Simulating Graphene-Based Photonic and Optoelectronic Devices

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COMSOL

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SECE, Purdue University

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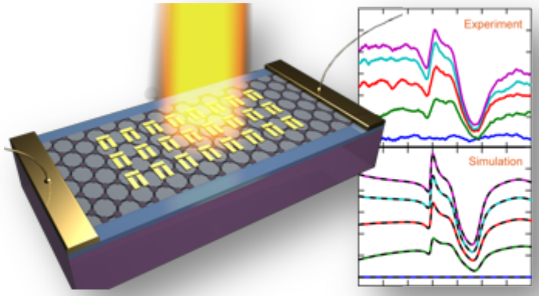
Agenda

- Optics Simulation with COMSOL Multiphysics®
- Simulating Graphene-Based Photonic and Optoelectronic Devices
- Live Demo
  - Graphene Frequency and Time Domain Modeling
- Q&A Session
- How To
  - Try COMSOL Multiphysics
  - Contact Us



Design of plasmonic antennas optimized using COMSOL Multiphysics

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Product Suite – COMSOL® 5.1

COMSOL Multiphysics®

COMSOL Server™

ELECTRICAL
- AC/DC Module
- RF Module
- Wave Optics Module
- Ray Optics Module
- MEMS Module
- Plasma Module
- Semiconductor Module

MECHANICAL
- Heat Transfer Module
- Structural Mechanics Module
- Nonlinear Structural Materials Module
- Geomechanics Module
- Fatigue Module
- Multibody Dynamics Module
- Acoustics Module

FLUID
- CFD Module
- Mixer Module
- Microfluidics Module
- Subsurface Flow Module
- Pipe Flow Module
- Molecular Flow Module

CHEMICAL
- Chemical Reaction Engineering Module
- Batteries & Fuel Cells Module
- Electrodeposition Module
- Corrosion Module
- Electrochemistry Module

MULTIPURPOSE
- Optimization Module
- Material Library
- Particle Tracing Module

INTERFACING
- LiveLink™ *for* MATLAB®
- LiveLink™ *for* Excel®
- CAD Import Module
- Design Module
- ECAD Import Module
- LiveLink™ *for* SOLIDWORKS®
- LiveLink™ *for* Inventor®
- LiveLink™ *for* AutoCAD®
- LiveLink™ *for* Revit®
- LiveLink™ *for* PTC® Creo® Parametric™
- LiveLink™ *for* PTC® Pro/ENGINEER®
- LiveLink™ *for* Solid Edge®
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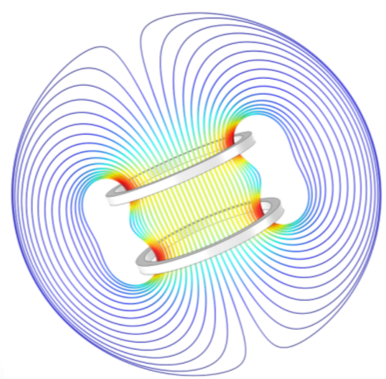
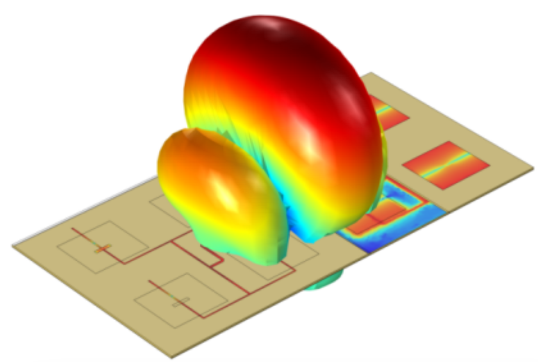
Electrical Simulations

- AC/DC current and field distribution
- Electromechanical machinery and electrical circuits
- RF and microwave components
- Wave propagation in optical media



Magnetic field in a Helmholtz coil



Microstrip patch antenna array

COMSOL Multiphysics®

COMSOL Server™

ELECTRICAL

AC/DC Module

RF Module

Wave Optics Module

Ray Optics Module

MEMS Module

Plasma Module

Semiconductor Module

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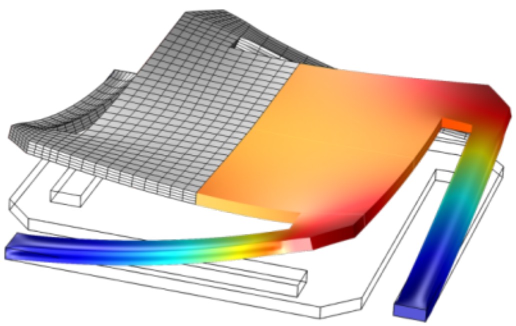
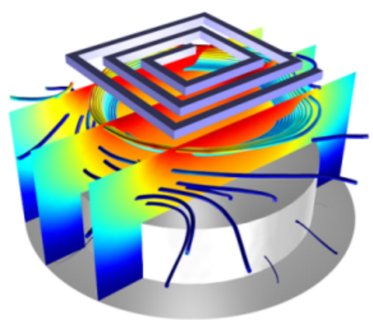
Electrical Simulations

- MEMS devices and sensors
- Low temperature plasma reactors
- Semiconductor devices
- Ray tracing in optically large systems



Prestressed micromirror



Inductively coupled plasma reactor

- COMSOL Multiphysics®
- COMSOL Server™

ELECTRICAL

- AC/DC Module
- RF Module
- Wave Optics Module
- Ray Optics Module
- MEMS Module
- Plasma Module
- Semiconductor Module

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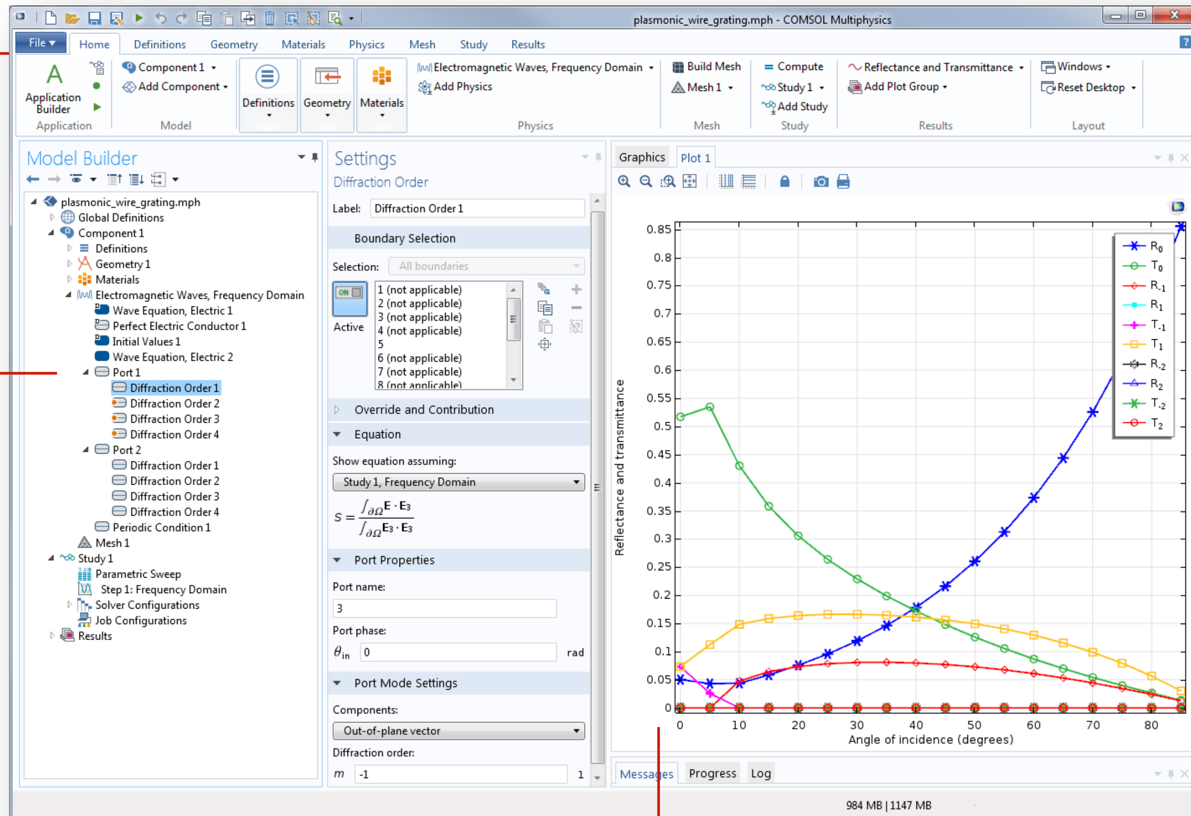
A Complete Simulation Environment



COMSOL Desktop®

Straightforward to use, the Desktop gives insight and full control over the modeling process

