipole approximation

fast and efficient

hardly applicable for layered structures

Theoretical consideration

Universal methods

- FDTD
- FEM

exact solution

too computationally expensive

Fourier modal method (Rigorous coupled-wave analysis)

specialized for layered periodic structures

too many diffraction orders should be taken into account

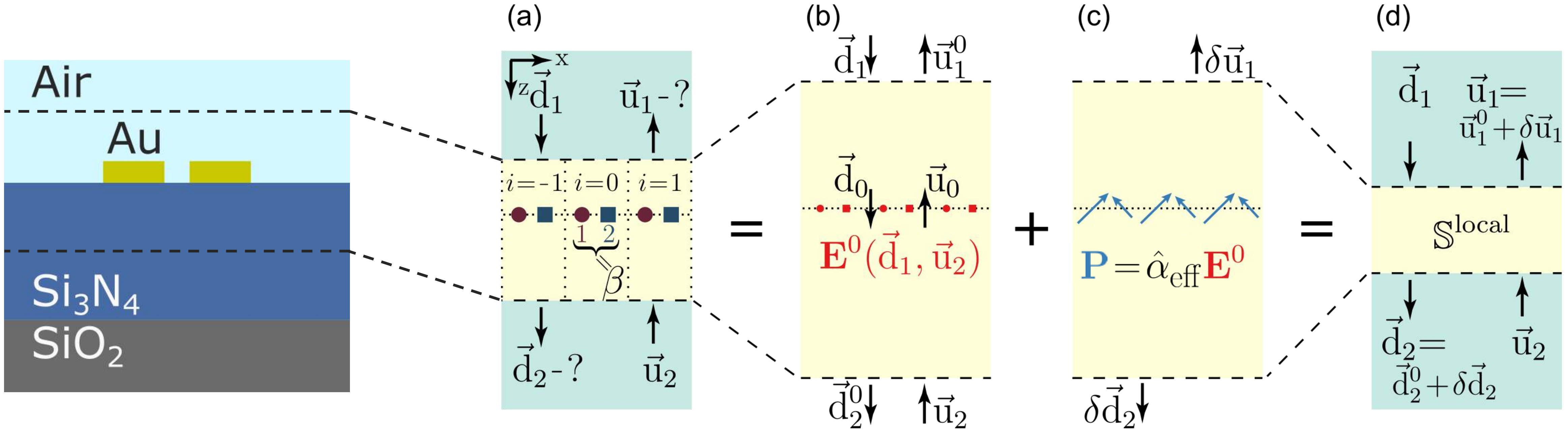
Discrete dipole approximation

fast and efficient

hardly applicable for layered structures

We **combine** approaches to consider **plasmonic lattices** inside **layered structures**

Scattering matrix calculation



$$\begin{bmatrix} \vec{d}_2 \\ \vec{u}_1 \end{bmatrix} = \mathbb{S}^{\rm local} \begin{bmatrix} \vec{d}_1 \\ \vec{u}_2 \end{bmatrix}$$

$$\mathbb{S} = \mathbb{S}^1 \otimes \mathbb{S}^2$$

$$\mathbb{S}_{11} = \mathbb{S}_{11}^2(\hat{I} - \mathbb{S}_{12}^1\mathbb{S}_{21}^2)^{-1}\mathbb{S}_{11}^1,$$
$$\mathbb{S}_{12} = \mathbb{S}_{12}^2 + \mathbb{S}_{11}^2(\hat{I} - \mathbb{S}_{12}^1\mathbb{S}_{21}^2)^{-1}\mathbb{S}_{12}^1\mathbb{S}_{22}^2,$$
$$\mathbb{S}_{21} = \mathbb{S}_{21}^1 + \mathbb{S}_{22}^1(\hat{I} - \mathbb{S}_{21}^2\mathbb{S}_{12}^1)^{-1}\mathbb{S}_{21}^2\mathbb{S}_{11}^1,$$
$$\mathbb{S}_{22} = \mathbb{S}_{22}^1(\hat{I} - \mathbb{S}_{21}^2\mathbb{S}_{12}^1)^{-1}\mathbb{S}_{22}^2.$$

Should we include interface into the local layer?

Dipole approximation validity

When our approximation breaks?

$$\begin{pmatrix} \mathbf{p} \\ \mathbf{m} \\ \hat{\mathbf{Q}} \end{pmatrix} = \begin{pmatrix} \hat{\alpha}_0^p & \hat{\alpha}_1^p & \dots \\ \hat{\alpha}_0^m & \hat{\alpha}_1^m & \dots \\ \hat{\alpha}_0^Q & \hat{\alpha}_1^Q & \dots \end{pmatrix} \begin{pmatrix} \mathbf{E} \\ \nabla \otimes \mathbf{E} \\ \dots \end{pmatrix}$$

Dipole approximation validity

When our approximation breaks?

$$\begin{pmatrix} \mathbf{p} \\ \mathbf{m} \\ \hat{\mathbf{Q}} \end{pmatrix} = \begin{pmatrix} \hat{\alpha}_0^p & \hat{\alpha}_1^p & \dots \\ \hat{\alpha}_0^m & \hat{\alpha}_1^m & \dots \\ \hat{\alpha}_0^Q & \hat{\alpha}_1^Q & \dots \end{pmatrix} \begin{pmatrix} \mathbf{E} \\ \nabla \otimes \mathbf{E} \\ \dots \end{pmatrix}$$

- Large particle
- High-multipole resonances

Dipole approximation validity

When our approximation breaks?

$$\begin{pmatrix} \mathbf{p} \\ \mathbf{m} \\ \hat{\mathbf{Q}} \end{pmatrix} = \begin{pmatrix} \hat{\alpha}_0^p & \hat{\alpha}_1^p & \dots \\ \hat{\alpha}_0^m & \hat{\alpha}_1^m & \dots \\ \hat{\alpha}_0^Q & \hat{\alpha}_1^Q & \dots \end{pmatrix} \begin{pmatrix} \mathbf{E} \\ \nabla \otimes \mathbf{E} \\ \dots \end{pmatrix}$$

- Large particle
- High gradients (near field)

Dipole approximation validity

When our approximation breaks?

$$\mathbf{E}^{\rm sc} = \hat{G}^p(\mathbf{r})\mathbf{p} + \hat{G}^m(\mathbf{r})\mathbf{m} + \hat{G}^Q(\mathbf{r})\hat{\mathbf{Q}} + \cdots$$

Dipole contribution might dominate in far-field, but not in the near-field

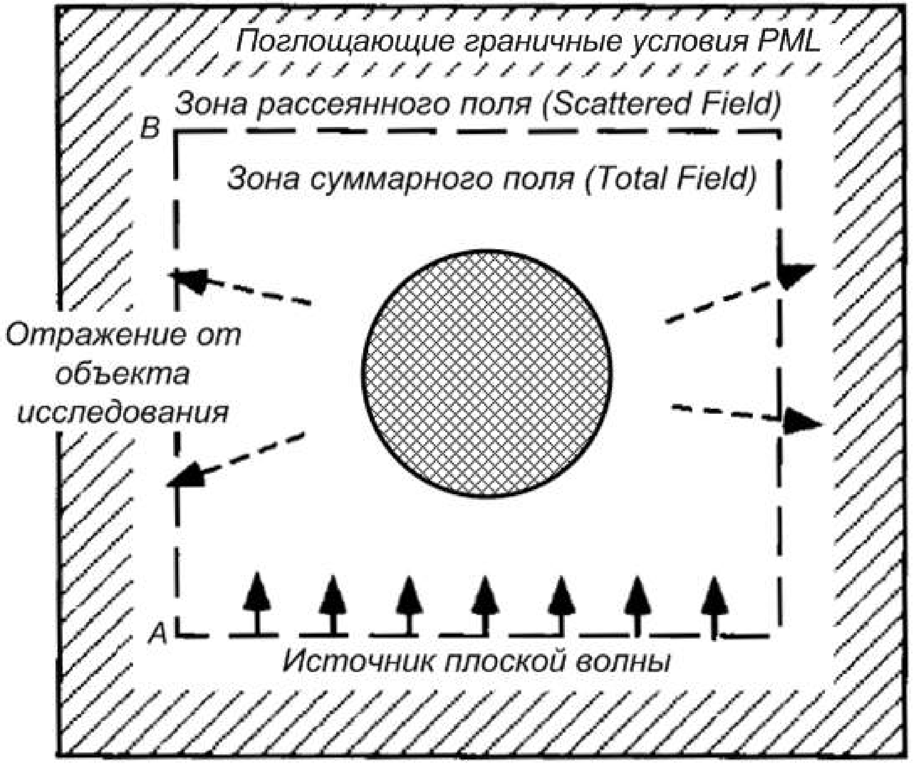
⇩

No interfaces and other particles in dipole near field!

⇩

Interface should be already accounted for in $\hat{\alpha}$ polarizability!

Total/Scattered fields formulation



https://ru.wikipedia.org/wikiФайл:Total_Field_-_Scattered_Field.png

$$\mathrm{rot}\mathbf{H} = \frac{4\pi}{c}\mathbf{j} + \frac{\partial \mathbf{D}}{c\partial t}$$

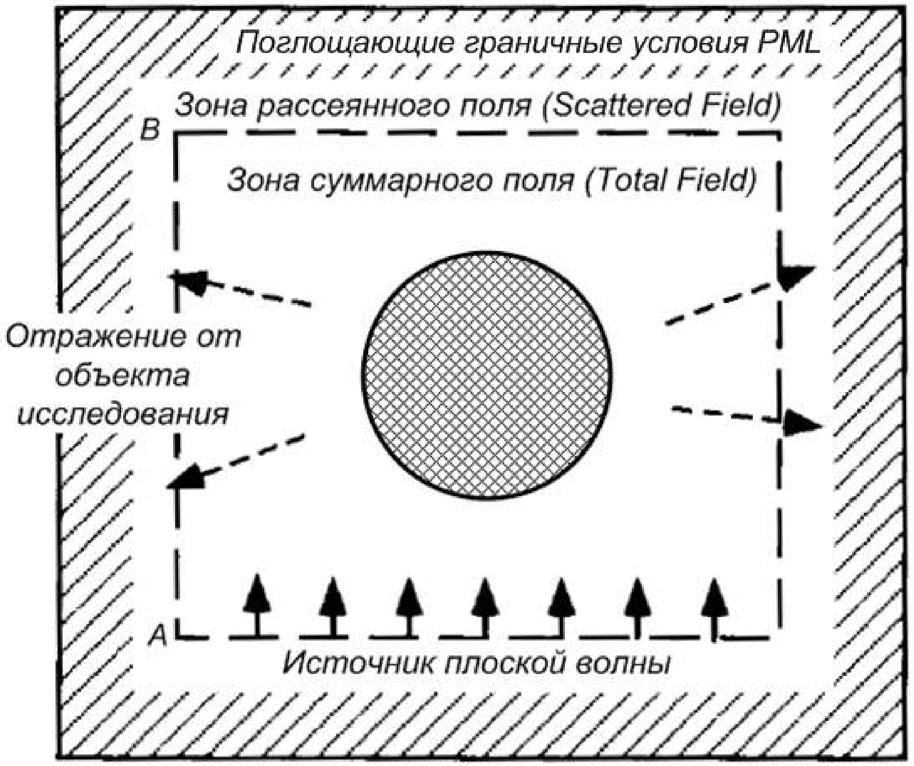
$$\mathrm{rot}\mathbf{H}_0 = -\frac{i\omega}{c}\varepsilon_{\mathrm{bg}}\mathbf{E}_0$$
$$\mathrm{rot}\mathbf{H}_{\mathrm{tot}} = -\frac{i\omega}{c}\varepsilon_{\mathrm{tot}}\mathbf{E}_{\mathrm{tot}}$$

$$\mathbf{E}_{\mathrm{tot}} = \mathbf{E}_0 + \mathbf{E}_{\mathrm{sc}}$$
$$\mathbf{H}_{\mathrm{tot}} = \mathbf{H}_0 + \mathbf{H}_{\mathrm{sc}}$$

1^{st} step

$$\mathrm{rot}\mathbf{H}_0 + \mathrm{rot}\mathbf{H}_{\mathrm{sc}} = -\frac{i\omega}{c}\left(\varepsilon_{\mathrm{bg}} + \Delta\varepsilon\right)\mathbf{E}_0 - \frac{i\omega}{c}\varepsilon_{\mathrm{tot}}\mathbf{E}_{\mathrm{sc}}$$

Total/Scattered fields formulation



https://ru.wikipedia.org/wikiФайл:Total_Field_-_Scattered_Field.png

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$$\mathbf{E}_{\mathrm{tot}} = \mathbf{E}_0 + \mathbf{E}_{\mathrm{sc}}$$

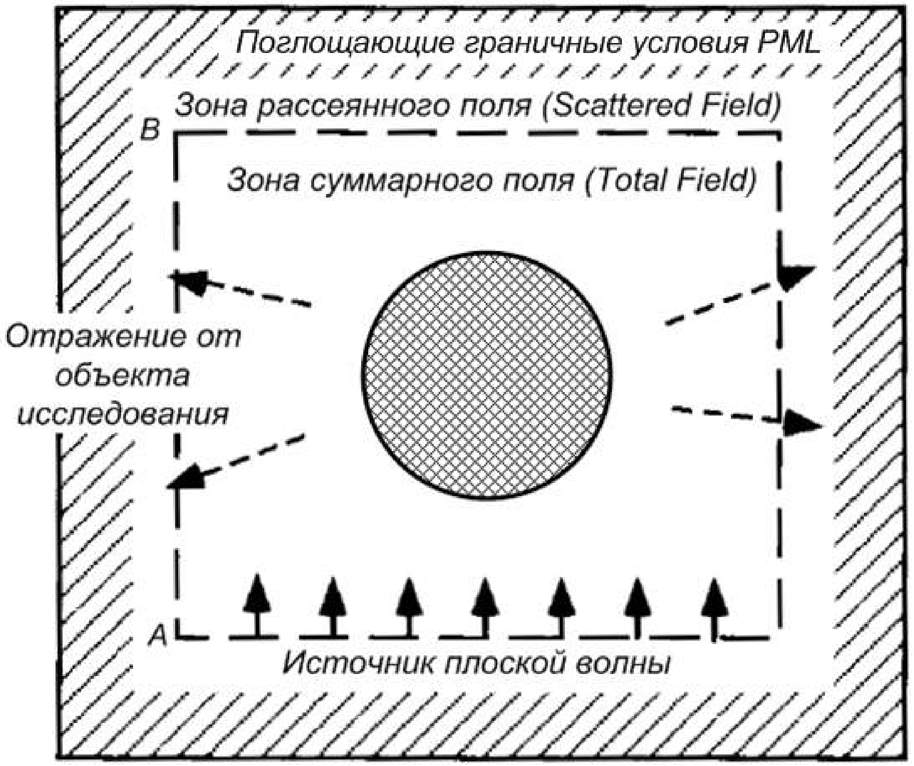
$$\mathbf{H}_{\mathrm{tot}} = \mathbf{H}_0 + \mathbf{H}_{\mathrm{sc}}$$

1st step

$$\mathrm{rot}\mathbf{H}_0 + \mathrm{rot}\mathbf{H}_{\mathrm{sc}} = -\frac{i\omega}{c}\left(\varepsilon_{\mathrm{bg}} + \Delta\varepsilon\right)\mathbf{E}_0 - \frac{i\omega}{c}\varepsilon_{\mathrm{tot}}\mathbf{E}_{\mathrm{sc}}$$

$$\mathrm{rot}\mathbf{H}_{\mathrm{sc}} = -\frac{i\omega}{c}\Delta\varepsilon\mathbf{E}_0 - \frac{i\omega}{c}\varepsilon_{\mathrm{tot}}\mathbf{E}_{\mathrm{sc}}$$

Total/Scattered fields formulation



https://ru.wikipedia.org/wikiФайл:Total_Field_-_Scattered_Field.png

$$\mathrm{rot}\mathbf{H} = \frac{4\pi}{c}\mathbf{j} + \frac{\partial \mathbf{D}}{c\partial t}$$

