Nano-Plasmonics: Material Models and Computational Methods

AG Theoretische Optik & Photonik

Kurt Busch

Humboldt-Universität zu Berlin, Institut für Physik, AG Theoretische Optik & Photonik

and

Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Berlin, Germany

Acknowledgments

Dr. Richard Diehl*

Dr. Michael König*

Dr. Jens Niegemann*

Dr. Christian Matyssek

Dr. Rogelio Rodriguez-Oliveros

Dr. Christian Wolff

Matthias Moeferdt

Dan-Nha Huynh

Julia Werra

Timo Köllner*

Christopher Prohm*

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SPP 1391

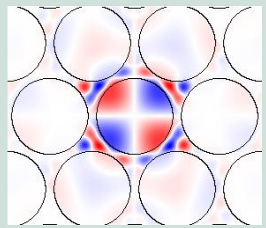
Hybrid Inorganic/Organic Systems for Opto-Electronics

Sonderforschungsbereich 951

Theoretical Optics & Photonics Group

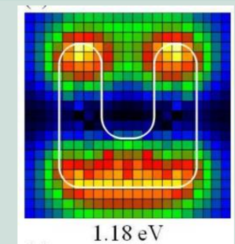
Periodic Nanostructures

Photonic Crystals
Functional Elements
Radiation Dynamics



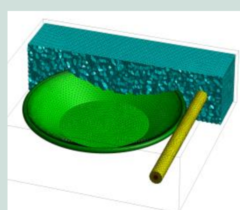
Metamaterials / Plasmonics

Coupling Mechanisms
EELS
Nonlinear Metal Optics



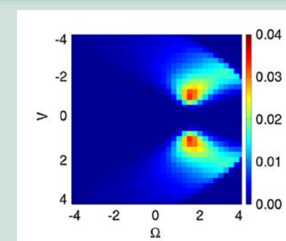
Method Development

Discontinuous Galerkin Methods
Fourier Modal Method
Operator Exponential Methods
Photonic Wannier Functions



Quantum Photonics

Few-Photon Transport
Counting Statistics
Quantum Field Theory



Outline

- Motivation
- Discontinuous Galerkin Time-Domain Approach
- Example: Electron Energy Loss Spectroscopy
- Advanced Modeling: Transition Metals (Magneto-Plasmonics)
- Advanced Modeling: Nonlinear Metal Optics
- Conclusions & Outlook

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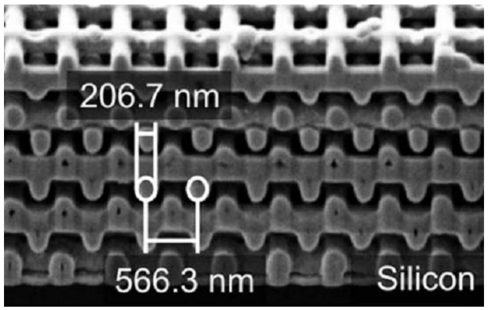
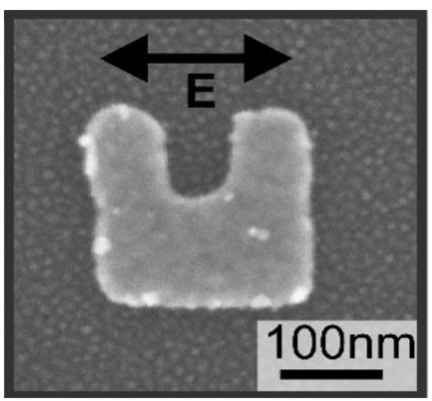
Nano-Photonics

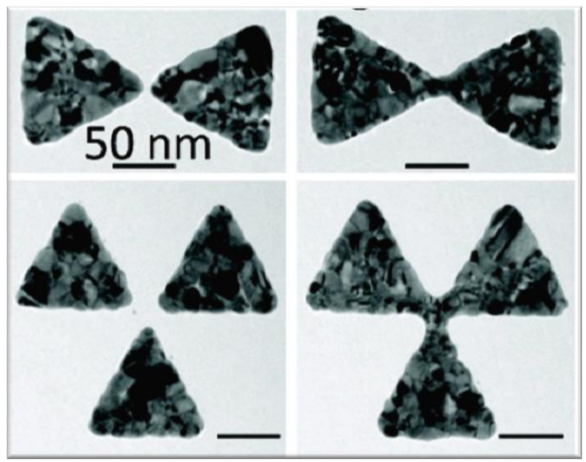
Accurate & Efficient Simulation of Nano-Photonics Systems



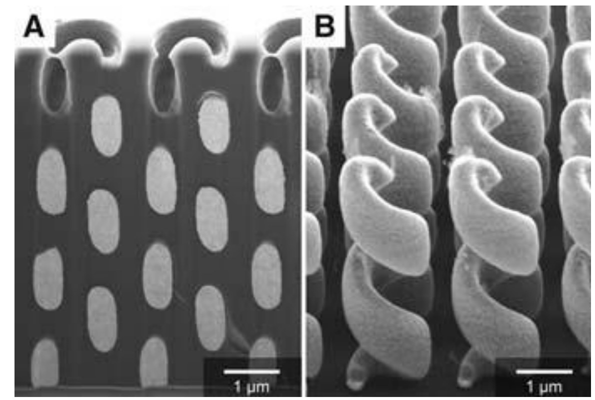
Opt. Lett. **35**, 1094 (2010)



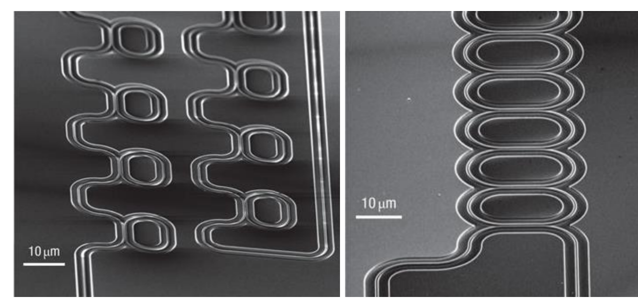
Nature Photonics **2**, 614 (2008)



Nano Letters **11**, 1323 (2011)

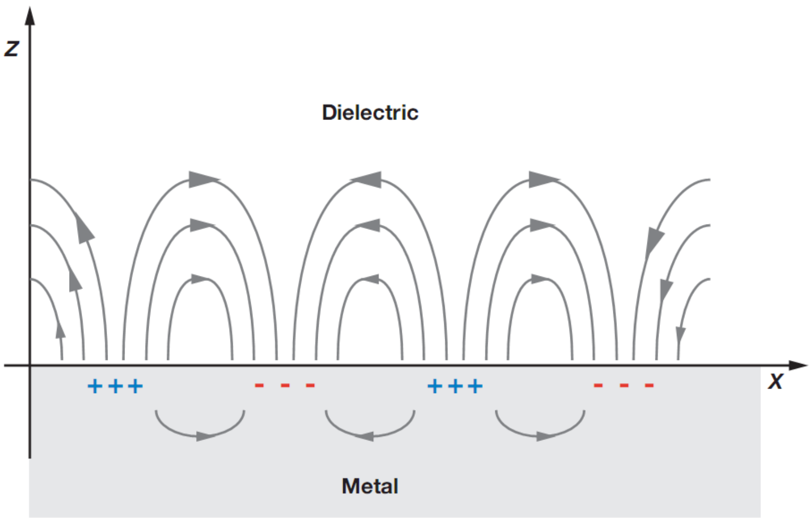


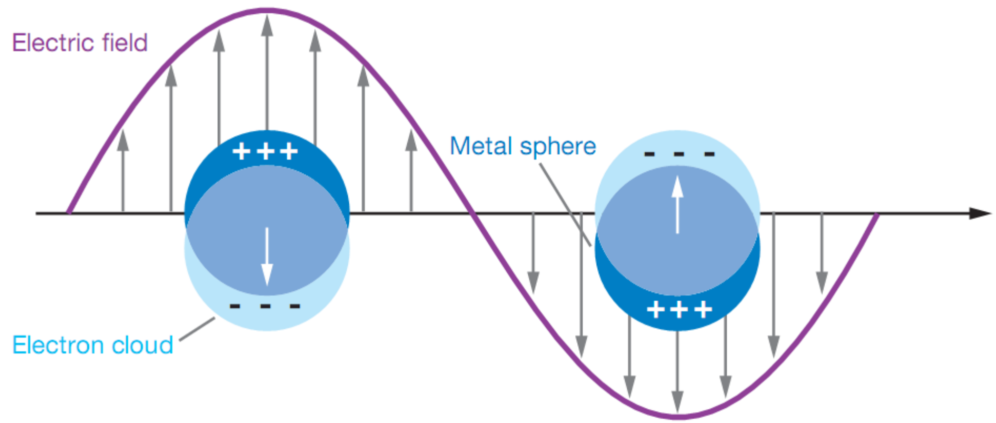
Science **325**, 1513 (2009)



Nature Photonics **1**, 65 (2007)

Nano-Plasmonics





Propagating Surface Plasmon Polariton

Localized Particle Plasmon Polariton

Graphs taken from Annu. Rev. Phys. Chem. **58**, 267 (2007)

Not to forget: Longitudinal (bulk) plasmons

Nano-Plasmonics: Challenges for Modeling

- Complex Objects: Shape and Material Properties
  - Geometry: Curved Surfaces, Tiny Gaps, Large Aspect Ratios
  - Light-Matter Interaction: Dispersive, Nonlinear, Active Materials
  - Strong Multiple Scattering Effects
  - Multiple Time- and Length-Scales

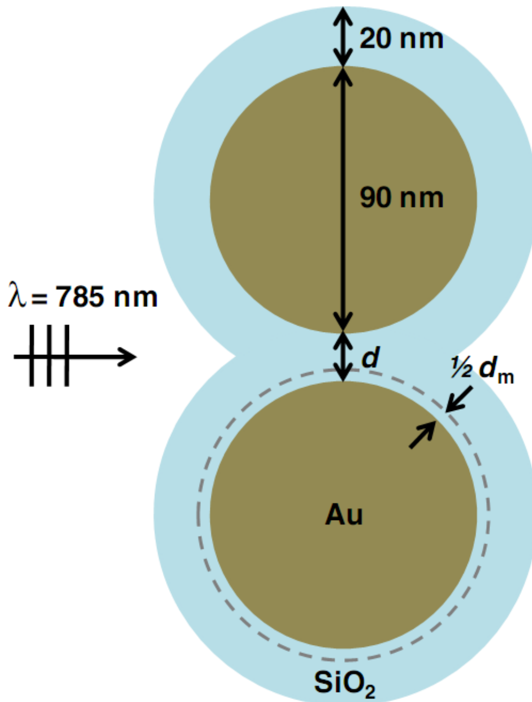
- Very Few Analytical Solutions Available

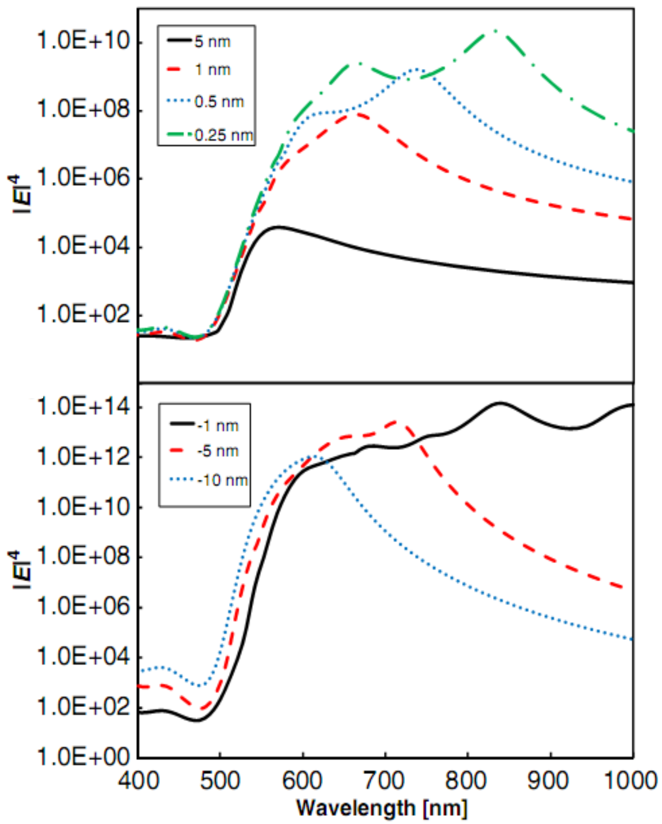
- Frequency-Domain Solvers
  - FEM, BEM, MMP, FMM (aka RCWA), DDA, GF, …

- Time-Domain
  - FDTD, (FVTD), (FETD), (MoL-TD)
  - MicPIC, DFT, TDDFT, Multi-Scale (Hybrid)

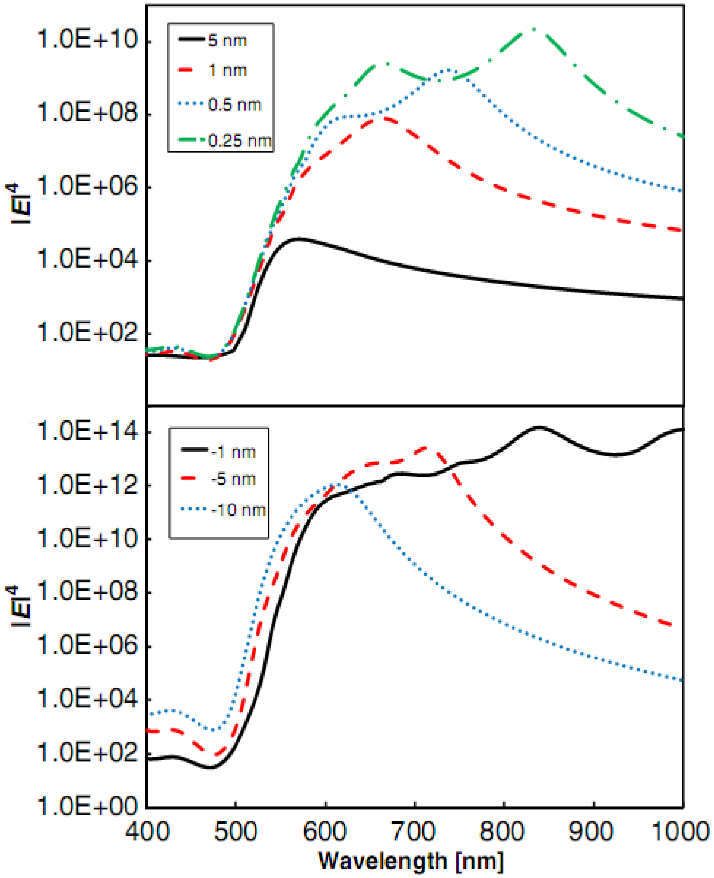
Do not trust Computers, Part I

The Gospel of the SERS Enhancement Factor:





Do not trust Computers, Part II

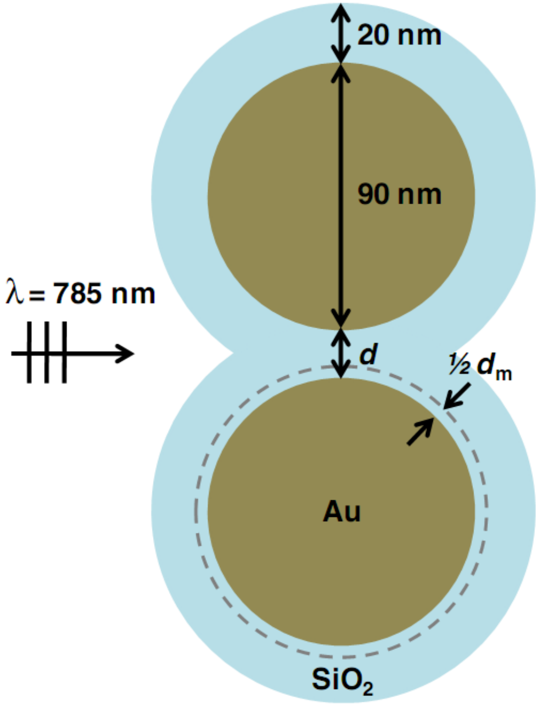


These EM enhancements are significantly larger than has been reported in most of the past EM studies of fused structures [6, 23, 35], and in fact they suggest that in these systems non-resonant SMSERS would be possible. The reason for this exotic behavior is that the crevice formed by the dimer overlap is incredibly sharp, yet the overlap is not severe enough to exclude the antenna position where strong localization of the EM enhancements occur.

EM-Field Enhancement:

$$\left(10^{14}\right)^{1/4} \approx 3 * 10^3$$

Do not trust Computers, Part III



- Fermi Wavelength of Gold (Longitudinal):

$$\lambda_F = 0.5 \text{ nm}$$

- Tranverse Length Scale:

$$\ell_T = \frac{v_F}{c}\lambda = \frac{1.4 * 10^6 \quad \text{m/s}}{3 * 10^8 \text{m/s}} 785 \quad \text{nm} \approx 3.6 \quad \text{nm}$$

- Typical Parameters:

$$I = \frac{P}{A} = \frac{10 \text{ mW}}{\pi (0.5 \ \mu\text{m})^2} = \frac{E_0^2}{376} = \frac{E_0^2}{Z_0}$$

$$E_0 \approx 2 * 10^6 \ \frac{\text{V}}{\text{m}} \ \rightarrow E \approx 6 * 10^9 \ \frac{\text{V}}{\text{m}}$$

Electron Tunneling, Nonlocal Effects, Local Heating, Nonlinear Optical Properties?

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Discontinuous Galerkin Time-Domain Approach

- Maxwell Equations in Flux-Conservative Form

$$\hat{\mathcal{Q}}\,\frac{\partial}{\partial t}\begin{pmatrix}\vec{E}\\ \vec{H}\end{pmatrix} + \nabla\cdot\vec{\mathcal{F}}(\vec{E},\vec{H}) = 0$$

$$\hat{\mathcal{Q}} = \begin{pmatrix}\epsilon(\vec{r}) & 0\\ 0 & \mu(\vec{r})\end{pmatrix} \qquad \mathcal{F}_i = \begin{pmatrix}-\mathbf{e}_i\times\vec{H}\\ \mathbf{e}_i\times\vec{E}\end{pmatrix}$$

- Tessalate Domain into Triangles/Tetrahedra

Discontinuous Galerkin Time-Domain Approach

- On each Element: Expand Fields into a Nodal Basis

$$\begin{pmatrix} \vec{E}^k(\vec{r},t) \\ \vec{H}^k(\vec{r},t) \end{pmatrix} \approx \tilde{\mathbf{q}}^k(\vec{r},t) = \sum_{j=1}^{N_p} \mathbf{q}^k(\vec{r}_j,t) L_j(\vec{r}) = \sum_{j=1}^{N_p} \tilde{\mathbf{q}}_j^k(t) L_j(\vec{r})$$

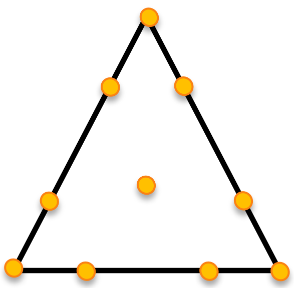
- Insert into the Maxwell Equations

$$\hat{\mathcal{Q}} \frac{\partial}{\partial t} \begin{pmatrix} \vec{E}^k \\ \vec{H}^k \end{pmatrix} + \nabla \cdot \vec{\mathcal{F}} \left(\vec{E}^k, \vec{H}^k \right) = \mathrm{Res.}$$

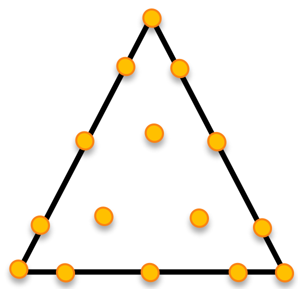
Discontinuous Galerkin Time-Domain Approach

- Choose Nodal Points to Minimize Interpolation Errors

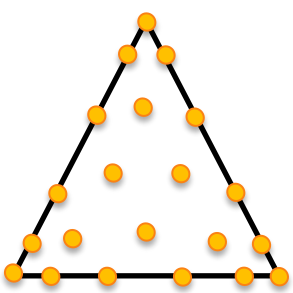
2D (Triangles)