Model Builder

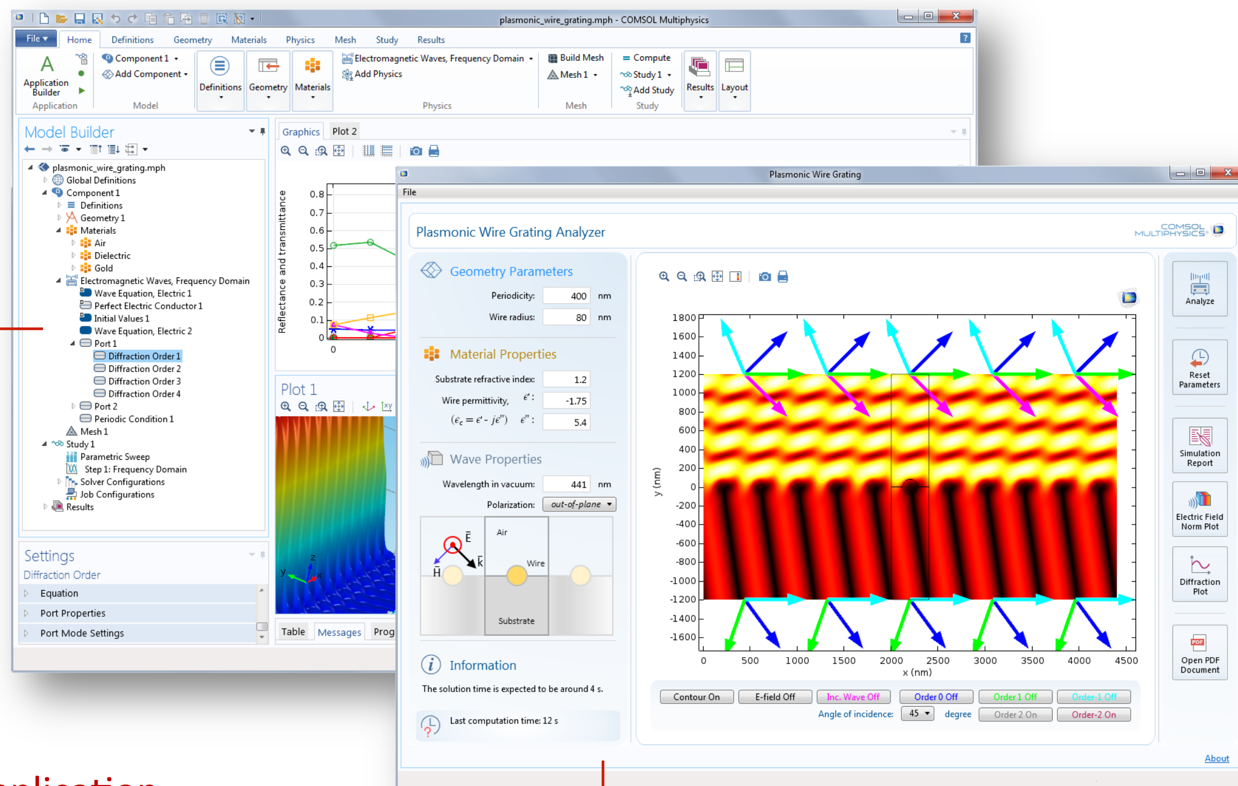
Provides instant access to any of the model settings

- CAD/Geometry
- Materials
- Physics
- Mesh
- Solve
- Results

Graphics Window

Ultrafast graphic presentation, stunning visualization

Application Design Tools



Application Builder

Provides all the tools needed to build and run simulation apps

- Form Editor
- Method Editor

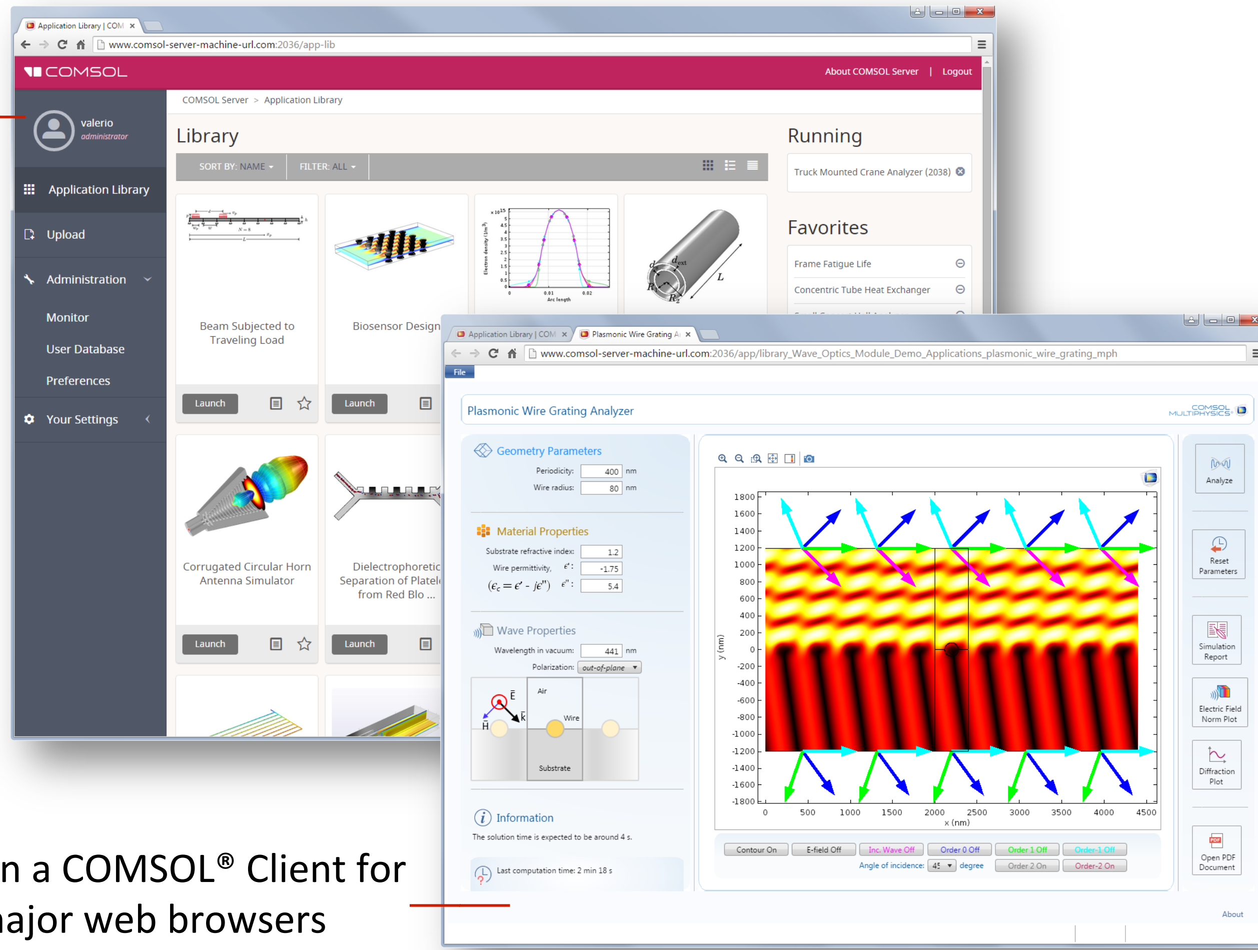
Simulation Application

Any COMSOL model can be turned into an app with its own interface using the tools provided in the Application Builder

Run Applications

COMSOL Server™

It's the engine for running COMSOL apps and the hub for controlling their deployment, distribution, and use



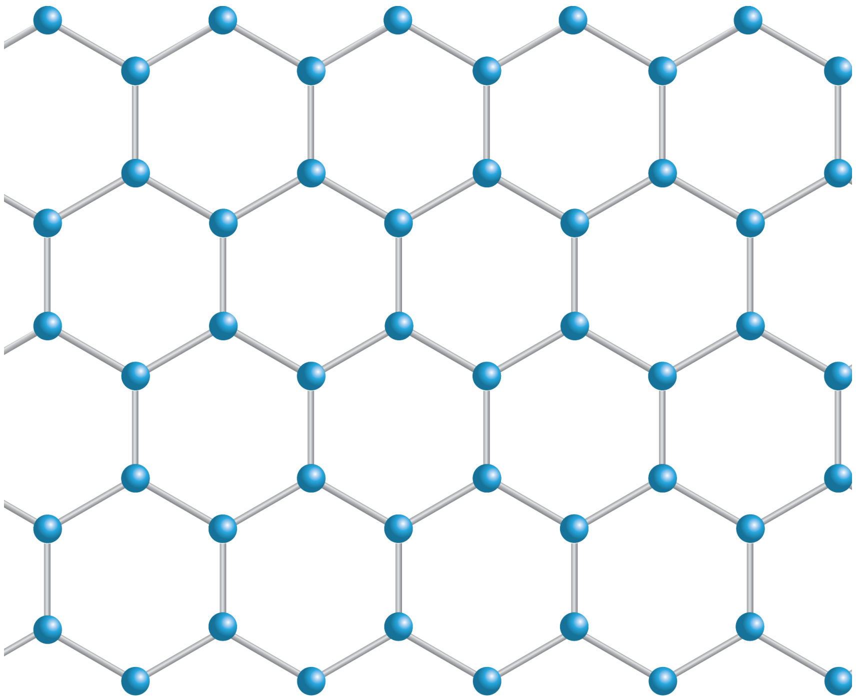
Simulation Apps

They can be run in a COMSOL® Client for Windows® and major web browsers

Microsoft and Windows are either registered trademarks or trademarks of Microsoft Corporation in the United States and/or other countries.