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$$\mathrm{rot}\mathbf{H}_{\mathrm{tot}} = -\frac{i\omega}{c}\varepsilon_{\mathrm{tot}}\mathbf{E}_{\mathrm{tot}}$$

$$\mathbf{E}_{\mathrm{tot}} = \mathbf{E}_0 + \mathbf{E}_{\mathrm{sc}}$$

$$\mathbf{H}_{\mathrm{tot}} = \mathbf{H}_0 + \mathbf{H}_{\mathrm{sc}}$$

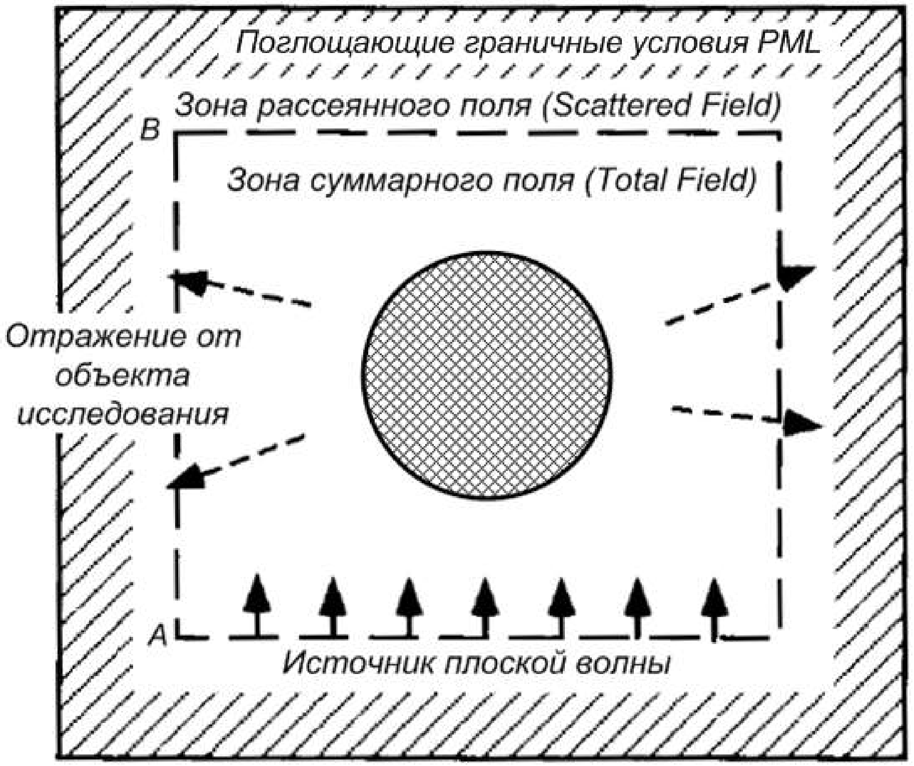
1st step

$$\mathrm{rot}\mathbf{H}_0 + \mathrm{rot}\mathbf{H}_{\mathrm{sc}} = -\frac{i\omega}{c}(\varepsilon_{\mathrm{bg}} + \Delta\varepsilon)\,\mathbf{E}_0 - \frac{i\omega}{c}\varepsilon_{\mathrm{tot}}\mathbf{E}_{\mathrm{sc}}$$

$$\mathrm{rot}\mathbf{H}_{\mathrm{sc}} = -\frac{i\omega}{c}\Delta\varepsilon\mathbf{E}_0 - \frac{i\omega}{c}\varepsilon_{\mathrm{tot}}\mathbf{E}_{\mathrm{sc}}$$

$$= \frac{4\pi}{c}\mathbf{j}_0$$

Total/Scattered fields formulation



https://ru.wikipedia.org/wikiФайл:Total_Field_-_Scattered_Field.png

$$\mathrm{rot}\mathbf{H} = \frac{4\pi}{c}\mathbf{j} + \frac{\partial \mathbf{D}}{c\partial t}$$

$$\mathrm{rot}\mathbf{H}_0 = -\frac{i\omega}{c}\varepsilon_{\mathrm{bg}}\mathbf{E}_0$$

$$\mathrm{rot}\mathbf{H}_{\mathrm{tot}} = -\frac{i\omega}{c}\varepsilon_{\mathrm{tot}}\mathbf{E}_{\mathrm{tot}}$$

$$\mathbf{E}_{\mathrm{tot}} = \mathbf{E}_0 + \mathbf{E}_{\mathrm{sc}}$$

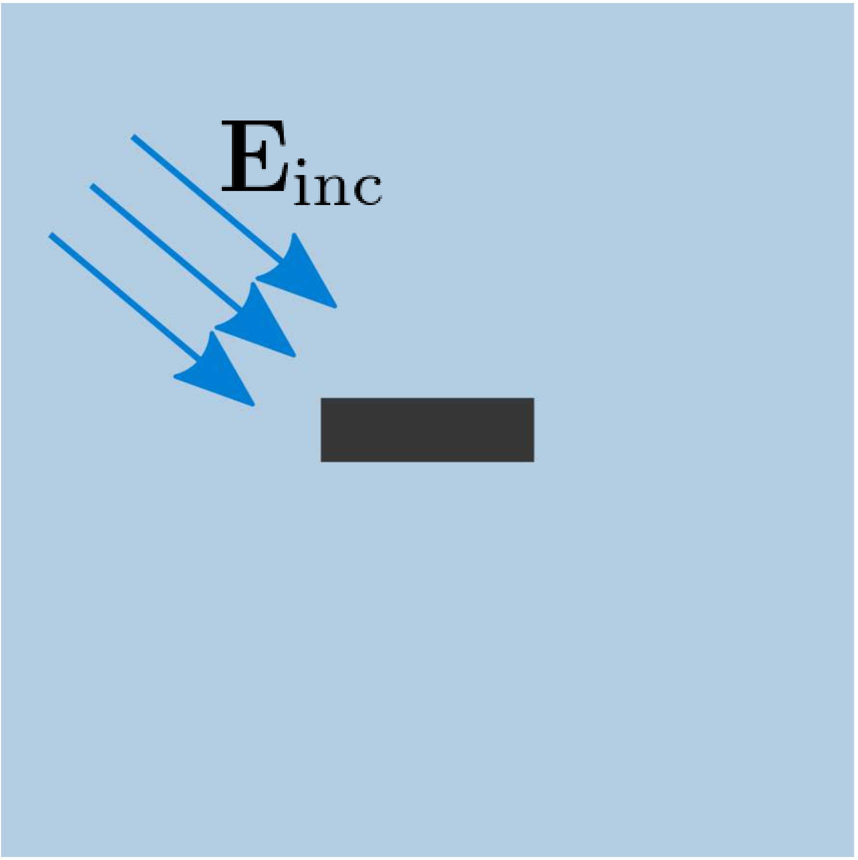
$$\mathbf{H}_{\mathrm{tot}} = \mathbf{H}_0 + \mathbf{H}_{\mathrm{sc}}$$

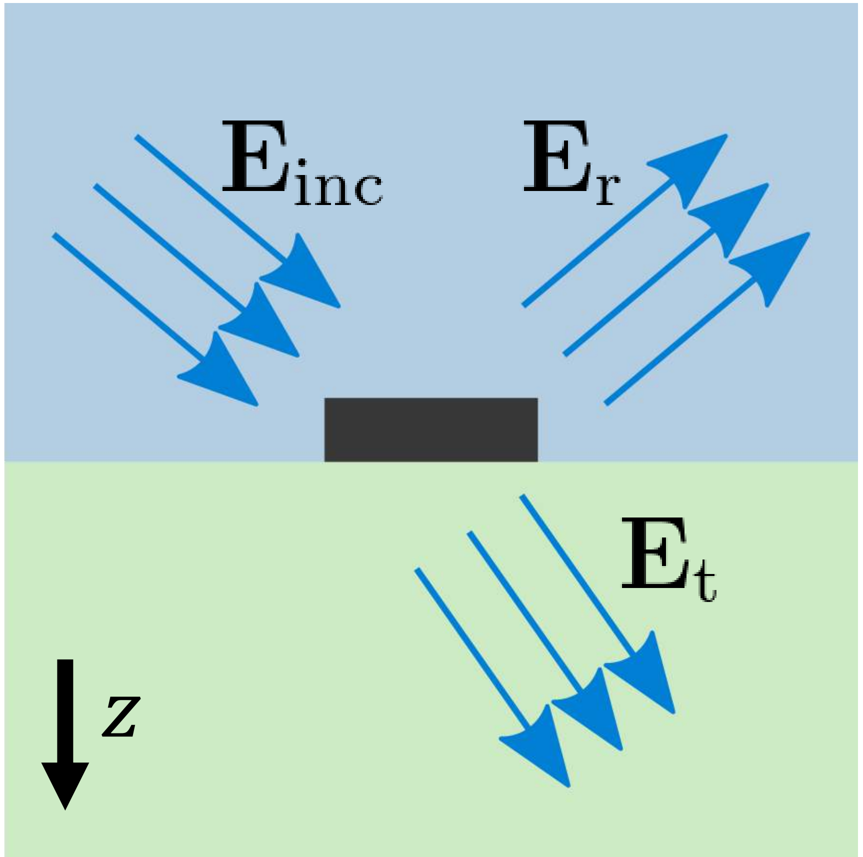
2nd step

$$\mathrm{rot}\mathbf{H}_{\mathrm{tot}} = -\frac{i\omega}{c}\Delta\varepsilon\mathbf{E}_{\mathrm{tot}} - \frac{i\omega}{c}\varepsilon_{\mathrm{bg}}\mathbf{E}_{\mathrm{tot}}$$

$$= \frac{4\pi}{c}\mathbf{j}_{\mathrm{tot}}$$

Polarizability tensor: examples





$$\mathbf{E}_0 = \mathbf{E}_{\rm inc}$$

$$\mathbf{E}_0 = \begin{cases} \mathbf{E}_{\rm inc} + \mathbf{E}_{\rm r} & \text{for} z < 0, \\ \mathbf{E}_{\rm t} & \text{for} z > 0. \end{cases}$$

Lattice sum calculation

$$\hat{G}^{ij}_{ee}(\mathbf{r}) = k_0^2 \left(\delta_{ij} + \frac{1}{k^2}\partial_i \partial_j \right) \frac{e^{ikr}}{r}$$

$r \to 0$

$$\hat{G} \propto \frac{1}{r^3}$$

sum in real space

$r \to \infty$

$$\hat{G} \propto \frac{e^{ikr}}{r}$$

sum in Fourier space

Ewald summation

Ewald, Paul P. *Annalen der physik* 369.3 (1921): 253-287.

Lattice sum calculation

Homogeneous environment

$$\hat{G}_{ee}^{ij}(\mathbf{r}) = k_0^2\left(\delta_{ij} + \frac{1}{k^2}\partial_i\partial_j\right)\frac{e^{ikr}}{r}$$

Ewald summation

$$\hat{G} \propto \frac{1}{r^3}$$

sum in real space

+

$$\hat{G} \propto \frac{e^{ikr}}{r}$$

sum in Fourier space

Interface

$$\hat{M}(\mathbf{k}_\parallel) = \frac{1}{4\pi^2}\int \hat{G}(\mathbf{r}_\parallel)e^{-i\mathbf{k}_\parallel\mathbf{r}_\parallel}d^2\mathbf{r}_\parallel$$

$$\hat{M} = \hat{M}^0 + \hat{M}^r$$

$$\hat{M}^{0,\pm} = \frac{ik_0^2}{2\pi k_z k_\parallel^2}\begin{pmatrix} k_y^2 & -k_xk_y & 0 \\ -k_xk_y & k_x^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{ik_0^2}{2\pi k^2 k_\parallel^2}\begin{pmatrix} k_x^2k_z & k_xk_yk_z & \mp k_xk_\parallel^2 \\ k_xk_yk_z & k_y^2k_z & \mp k_yk_\parallel^2 \\ \mp k_xk_\parallel^2 & \mp k_yk_\parallel^2 & k_\parallel^4/k_z \end{pmatrix}$$

sum in Fourier space

Lattice sum calculation

Homogeneous environment

$$\hat{G}_{ee}^{ij}(\mathbf{r}) = k_0^2\left(\delta_{ij} + \frac{1}{k^2}\partial_i\partial_j\right)\frac{e^{ikr}}{r}$$

Ewald summation

$\hat{G} \propto \frac{1}{r^3}$ + $\hat{G} \propto \frac{e^{ikr}}{r}$

sum in real space

sum in Fourier space

Interface

$$\hat{M}(\mathbf{k}_\parallel) = \frac{1}{4\pi^2}\int \hat{G}(\mathbf{r}_\parallel)e^{-i\mathbf{k}_\parallel\mathbf{r}_\parallel}d^2\mathbf{r}_\parallel$$

$$\hat{M} = \hat{M}^0 + \hat{M}^r$$

$$\hat{M}^{0,\pm} = \frac{ik_0^2}{2\pi k_z k_\parallel^2}\begin{pmatrix} k_y^2 & -k_xk_y & 0 \\ -k_xk_y & k_x^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{ik_0^2}{2\pi k^2 k_\parallel^2}\begin{pmatrix} k_x^2k_z & k_xk_yk_z & \mp k_xk_\parallel^2 \\ k_xk_yk_z & k_y^2k_z & \mp k_yk_\parallel^2 \\ \mp k_xk_\parallel^2 & \mp k_yk_\parallel^2 & k_\parallel^4/k_z \end{pmatrix}$$

sum in Fourier space

Lattice sum calculation

Homogeneous environment

$$\hat{G}^{ij}_{ee}(\mathbf{r}) = k_0^2 \left(\delta_{ij} + \frac{1}{k^2} \partial_i \partial_j \right) \frac{e^{ikr}}{r}$$

Ewald summation

$$\hat{G} \propto \frac{1}{r^3}$$

+

$$\hat{G} \propto \frac{e^{ikr}}{r}$$

sum in real space

sum in Fourier space

Interface

$$\hat{M}(\mathbf{k}_\parallel) = \frac{1}{4\pi^2} \int \hat{G}(\mathbf{r}_\parallel) e^{-i\mathbf{k}_\parallel \mathbf{r}_\parallel} d^2\mathbf{r}_\parallel$$

$$\hat{M} = \hat{M}^0 + \hat{M}^r$$

$$\hat{M}^r = e^{2ik_z h} \left[r_s(k_\parallel) \frac{ik_0^2}{2\pi k_z k_\parallel^2} \begin{pmatrix} k_y^2 & -k_x k_y & 0 \\ -k_x k_y & k_x^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} - r_p(k_\parallel) \frac{ik_0^2}{2\pi k^2 k_\parallel^2} \begin{pmatrix} k_x^2 k_z & k_x k_y k_z & k_x k_\parallel^2 \\ k_x k_y k_z & k_y^2 k_z & k_y k_\parallel^2 \\ -k_x k_\parallel^2 & -k_y k_\parallel^2 & -k_\parallel^4 / k_z \end{pmatrix} \right]$$

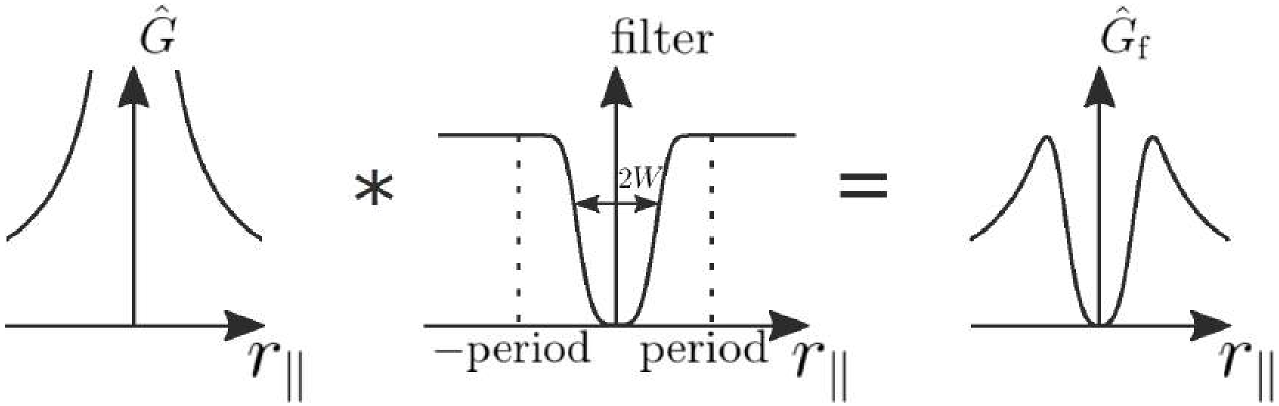
sum in Fourier space

Lattice sum calculation

Poisson summation

$$\hat{C}(\mathbf{k}_\parallel) = \sum_{j \neq i} \hat{G}(\mathbf{r}_i, \mathbf{r}_j) e^{-i\mathbf{k}_\parallel (\mathbf{r}_i - \mathbf{r}_j)}$$

zero term is missed



$$\hat{C}(\mathbf{k}_\parallel) = \sum_j \hat{G}_\mathrm{f}(\mathbf{t}_j) e^{-i\mathbf{k}_\parallel \mathbf{t}_j} = \frac{4\pi^2}{s} \sum_j \hat{M}_\mathrm{f}(\mathbf{k}_\parallel + \mathbf{g}_j)$$

sum over lattice nodes — sum over diffraction orders

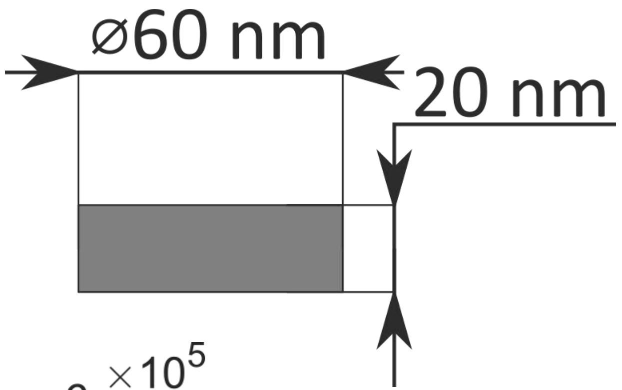
$$\hat{M}_\mathrm{f}(\mathbf{k}_\parallel) = \frac{1}{4\pi^2} \int \hat{G}_\mathrm{f}(\mathbf{r}) e^{-i\mathbf{k}_\parallel \mathbf{r}} d^2\mathbf{r}$$