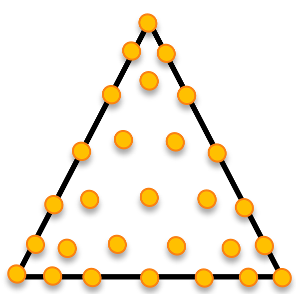
3rd order, 10 points



4th order, 15 points

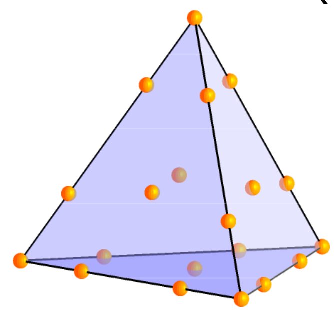


5th order, 21 points

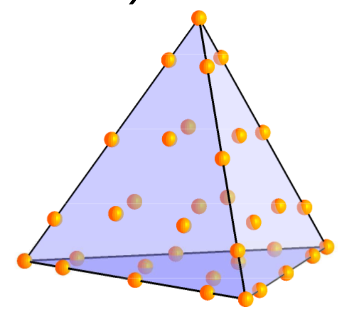


6th order, 28 points

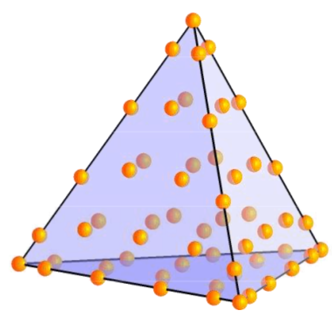
3D (Tetrahedra)



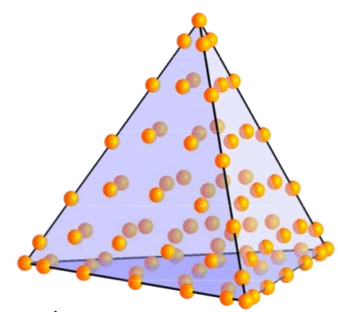
3rd order, 20 points



4th order, 35 points



5th order, 56 points



6th order, 84 points

T. Warburton, Eng. Math. **56**(3),247-262 (2006)

Discontinuous Galerkin Time-Domain Approach

- Strong Formulation on Each Element

$$\int_{D^k} \mathrm{d}^3 r \left[\hat{\mathcal{Q}} \frac{\partial}{\partial t} \begin{pmatrix} \vec{E}^k \\ \vec{H}^k \end{pmatrix} + \nabla \cdot \vec{\mathcal{F}} \right] L_j(\vec{r}) = 0$$

- Coupling between Elements: Penalty Term

$$\int_{D^k} \mathrm{d}^3 r \left[\hat{\mathcal{Q}} \frac{\partial}{\partial t} \begin{pmatrix} \vec{E} \\ \vec{H} \end{pmatrix} + \nabla \cdot \vec{\mathcal{F}} \right] L_j(\vec{r}) = \oint_{\partial D^k} \mathrm{d}\vec{A} \cdot \vec{\mathcal{P}}^k$$

Discontinuous Galerkin Time-Domain Approach

- Strong Formulation on Each Element

$$\int_{D^k} \mathrm{d}^3 r \left[\hat{\mathcal{Q}} \frac{\partial}{\partial t} \begin{pmatrix} \vec{E} \\ \vec{H} \end{pmatrix} + \nabla \cdot \vec{\mathcal{F}} \right] L_j(\vec{r}) = \oint_{\partial D^k} \mathrm{d}\vec{A} \left(\vec{\mathcal{F}} - \vec{\mathcal{F}}^* \right) L_j(\vec{r})$$

- Explicit Time-Stepping Scheme

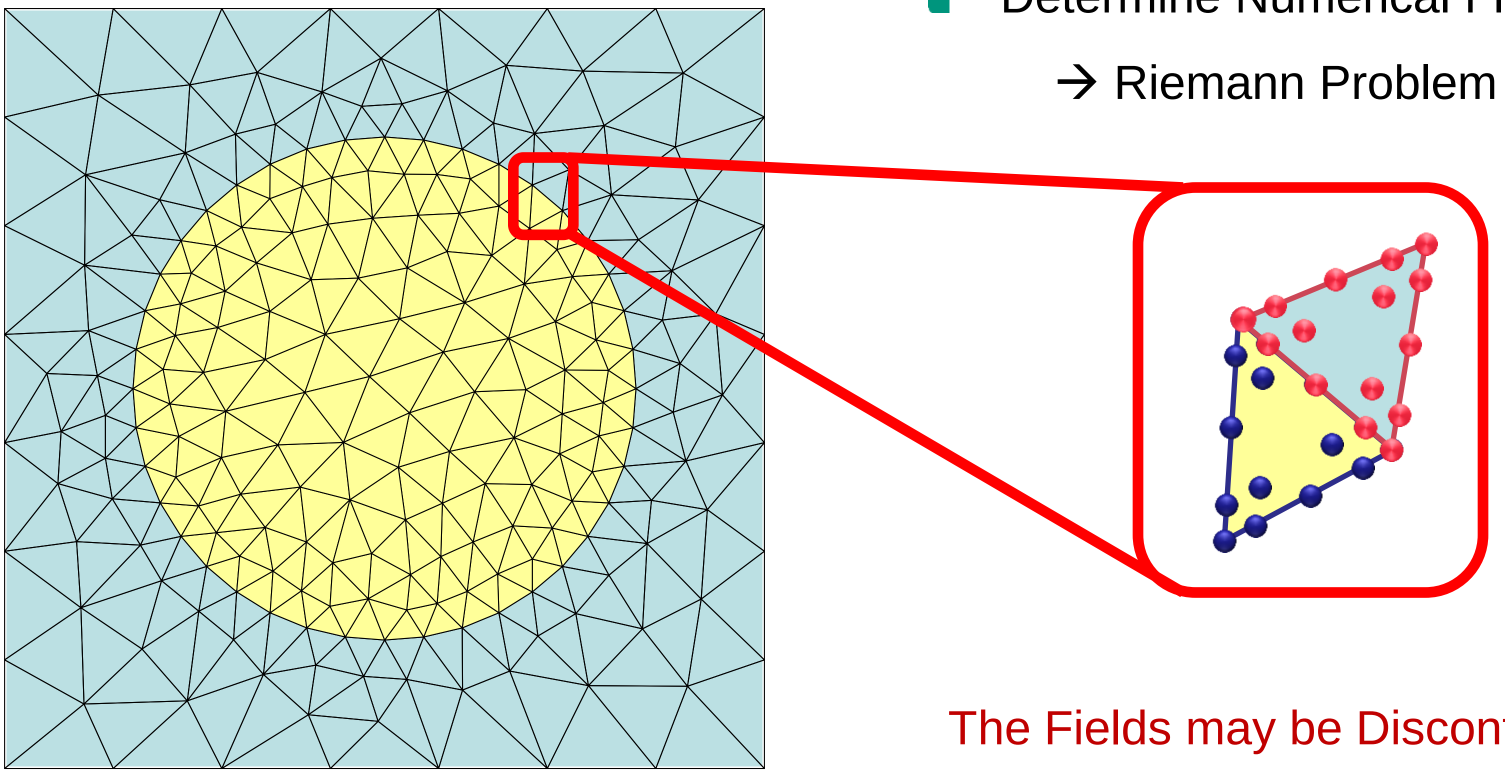
$$\frac{\partial}{\partial t} \begin{pmatrix} \vec{E}_{\mathrm{N}} \\ \vec{H}_{\mathrm{N}} \end{pmatrix} = \mathcal{H} \begin{pmatrix} \vec{E}_{\mathrm{N}} \\ \vec{H}_{\mathrm{N}} \end{pmatrix}$$

J. Hesthaven and T. Warburton,
J. Comput. Phys. **181**, 186 (2002)

Discontinuous Galerkin Time-Domain Approach

- Determine Numerical Flux

  → Riemann Problem



The Fields may be Discontinuous:

Values on the Edges stored Twice

J. Hesthaven and T. Warburton, Nodal Discontinuous Galerkin Methods, Springer (2008)

Required Add-Ons

- Total Field / Scattered Field Framework

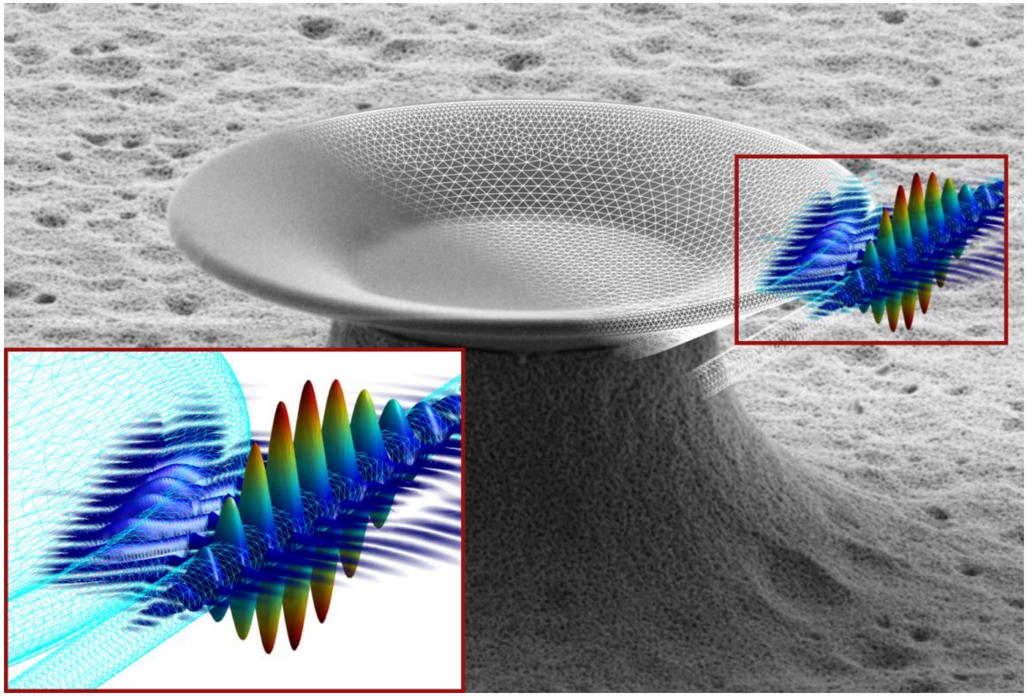
- Sources

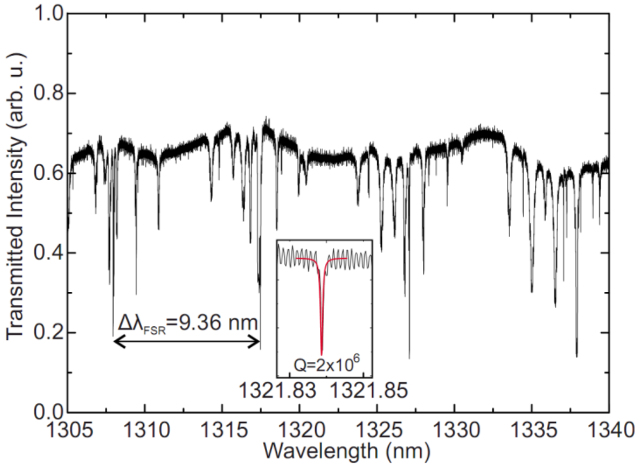
- “Absorbing Boundaries“:
  - Uniaxial Perfectly Matched Layers
  - Complex Frequency-Shifted PMLs

- Dispersive Materails: Auxiliary Differential Equations

- Nice to have:
  - Curved Elements
  - Flexible Time-Stepping Methods
  - Anisotropic Materials

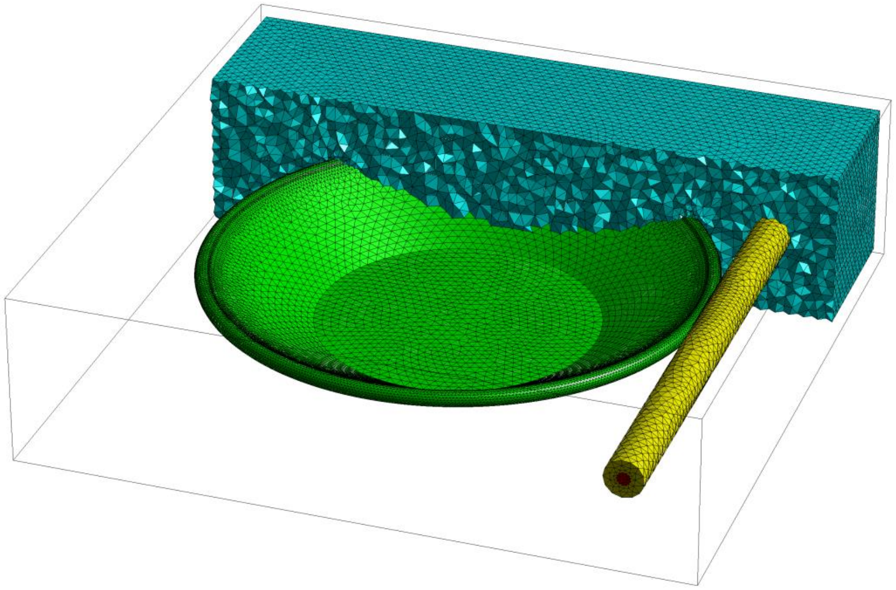
Performance of the DGTD-Approach





Courtesy of R. Diehl (REM picture from Appl. Phys. Lett. **96**, 013303 (2010))

Performance of the DGTD-Approach



- Domain: 51x50x13 μm
- 690.000 Tetrahedra
- DOF = 6*[(n+2)*(n+3)*(n+4)/6]*N
- 4^{th}-Order Polynomials:
  - $2.1*10^8$ DOF:
    → 9 GByte RAM
  - 10 Roundtrips at λ = 1.3 μm:
    → 12 d CPU time on a single 12-core node
  - GPU acceleration:
    → Speedup factor ~30

J. Niegemann et al., Photonics and Nanostructures **7**, 2 (2009)

K. Stannigel et al., Optics Express **17**, 14934 (2009)

R. Diehl et al., J. Comput. Theor. Nanosci. **7**, 1572 (2010)

M. König et al., Photonics and Nanostructures **8**, 303 (2010)

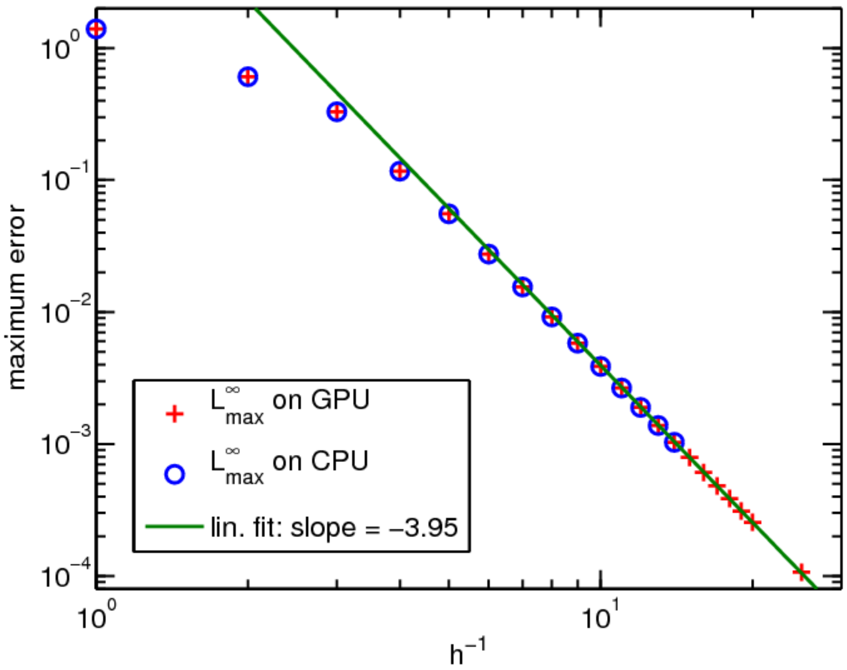
M. König et al., Optics Express **19**, 4618 (2011)

C. Matyssek et al., Photonics and Nanostructures **9**, 367 (2011)

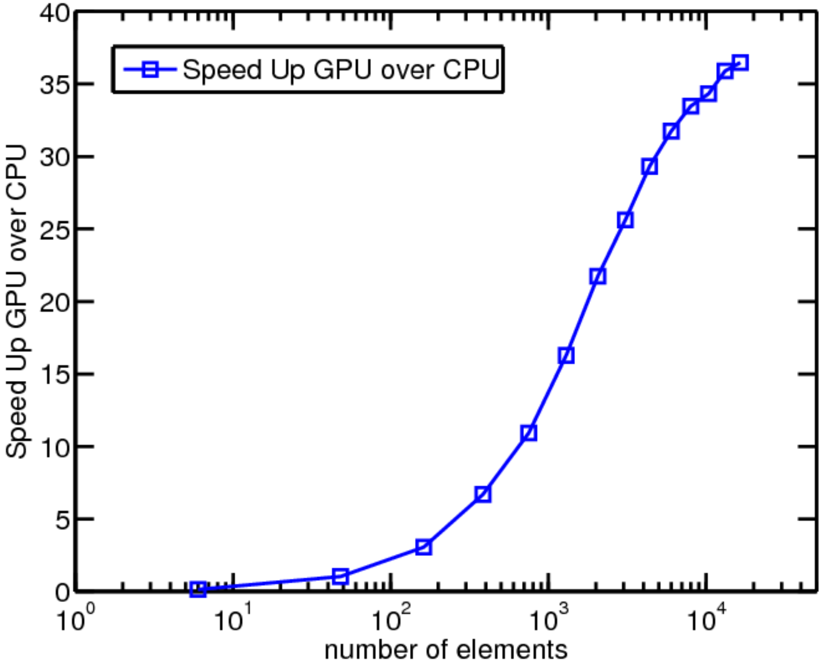
J. Niegemann et al., J. Comput. Phys. **231**, 364 (2012)

Review: K. Busch, M. König, J. Niegemann, Laser & Photonics Reviews **5**, 773 (2011)

DGTD on GPUs



Courtesy of Richard Diehl



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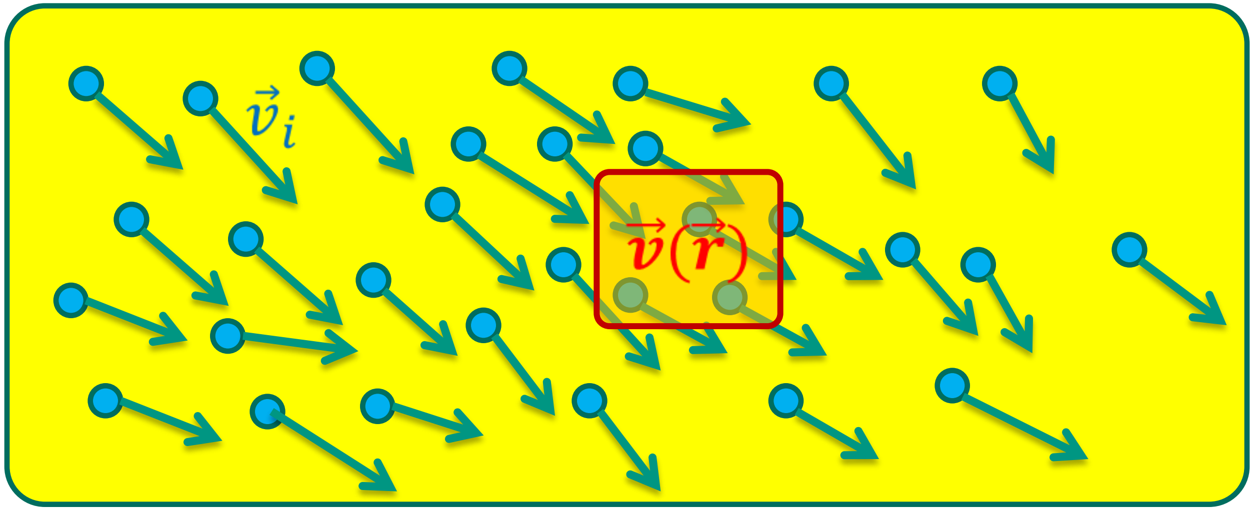
Modeling the Conduction Electrons in Metals

- Assume Free Electron Gas



- Standard Model: Constant Density → Drude Model

- Fixed Jellium Background $\rho^+(\vec{r})$ and varying Electron Density $\rho(\vec{r},t)$

$$\bar{\rho}(\vec{r},t) = \rho^+(\vec{r}) - \rho(\vec{r},t)$$

Drude Model of Free Electrons

- Free Electrons with Velocity $\vec{v}$

$$(\partial_t + \gamma)\,\vec{v} = -\frac{e}{m}\left(\vec{E} + \vec{v} \times \vec{H}\right)$$

- Continuum Description

- Coupling to Maxwell‘s Equations

Modeling the Conduction Electrons in Metals

- Free Electrons with Velocity $\vec{v}$

Nonrelativistic Limit

$$(\partial_t + \gamma)\,\vec{v} = -\frac{e}{m}\left(\vec{E} + \vec{v} \times \vec{H}\right)$$

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Modeling the Conduction Electrons in Metals