Graphene

- Discovered in 2004
  - Only 1 atom thick (Carbon)
  - 2D material in a honeycomb lattice
  - Nobel Prize in 2010
- Exciting material properties
  - Nearly transparent
  - Flexible
  - High electrical conductivity
  - High thermal conductivity
  - Stronger than steel
- Exotic material properties
  - Linear dispersion curve
  - Charge carries act as massless particles



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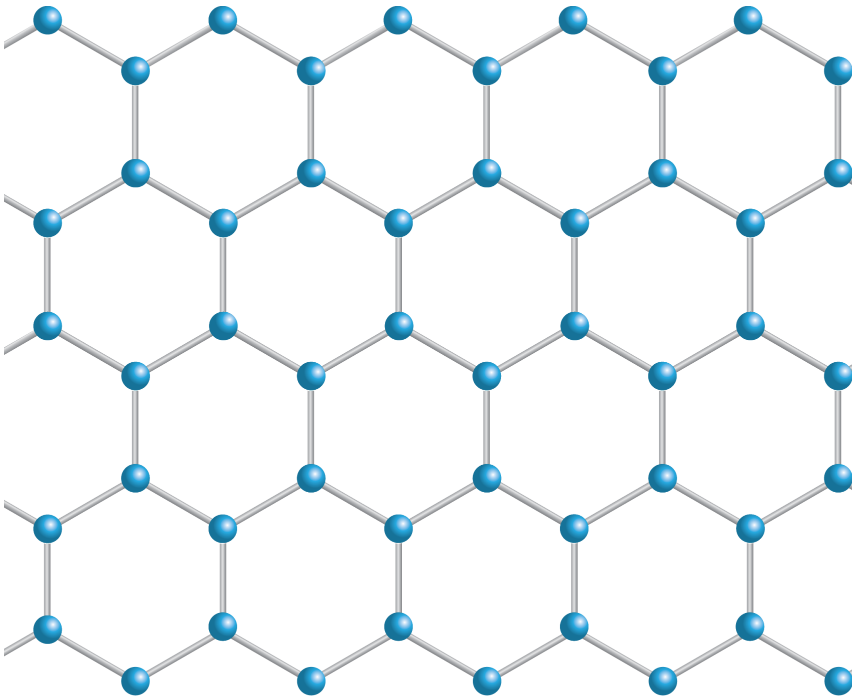
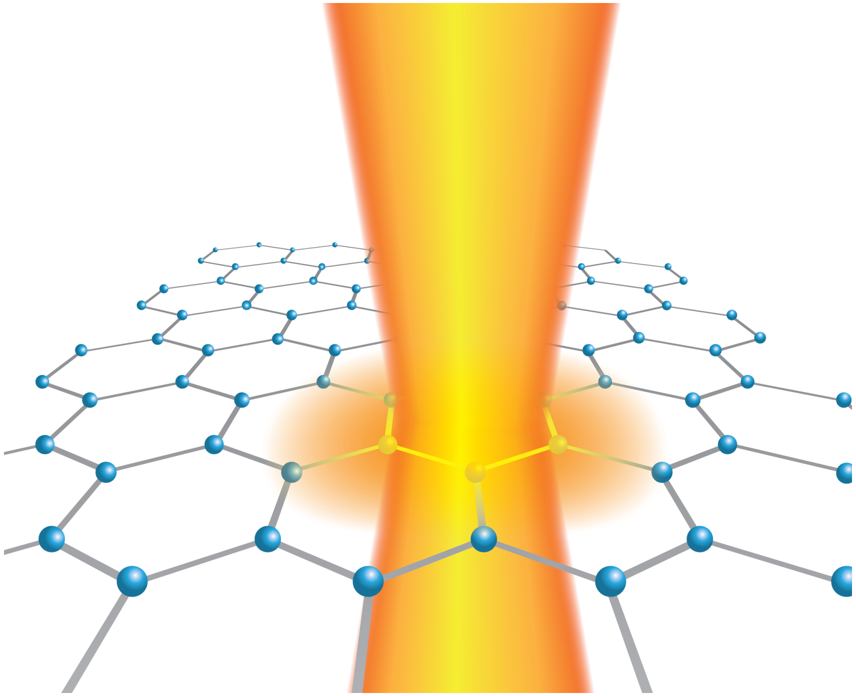
COMSOL and Graphene

- Graphene defies out intuition
  - Only 1 atom thick
- User-defined equations
  - Add in your own physics
- Physics and material properties can be assigned to any geometry and dimension
  - Treat thin layers as boundaries
- Flexibility in modeling
  - Explicit control of physics couplings



Why Simulate Graphene and Graphene-Based Devices?

- Graphene defies our intuition
  - Only 1 atom thick
- Conception and understanding
  - Enables innovation
- Design and optimization
  - Achieve the highest possible performance
- Testing and verification
  - Virtual testing is much faster than testing physical prototypes



Poll Question

- Are you currently simulating graphene applications?
  - Yes, I'm using my own code.
  - Yes, I'm using an off-the-shelf software.
  - Yes, I'd like to see how it's done in COMSOL.
  - No, I'd like to learn what is possible to simulate.

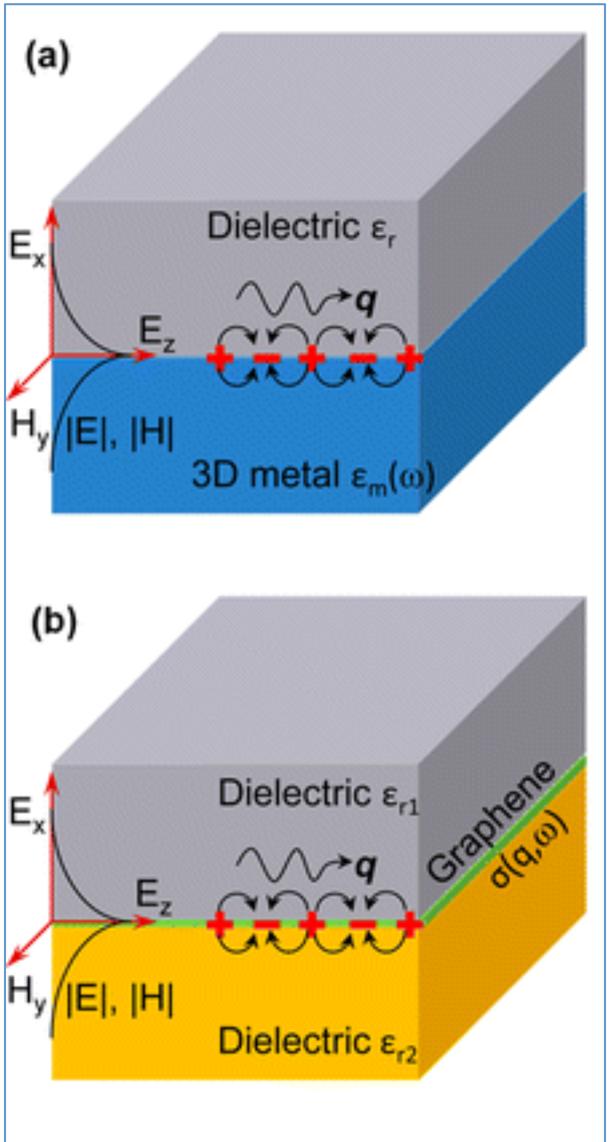
Simulating Graphene-Based Photonic and Optoelectronic Devices

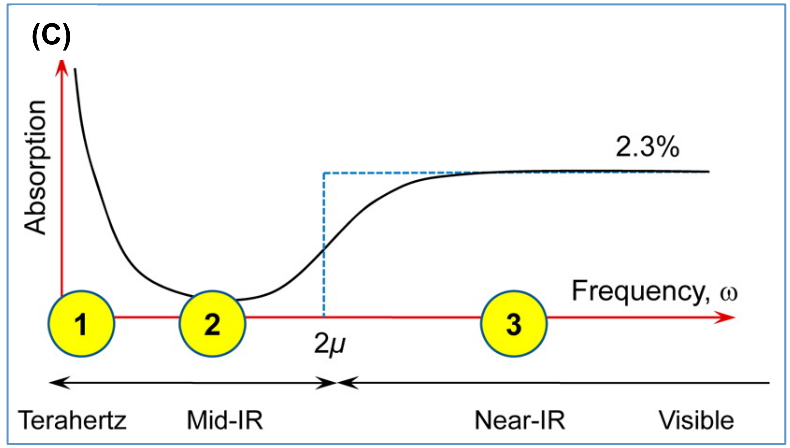
Alexander Kildishev

Associate Professor, Birck Nanotechnology Center,
School of Electrical and Computer Engineering, Purdue University