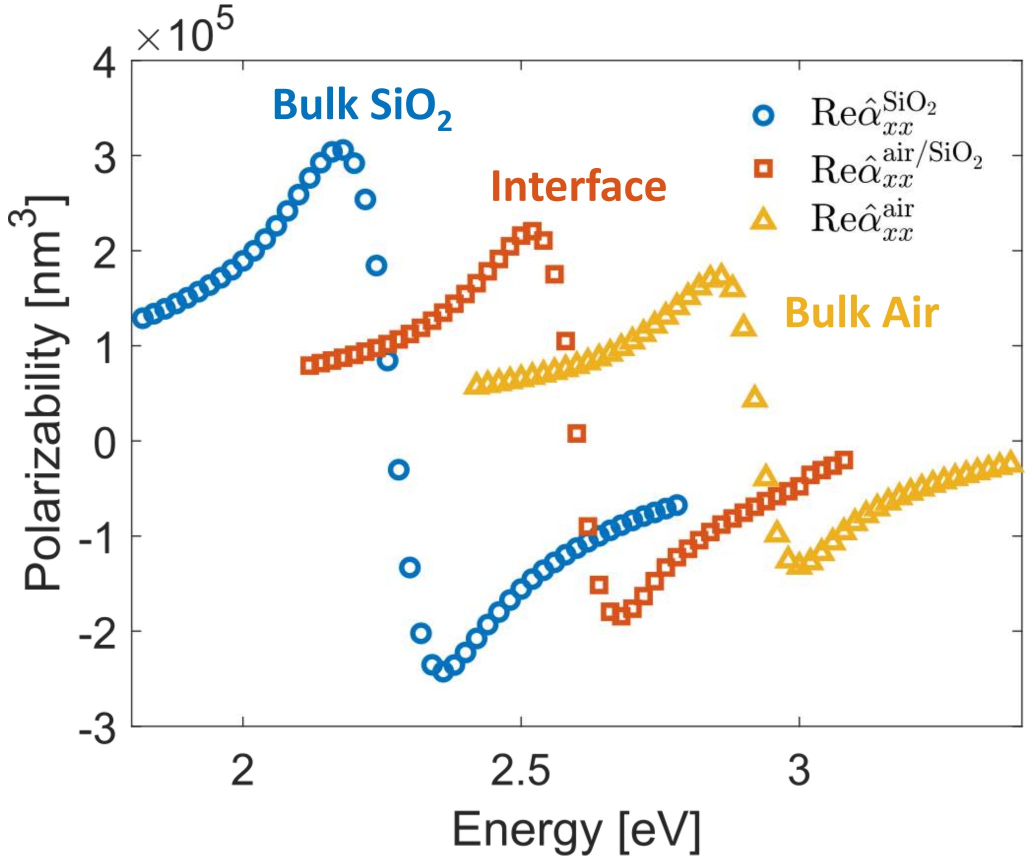
$\mathbf{g}_j$ - reciprocal lattice vector