- Free Electrons with Velocity $\vec{v}$

Nonrelativistic Limit

$$(\partial_t + \gamma)\,\vec{v} = -\frac{e}{m}\left(\vec{E} + \vec{v} \times \vec{H}\right)$$

- Continuum Description $\vec{j} = \rho_0 \vec{v}(\vec{r}, t)$

$$(\partial_t + \gamma)\,\vec{j} = -\omega_p^2 \vec{E}$$

- Coupling to Maxwell‘s Equations

Modeling the Conduction Electrons in Metals

- Free Electrons with Velocity $\vec{v}$

Nonrelativistic Limit

$$(\partial_t + \gamma)\,\vec{v} = -\frac{e}{m}\left(\vec{E} + \vec{v} \times \vec{H}\right)$$

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$$(\partial_t + \gamma)\,\vec{j} = -\omega_p^2 \vec{E}$$

- Coupling to Maxwell‘s Equations

$$\partial_t\,\vec{E} = \frac{1}{\epsilon}\vec{\nabla} \times \vec{H} - \vec{j}$$

$$\partial_t\,\vec{H} = -\,\frac{1}{\mu}\vec{\nabla} \times \vec{E}$$

Modeling the Conduction Electrons in Metals

- Free Electrons with Velocity $\vec{v}$

Nonrelativistic Limit

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$$(\partial_t + \gamma)\,\vec{j} = -\omega_p^2 \vec{E}$$

- Coupling to Maxwell‘s Equations

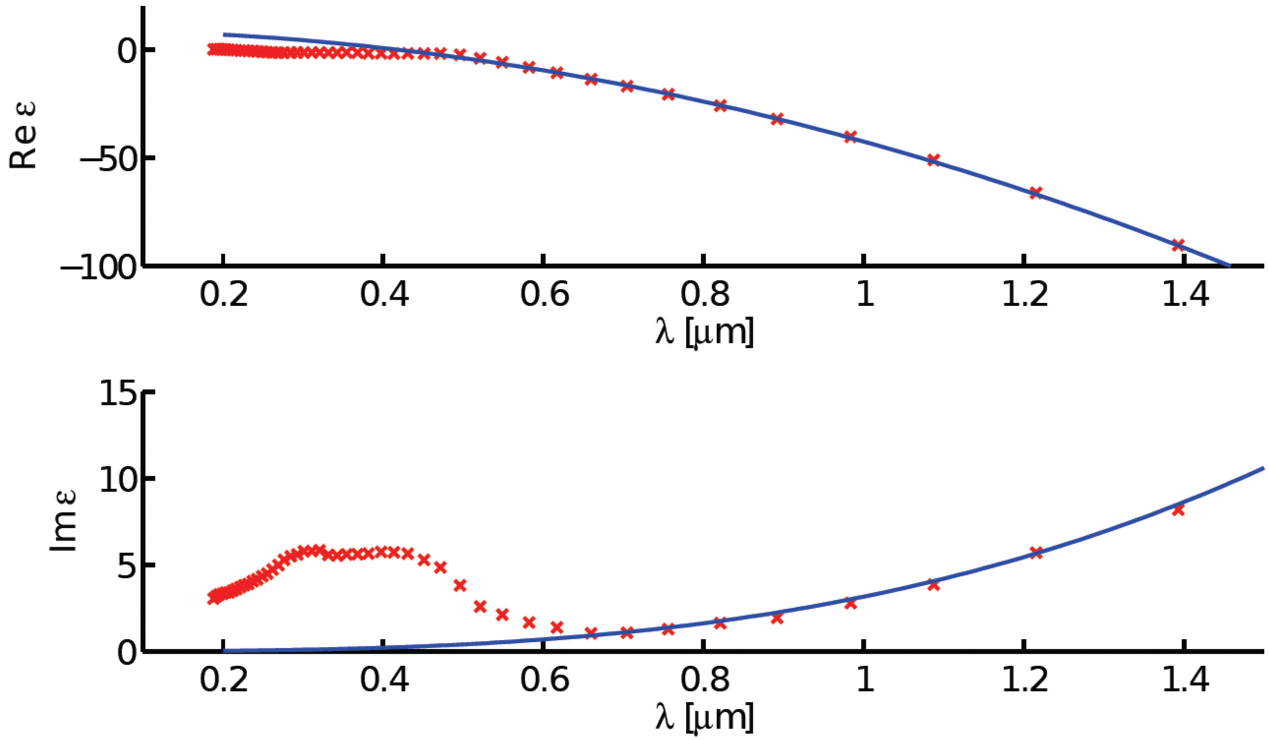
$$\partial_t\,\vec{E} = \frac{1}{\epsilon}\vec{\nabla} \times \vec{H} - \vec{j}$$

$$\partial_t\,\vec{H} = -\,\frac{1}{\mu}\vec{\nabla} \times \vec{E}$$

Linear and Local Model for the Optical Response of Metals

Modeling the Conduction Electrons in Metals

- Dielectric Function of Gold: Good Description in the Infrared (and Visible)

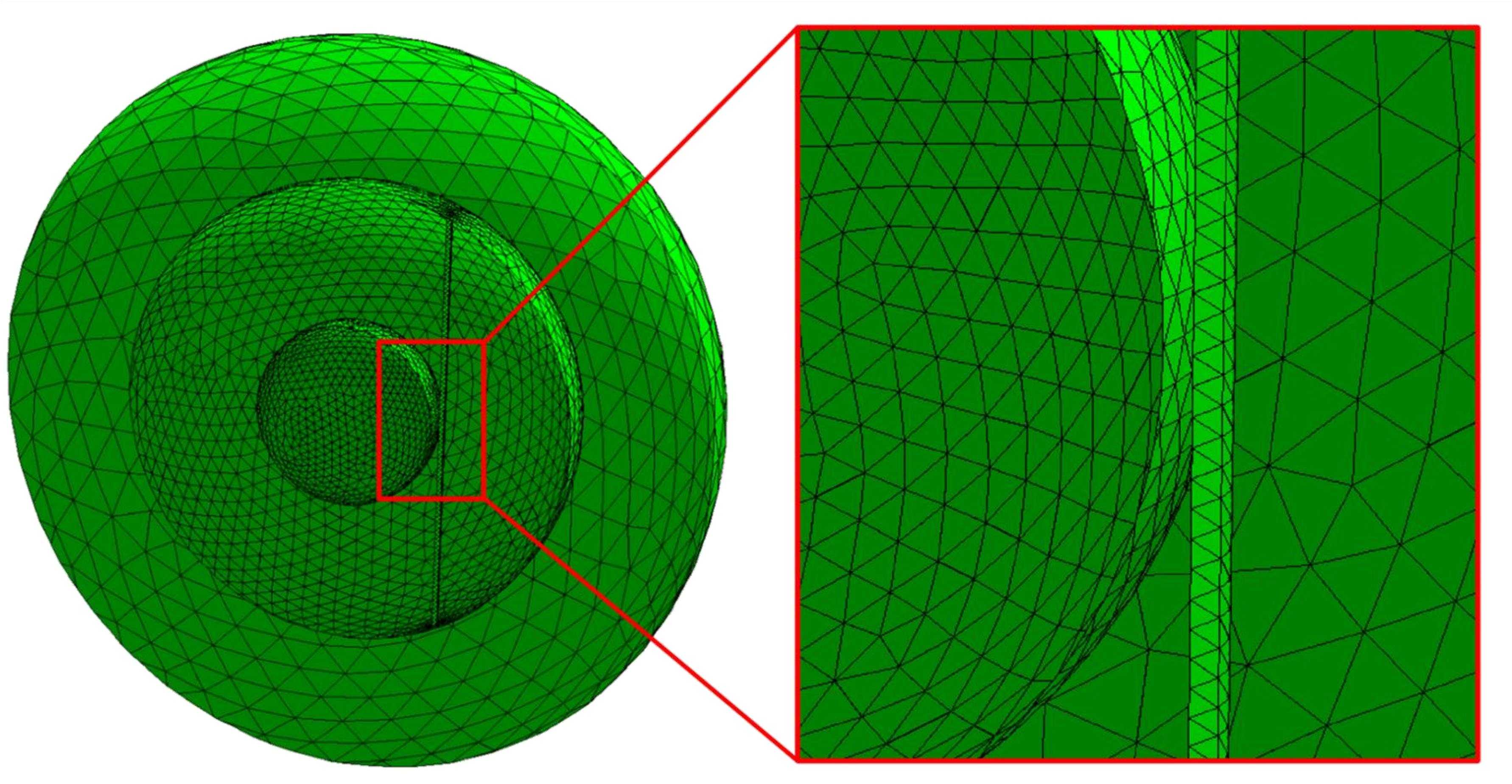


- Allows to Determine the Parameters γ, ω_p from Experiment

P. B. Johnson and R. W. Christy, Phys. Rev. B 6, 4370 (1972)

Electron Energy Loss Spectroscopy via DGTD

- Aluminum-Nanosphere, Radius 10nm



Electron Energy Loss Spectroscopy via DGTD

- Electron Energy Loss

$$\Delta E = \int_0^\infty d\omega \; \hbar\omega P(\omega) \sim 5 \ldots 25\text{eV}$$

- Electron Energy Loss Probability

$$P(\omega) = \frac{e}{\pi\hbar\omega} \int dt \; \Re\{e^{-i\omega t}\vec{v} \cdot \vec{E}^{\text{ind}}(\vec{r}_e(t), \omega)\}$$

- Scattering Angle

$$\theta_E \approx \frac{\Delta E}{E} \cdot \quad 0.1\,\text{mrad}$$

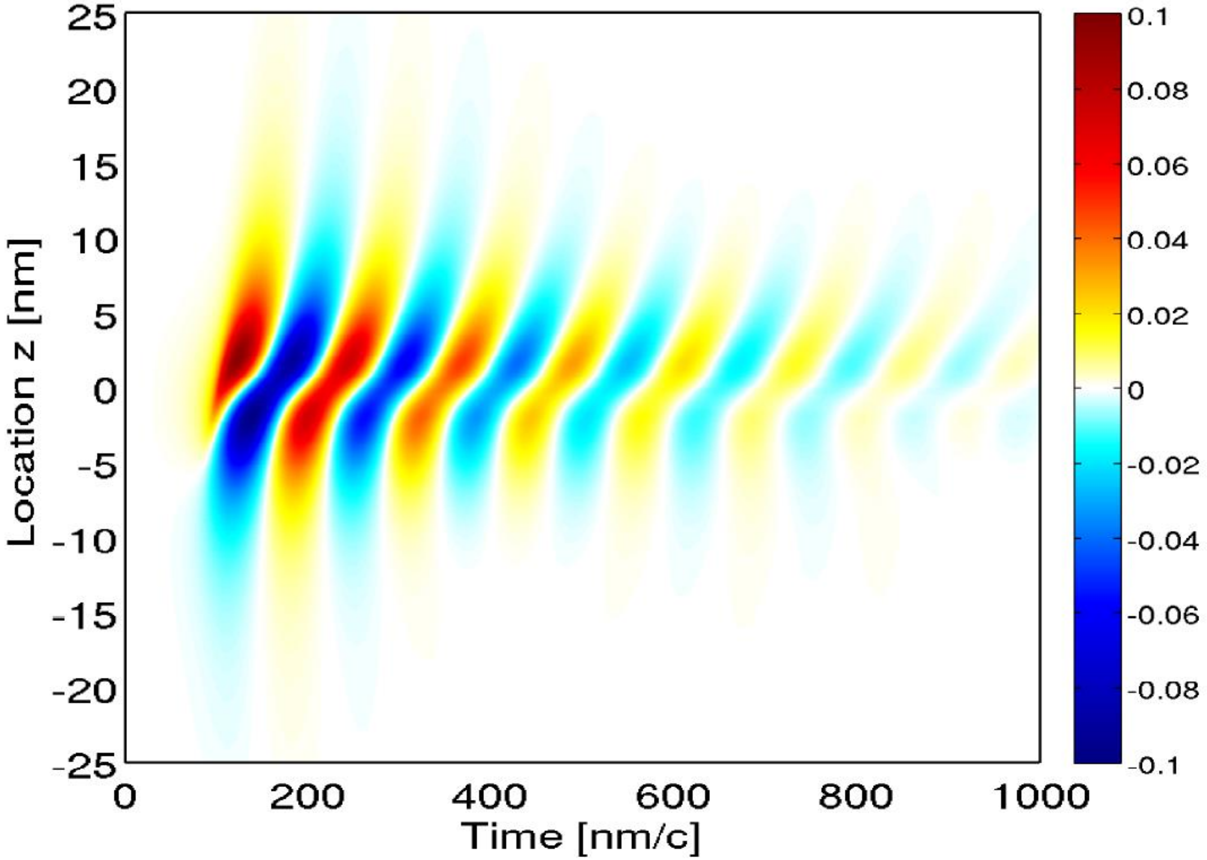
→ No-Recoil Approximation: $\vec{v}(t) = \text{const.}$

Beyond No-Recoil Approximation: PIC

Electron Energy Loss Spectroscopy via DGTD

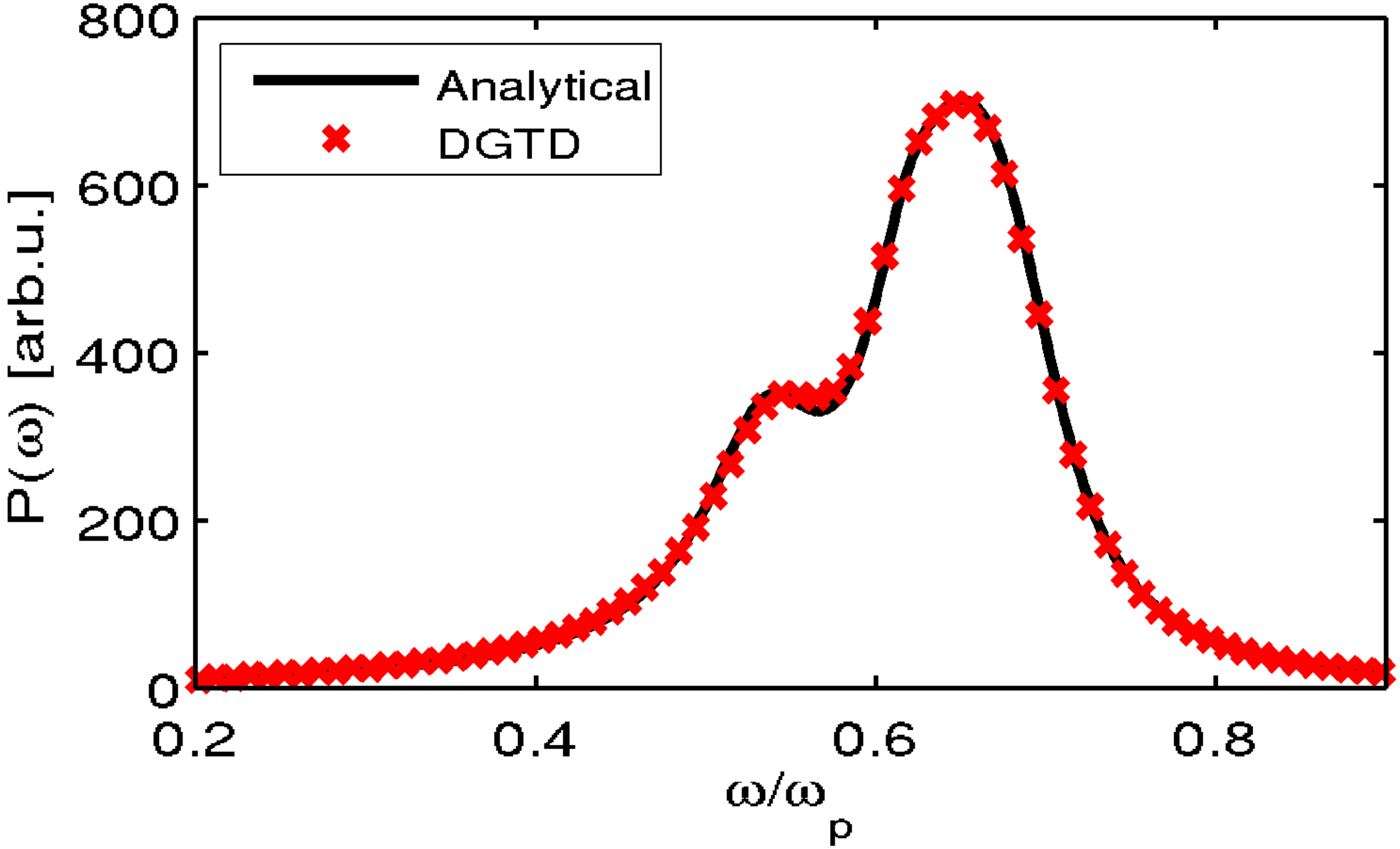
Movie: EELS on a single aluminium sphere

Electron Energy Loss Spectroscopy via DGTD



$$P(\omega) = \frac{e}{\pi\hbar\omega}\int dz\ \Re\{e^{-i\omega(z-z_0)/v}\vec{E}_z^{\,\mathrm{ind}}(z,\omega)\}$$