Graphene Plasmonics: Optical Dispersion

Low & Avouris, ACS Nano, 2014, 8 (2), 1086–1101





$$\sigma(\omega) = \frac{2e^2\omega_T}{\pi\hbar}\frac{i}{\omega + i\tau^{-1}}\log\left[2\cosh\left(\frac{\omega_F}{2\omega_T}\right)\right]$$

Intraband term

$$+\frac{e^2}{4\hbar}\left[H\left(\frac{\omega}{2}\right) + i\frac{2\omega}{\pi}\int_0^\infty \frac{H\left(\frac{\omega'}{2}\right) - H\left(\frac{\omega}{2}\right)}{\omega^2 - \omega'^2}d\omega'\right]$$

Interband term (not TD-friendly)

$$H(\omega) = \sinh(\omega/\omega_T)/[\cosh(\omega_F/\omega_T) + \cosh(\omega/\omega_T)]$$

$$\omega_F = E_F/\hbar \quad \omega_T = k_B T/\hbar$$

ω is the frequency of incident light, e is the charge of an electron, τ is the Drude relaxation rate, T is the temperature, and k_B is the Boltzmann constant

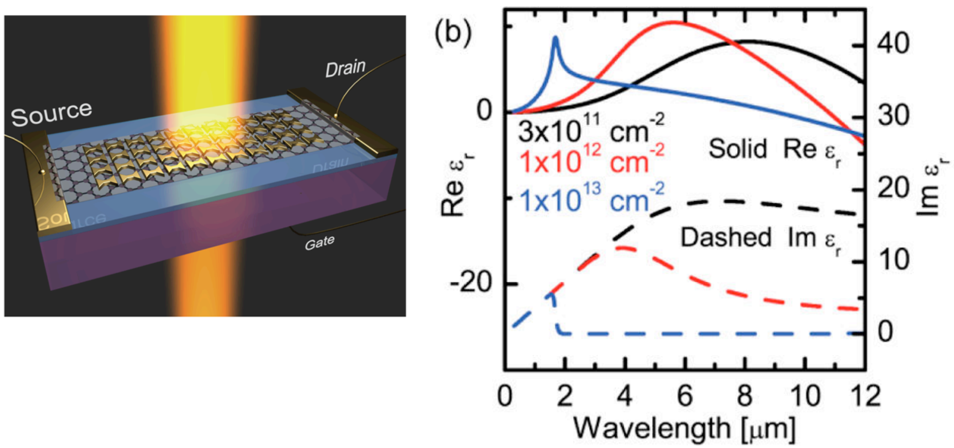
Falkovsky, L. *Optical properties of graphene*, 2008; IOP Publishing: p. 012004.

Graphene Plasmonics: Applications

NANO LETTERS
Letter
pubs.acs.org/NanoLett

Electrically Tunable Damping of Plasmonic Resonances with Graphene

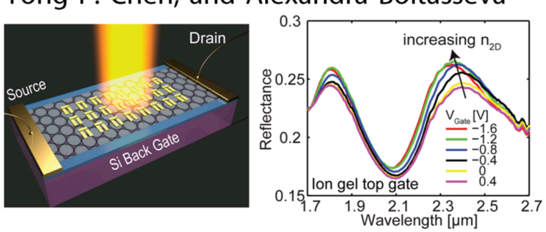
Naresh K. Emani, Ting-Fung Chung, Xingjie Ni, Alexander V. Kildishev,
Yong P. Chen, and Alexandra Boltasseva



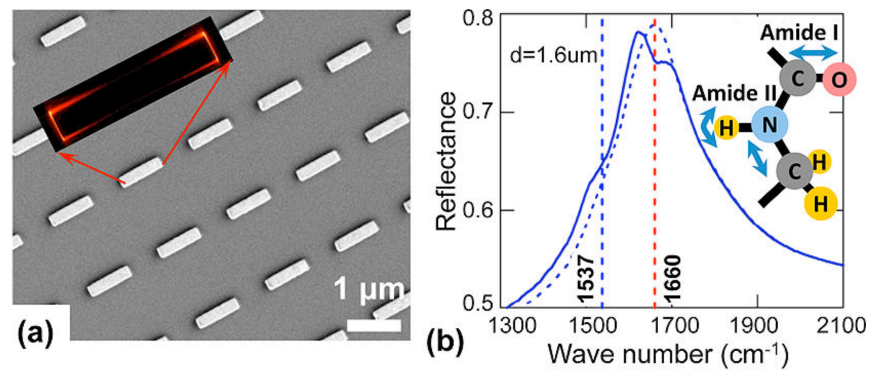
NANO LETTERS
Letter
pubs.acs.org/NanoLett

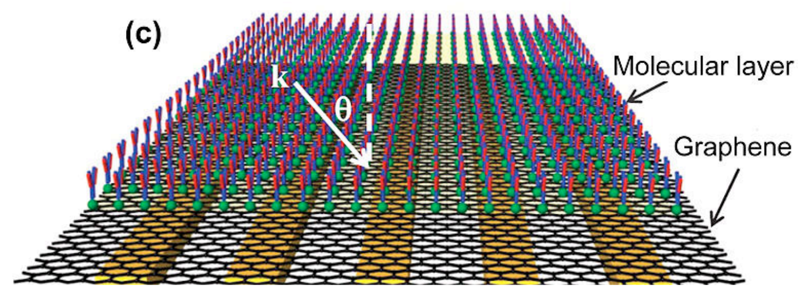
Electrical Modulation of Fano Resonance in Plasmonic Nanostructures Using Graphene

Naresh K. Emani, Ting-Fung Chung, Alexander V. Kildishev, Vladimir M. Shalaev,
Yong P. Chen, and Alexandra Boltasseva



Adato, *et al.*, Proc. Acad. Sci. U.S.A. 106, 19227, 2009
(The Altug Group, Boston University)





Low & Avouris, ACS Nano, 2014, 8 (2), 1086–1101

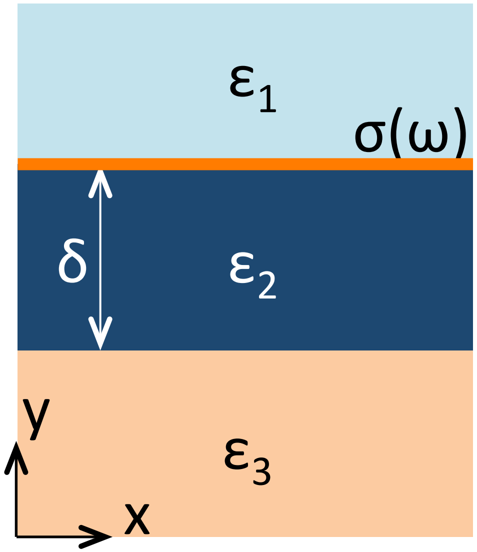
Modeling Challenges

- Frequency Domain Modeling: As graphene is a material with reduced dimensionality and chemically or electrically tunable optical dispersion (plasmonic properties) – specific methods are necessary

- Time Domain Modeling: RPA does not provide an easy way to implement the time-domain analysis of tunable nanostructured plasmonic graphene elements and hybrid SLG-metal devices in real time – better causal models are desirable

- Advanced Modeling Problems: coupling with polar substrates, non-linear graphene plasmonics, quantum effects in nano-structured graphene, etc

Frequency Domain Modeling: Validation Effort



φ	Angle of incidence
δ	Spacer layer thickness
$\varepsilon_i, i \in \overline{1,3}$	Relative permittivity in i-th media
$\sigma(\omega)$	Surface conductivity
$k_i = \frac{2\pi}{\lambda}\sqrt{\varepsilon_i - \varepsilon_1 \sin^2 \varphi}$	X-component of wave vector

The Modified Fresnel Equations (p-polarization)

$$\boxed{r_{12}^{\pm} = \frac{\varepsilon_2 k_1 + \xi - \varepsilon_1 k_2}{\varepsilon_2 k_1 + \xi + \varepsilon_1 k_2}, r_{12}^{\mp} = \frac{\varepsilon_2 k_1 - \xi + \varepsilon_1 k_2}{\varepsilon_2 k_1 + \xi + \varepsilon_1 k_1}, r_{12}^{=} = \frac{\varepsilon_2 k_1 - \xi - \varepsilon_1 k_1}{\varepsilon_2 k_1 + \xi + \varepsilon_1 k_2}, r_{23} = \frac{\varepsilon_3 k_2 - \varepsilon_2 k_3}{\varepsilon_3 k_2 + \varepsilon_2 k_3}, \xi = \sigma(\omega) k_2 k_3 / (\omega \varepsilon_0)}$$