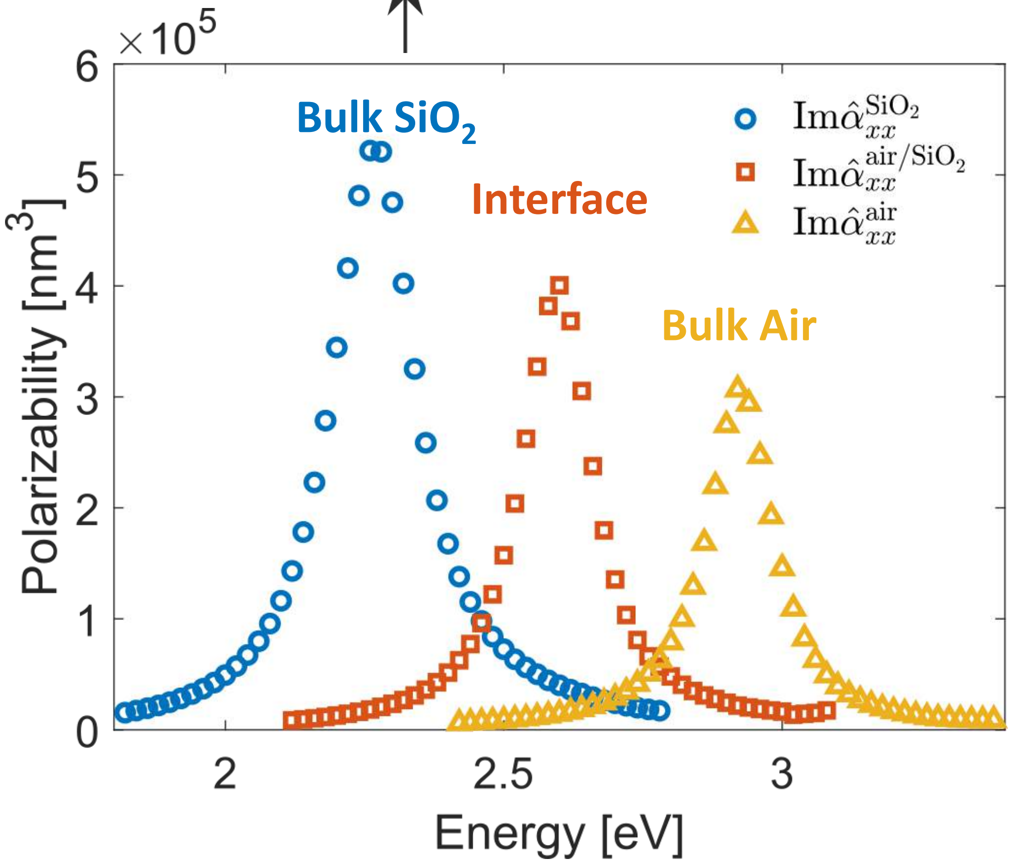
s - area of a unit cell

Polarizability tensor: FEM

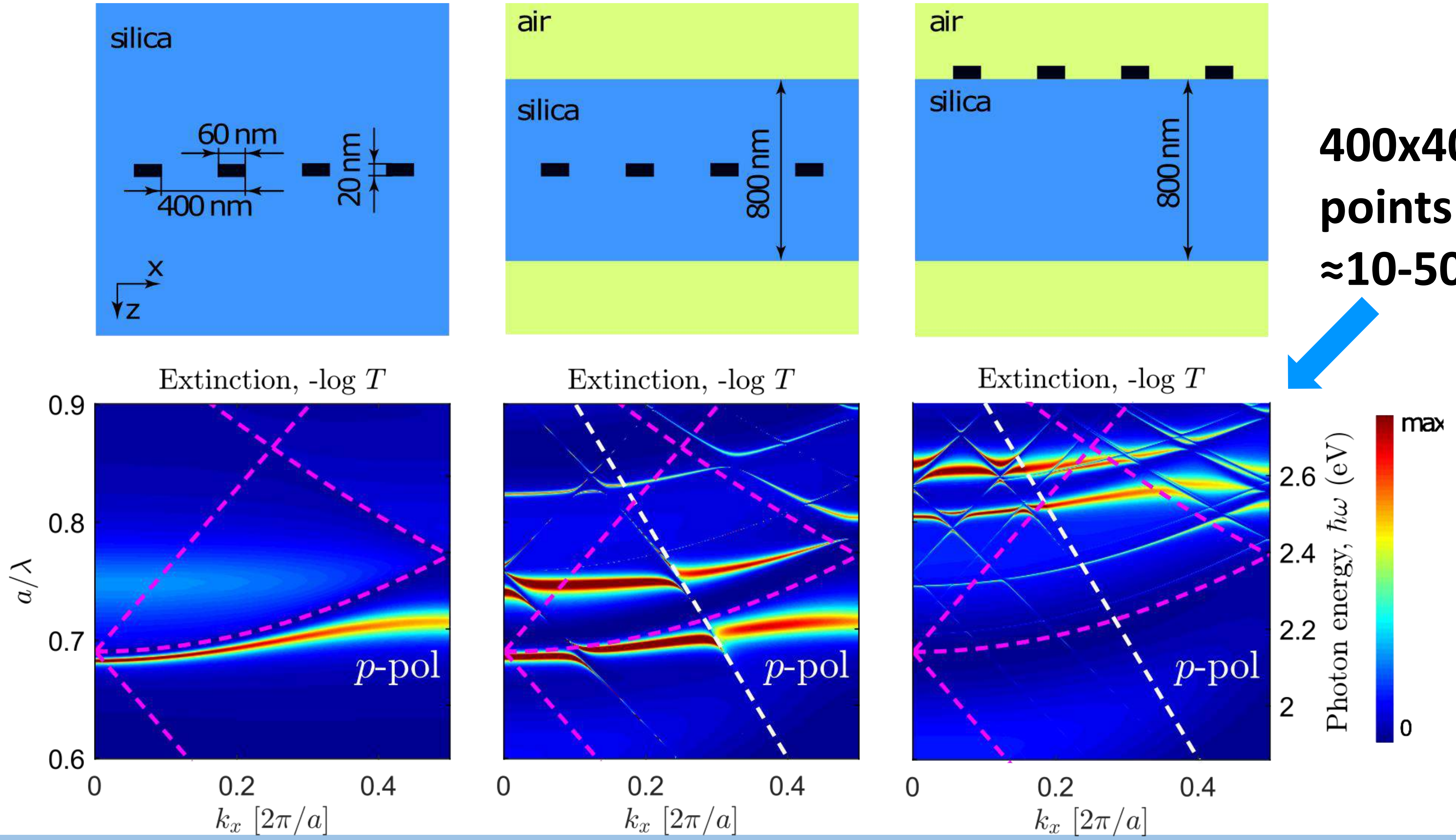
Silver nanodisk





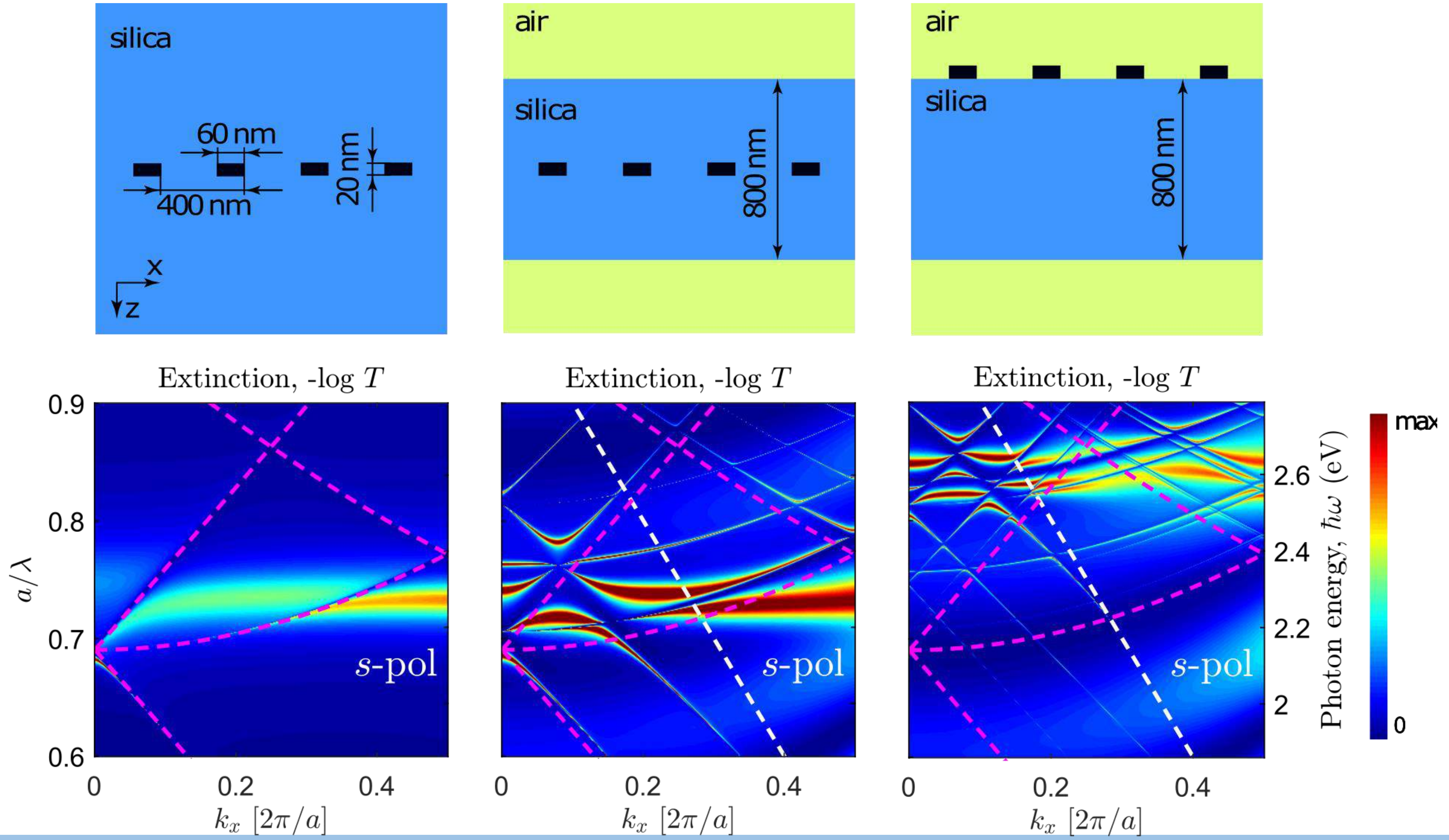


Spectra of plasmonic lattices

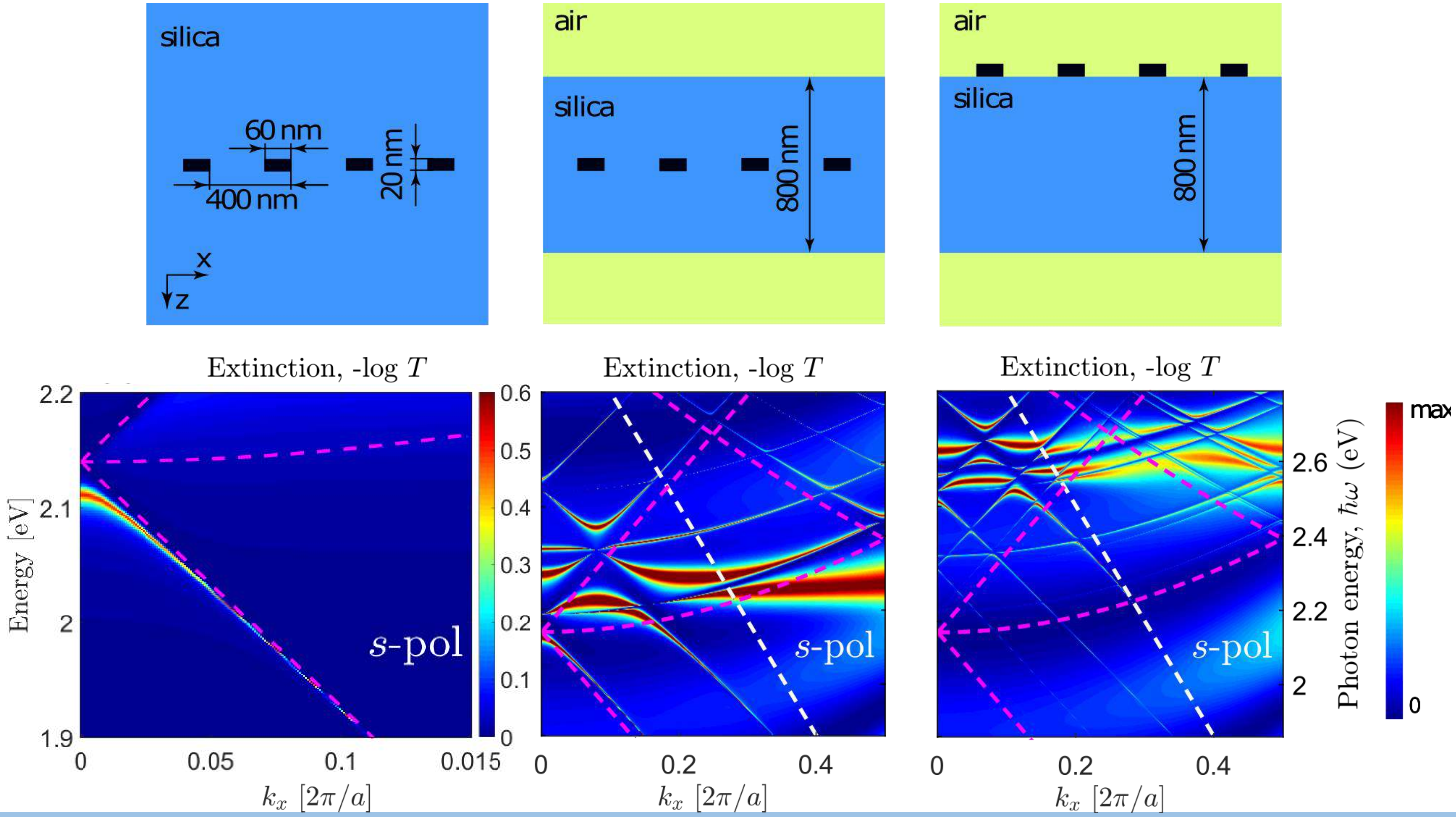


400x400 points ≈10-50ms

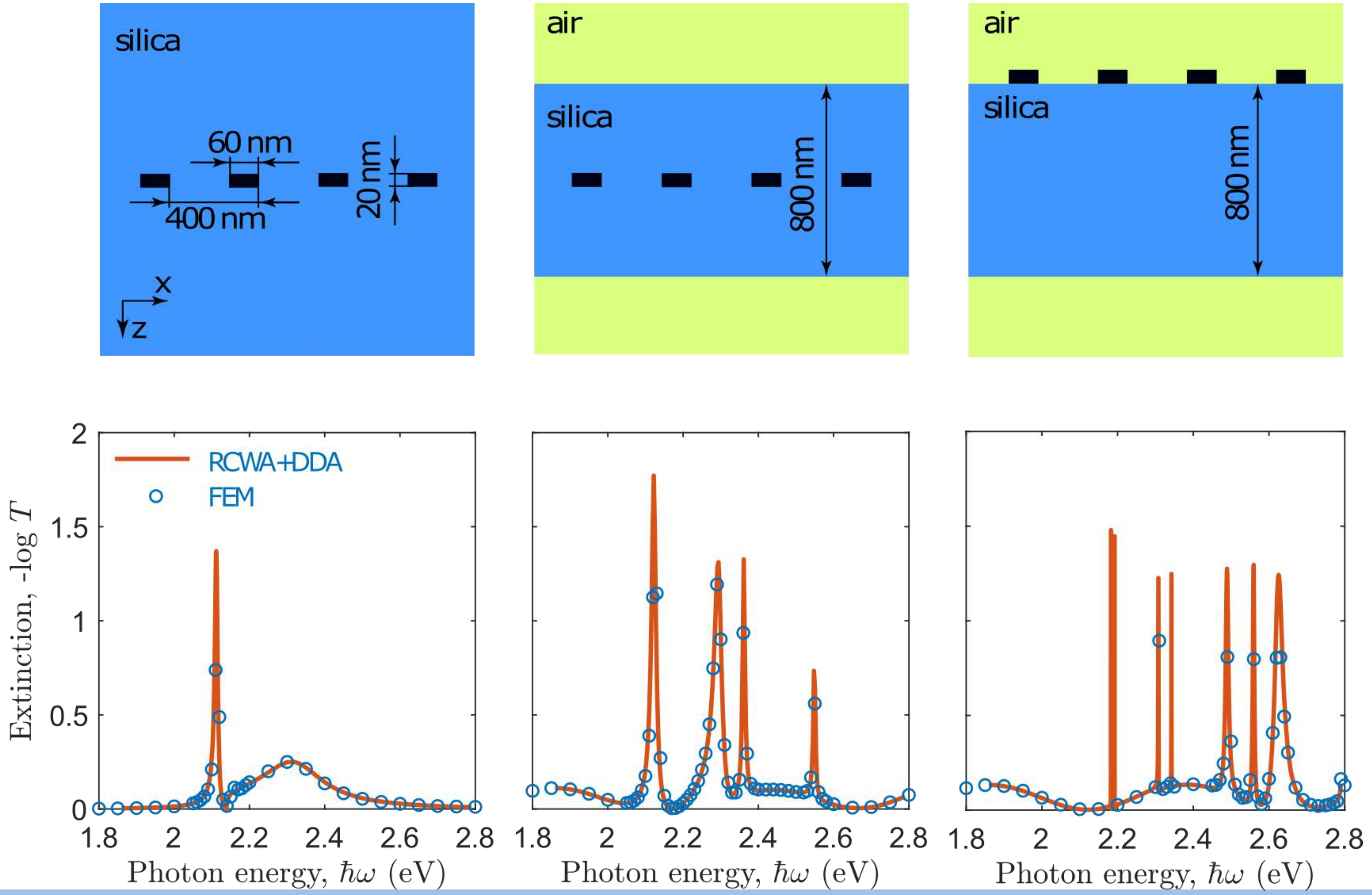
Spectra of plasmonic lattices



Spectra of plasmonic lattices

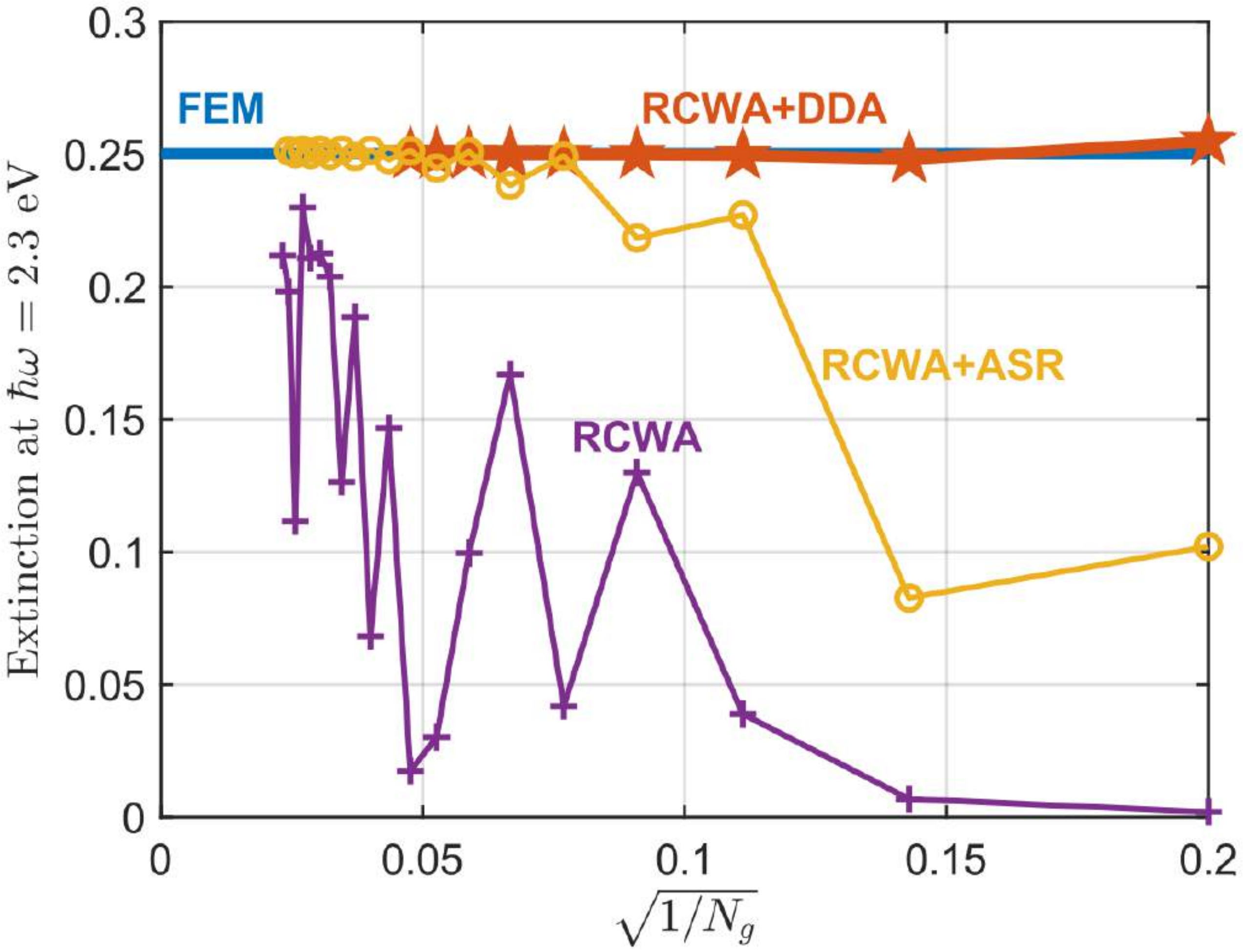


Spectra of plasmonic lattices



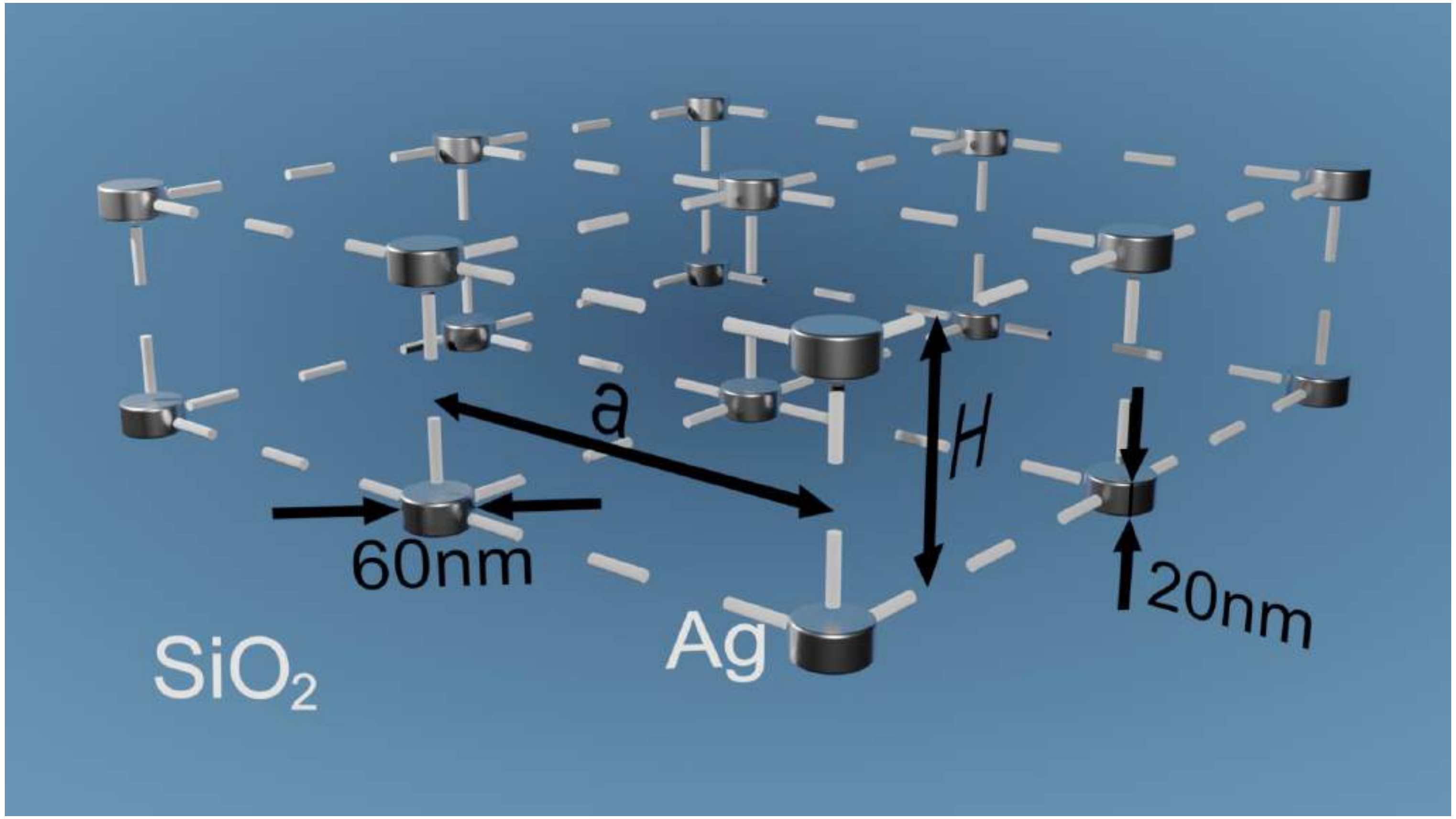
[I.M. Fradkin, S.A. Dyakov, and N.A. Gippius, Phys. Rev. B 99, 075310]

Remarks and questions



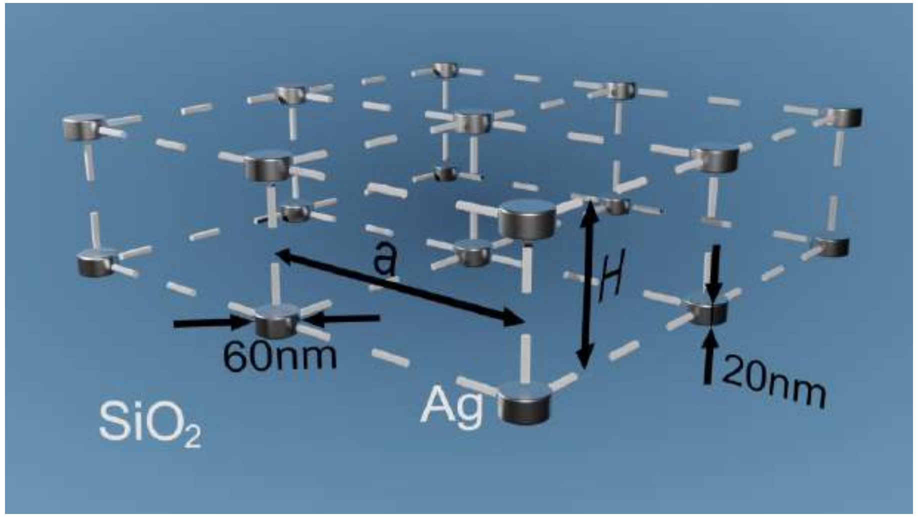
- **FEM** *calculations conducted in COMSOL Multiphysics.*
- **RCWA+DDA** *calculations from this study.*
- **RCWA** calculations (based on the original works of Prof. Gippius and Tikhodeev).
- **RCWA+ASR** calculations conducted by Prof. Thomas Weiss.

Stack of plasmonic lattices



[I.M. Fradkin, S.A. Dyakov, and N.A. Gippius, Phys. Rev. Applied **14**, 054030]

Dipole model



Equations on dipole moments:

$$\begin{pmatrix} \mathbf{P}_1 \\ \mathbf{P}_2 \end{pmatrix} = \begin{pmatrix} \hat{\alpha} & 0 \\ 0 & \hat{\alpha} \end{pmatrix} \begin{pmatrix} \mathbf{E}_1^{\mathrm{bg}} \\ \mathbf{E}_2^{\mathrm{bg}} \end{pmatrix}$$

$$\begin{pmatrix} \mathbf{P}_1 \\ \mathbf{P}_2 \end{pmatrix} = \begin{pmatrix} \hat{\alpha} & 0 \\ 0 & \hat{\alpha} \end{pmatrix} \left[\begin{pmatrix} \mathbf{E}_1^0 \\ \mathbf{E}_2^0 \end{pmatrix} + \begin{pmatrix} \hat{C}_{11} & \hat{C}_{12} \\ \hat{C}_{21} & \hat{C}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{P}_1 \\ \mathbf{P}_2 \end{pmatrix} \right]$$

Symmetry

$$\mathbf{P} \rightarrow P^x$$
$$C_{11}^{xx} = C_{22}^{xx}$$
$$C_{12}^{xx} = C_{21}^{xx}$$

Change of the basis:

$$\begin{pmatrix} P_{\mathrm{A}} \\ P_{\mathrm{B}} \end{pmatrix} = \frac{\alpha_{xx}}{\sqrt{2}} \begin{pmatrix} E_1^{0x} + E_2^{0x} \\ E_1^{0x} - E_2^{0x} \end{pmatrix} + \alpha_{xx} \begin{pmatrix} C_{11}^{xx} + C_{12}^{xx} & 0 \\ 0 & C_{11}^{xx} - C_{12}^{xx} \end{pmatrix} \begin{pmatrix} P_{\mathrm{A}} \\ P_{\mathrm{B}} \end{pmatrix}$$

$$\begin{pmatrix} P_{\mathrm{A}} \\ P_{\mathrm{B}} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} P_1^x \\ P_2^x \end{pmatrix}$$

The solution separates into **even (A)** and **odd (B)** modes

Amplitudes of even (A) and odd (B) mode:

$$P_{\mathrm{A}} = \frac{E_1^{0x}(1 + e^{ikH})/\sqrt{2}}{\alpha_{xx}^{-1} - (C_{11}^{xx} + C_{12}^{xx})} \qquad P_{\mathrm{B}} = \frac{E_1^{0x}(1 - e^{ikH})/\sqrt{2}}{\alpha_{xx}^{-1} - (C_{11}^{xx} - C_{12}^{xx})}$$