Electron Energy Loss Spectroscopy via DGTD

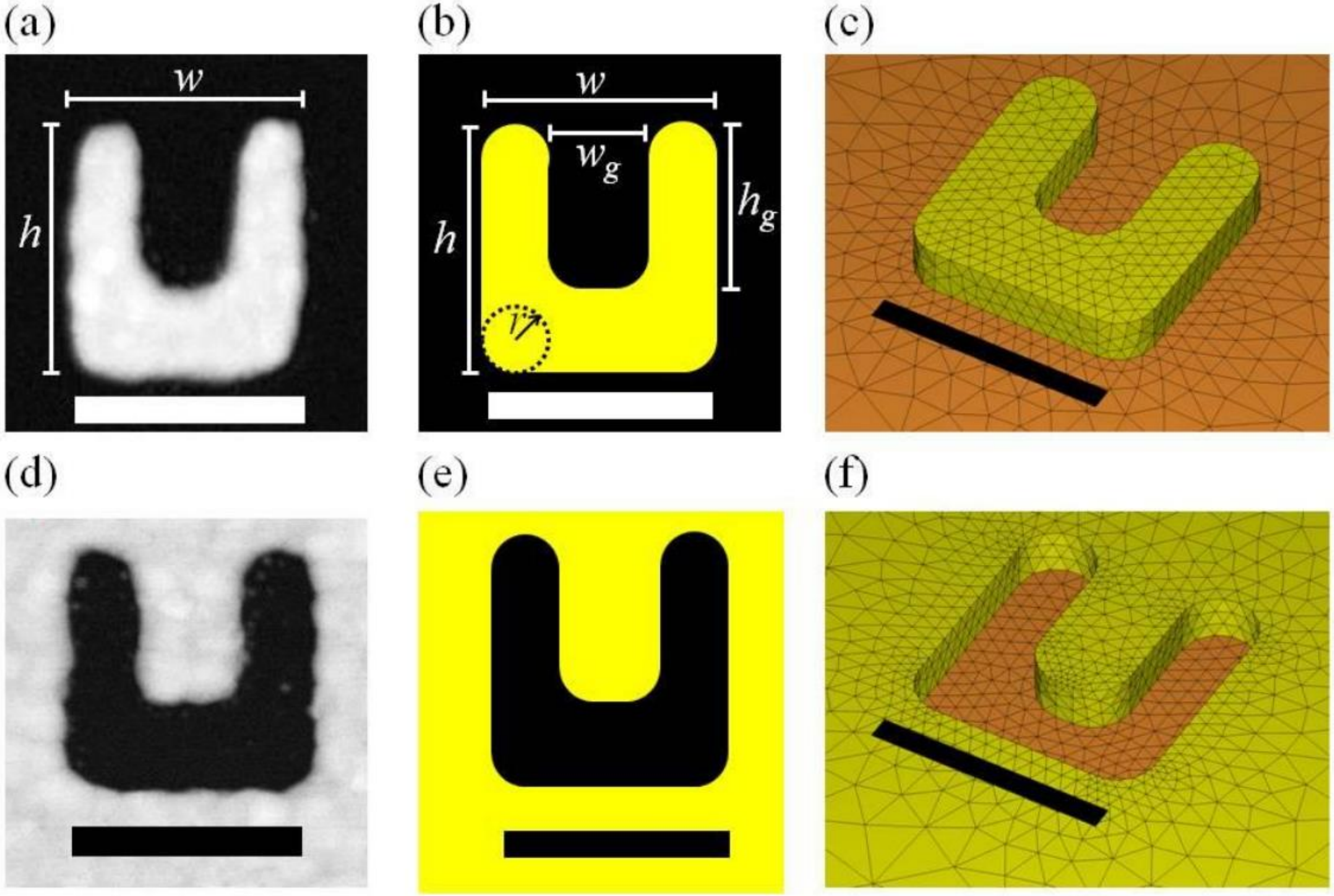


C. Matyssek, J. Niegemann, W. Hergert, K. Busch,
Photonics and Nanostructures **9**, 367 (2011)

Electron Energy Loss Spectroscopy via DGTD

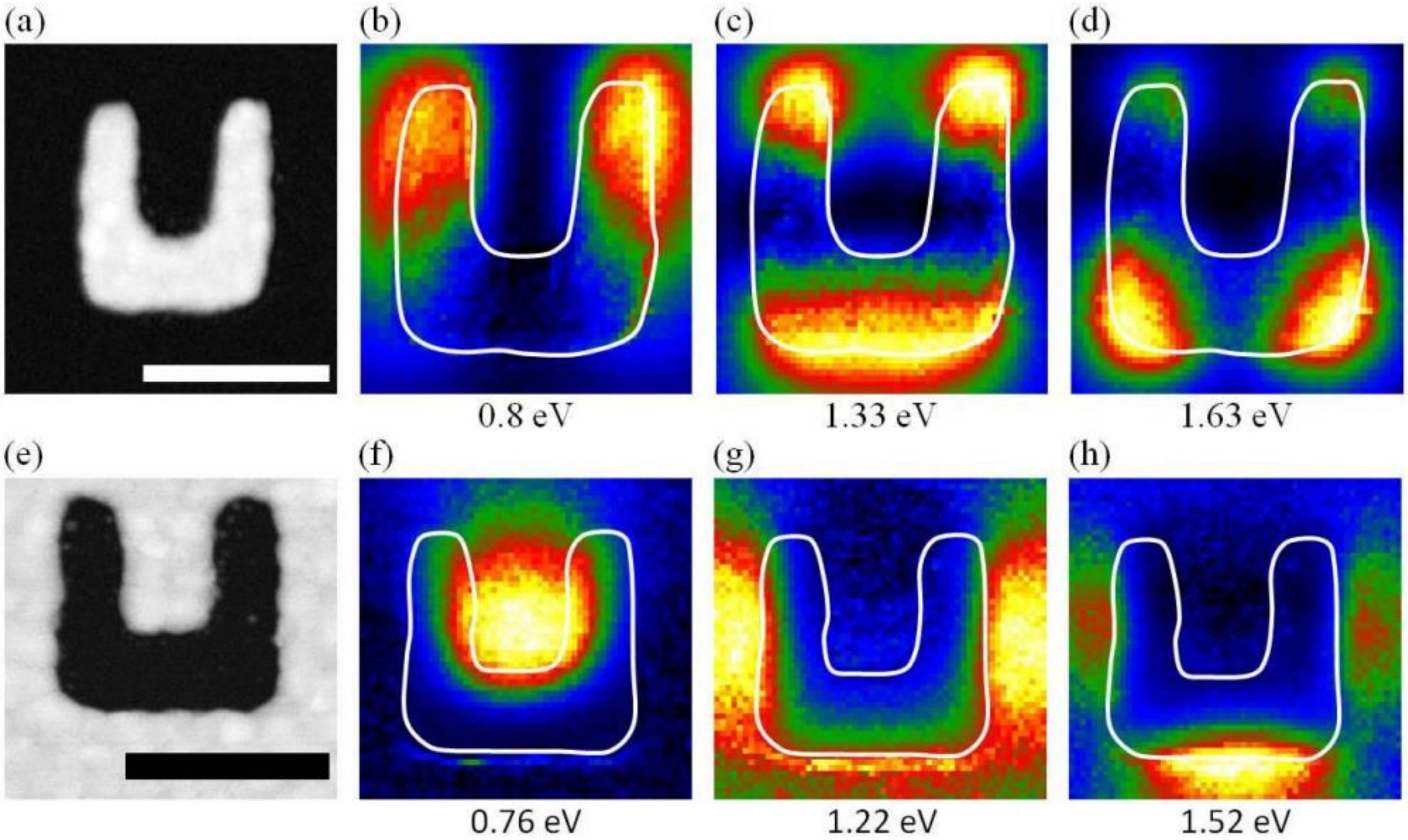
Movie: EELS on an aluminium sphere dimer

EELS: Experiment and Theory



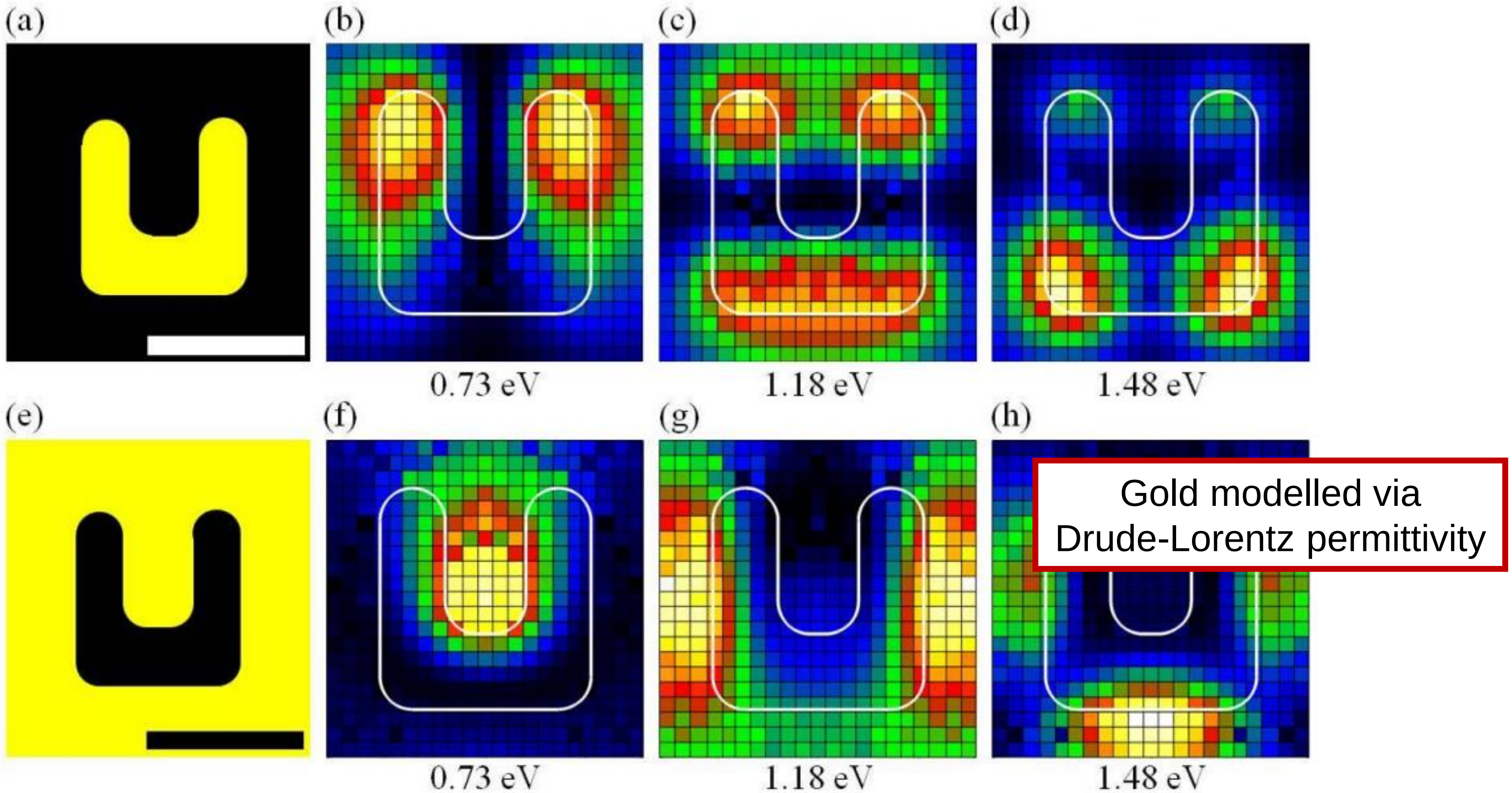
F. von Cube et al., Optical Materials Express **1**, 1009 (2011)

EELS: Experiment and Theory



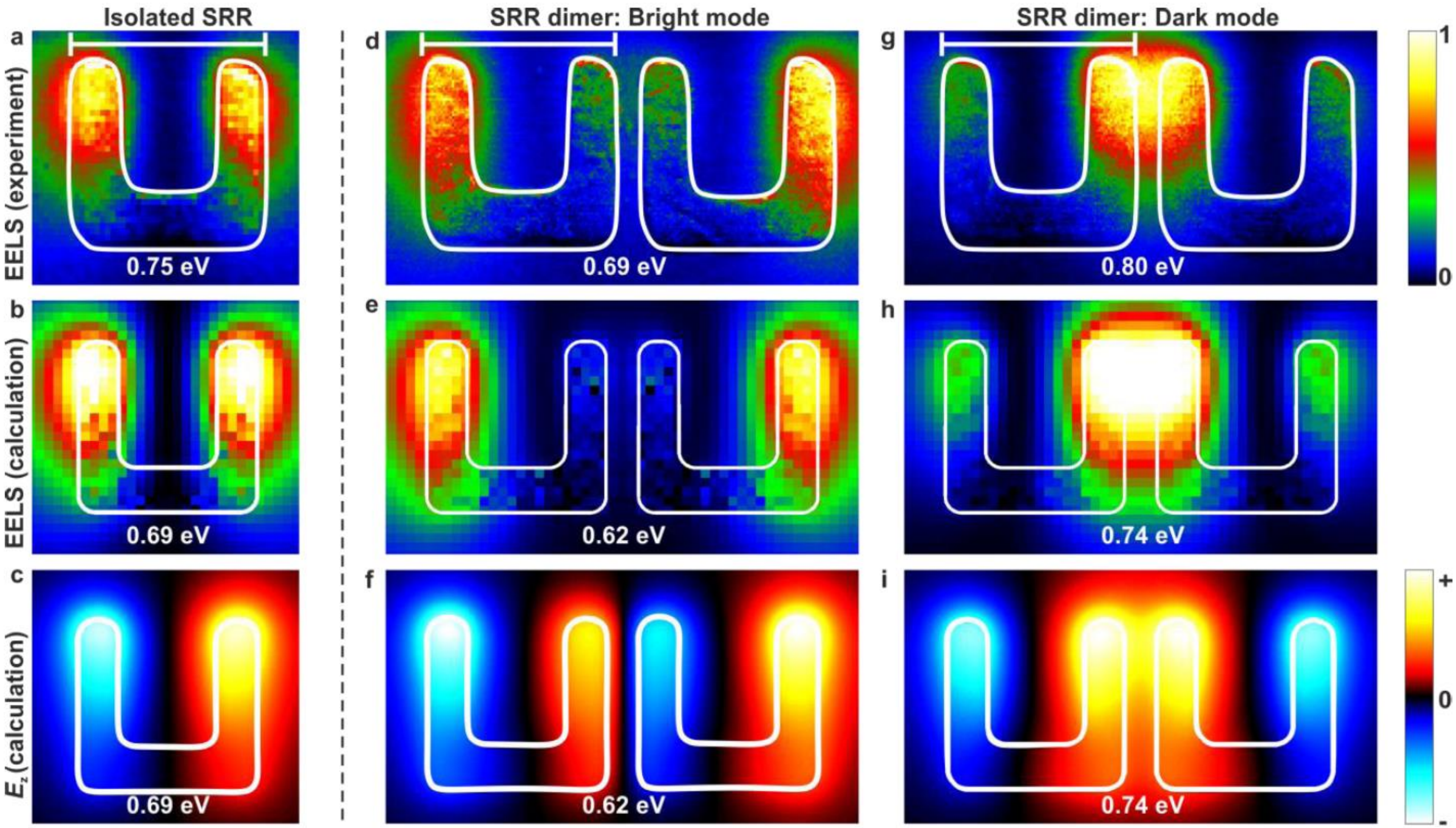
F. von Cube et al., Optical Materials Express **1**, 1009 (2011)

EELS: Experiment and Theory



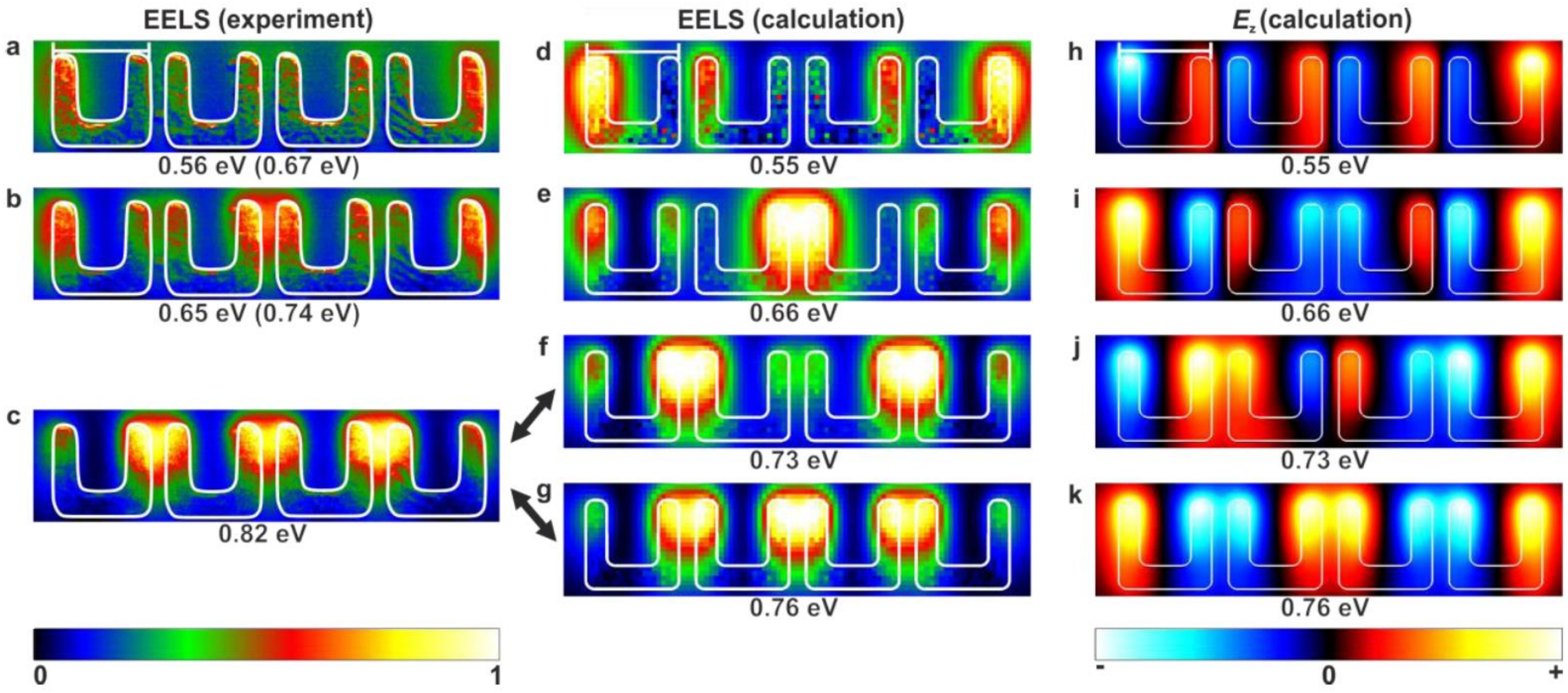
F. von Cube et al., Optical Materials Express **1**, 1009 (2011)

EELS: Coupling between Split-Ring Resonators



F. von Cube et al., Nano Lett. **13**, 703 (2013)

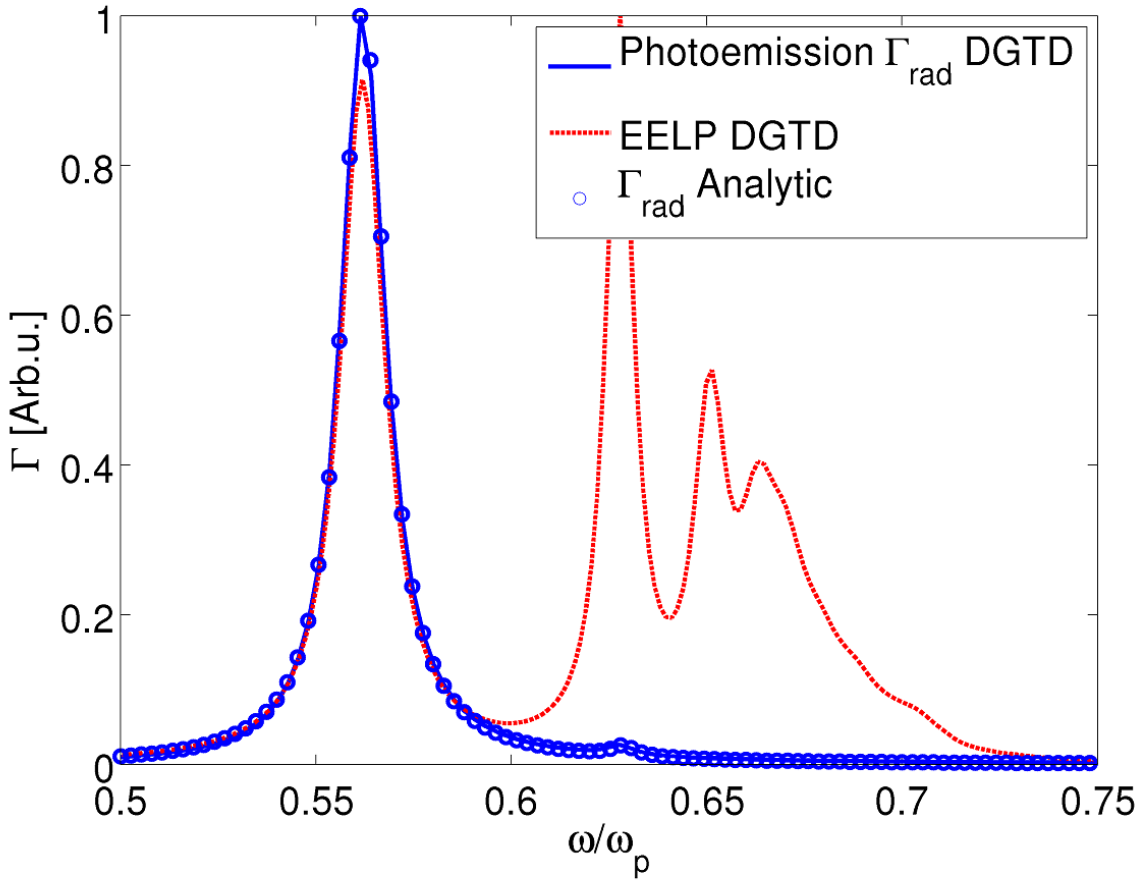
EELS: Coupling between Split-Ring Resonators