The Modified Drude Equation

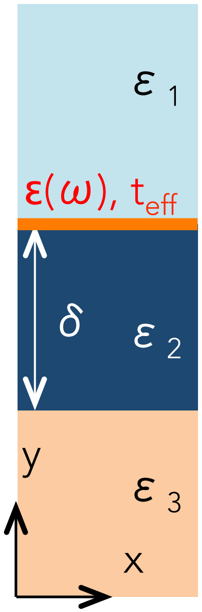
$$\boxed{r = \frac{r_{12}^{\pm} + r_{12}^{\mp} r_{23} e^{\iota 2 k_2 \delta}}{1 + r_{12}^{=} r_{23} e^{\iota 2 k_2 \delta}}}$$

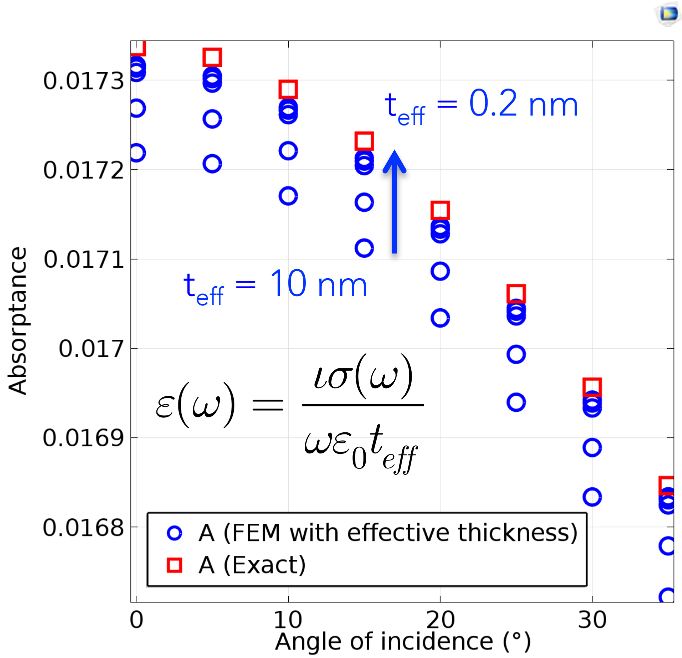
The Modified Voight Equation

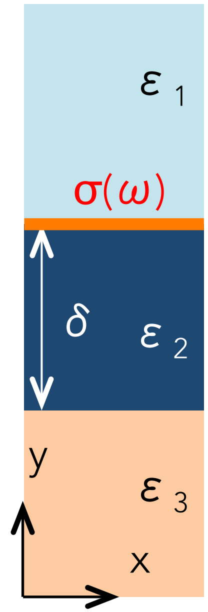
$$\boxed{t = \frac{t_{12}^{=} t_2 e^{i k_1 \delta}}{1 + r_{12}^{=} r_{23} e^{i 2 k_1 \delta}}, \quad \left(t_{12}^{=} = 1 + r_{12}^{=}, t_{23} = 1 + r_{23}\right)}$$

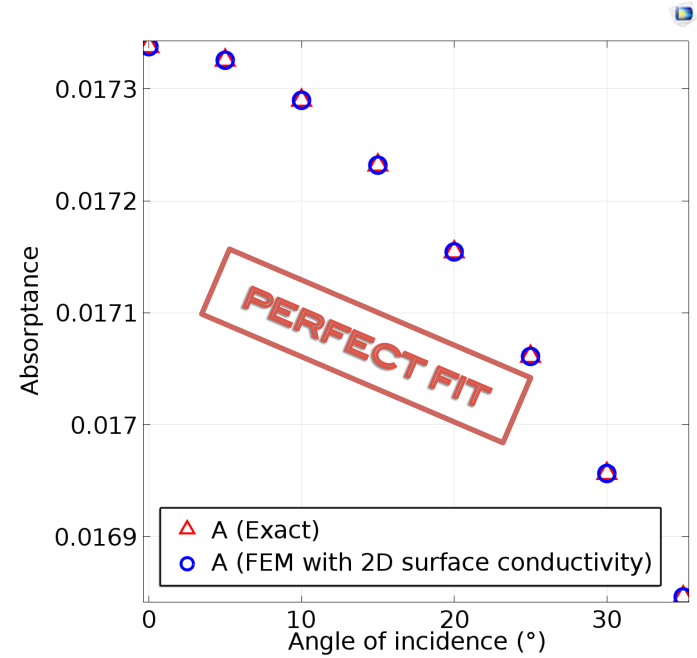
Drude P. Ueber Oberflächenschichten. II. Theil. Annalen der Physik 1889, 272:865-897.

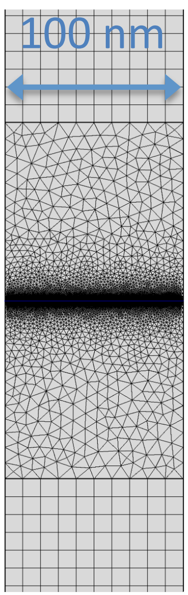
FD Modeling: "thin layer" vs. "surface current"











Single scan with t_{eff} = 0.2 nm

Free-space λ = 6 μm

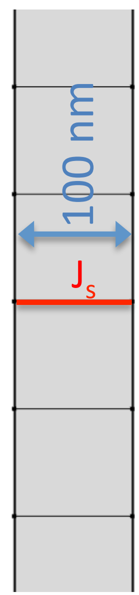
δ = 0.3 μm, ε_2 – silica

ε_3 – glass substrate

Angle of incidence: (0°: 5°: 35°)

Number of DOF: 241721

Solution time (8 angles): 35 s



Single scan with 2D conductivity

Free-space λ = 6 μm

δ = 0.3 μm, ε_2 – silica

ε_3 – glass substrate

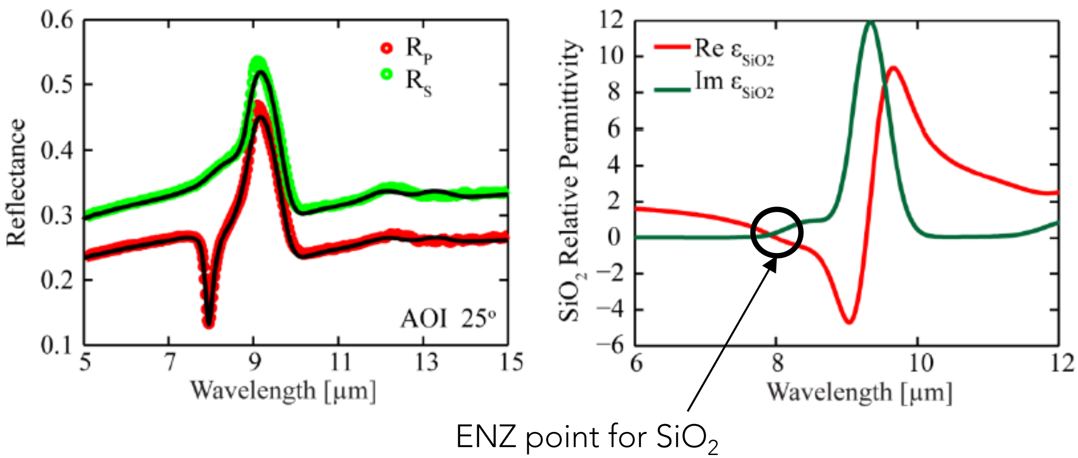
Angle of incidence: (0°: 5°: 35°)

Number of DOF: 278 (vs. 241721)

Solution time (8 angles): 2 s (vs. 35 s)