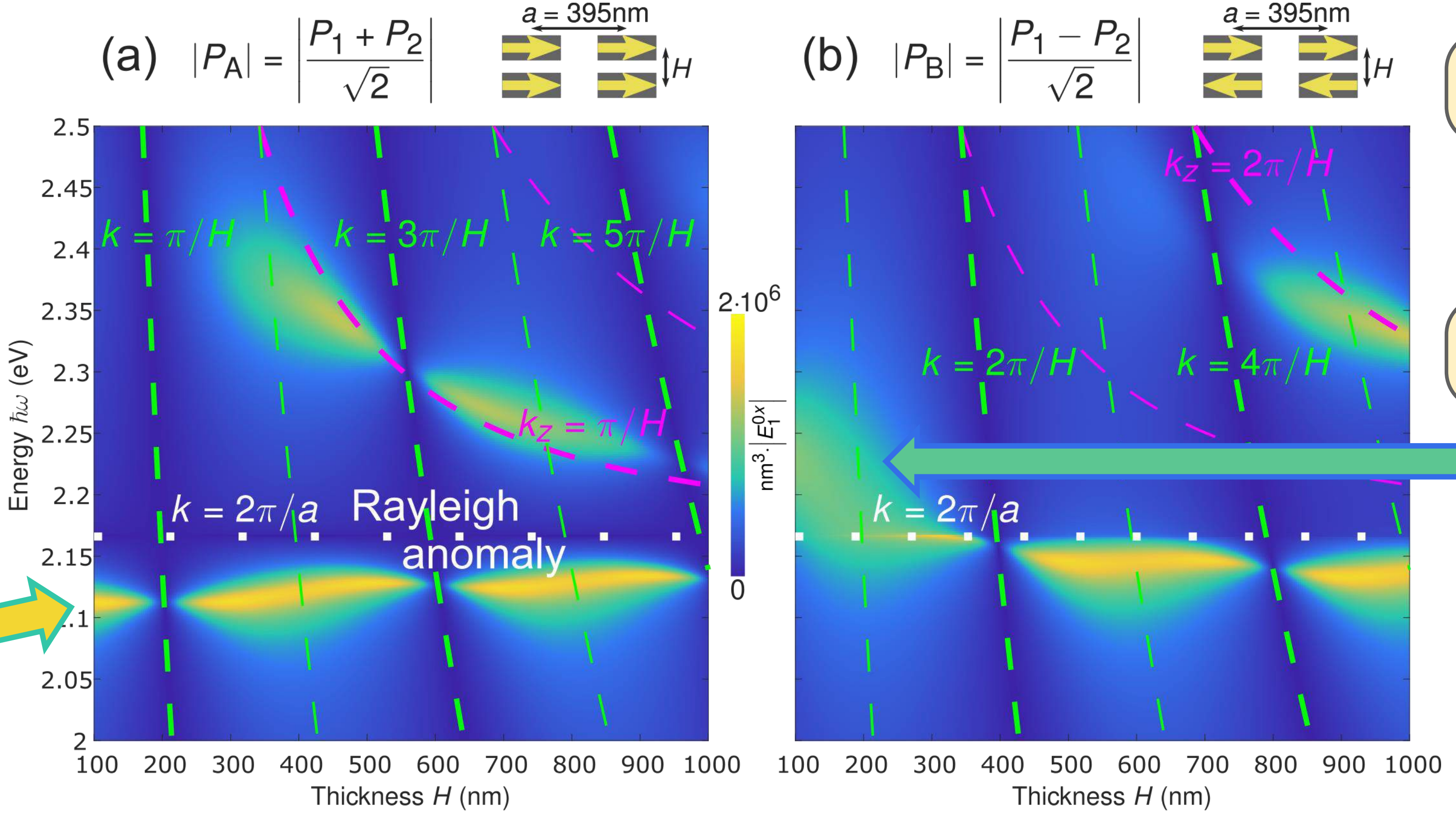
Spectra of plasmonic lattices stack

even modes | **odd** modes

$$C_{11}^{xx} = C_{12}^{xx}$$

$$\mathrm{Re}\,\alpha_{xx}^{-1} = 2C_{11}^{xx}$$

Ordinary lattice plasmon



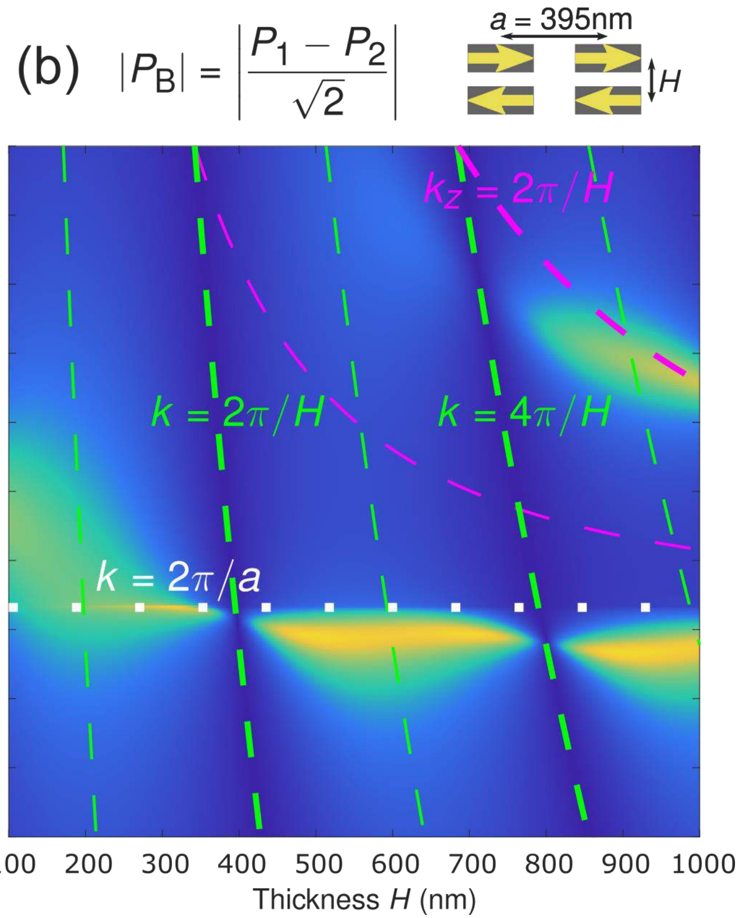
$$C_{11}^{xx} = C_{12}^{xx}$$

$$\mathrm{Re}\,\alpha_{xx}^{-1} = 0$$

Localized plasmon

$$P_A = \frac{E_1^{0x}(1 + e^{ikH})/\sqrt{2}}{\alpha_{xx}^{-1} - (C_{11}^{xx} + C_{12}^{xx})} \qquad P_B = \frac{E_1^{0x}(1 - e^{ikH})/\sqrt{2}}{\alpha_{xx}^{-1} - (C_{11}^{xx} - C_{12}^{xx})}$$

Spectra of plasmonic lattices stack



$$P_{\rm B} = \frac{E_1^{0x}(1 - e^{ikH})/\sqrt{2}}{\alpha_{xx}^{-1} - (C_{11}^{xx} - C_{12}^{xx})}$$

$$C_{11}^{xx} = \frac{4\pi}{s}\frac{ik_0^2}{k_z} + \tilde{C}_{11}^{xx} \qquad C_{12}^{xx} = \frac{4\pi}{s}\frac{ik_0^2}{k_z}e^{ik_zH} + \tilde{C}_{12}^{xx}(H)$$

$$\alpha_{xx}^{-1} - C_{11}^{xx} + C_{12}^{xx} =$$

$$\alpha_{xx}^{-1} + \frac{4\pi}{s}\frac{ik_0^2}{k_z}(e^{ik_zH} - 1) - \tilde{C}_{11}^{xx} + \tilde{C}_{12}^{xx}(H) \approx$$

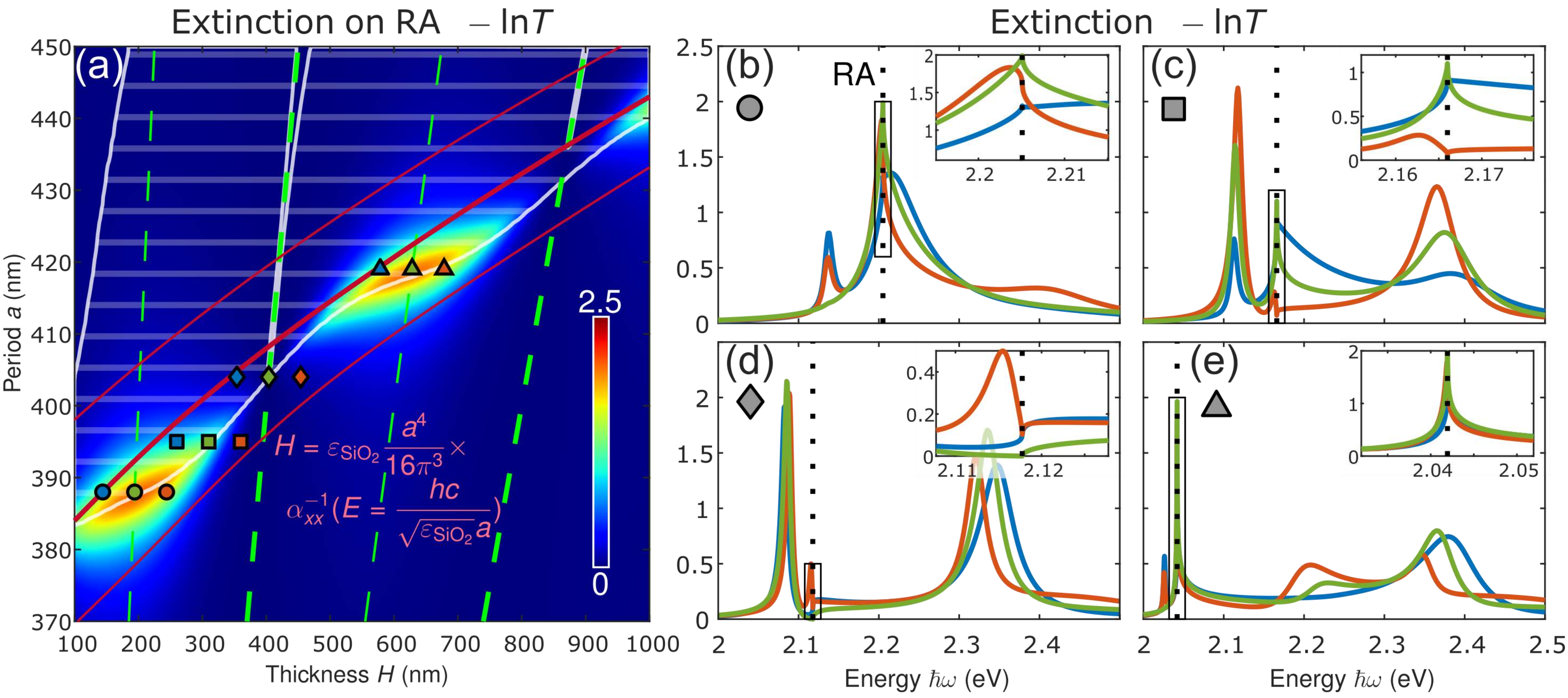
$$\alpha_{xx}^{-1} - \frac{4\pi k_0^2}{s}H - \frac{4\pi k_0^2}{s}ik_zH^2/2 - \tilde{C}_{11}^{xx} + \tilde{C}_{12}^{xx}(H)$$

Indeterminate term

Determines resonance condition

Derivative discontinuity

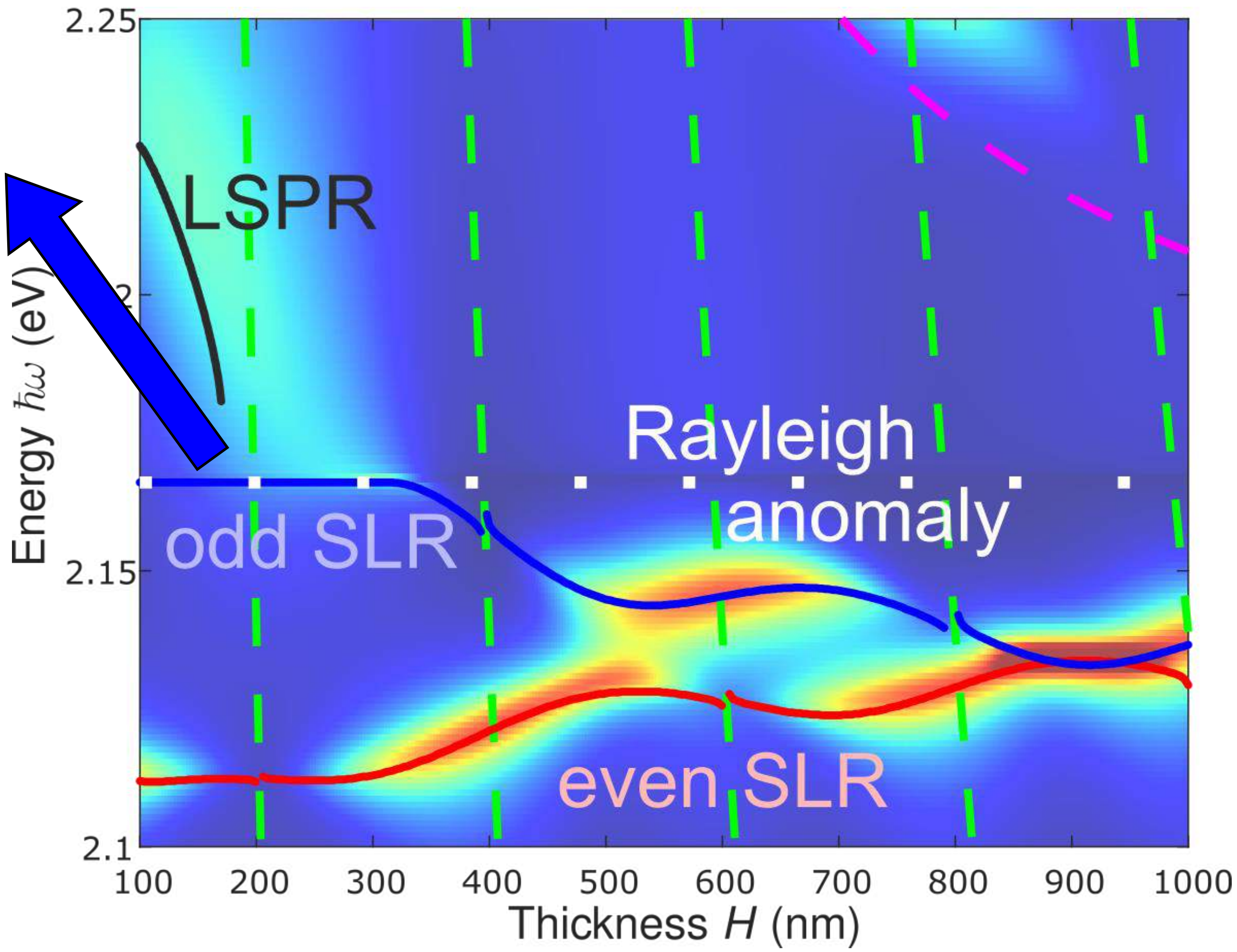
Spectra of plasmonic lattices stack



Dispersion of plasmonic modes

Resonance is pinned to the Rayleigh anomaly for the wide range of thicknesses

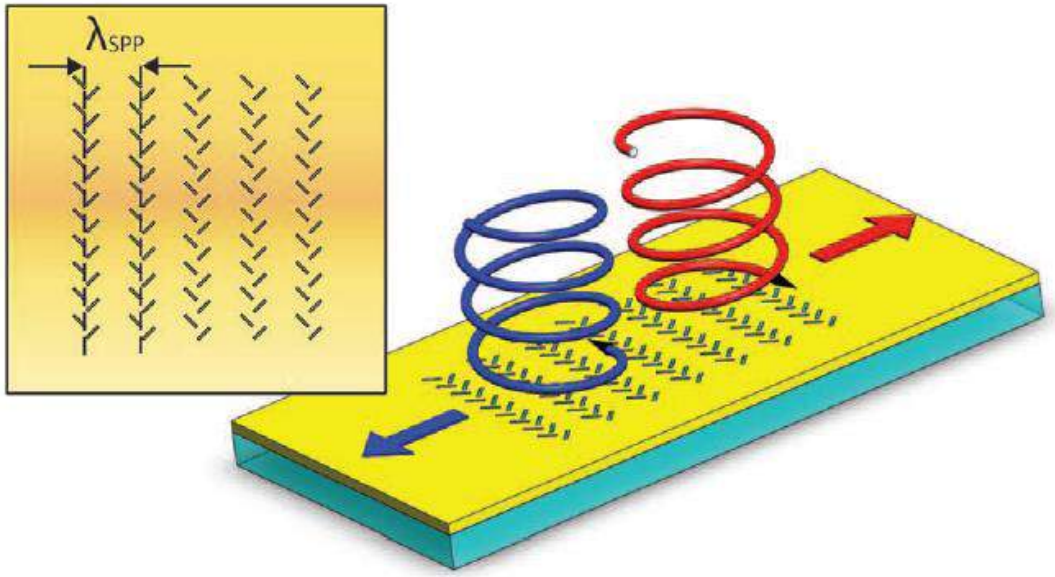
Energy is determined just by a period, which is most stably reproduced quantity in experiment