F. von Cube et al., Nano Lett. **13**, 703 (2013)

Cathodoluminescence via DGTD

- Gold-Nanosphere, Radius 10nm

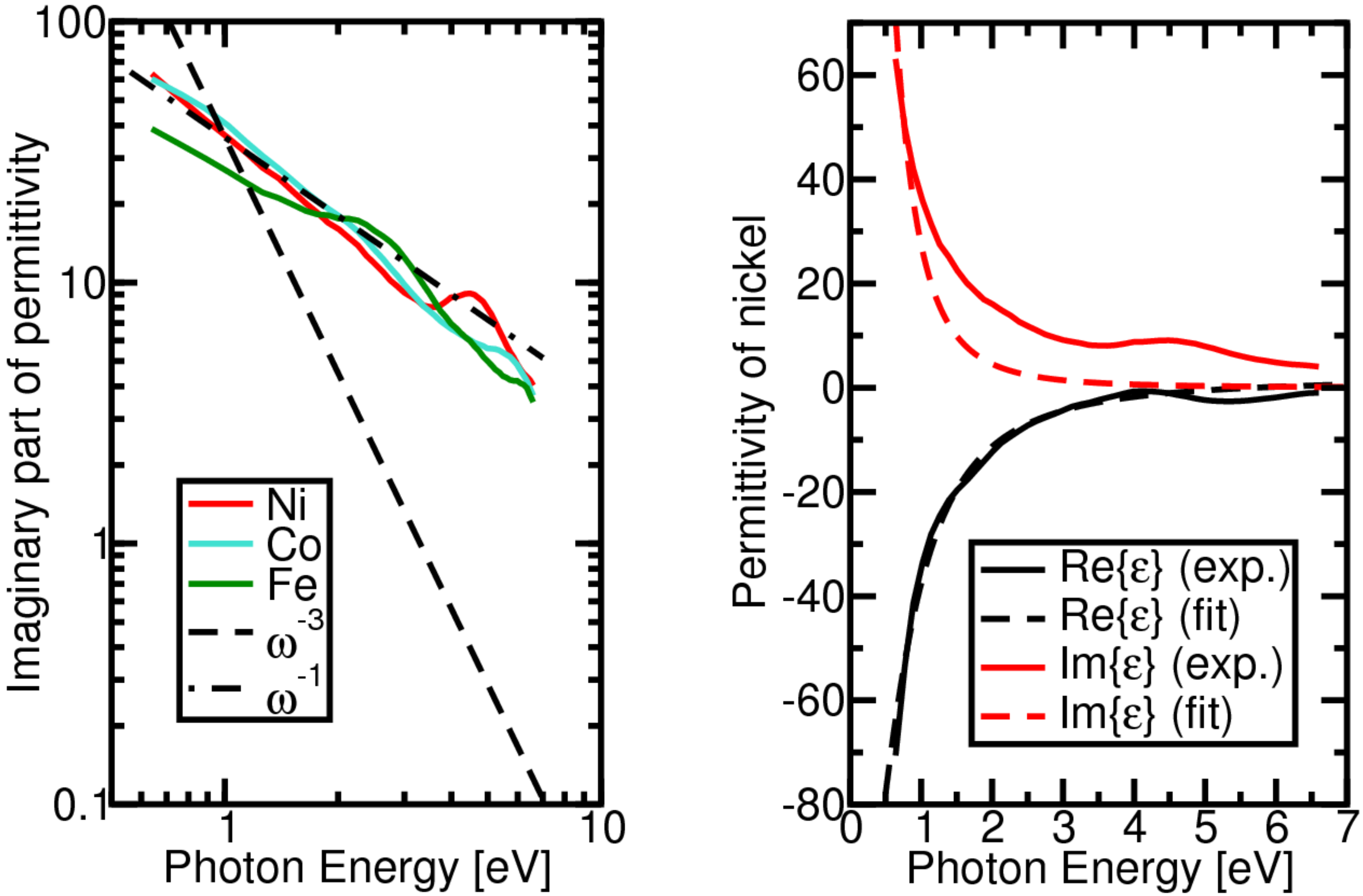


Courtesy of Christian Matyssek

Outline

- Motivation
- Discontinuous Galerkin Time-Domain Approach
- Example: Electron Energy Loss Spectroscopy
- Advanced Modeling: Transition Metals (Magneto-Plasmonics)
- Advanced Modeling: Nonlinear Metal Optics
- Conclusions & Outlook

Magneto-Optics: Transition Metal Modeling



Transition Metals: Isotropic Response

- Drude Model

$$(\partial_t + \gamma)\,\vec{j} = -\omega_p^2 \vec{E}$$

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- Transition Metals: Correlated Electron Dynamics leads to Memory Effects

$$(\partial_t + \gamma)\,\vec{j} = \int_0^\infty \mathrm{d}s\, Z(s)\vec{E}(t-s)$$

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$$\tau = \ell_c / v_F \approx 1 \text{ fsec}$$

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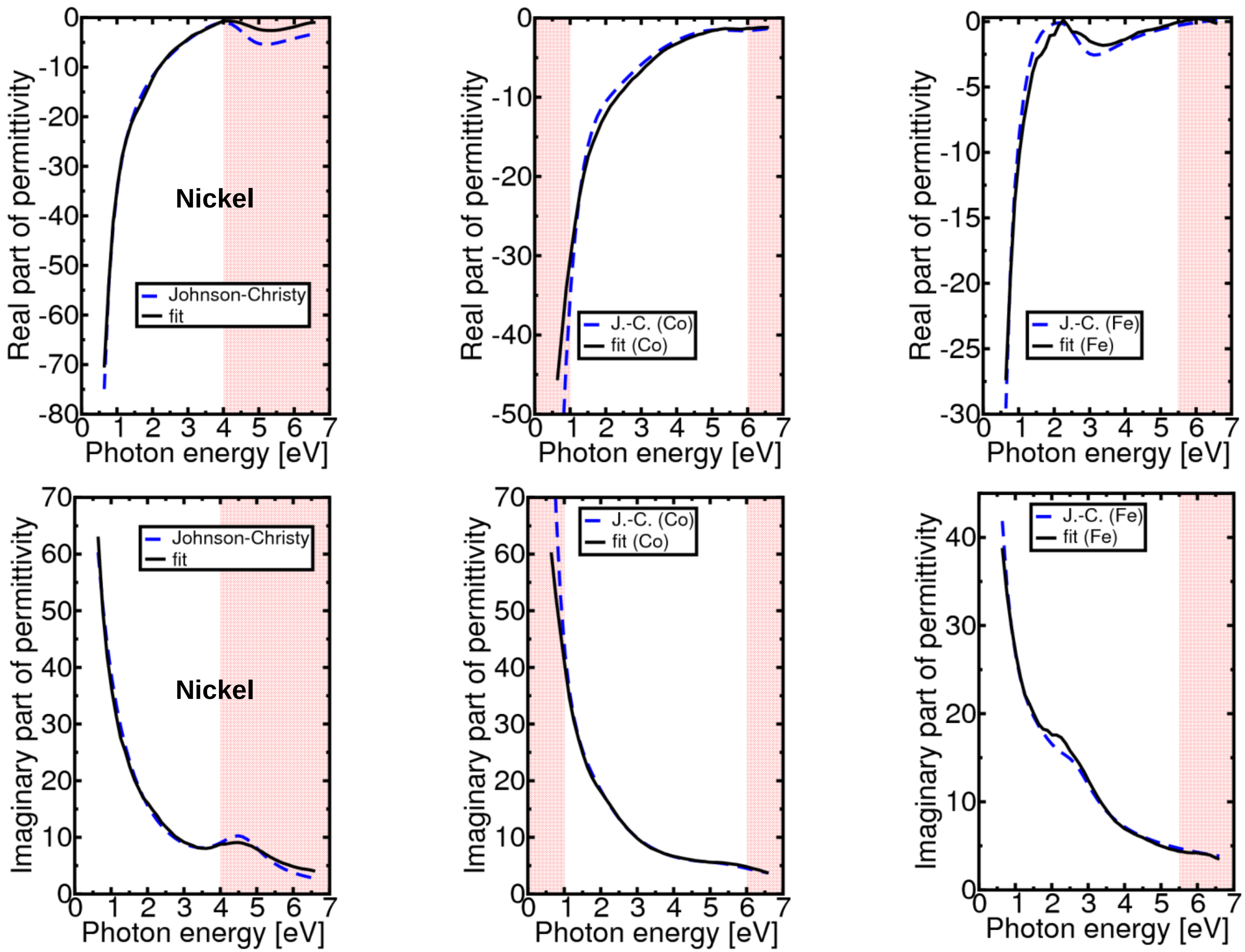
- Drude Model plus Retardation

$$(\partial_t + \gamma)\,\vec{j} = -\omega_p^2\,(1 + \tau\partial_t)\,\vec{E}$$

→ Additional Fit Parameter: τ (isotropic response)

Transition Metals: Isotropic Response



Transition Metals: Magneto-Optic Response

- Drude Model plus Retardation

$$(\partial_t + \gamma)\,\vec{j} = -\omega_p^2\,(1 + \tau\partial_t)\,\vec{E}$$

- Primary Source of Anisotropic Behavior: Lorentz Force

$$(\partial_t + \gamma)\,\vec{j} = -\omega_p^2\,(1 + \tau\partial_t)\,\vec{E} + \vec{\;} \times \vec{j}$$

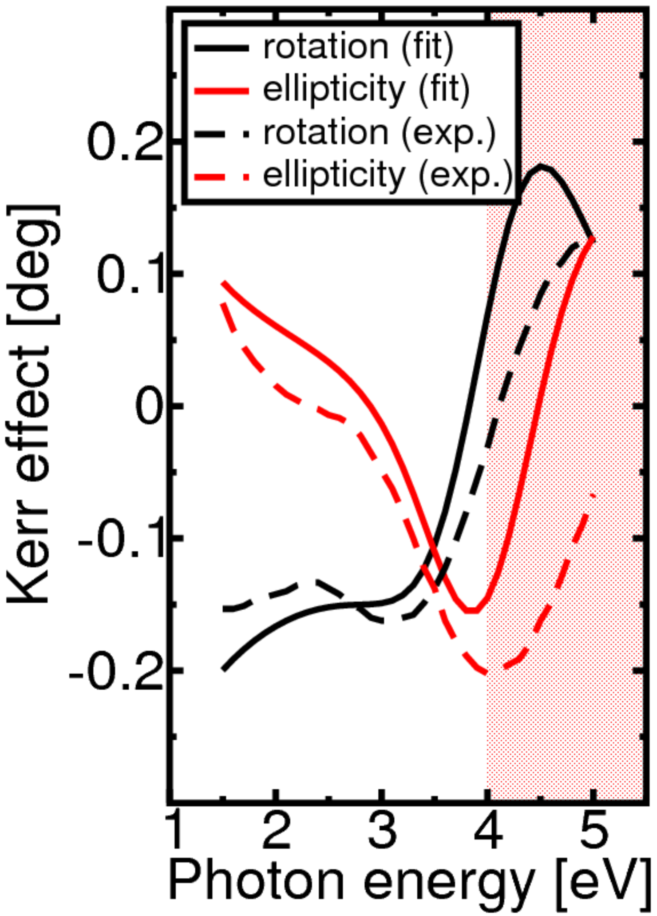
$$\vec{\;} = -\frac{e}{m}\vec{B}_{\mathrm{ext}}$$

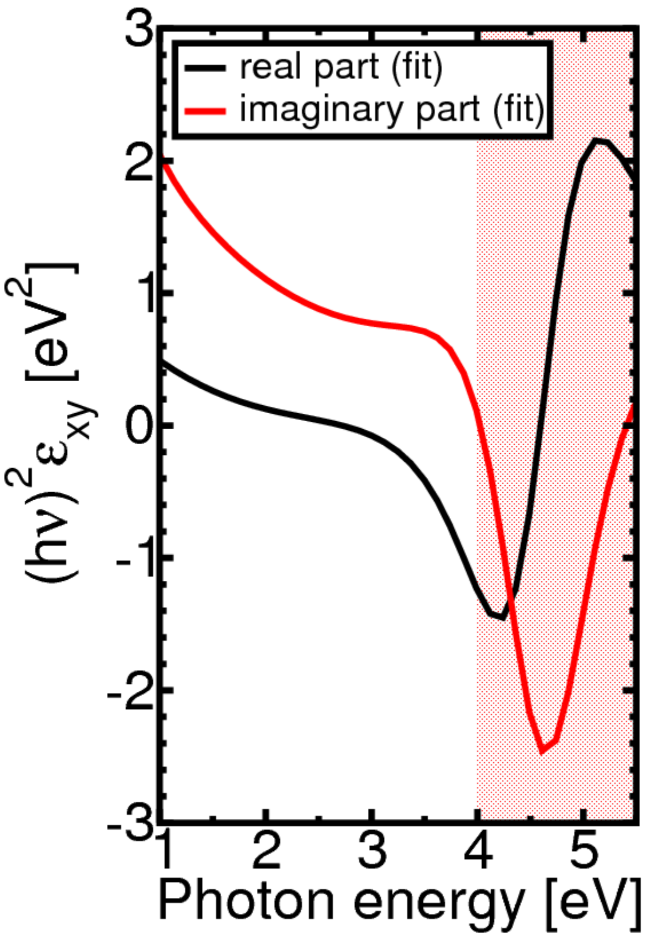
→ Additional Fit Parameter: e/m (magneto-optic response)

- Higher-Order Corrections: Spin-Orbit Coupling (Ongoing Work)

- Methodology also Applicable to Lorentz-Oscillator Model
  → Interband Transitions

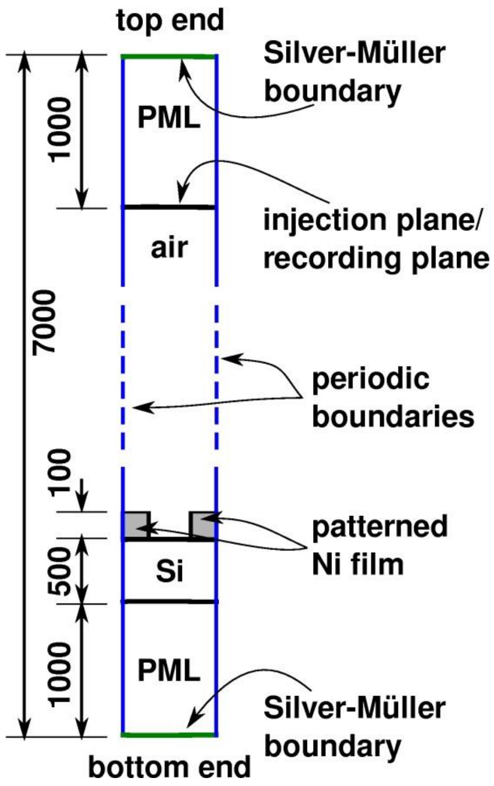
Nickel: Magneto-Optic Response

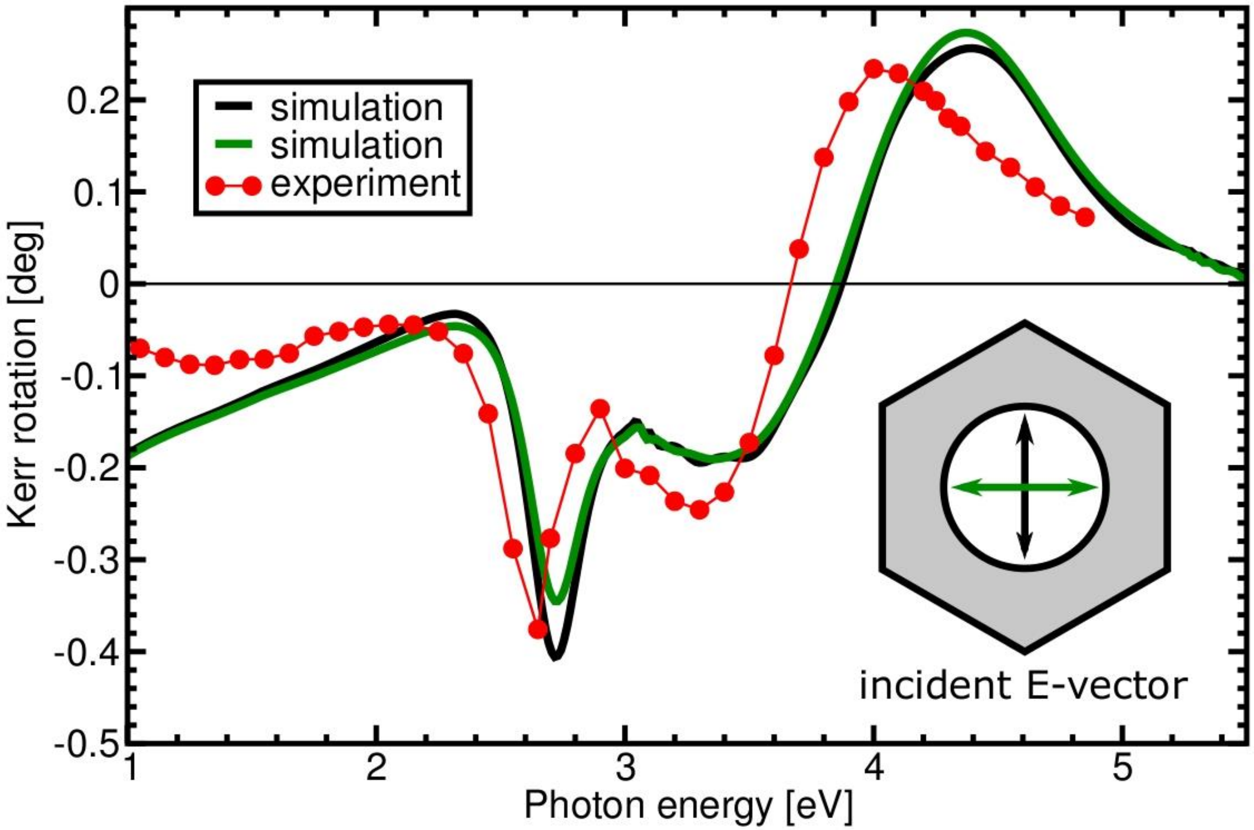




C. Wolff et al., Opt. Express, in press

Magneto-Optics of Nickel Anti-Dot Arrays





C. Wolff et al., Opt. Express, in press

Experimental data courtesy of G. Ctistis: Opt. Express **23**, 23867 (2011)

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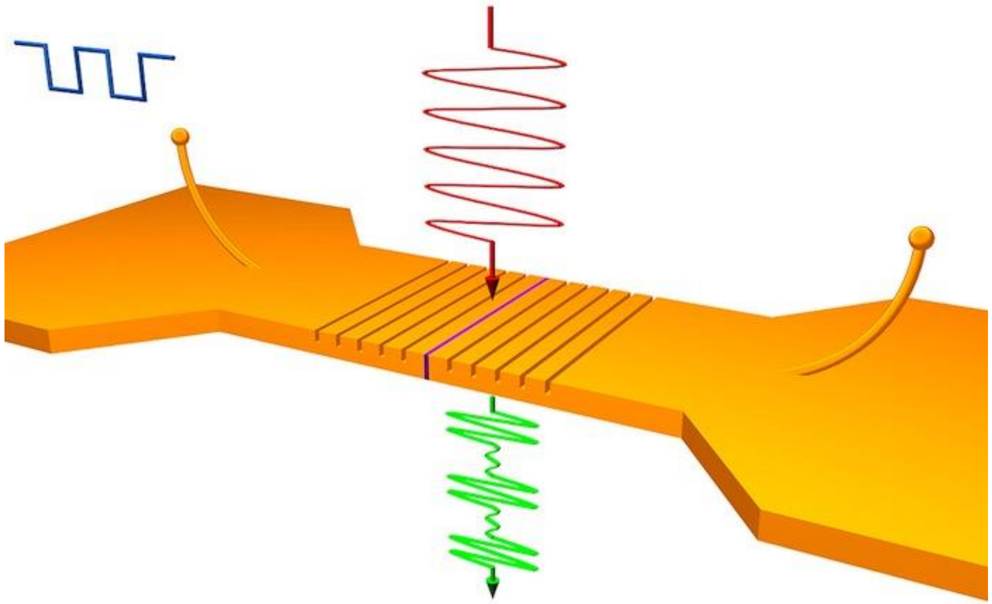
Nonlinear Metal Optics



W. Cai et al., Science **333**, 1720 (2011)

Hydrodynamic Model of Free Electrons

- Electron charge density no longer fixed. Instead

$$\bar{\rho}(\vec{r},t) = \rho^{+}(\vec{r}) - \rho(\vec{r},t)$$

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$$(\partial_t + \gamma)\,\vec{j} + \vec{\nabla} \cdot \left(\frac{\vec{j} \quad \vec{j}}{\rho} \right) = -\frac{e}{m}\left(\rho\vec{E} + \vec{j} \times \vec{H}\right) - \frac{1}{m}\vec{\nabla} p$$

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- Closure: Thomas-Fermi Pressure

$$p(\rho) = e\frac{(2\pi^2)^{2/3}\hbar^2}{5m}\rho^{5/3}$$

J. Sipe et al.,
Phys. Rev. B **21**, 4389 (1980)

Hydrodynamic Model of Free Electrons

- **Rigorous Derivation** from the Boltzmann Equation

- **Nonlocal** and **Nonlinear** Terms

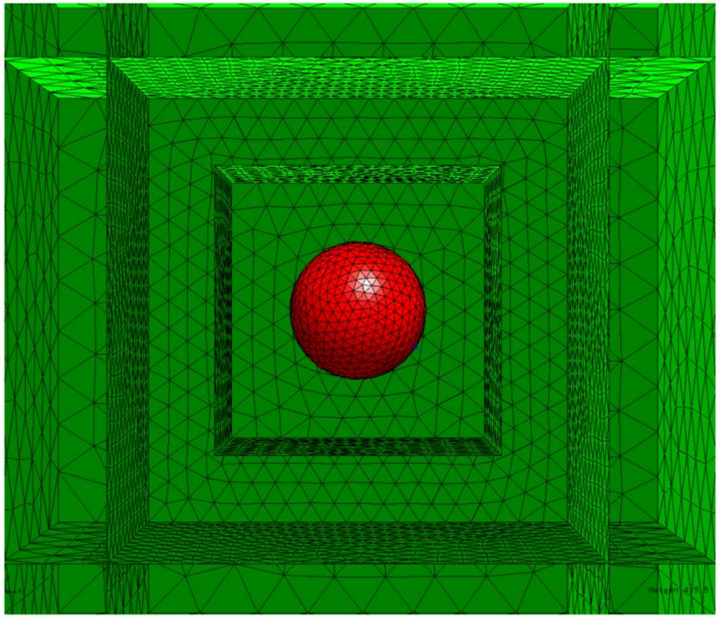
$$(\partial_t + \gamma)\,\vec{j} + \vec{\nabla}\cdot\left(\frac{\vec{j}\quad\vec{j}}{\rho}\right) = -\frac{e}{m}\left(\rho\vec{E} + \vec{j}\times\vec{H}\right) - \frac{1}{m}\vec{\nabla}p$$