Frequency Domain Modeling: the case of SLG

Ellipsometry for SiO_2 WITHOUT graphene*



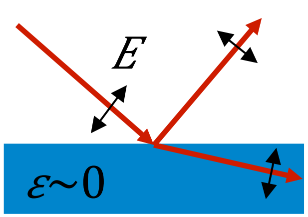
Modeling Approaches

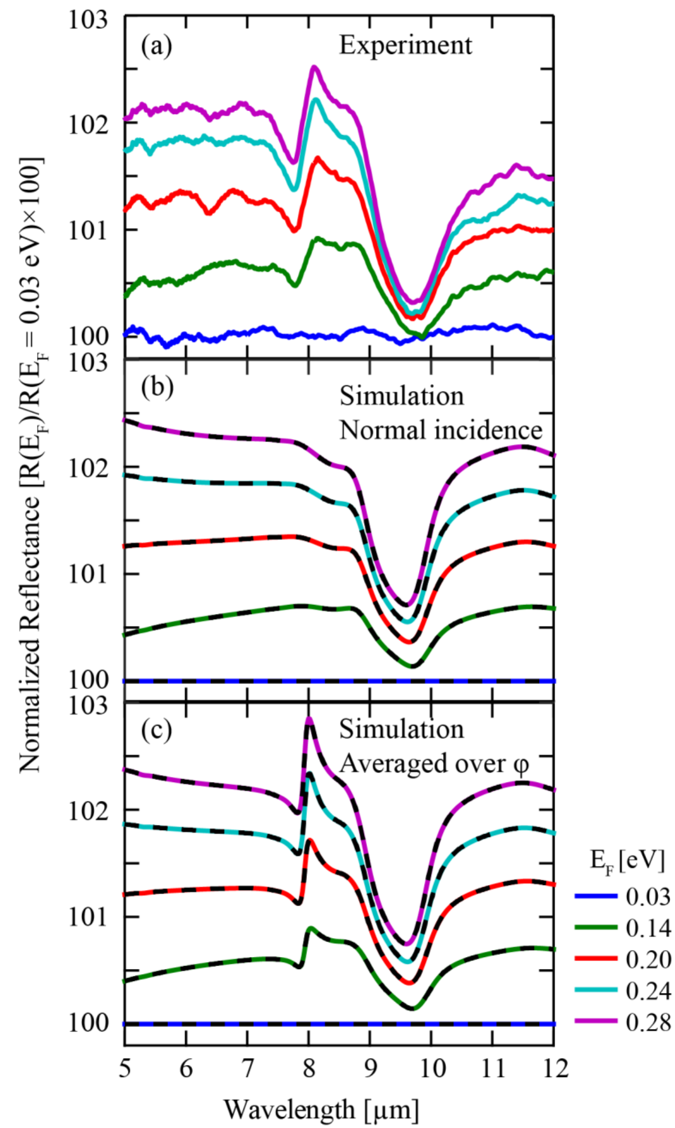
(1) 2D conductivity, $\sigma(\omega)$

(2) Permittivity ε of an effective layer with thickness t_{eff}

$$\varepsilon(\omega) = \iota\sigma(\omega)/(\omega\varepsilon_0 t_{eff})$$

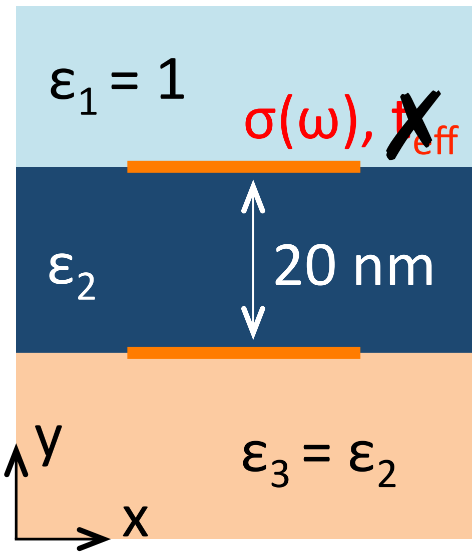
(3) Angular averaging



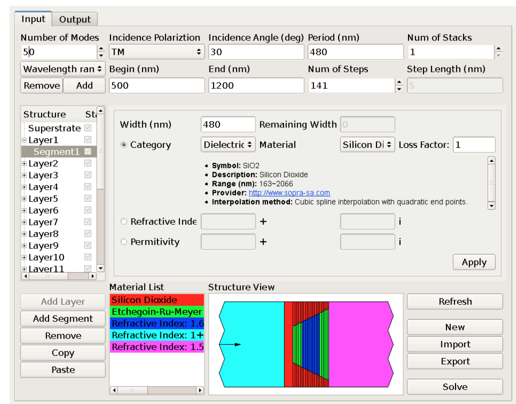


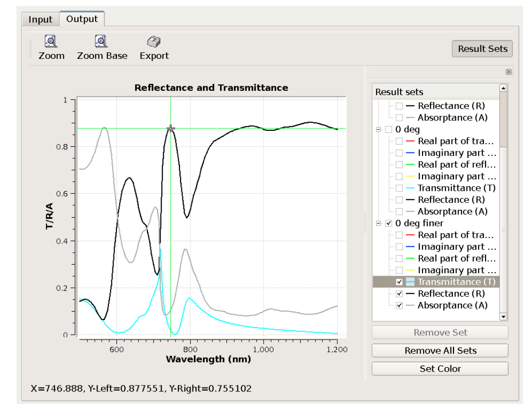
*Ellipsometry data from J. A. Woollam

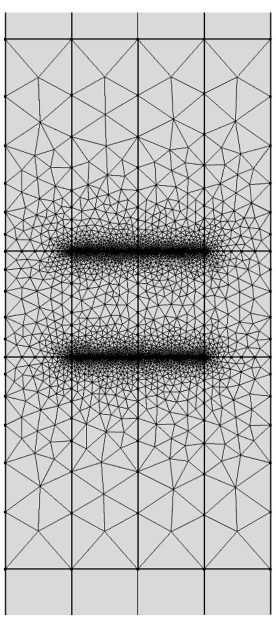
FD Modeling: the case of nanostructured graphene