We find eigenenergies as follows:

$$\max\arg |P_{\mathrm{A}}(E)|$$
$$\max\arg |P_{\mathrm{B}}(E)|$$

Routing waveguide modes

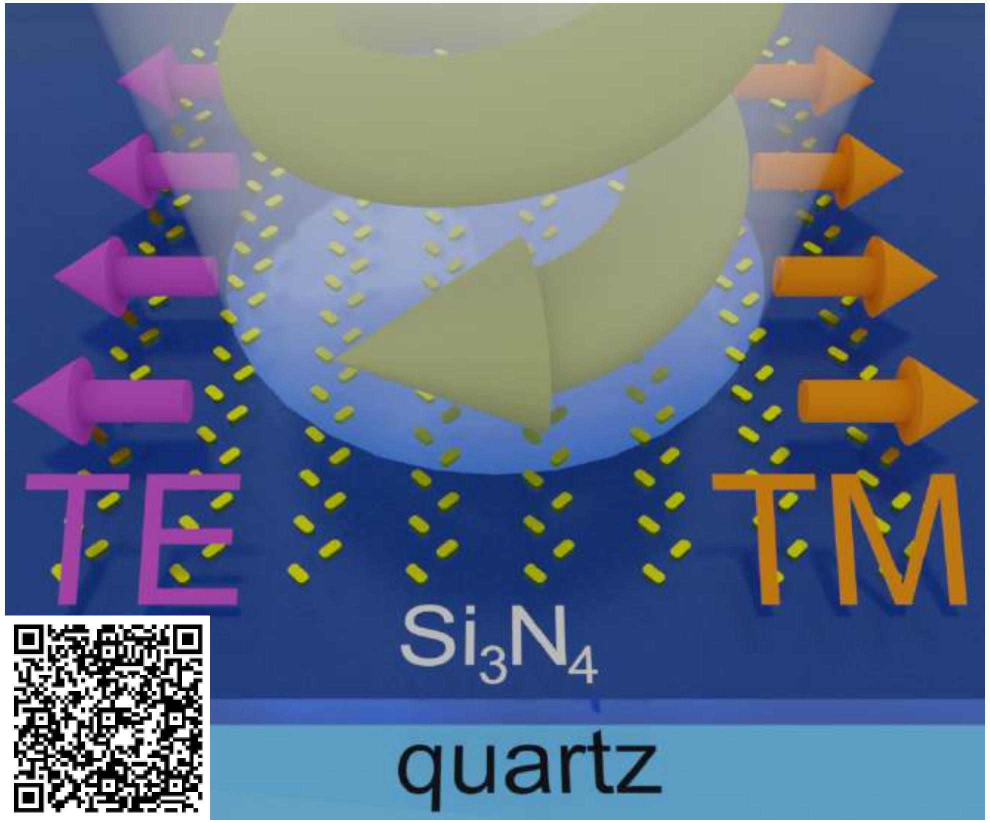


[Lin, J., Mueller, J. B., Wang, Q., Yuan, G., Antoniou, N., Yuan, X. C., & Capasso, F., 2013, *Science, 340*(6130), 331-334.]

Vladimir Kulakovskiy

Andrey Demenev

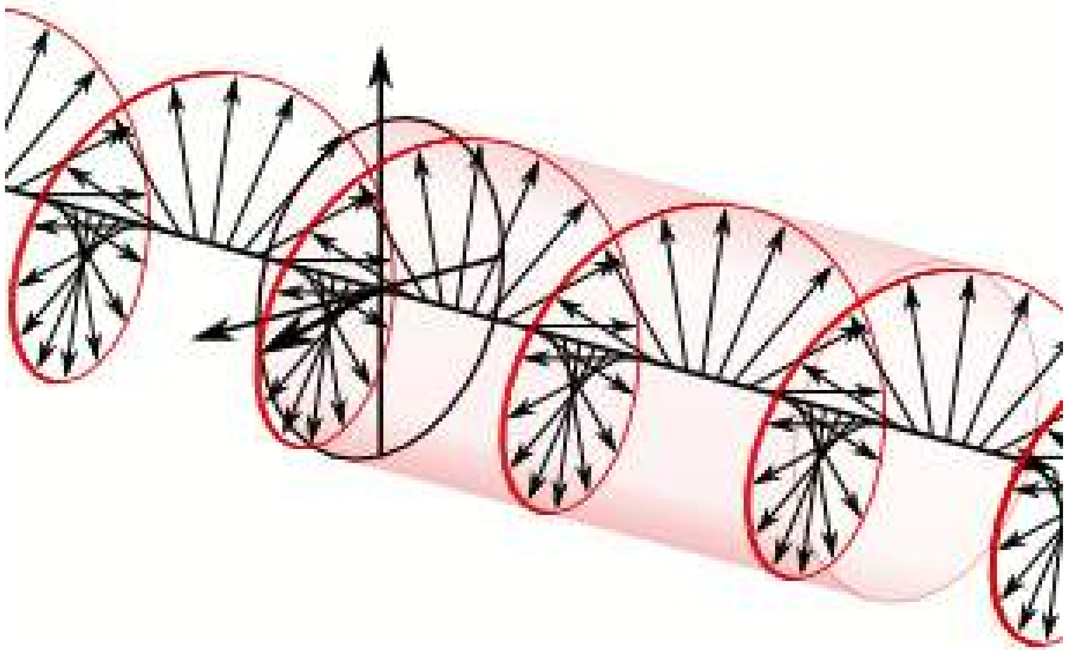
Vladimir Antonov



Fradkin, Ilia M., et al., *Advanced Optical Materials* (2024): 2303114.

Routing waveguide modes

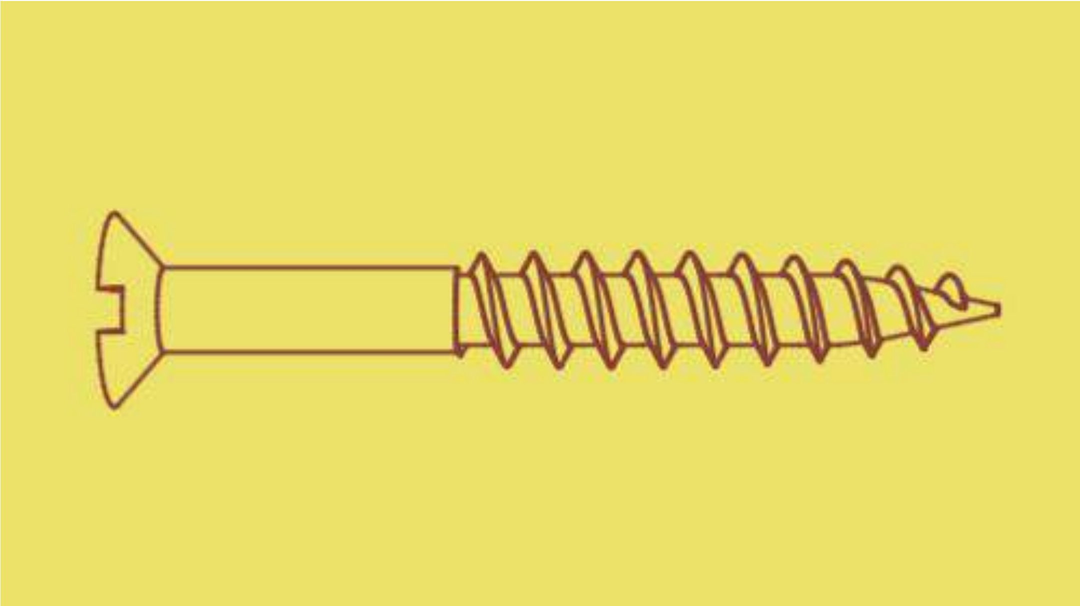
What is the handedness?



https://ru.wikipedia.org

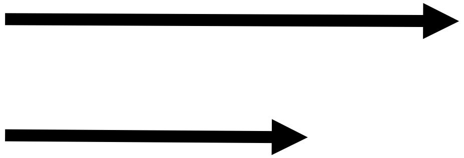
Routing waveguide modes

Right-handed screw



$\vec{\omega}$

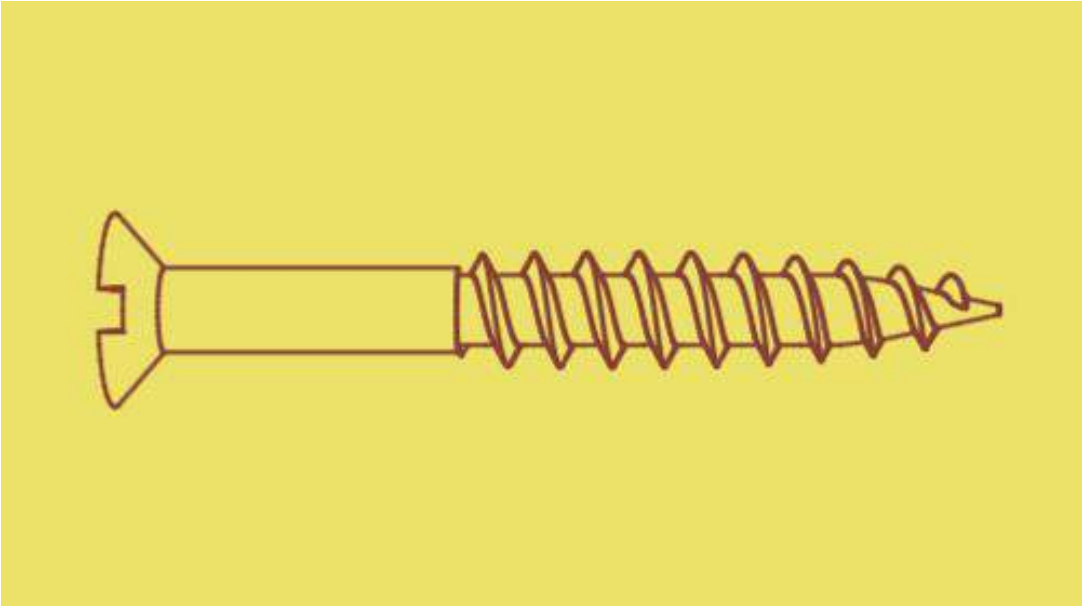
$\vec{v}$



https://fruitnice.ru

Routing waveguide modes

Right-handed screw

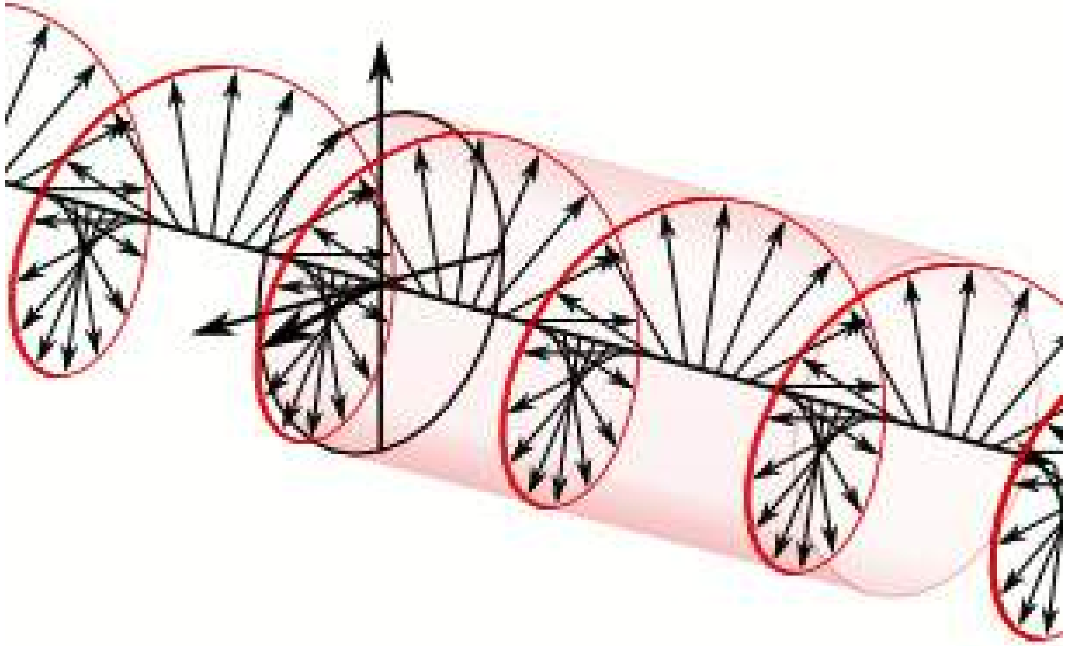


$\vec{\omega}$ ⟶

$\vec{v}$ ⟶

https://fruitnice.ru

What is the handedness?