- Perturbation Theory: $\vec{E}(\vec{r},\omega) = \vec{E}_0 + \vec{E}_1\,e^{i\omega t} + \vec{E}_2\,e^{2i\omega t}$
  - 0th Order: Thomas-Fermi Model (Static Electron Density Distribution)
  - 1st Order: Drude Model → **Fixes all Free Parameters**
  - Higher Orders: Higher-Harmonic Generation (SHG, THG)

- Quantum Mechanical Generalization

  G. Manfredi and F. Haas, Phys. Rev. B **64**, 075316 (2001)

Nonlinear Optics of Metal Nano-Structures



- Maxwell‘s Equations

$$\partial_t \vec{E} = \frac{1}{\epsilon}\vec{\nabla} \times \vec{H} - \vec{j}$$

$$\partial_t \vec{H} = -\frac{1}{\mu}\vec{\nabla} \times \vec{E}$$

$$\vec{\nabla} \cdot \vec{E} = \bar{\rho}$$

$$\vec{\nabla} \cdot \vec{H} = 0$$

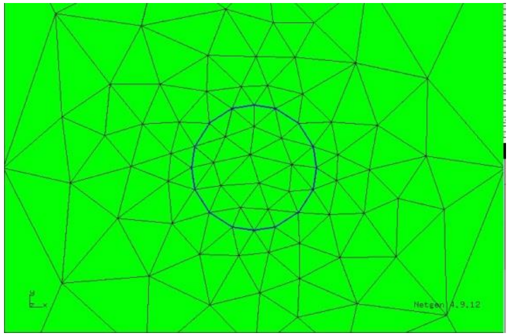
- Free Electrons as a Plasma („Hard Wall BCs“)

$$\partial_t \rho + \nabla \cdot \vec{j} = 0$$

$$(\partial_t + \gamma)\,\vec{j} + \nabla \cdot \left(\frac{\vec{j}\quad\vec{j}}{\rho}\right) = -\frac{e}{m}\left(\rho\vec{E} + \vec{j} \times \vec{H}\right) - \frac{1}{m}\nabla p$$

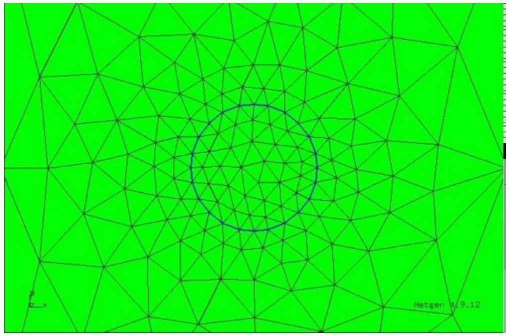
$$p(\vec{r}, t) = \zeta\left[\rho(\vec{r}, t)\right]^{5/3}$$

Gold Cylinder: Radius 5 nm



h_{max} = 5.0 nm

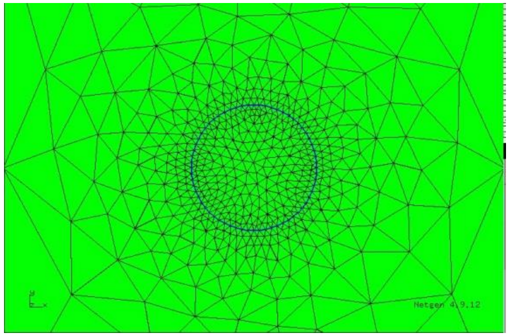
Movie (h_{max} = 5.0 nm, p = 3)



h_{max} = 3.0 nm

Movie (h_{max} = 3.0 nm, p = 3)

Need to resolve the longitudinal (bulk) plasmons



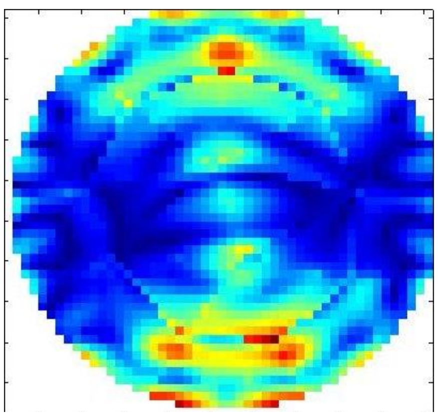
h_{max} = 1.0 nm

Movie (h_{max} = 1.0 nm, p = 3)

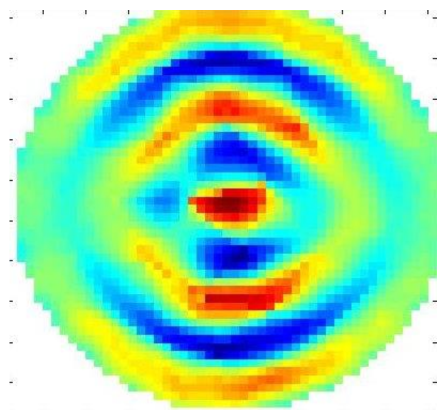
Resolving Longitudinal (Bulk) Plasmons

Movie: h_{max} = 5.0 nm vs. h_{max} = 1.0 nm

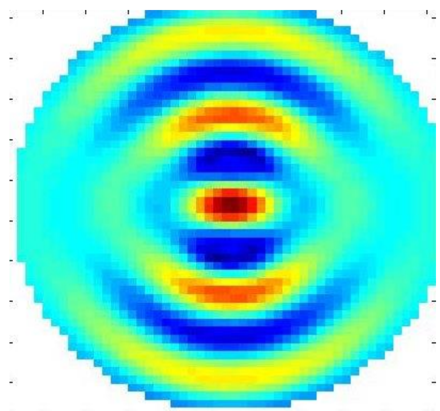
Electron Density @Second Harmonic



h_{max} = 5.0 nm



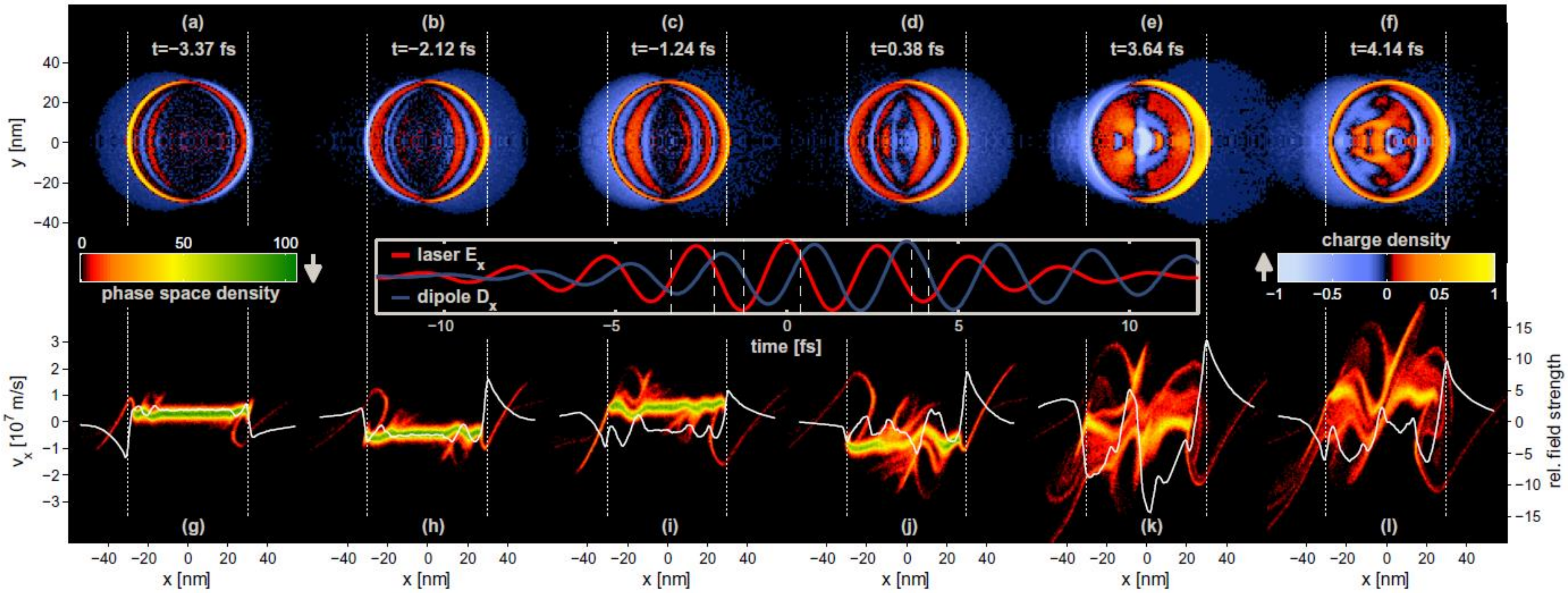
h_{max} = 3.0 nm



h_{max} = 1.0 nm

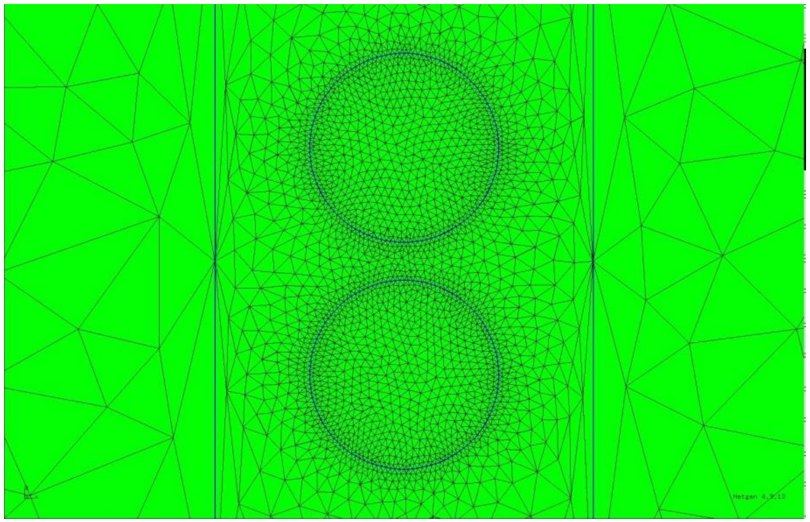
Courtesy of Christian Wolff

Resolving Longitudinal (Bulk) Plasmons



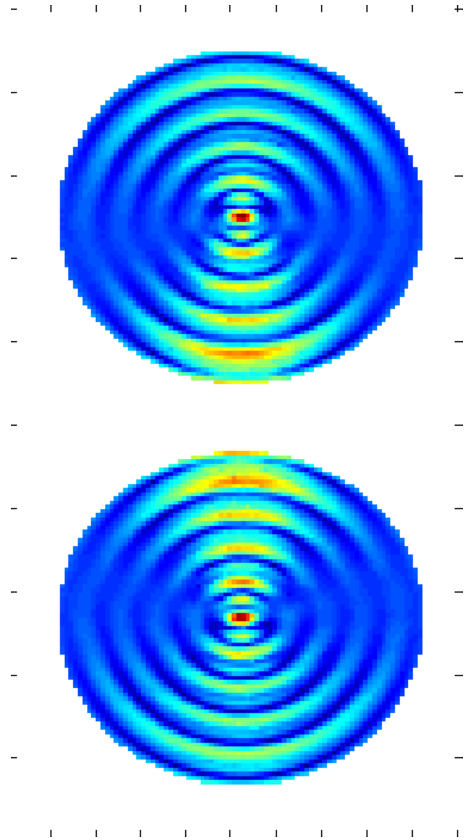
MicPIC computations from the group of Thomas Fennel:
New J. Phys. **14**, 065011 (2012)

Gold Dimer (Cylinder Radius 10 nm)

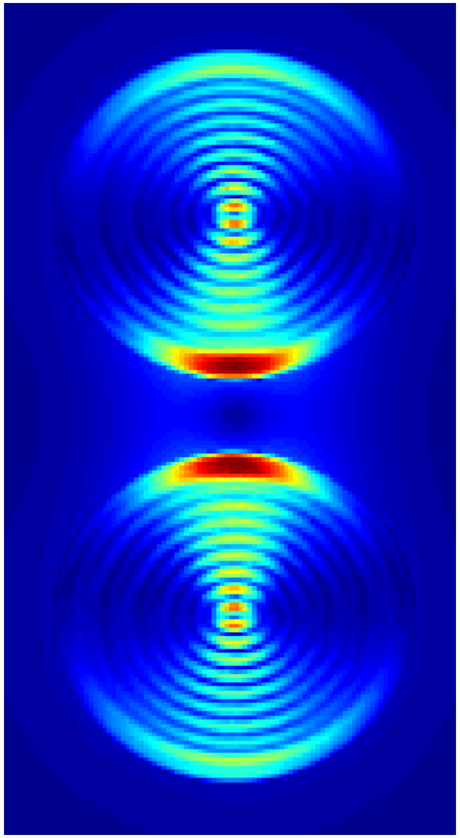


Movie: E_0 = 2*10^{10} V/m, Gap = 4 nm

Courtesy of Christian Wolff

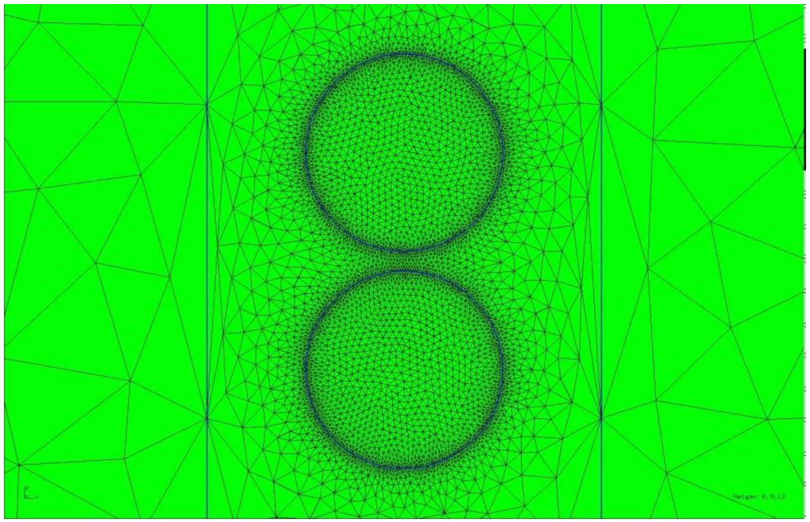


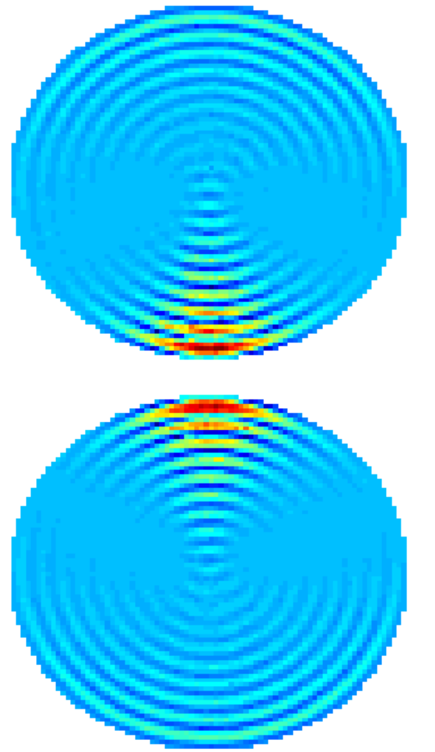
Electron Density
@SHG



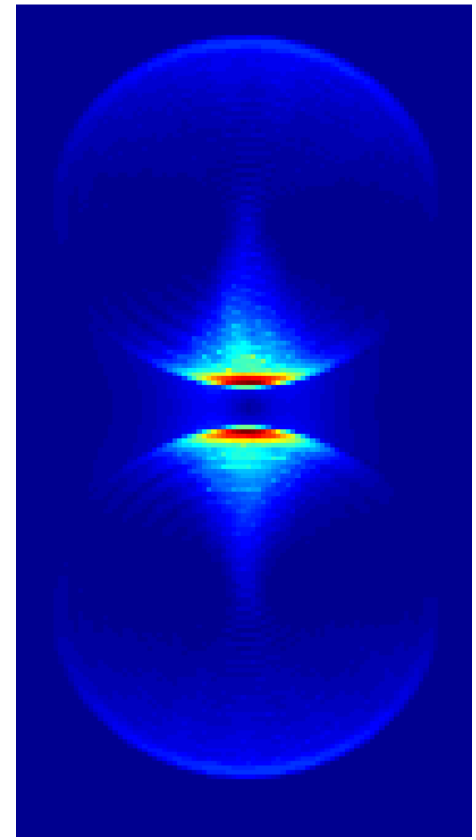
|Electric Field|
@SHG

Gold Dimer (Cylinder Radius 20 nm)





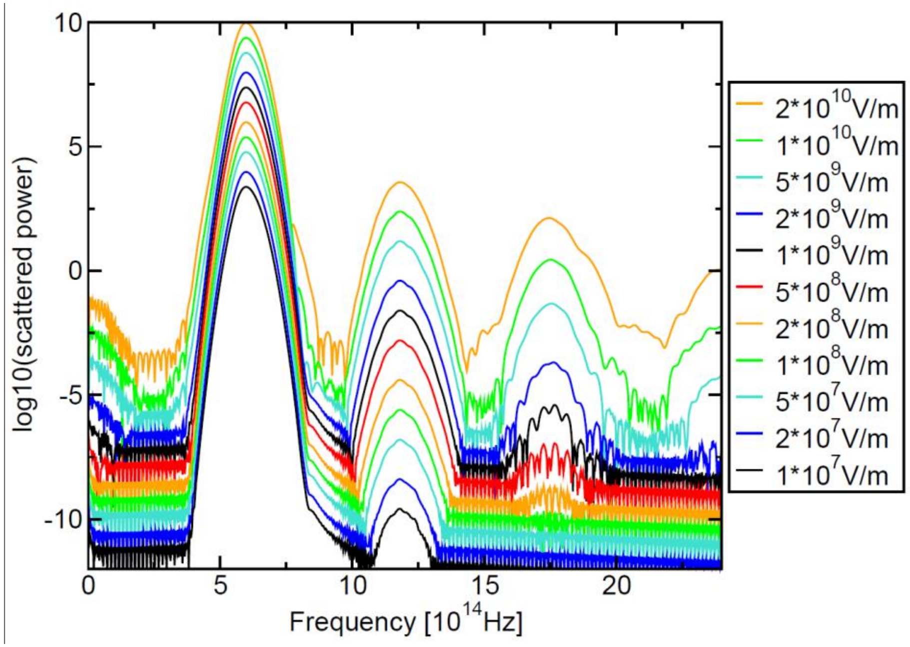
Electron Density
@SHG



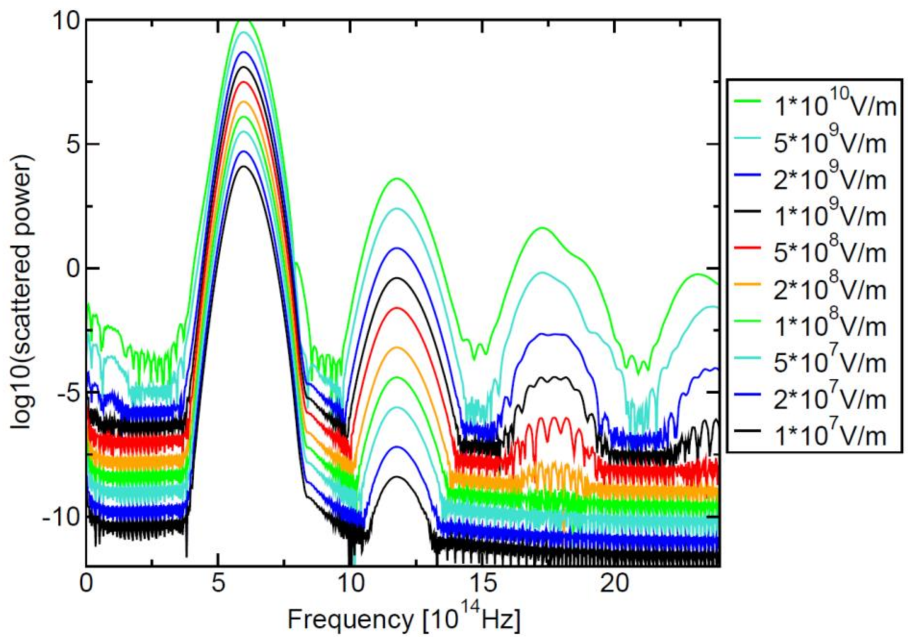
|Electric Field|
@SHG

Courtesy of Christian Wolff

Gold Dimer: Nonlinear Spectra



Radius 10 nm, Gap = 4 nm



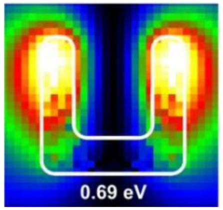
Radius 20 nm, Gap = 4 nm

Courtesy of Christian Wolff

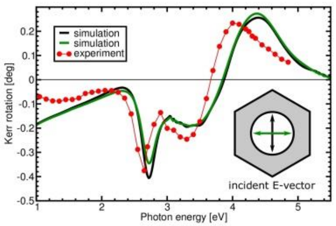
Conclusions & Outlook

- Discontinuous Galerkin Time-Domain Approach

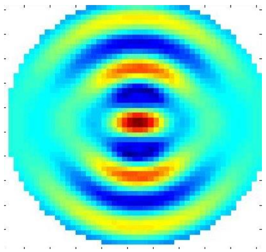
- Examples
  - Electron Energy Loss Spectroscopy
  - Cathodoluminescence