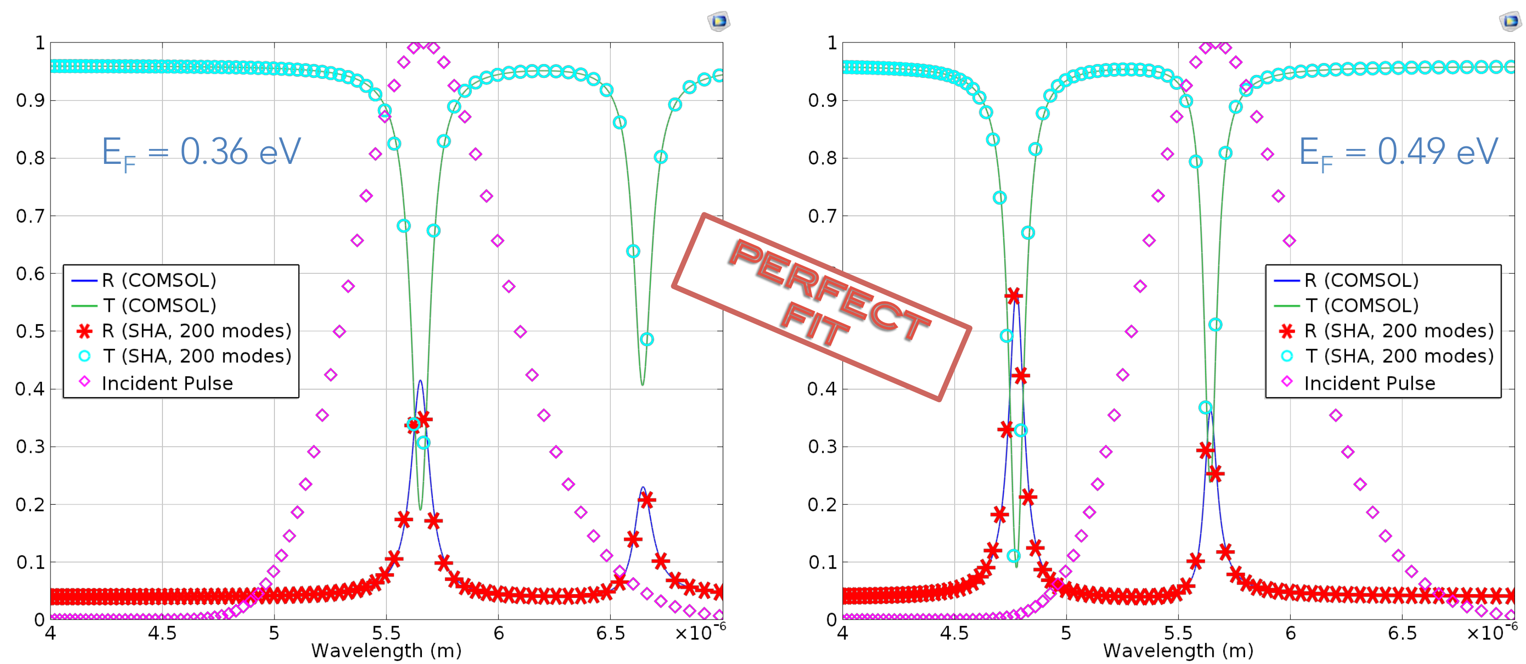


https://nanohub.org/tools/sha2d







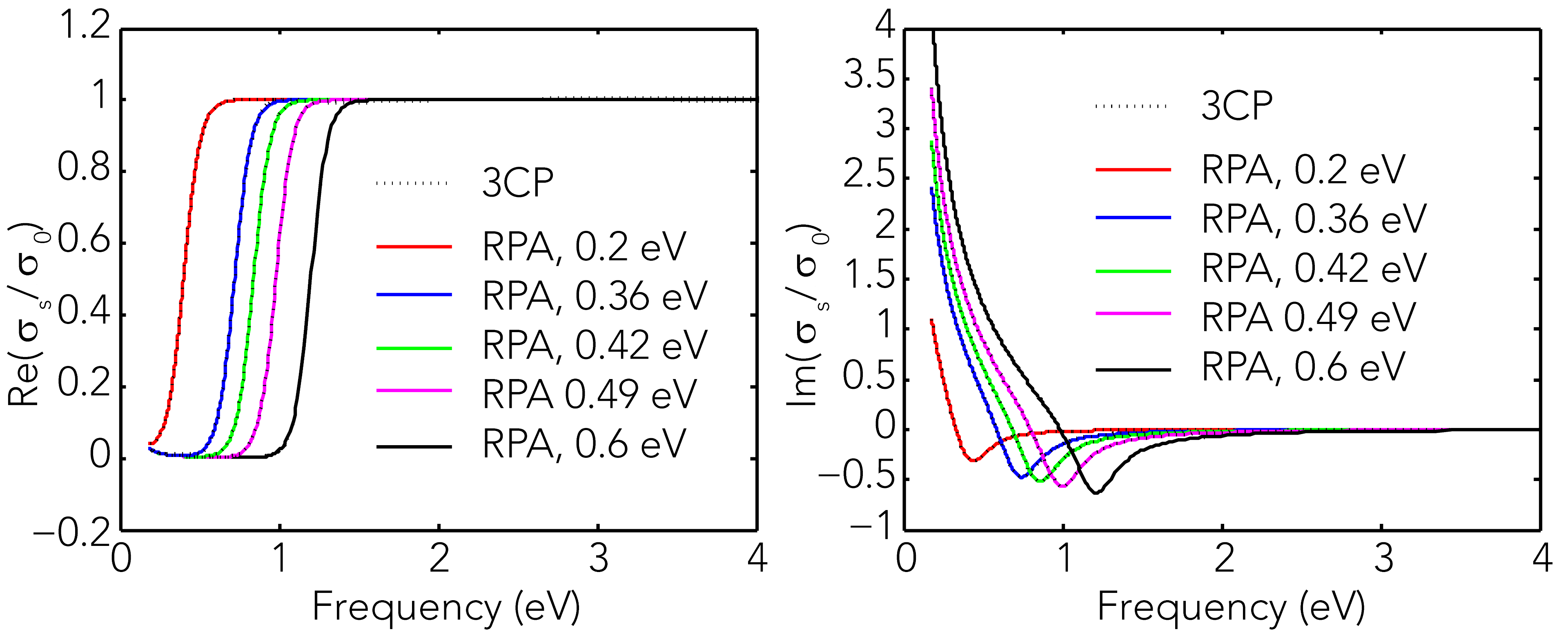


TD Modeling: Optical Dispersion

Padé approximation – summation of three Critical Points Terms

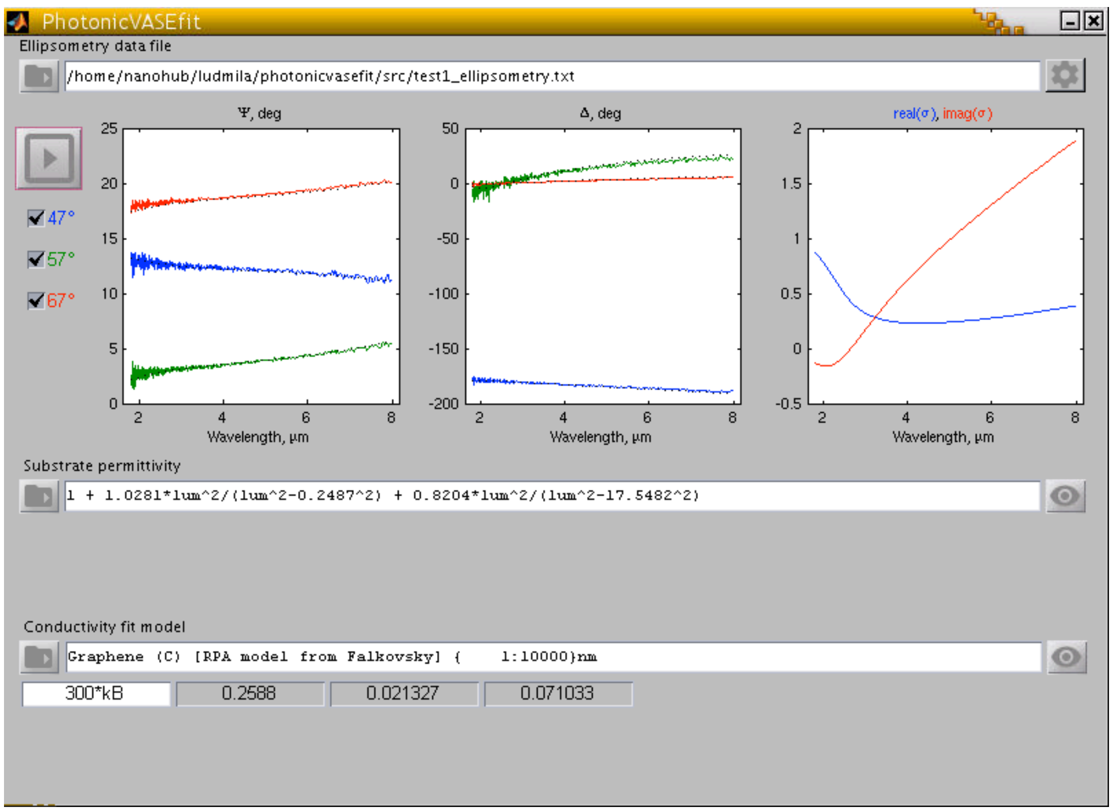
$$\boxed{\sigma_s = \sigma_0\left(1 + \frac{a_{1,0} - \iota\omega a_{1,1}}{b_{1,0} - \iota\omega b_{1,1} - \omega^2} + \frac{a_{2,0} - \iota\omega a_{2,1}}{b_{2,0} - \iota\omega b_{2,1} - \omega^2} + \frac{a_{3,0} - \iota\omega a_{3,1}}{b_{3,0} - \iota\omega b_{3,1} - \omega^2}\right)}$$

$$\boxed{\sigma_0 = \frac{e^2}{4\hbar}}$$



TD Modeling: Optical Dispersion

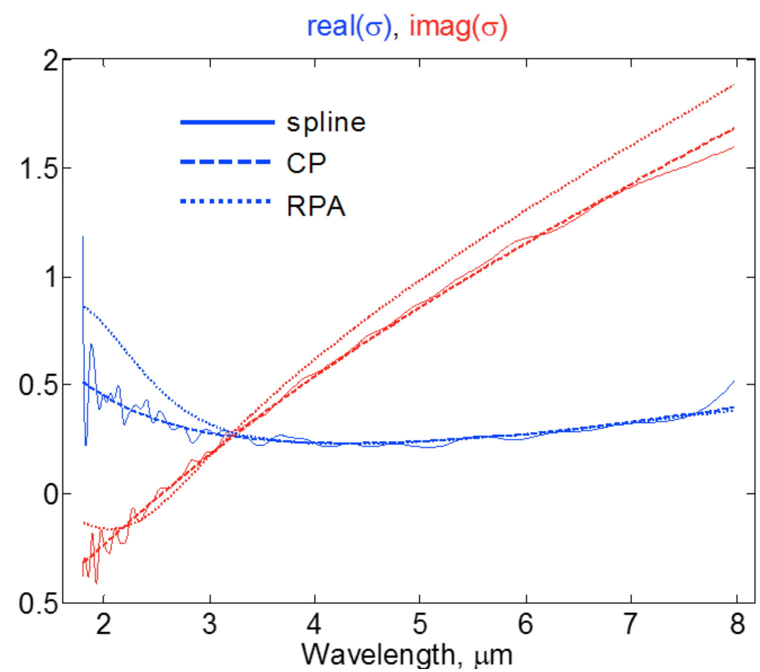
PhotonicVASEfit tool available at
https://nanoHUB.org/tools/photonicVASEfit



Spline – very good fit, slow (too many parameters ~100), does not represent physics, fictitious oscillations

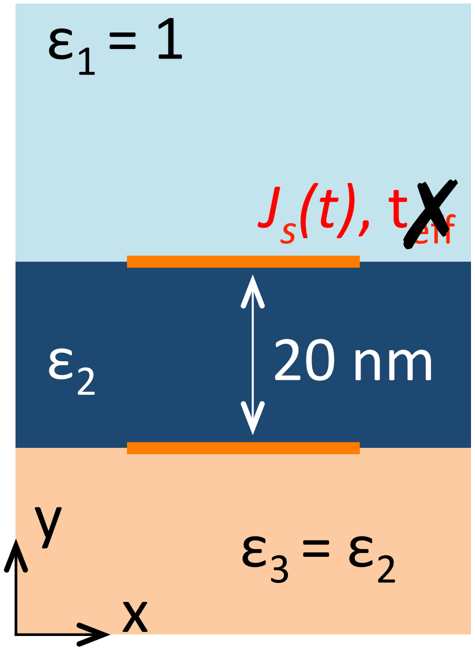
RPA – physical parameters, T, E_F, γ retrieval, slow (iterative integration)