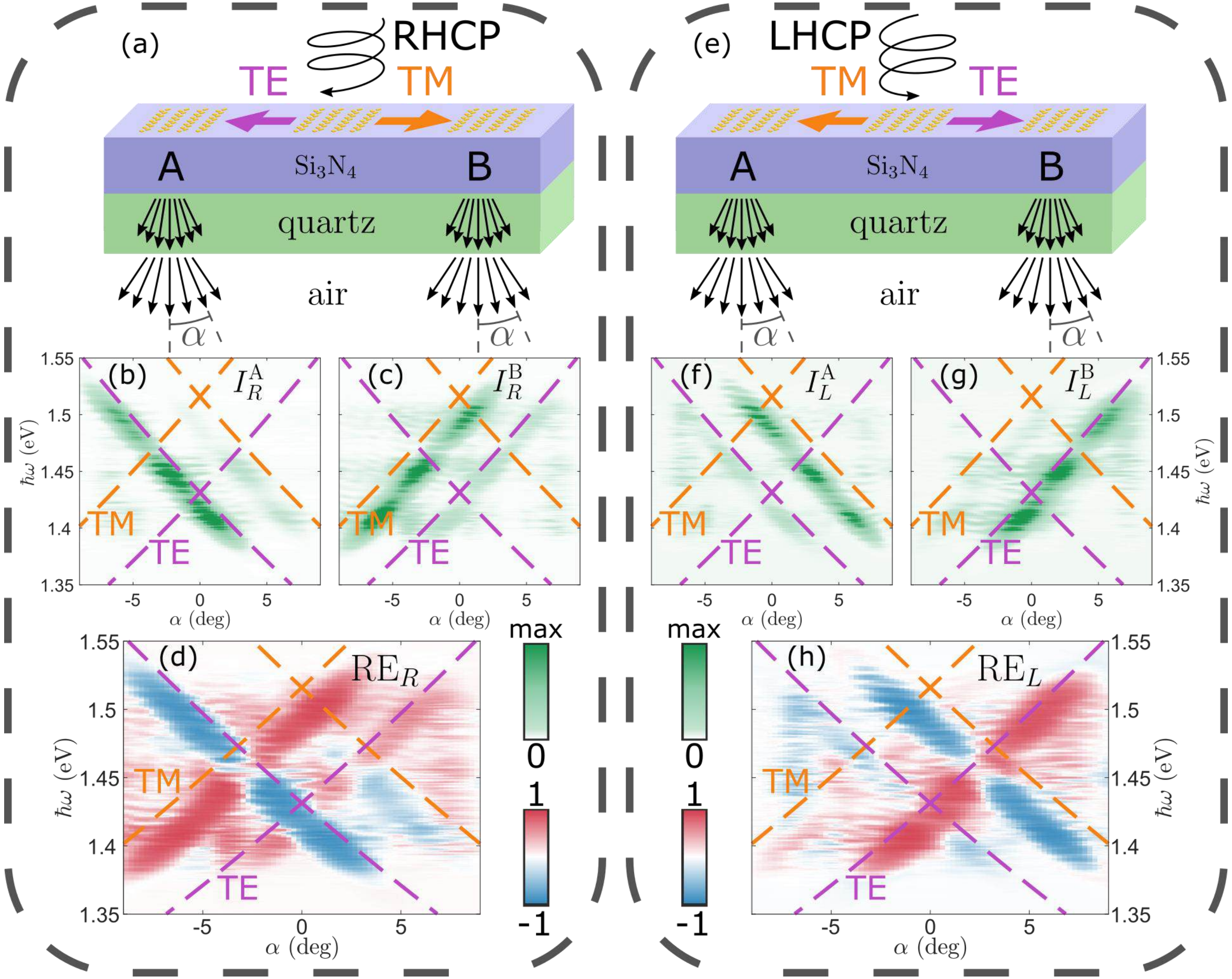


$\vec{\omega}$ ⟶

$\vec{v}$ ⟶

https://ru.wikipedia.org

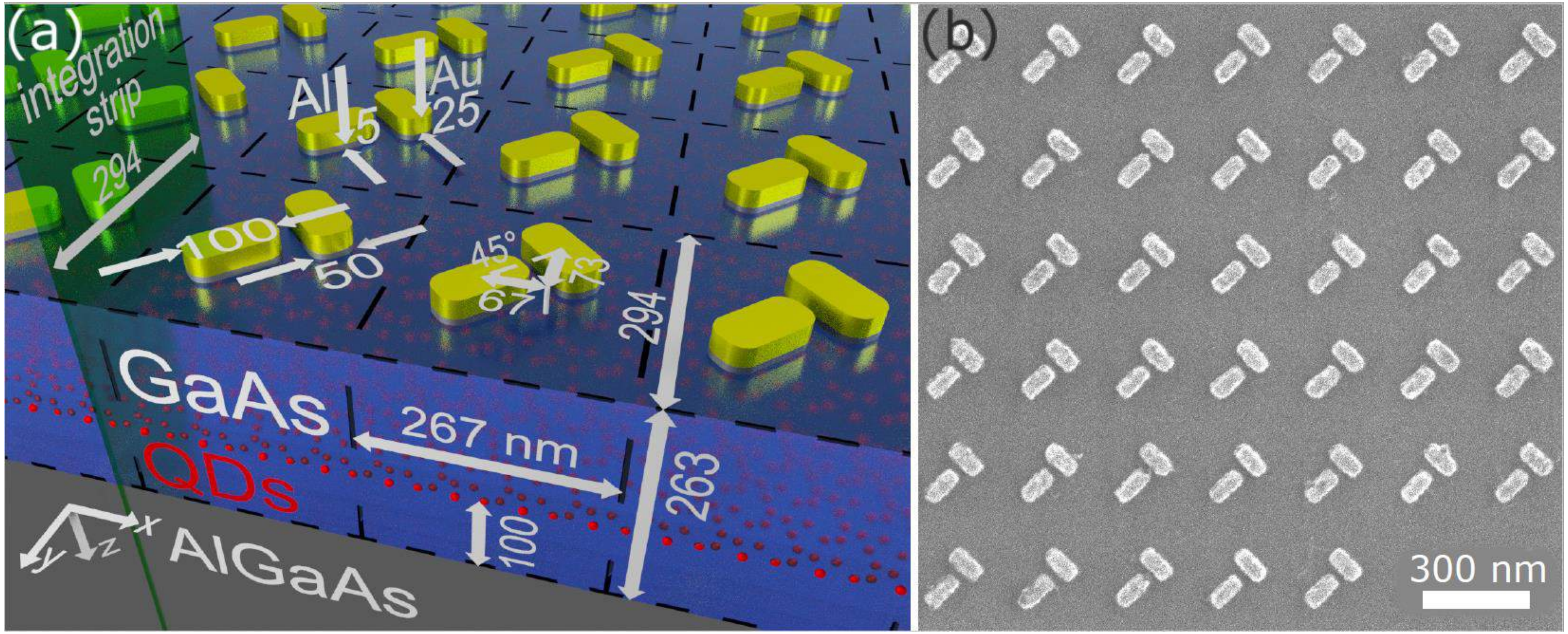
Routing waveguide modes



Routing Efficiency 95%

Degree of Circular Polarization 97%

Spontaneous emission control



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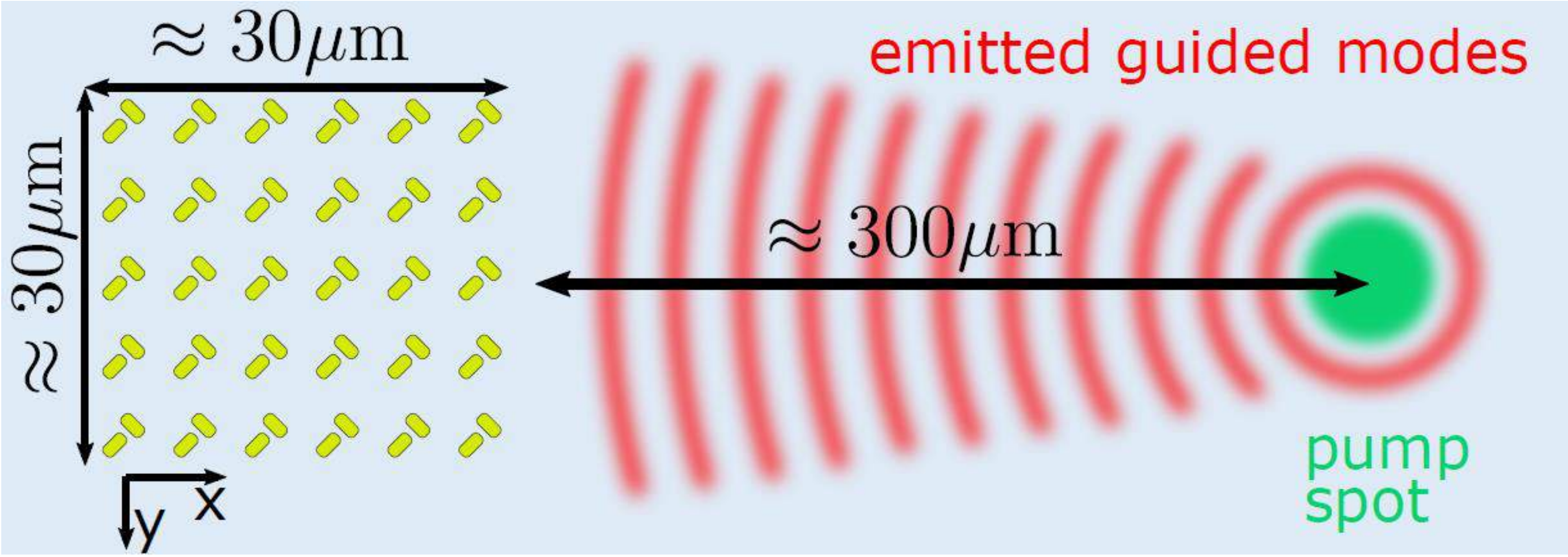
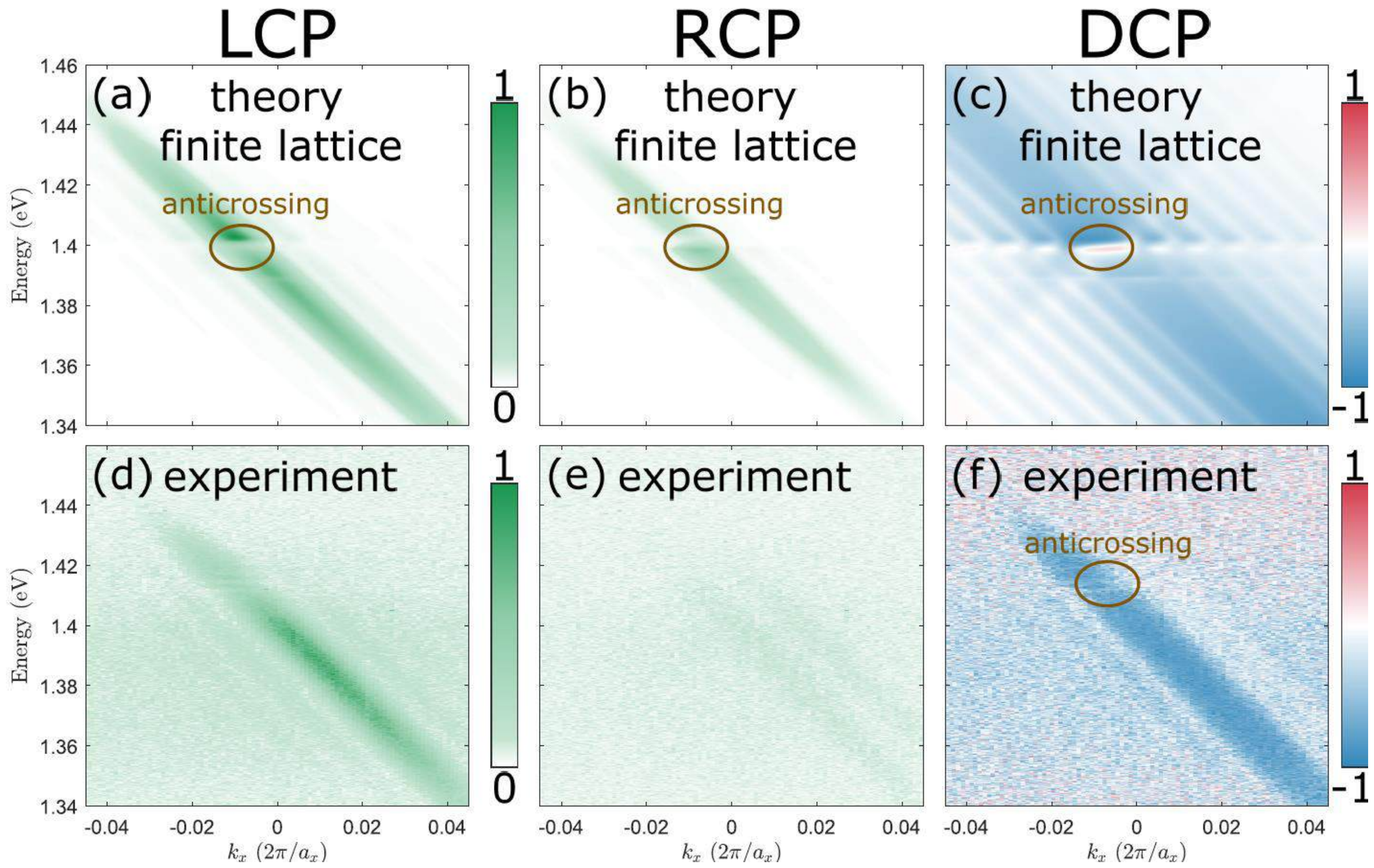
Fradkin, I. M., Demenev, A. A., Kulakovskii, V. D., Antonov, V. N., & Gippius, N. A. *Appl. Phys. Lett.*, 2022, *120*, 17, 171702.

Photoluminescense



Photoluminescense



Degree of Circular Polarization 80%

Conclusions

- Lattices of plasmonic nanoparticles support **hybrid optical modes**
- Discrete **dipole approximation** + **scattering matrix** = efficient numerical approach
- Coupling via **waveguide modes** and **Rayleigh anomalies** is strongly **different**
- Grating coupler of plasmonic nanoparticles routs waveguide modes (**95% routing efficiency**) and provides circularly-polarized outcoupling (**97% degree of circular polarization**)

Thank you for your attention!

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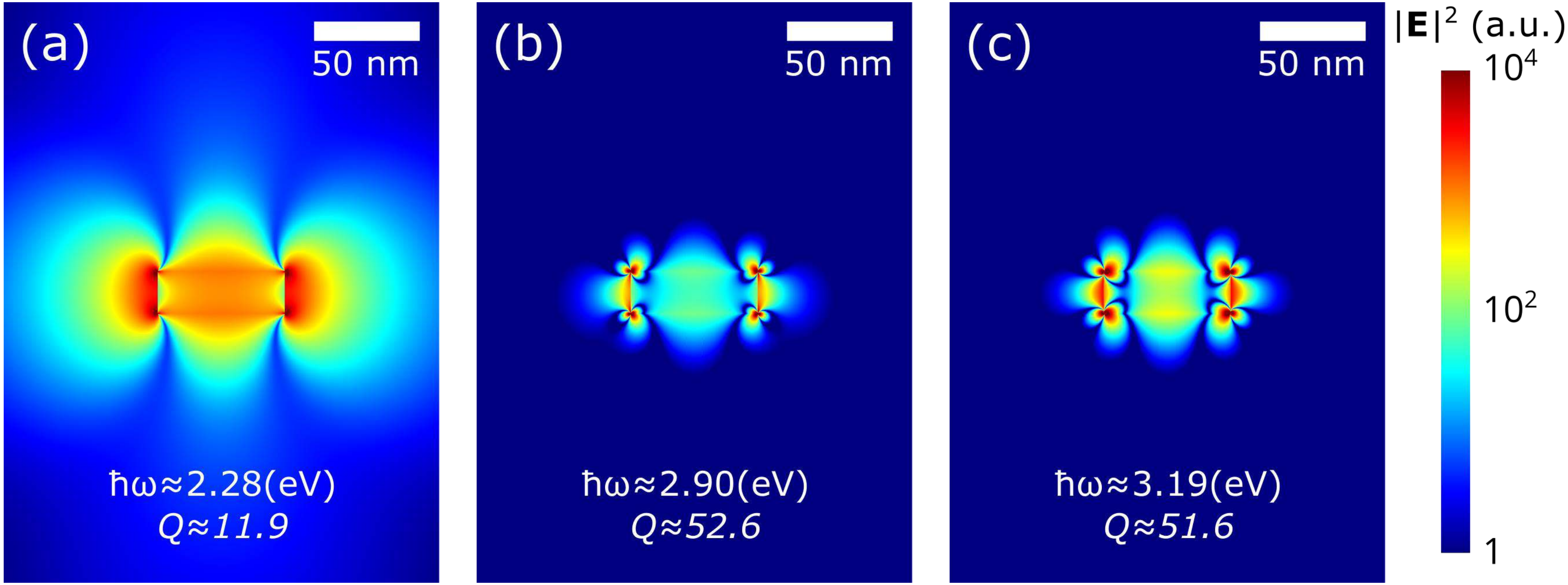
Clover