- Transition Material Modeling
  - Isotropic Response: Drude Model plus Retardation
  - Magneto-Optic Response



- Nonlinear Hydrodynamic Model for Conduction Electrons
  - Particle Plasmon Polaritons & Bulk Plasmons
  - Wave Mixing
  - Outlook: “Soft Walls“



Hydrodynamic Model – Treatment of Surfaces

$$\partial_t \rho + \nabla \cdot \vec{j} = 0$$

$$(\partial_t + \gamma)\,\vec{j} + \nabla \cdot \left(\frac{\vec{j} \quad \vec{j}}{\rho} \right) = -\frac{e}{m}\left(\rho \vec{E} + \vec{j} \times \vec{H}\right) - \frac{1}{m}\nabla p$$

$$p(\vec{r},t) = \zeta\,[\rho(\vec{r},t)]^{5/3} \qquad \zeta = \frac{\hbar^2}{5m}\left(3\pi^2\right)^{3/2}$$

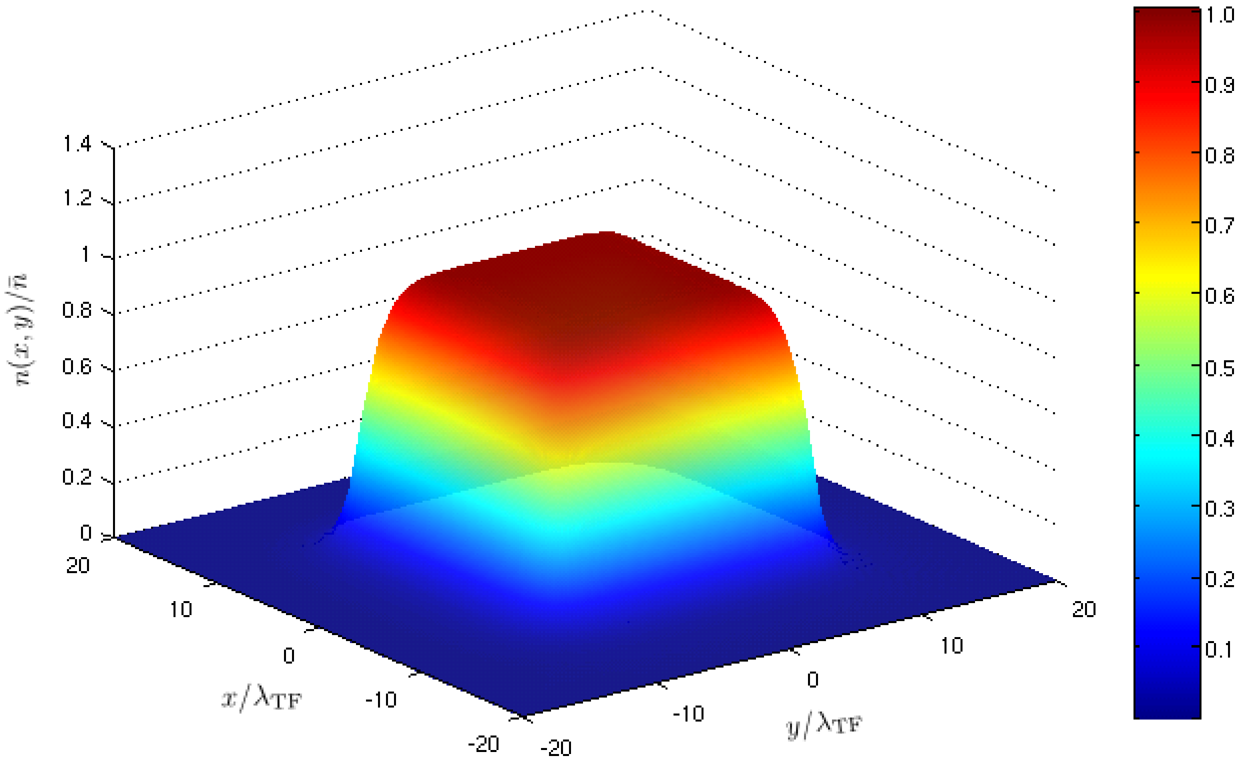
- Initial Condition: 0th-Order Equation

$$\boldsymbol{\nabla} \cdot \vec{E}_0(\vec{r}) = -e\left(\rho_0(\vec{r}) - \rho^+(\vec{r})\right)$$

$$\boldsymbol{\nabla} \rho_0(\vec{r}) = -\frac{3e}{5\zeta}\,\rho_0^{1/3}(\vec{r})\,\vec{E}_0(\vec{r})$$

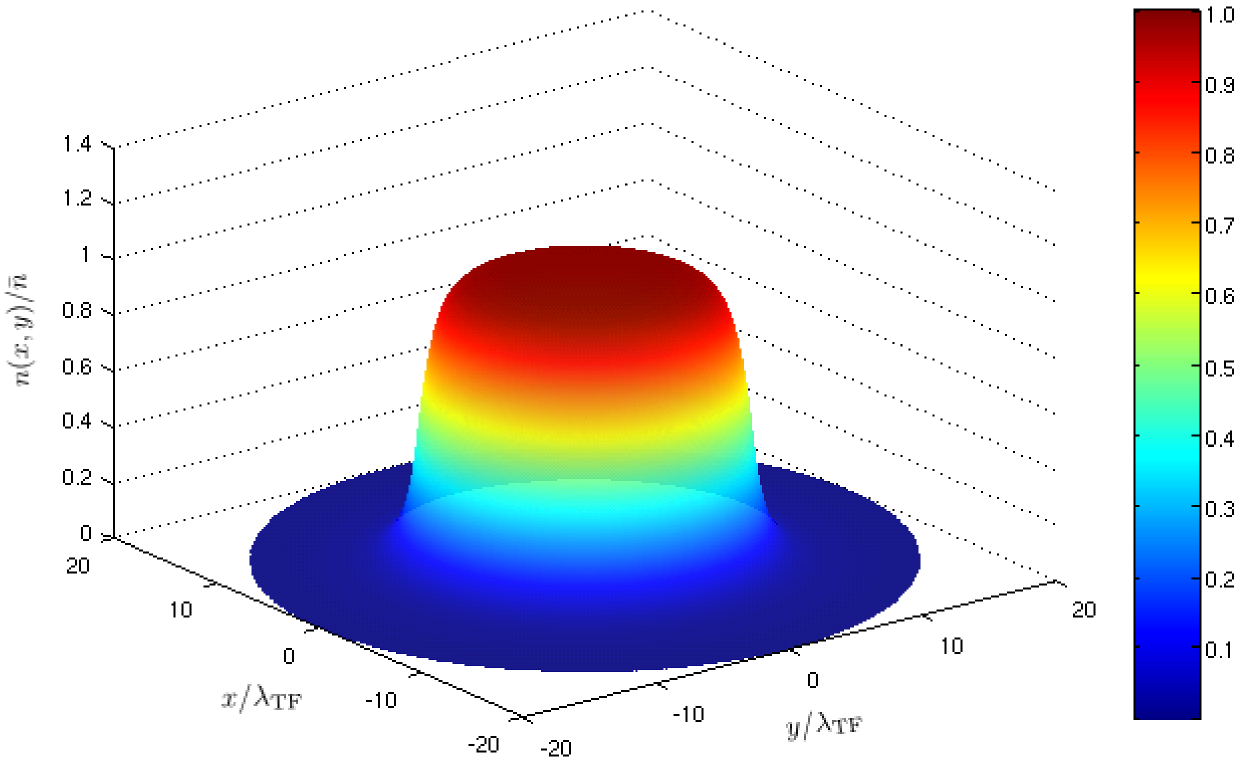
$$\lambda_{\mathrm{TF}} = \left(\frac{\pi^4}{3\bar{n}}\right)^{1/6}\left(\frac{\epsilon_0 \hbar^2}{m e^2}\right)^{1/2}$$

Hydrodynamic Model – Equilibrium Density



Courtesy of Timo Köllner

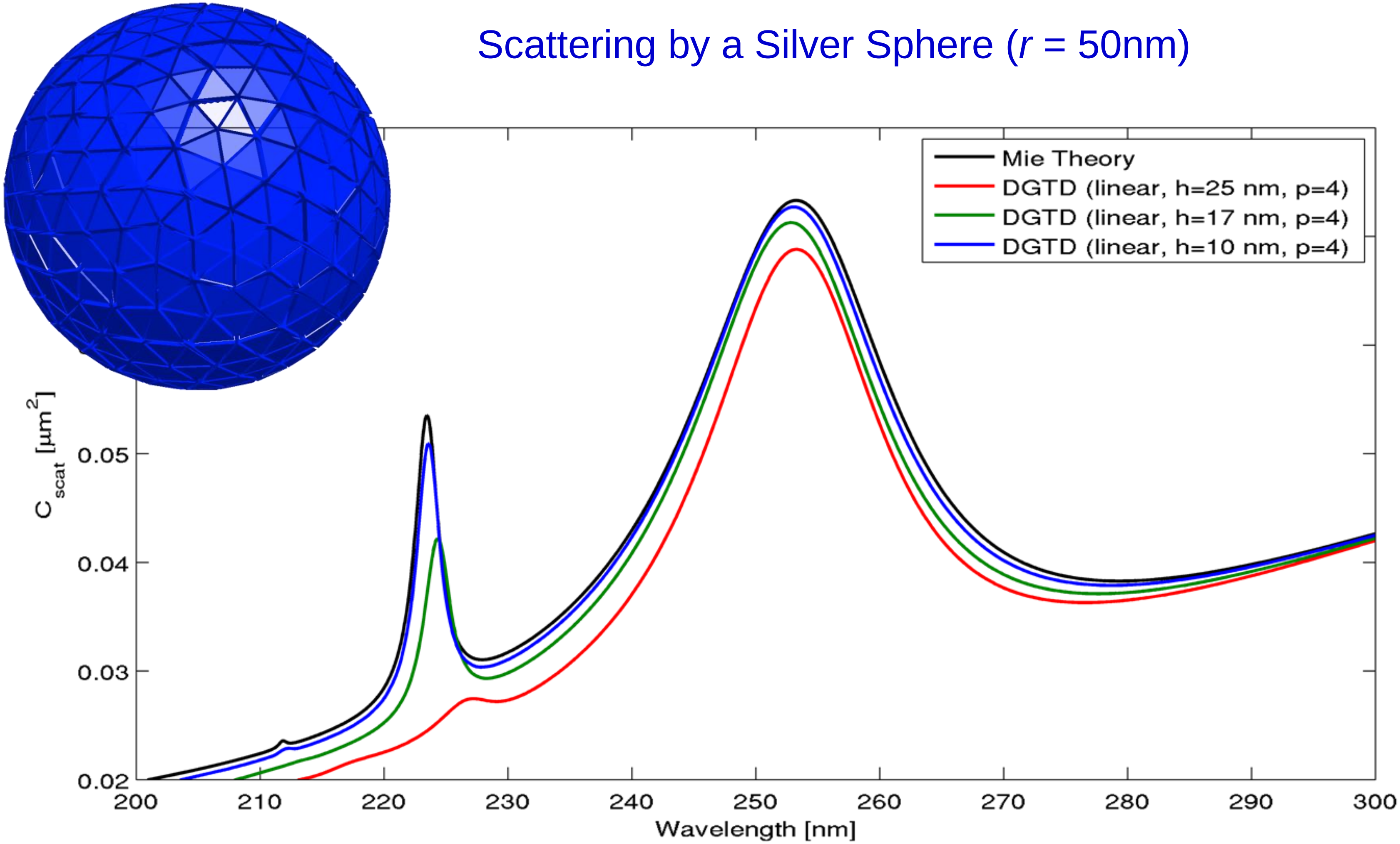
Hydrodynamic Model – Equilibrium Density



Courtesy of Timo Köllner

Straight-Sided vs. Curvilinear Elements

Scattering by a Silver Sphere (r = 50nm)



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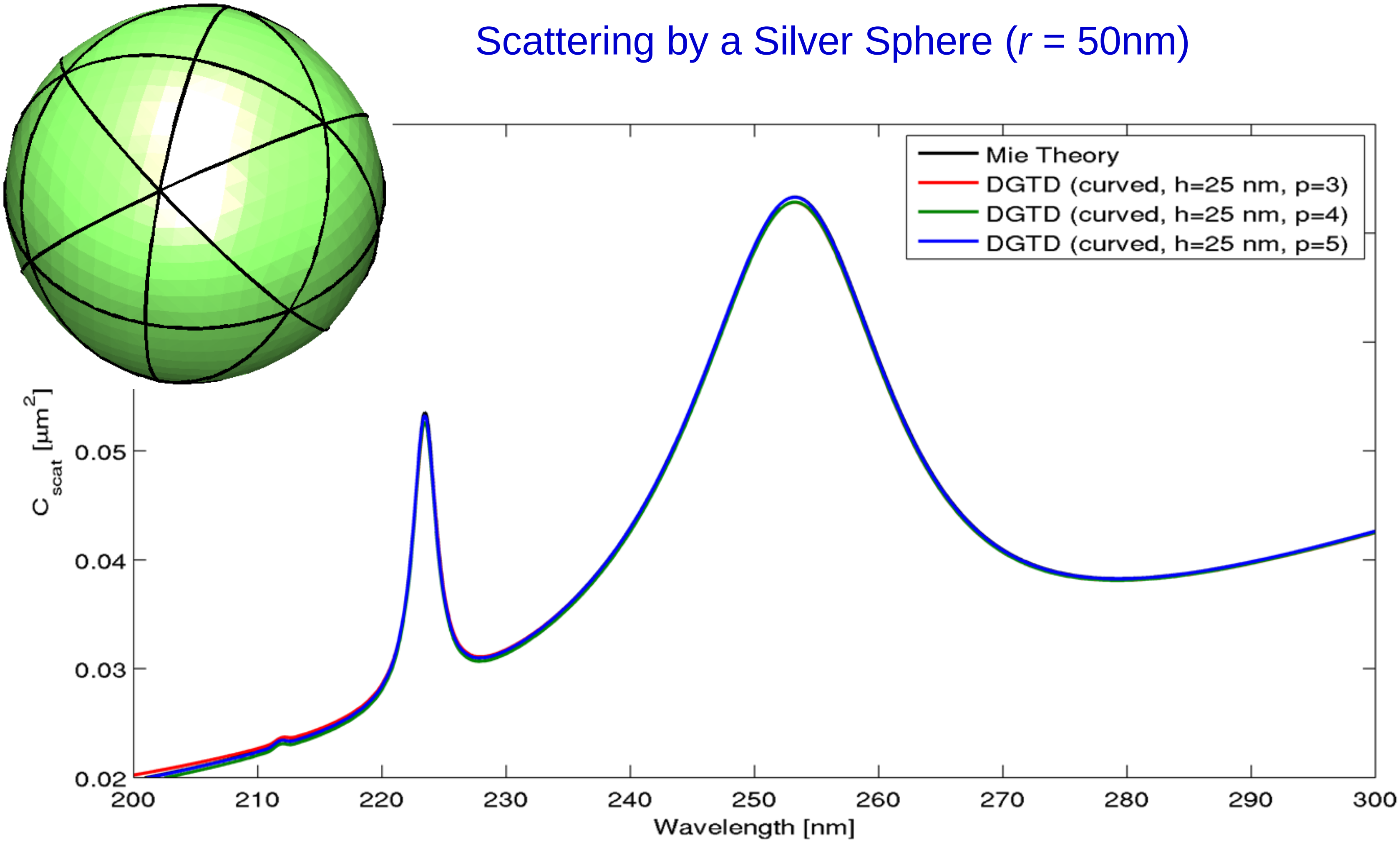
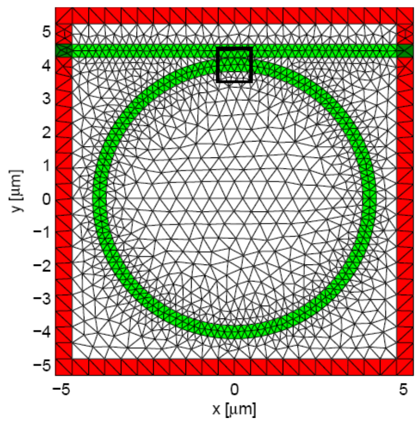
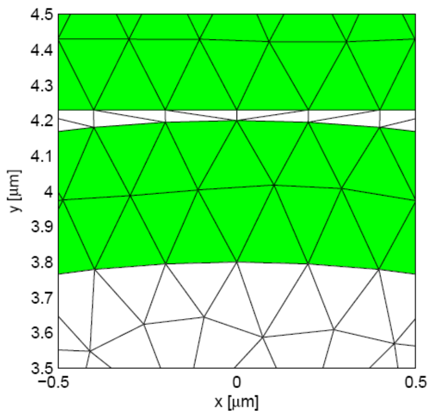
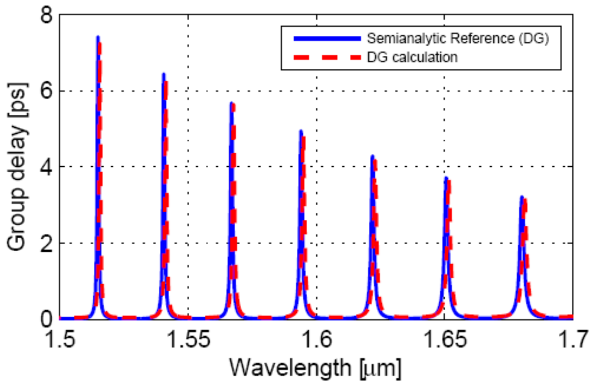


Performance of the DGTD-Approach



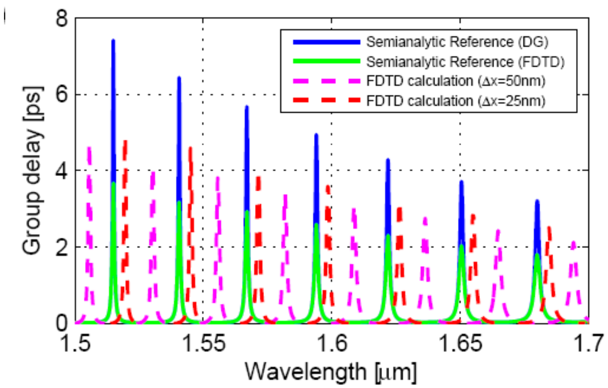




Comparison with FDTD:

MEEP: Memory ~100, Speed ~8

Commercial Codes: Even worse



J. Niegemann, W. Pernice, and K. Busch, J. Opt. A **11**, 114015 (2009)

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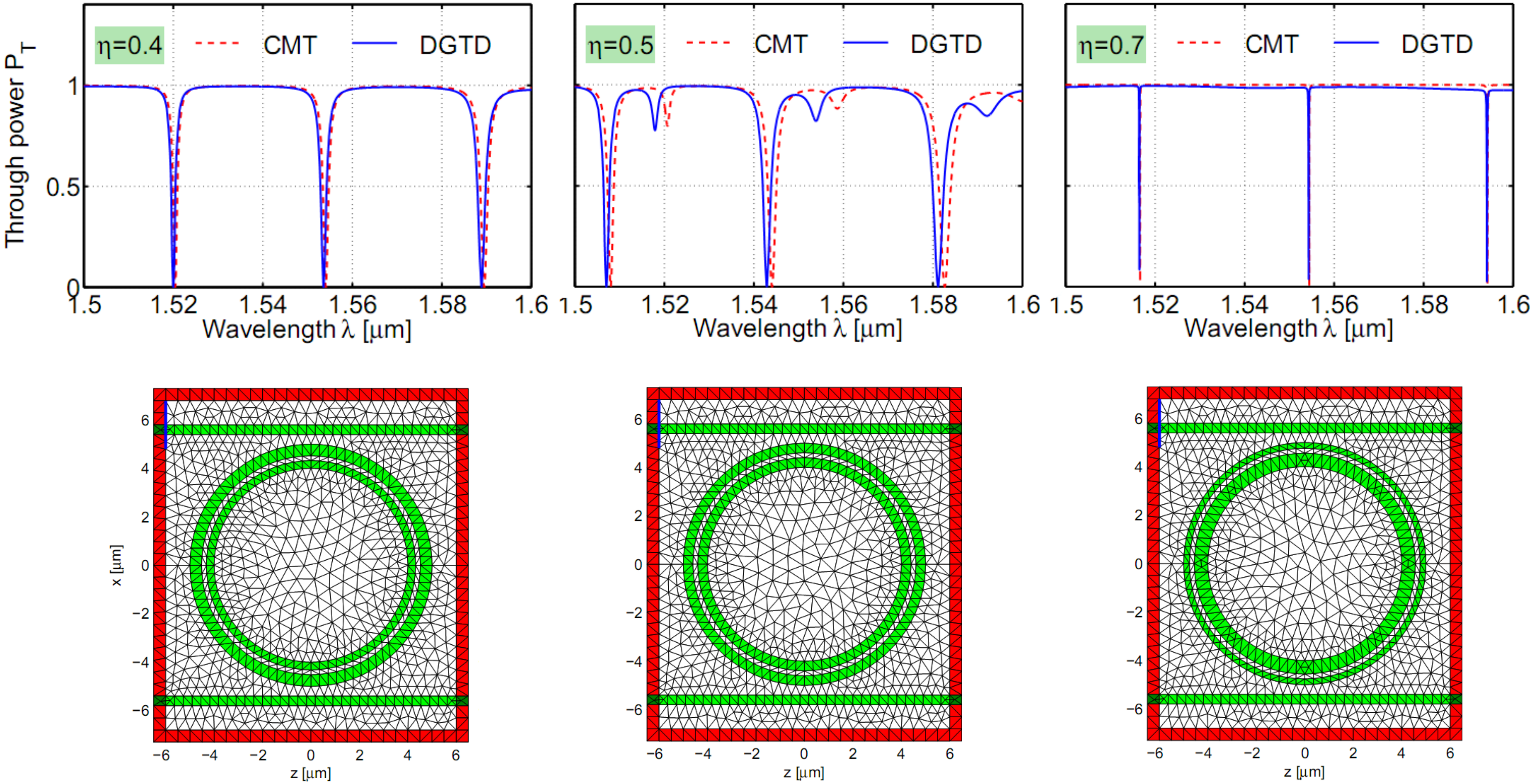
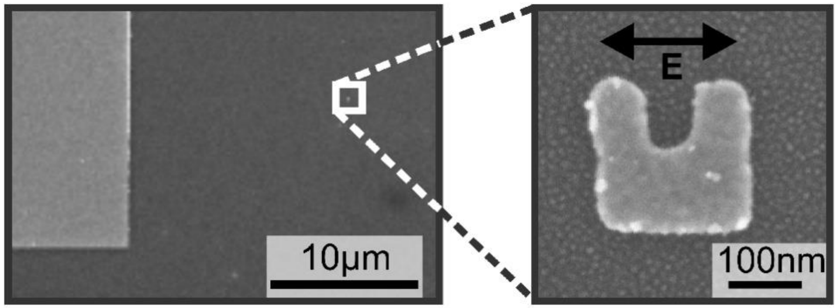
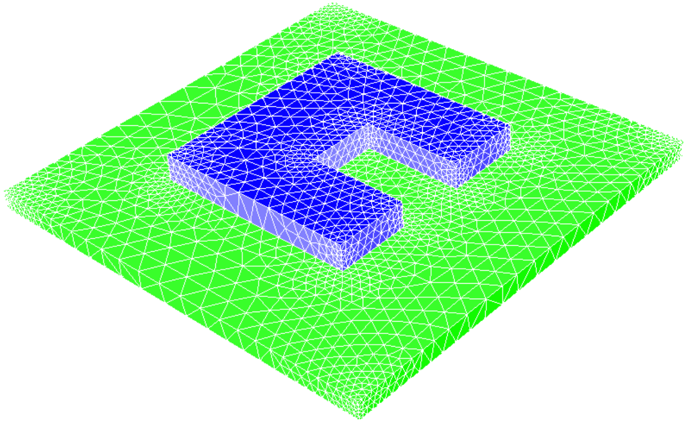
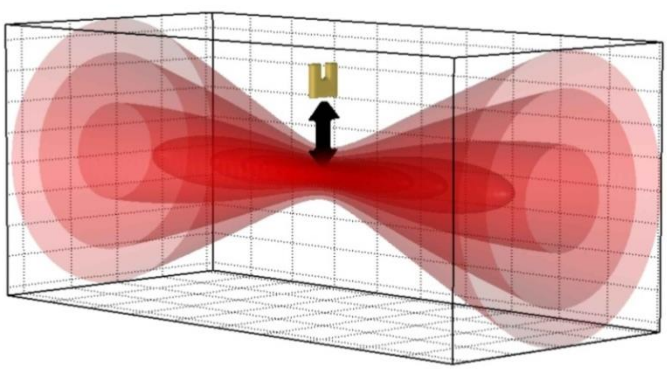


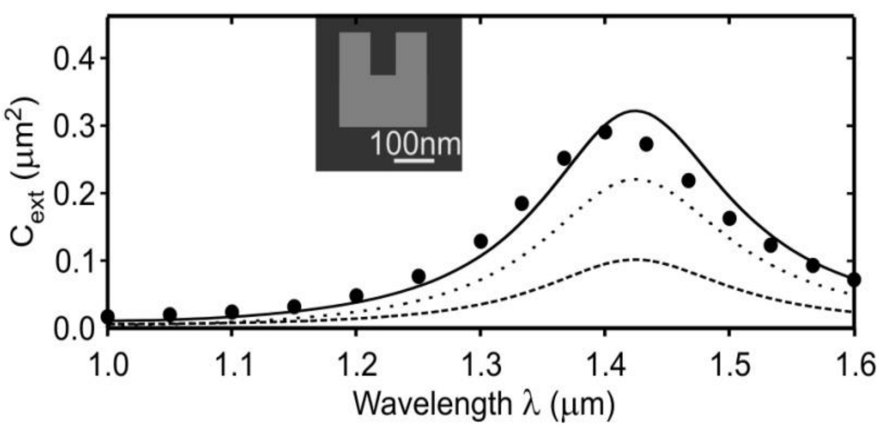
K. R. Hiremath, J. Niegemann, and K. Busch, Optics Express **19**, 8641 (2011)

Metamaterials: Single-Particle Spectroscopy



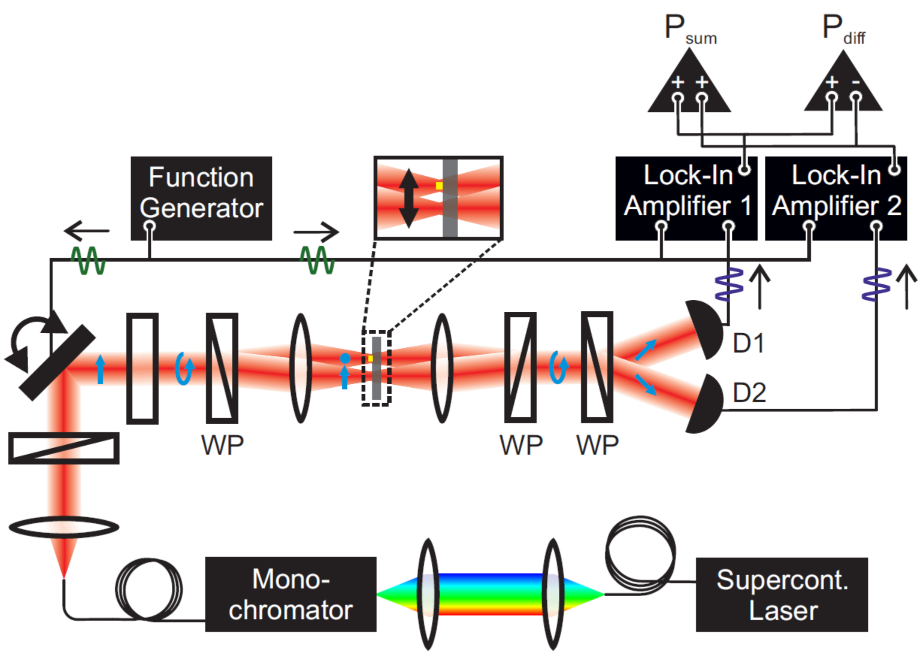


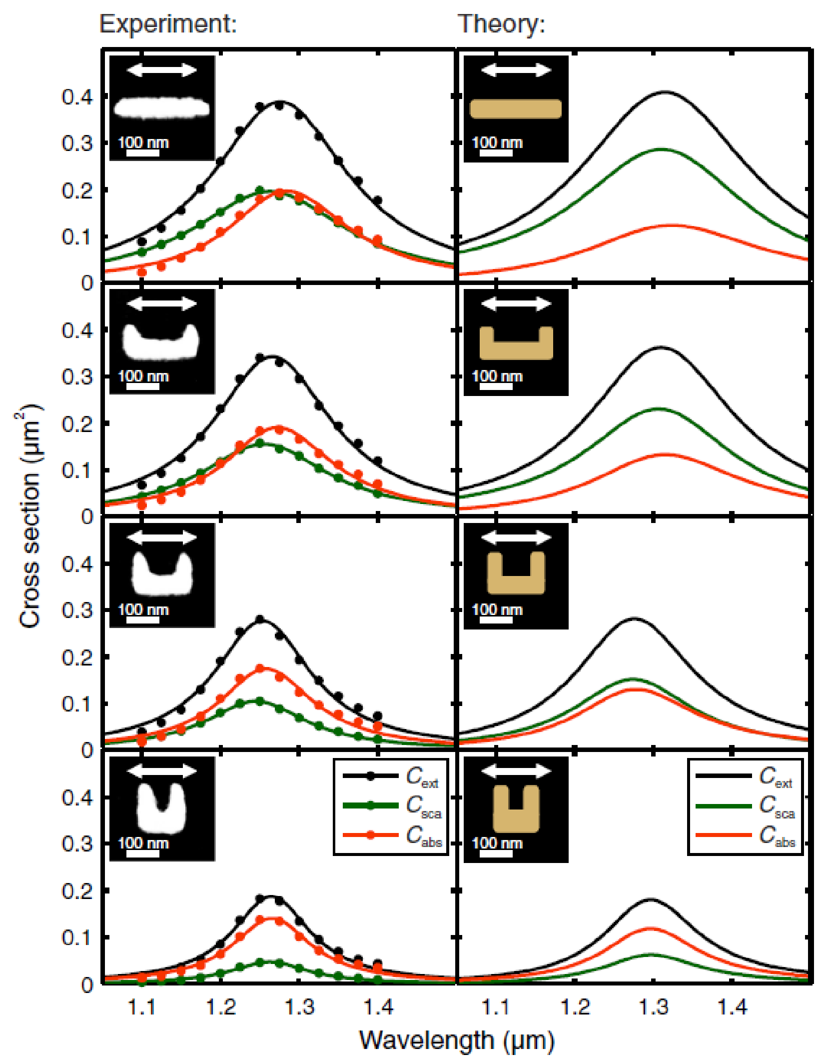




M. Husnik et al., Nature Photonics **2**, 614 (2008)

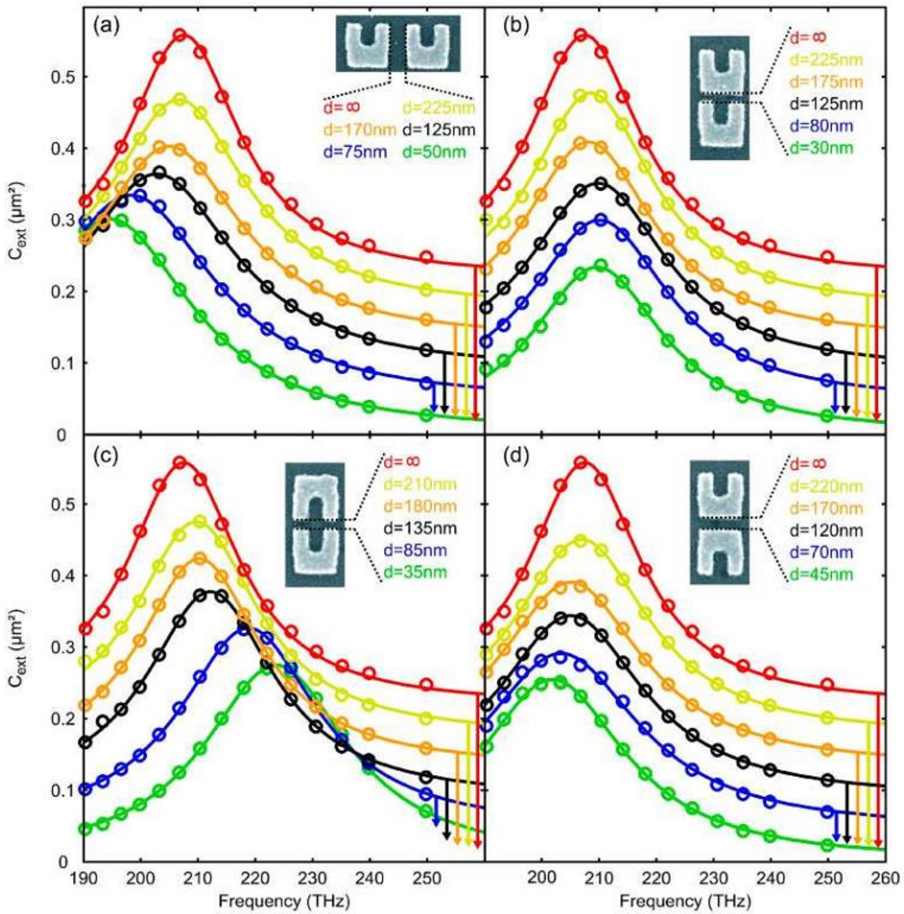
Metamaterials: Single-Particle Spectroscopy

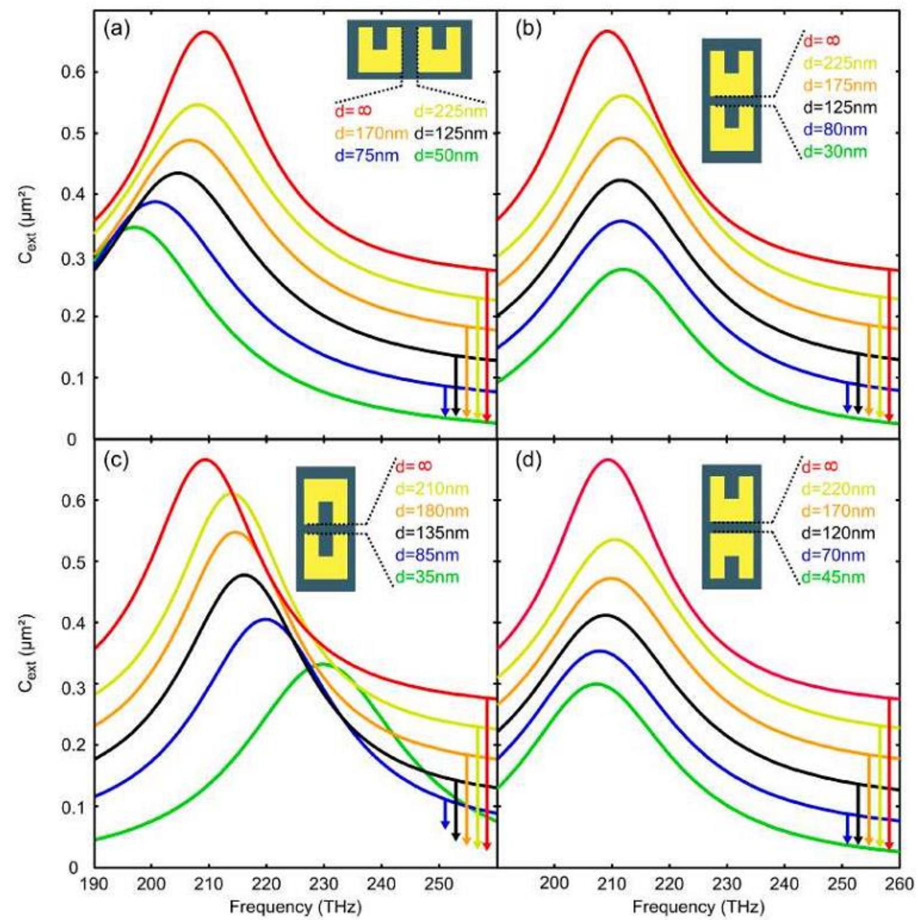




M. Husnik et al., Phys. Rev. Lett. **109**, 233902 (2012)

Interaction between SRRs: Experiment vs. Theory





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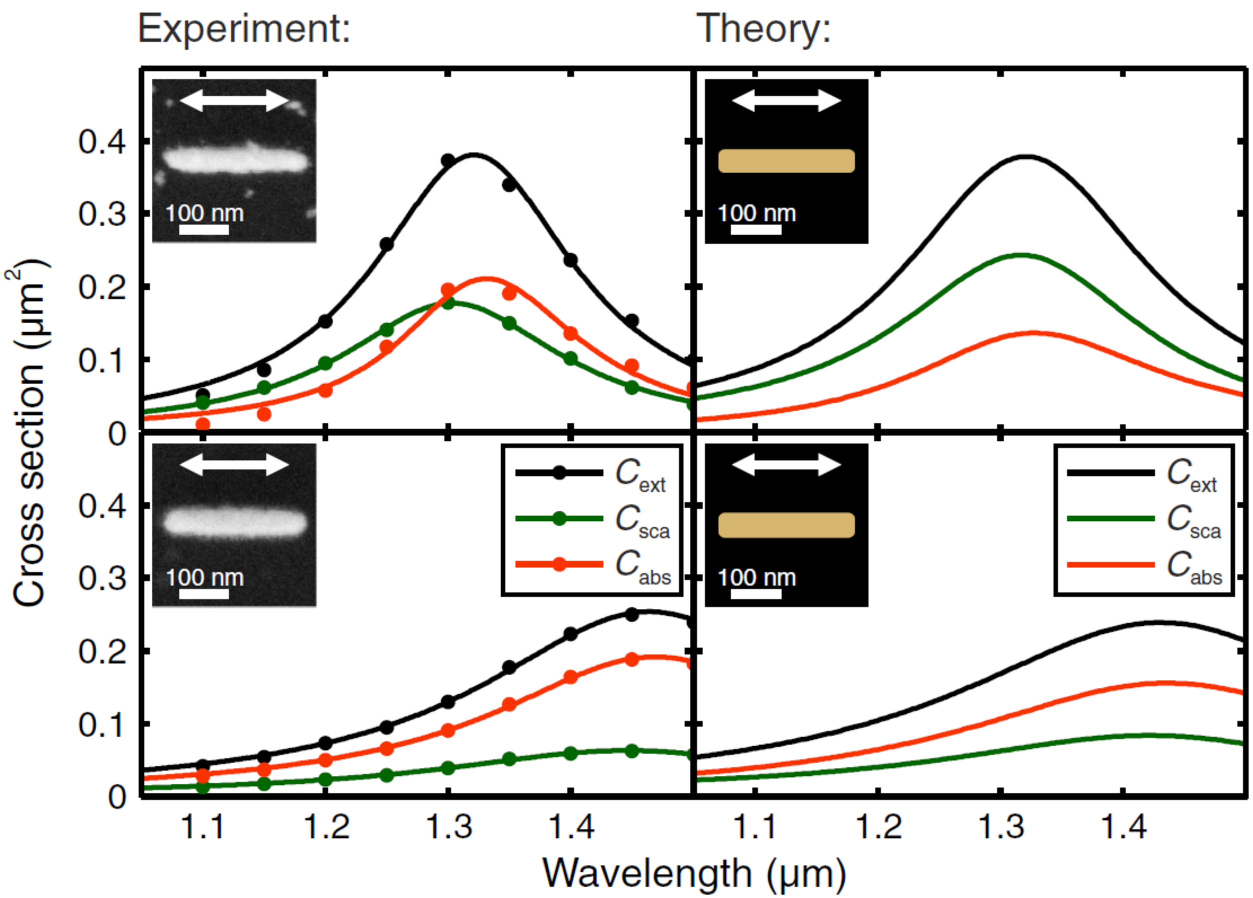
Role of Resistance



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