Polarizability tensor

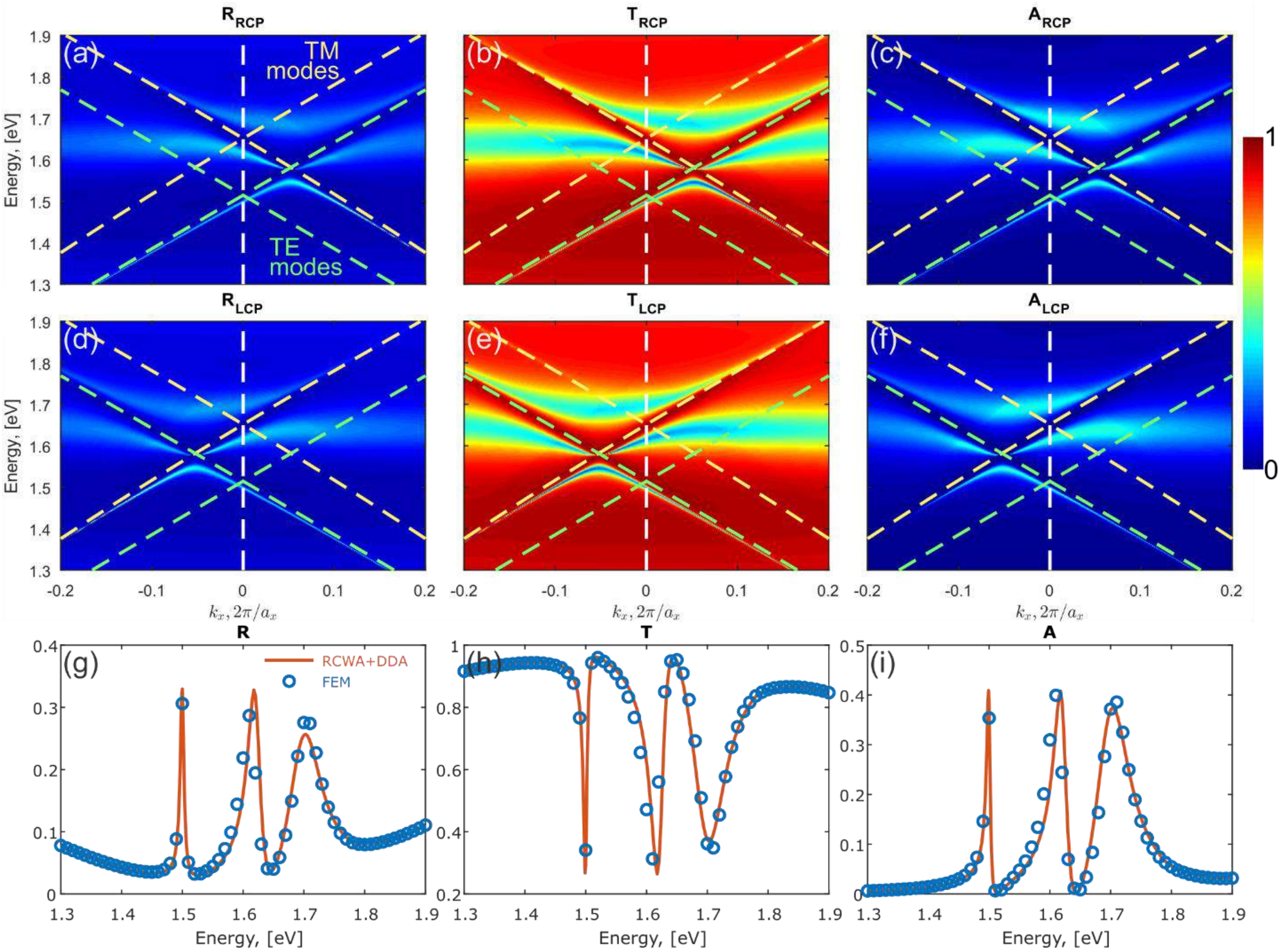
LSPR | LSPR + edge plasmons



Spectra of lattice with basis

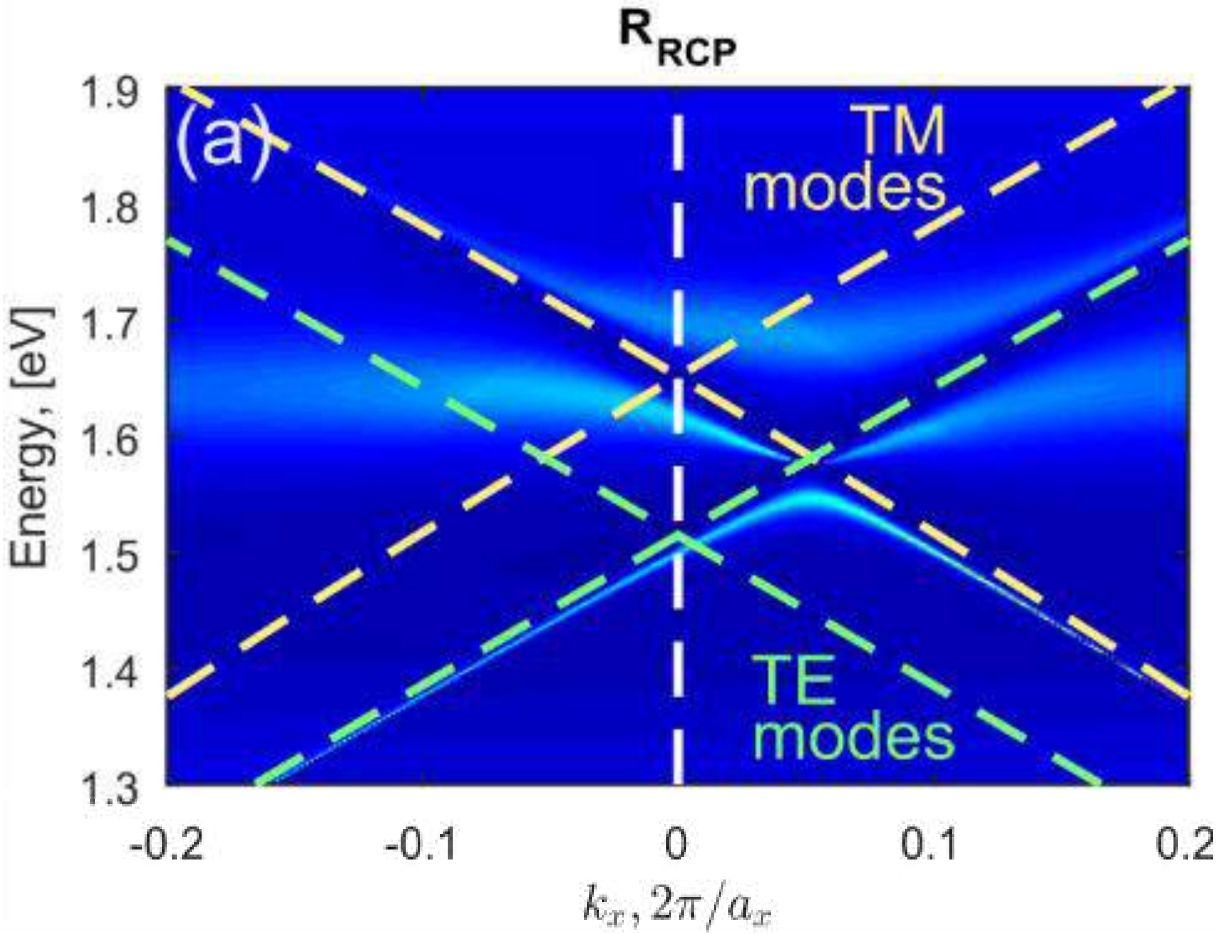
Right-hand Circular Polarization

Left-hand Circular Polarization



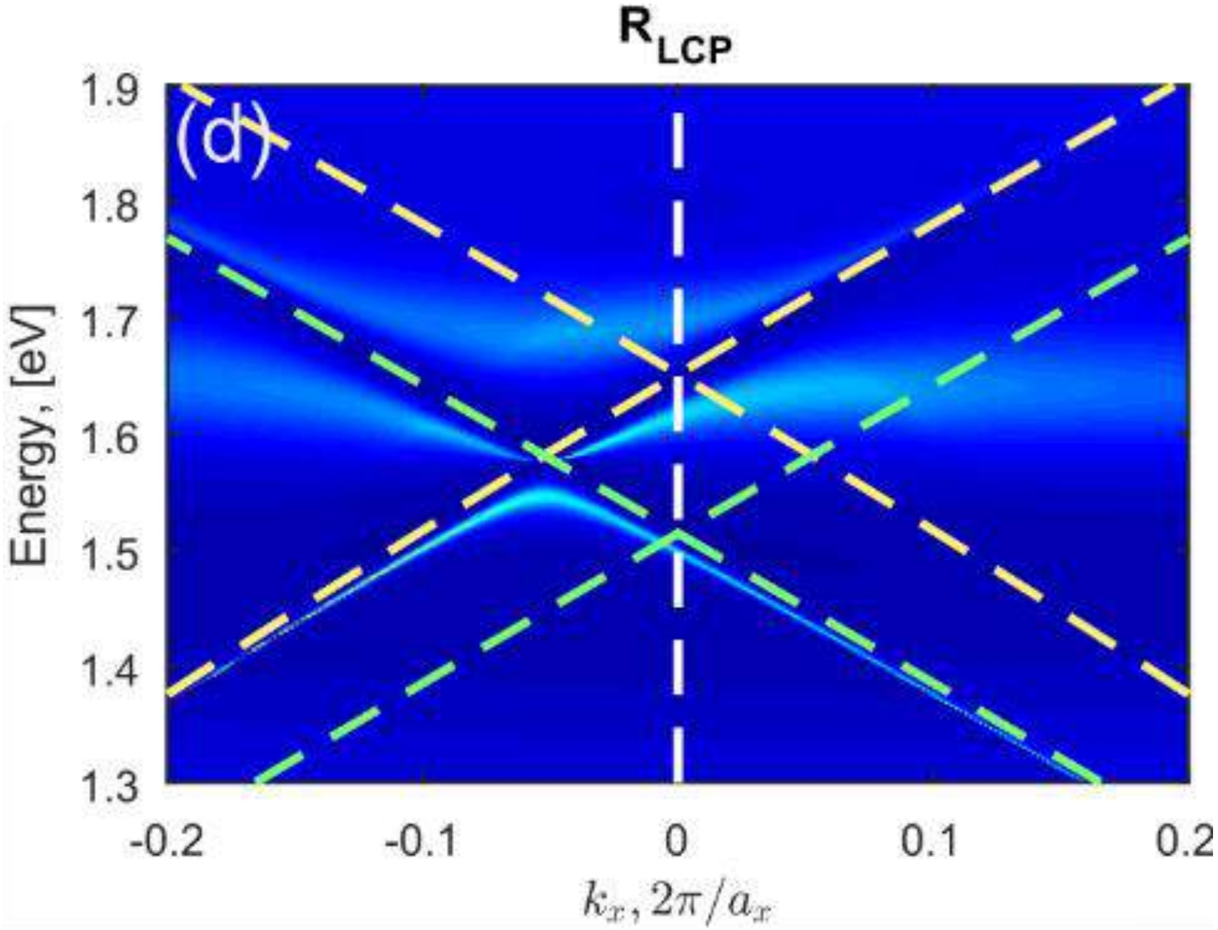
Spectra of lattice with basis

Right-hand Circular Polarization



Spectra of lattice with basis

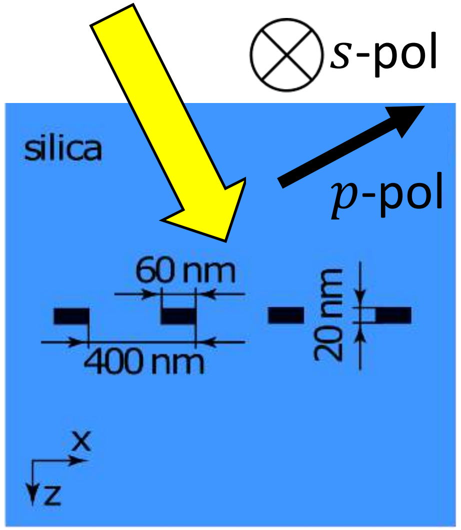
Left-hand Circular Polarization

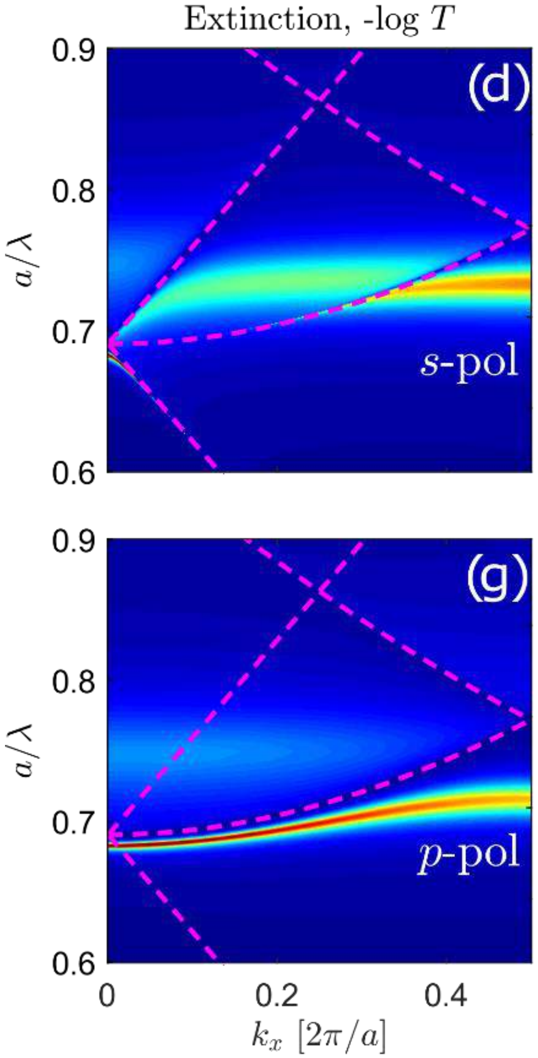


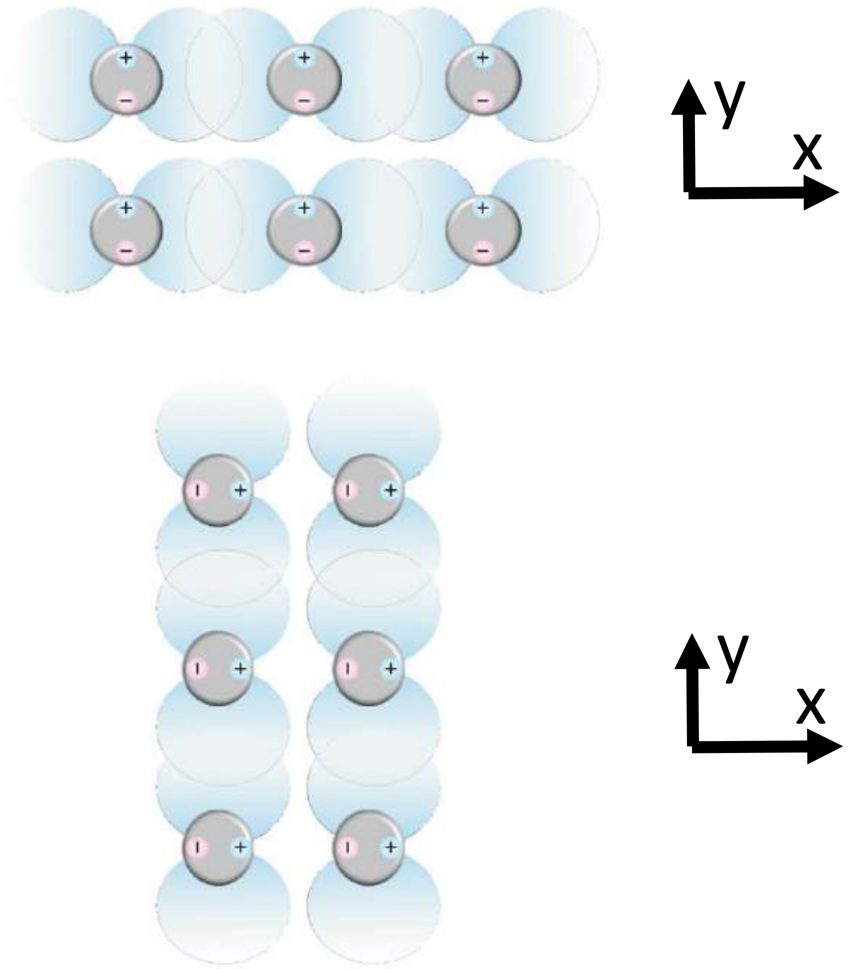
Remarks and questions

13. Some details of the geometry of interaction of light with the lattice of plasmonic particles (Ch.2) are missing.

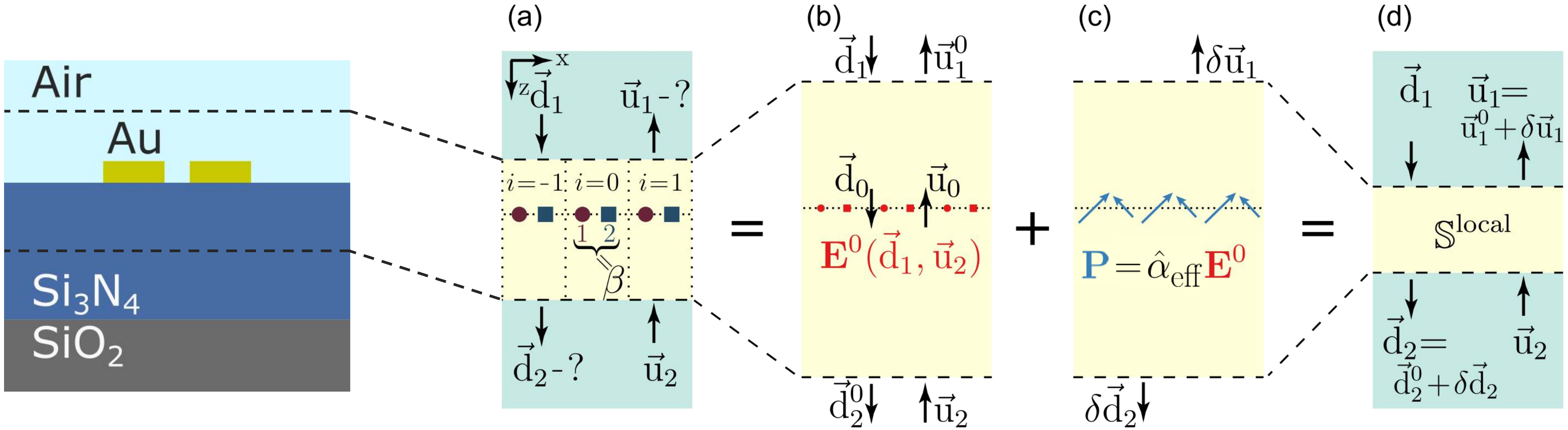
Indeed, it would have been very useful to describe more details of light interaction with simple lattice of plasmonic nanoparticles.







Scattering matrix calculation



$$\begin{pmatrix} \mathbf{E}^{bg}_{\beta=1} \\ \mathbf{E}^{bg}_{\beta=2} \\ \vdots \end{pmatrix} = \begin{pmatrix} \mathbf{E}^{0}_{\beta=1} \\ \mathbf{E}^{0}_{\beta=2} \\ \vdots \end{pmatrix} + \begin{pmatrix} \hat{C}_{11} & \hat{C}_{12} & \vdots \\ \hat{C}_{21} & \hat{C}_{22} & \vdots \\ \dots & \dots & \ddots \end{pmatrix} \begin{pmatrix} \hat{\alpha}_1 & 0 & 0 \\ 0 & \hat{\alpha}_2 & 0 \\ 0 & 0 & \ddots \end{pmatrix} \begin{pmatrix} \mathbf{E}^{bg}_{\beta=1} \\ \mathbf{E}^{bg}_{\beta=2} \\ \vdots \end{pmatrix}$$

$$\hat{C}_{\beta\gamma}(\mathbf{k}_\parallel) = \begin{cases} \sum_{j\neq i} \hat{G}(\mathbf{r}_{\beta,i}, \mathbf{r}_{\beta,j}) e^{i\mathbf{k}_\parallel(\mathbf{r}_{\beta,j}-\mathbf{r}_{\beta,i})} & \text{for } \beta = \gamma \\ \sum_{j} \hat{G}(\mathbf{r}_{\beta,i}, \mathbf{r}_{\gamma,j}) e^{i\mathbf{k}_\parallel(\mathbf{r}_{\gamma,j}-\mathbf{r}_{\gamma,i})} & \text{for } \beta \neq \gamma \end{cases}$$

We solve the equations for several particles in unit cell.

$$\hat{\alpha}_{\text{eff}} = \begin{pmatrix} \hat{\alpha}_1 & 0 & 0 \\ 0 & \hat{\alpha}_2 & 0 \\ 0 & 0 & \ddots \end{pmatrix} \times \left[\hat{I} - \begin{pmatrix} \hat{C}_{11} & \hat{C}_{12} & \vdots \\ \hat{C}_{21} & \hat{C}_{22} & \vdots \\ \dots & \dots & \ddots \end{pmatrix} \begin{pmatrix} \hat{\alpha}_1 & 0 & 0 \\ 0 & \hat{\alpha}_2 & 0 \\ 0 & 0 & \ddots \end{pmatrix} \right]^{-1}$$

And obtain generalized **effective polarizability** tensor