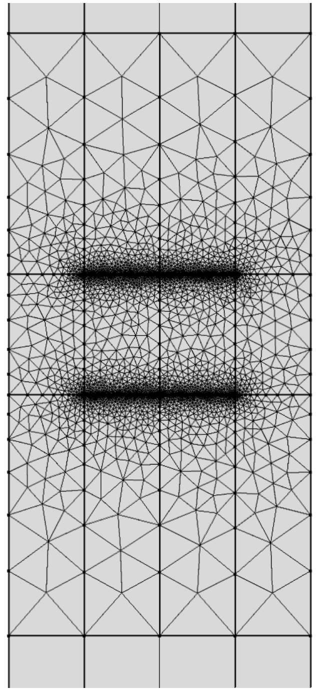
Critical points – good fit, only 4 parameters, causal (TD-friendly), fast



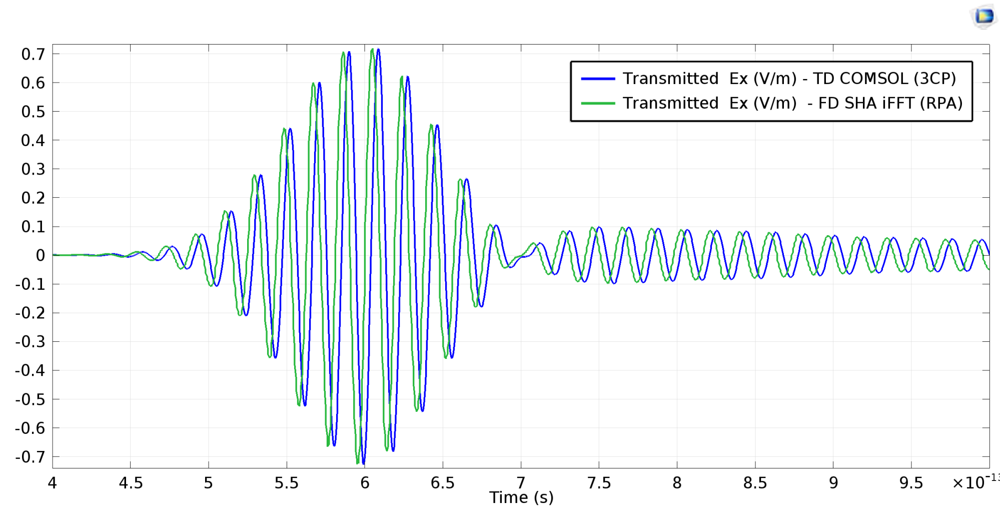
L. Prokopeva; A. V. Kildishev (2015), "PhotonicVASEfit: VASE fitting tool," https://nanohub.org/resources/photonicvasefit. (DOI: 10.4231/D3W08WH6M)

Time-domain SLG Modeling: Multiphysics in Action





Good agreement between the TD (Comsol, 3CP) and FD iFFT (SHA, RPA) models



$$J_s = \sigma_0 E_x + J_1 + J_2 + J_3$$

$$\mathbf{n} \times \left(\mathbf{H}_1 - \mathbf{H}_2 \right) = \hat{\mathbf{e}}_x J_s$$

$$\nabla \times \left(\nabla \times \mathbf{A} \right) + \mu_0 \sigma \frac{\partial}{\partial t} \left(\varepsilon_0 \varepsilon_r \frac{\partial \mathbf{A}}{\partial t} \right) = \mathbf{0}$$

+

$$\begin{cases} \underbrace{\frac{1}{b_{1,0}}}_{e_a} \frac{d^2 J_1}{dt^2} + \underbrace{\frac{b_{1,1}}{b_{1,0}}}_{d_a} \frac{dJ_1}{dt} = \underbrace{\left(\frac{a_{1,0}}{b_{1,0}} E_x + \frac{a_{1,1}}{b_{1,0}} \right) \sigma_0 - J_1}_{f} \\ \frac{1}{b_{2,0}} \frac{d^2 J_2}{dt^2} + \frac{b_{2,1}}{b_{2,0}} \frac{dJ_2}{dt} = \left(\frac{a_{2,0}}{b_{2,0}} E_x + \frac{a_{2,1}}{b_{2,0}} \right) \sigma_0 - J_2 \\ \frac{1}{b_{3,0}} \frac{d^2 J_3}{dt^2} + \frac{b_{3,1}}{b_{3,0}} \frac{dJ_3}{dt} = \left(\frac{a_{3,0}}{b_{3,0}} E_x + \frac{a_{3,1}}{b_{3,0}} \right) \sigma_0 - J_3 \end{cases}$$

SUMMARY

- Frequency Domain Modeling:
  - surface current (J_s) - an efficient method of choice for modeling graphene in COMSOL Multiphysics
  - successfully validated with optical experiments and other numerical methods

- PhotonicVASEfit - a complementary tool for graphene modeling with COMSOL:
  - fitting optical constants of materials to the data from Variable Angle Spectroscopic Ellipsometry (VASE) - is now available at https://nanoHUB.org/tools/photonicVASEfit
  - supports RPA, Splines, Critical Points models and most general user-defined functions

- Time Domain Multiphysics Modeling:
  - modeling of the broad-band dispersion of graphene in TD using COMSOL is shown
  - The method is based on causal Padé approximants (Critical Points)
  - Future Plans: Extend to temperature control, quantum emitters, etc

- Other things to do – future plans:
  - coupling with polar substrates, quantum emitters, non-linear graphene plasmonics;
  - quantum effects in nano-structured graphene;
  - etc…

Live Demo

1. Comparison between COMSOL and theory treating graphene as a thin, bulk material
2. Comparison between COMSOL and theory treating graphene as a 2D surface current
3. Nanostructured graphene - frequency domain
4. Nanostructured graphene - time domain

Files can be downloaded from COMSOL's Model Exchange at http://www.comsol.com/community/exchange/361/

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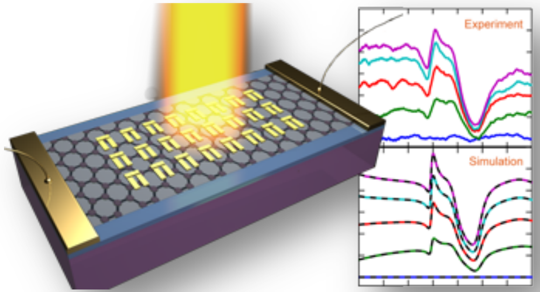

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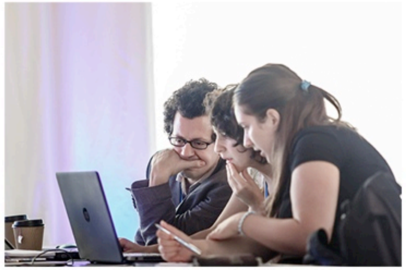

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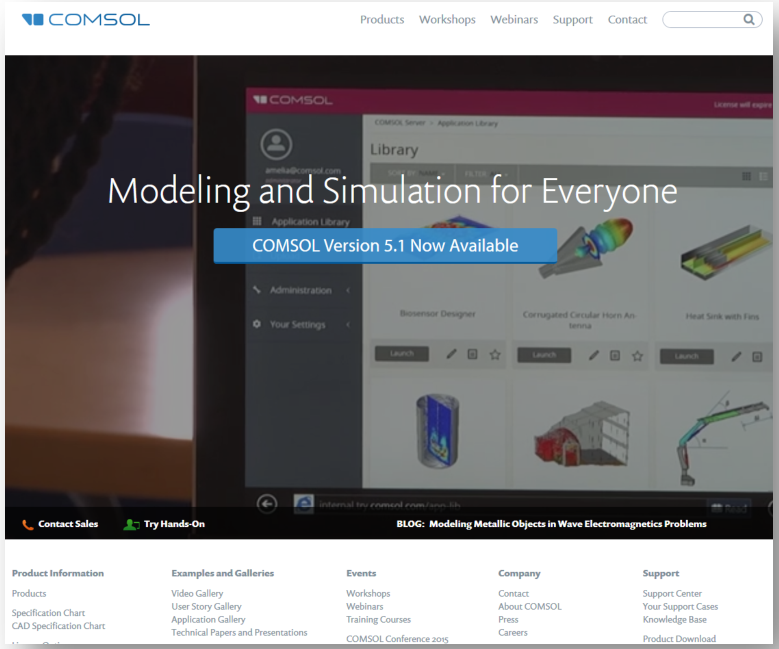

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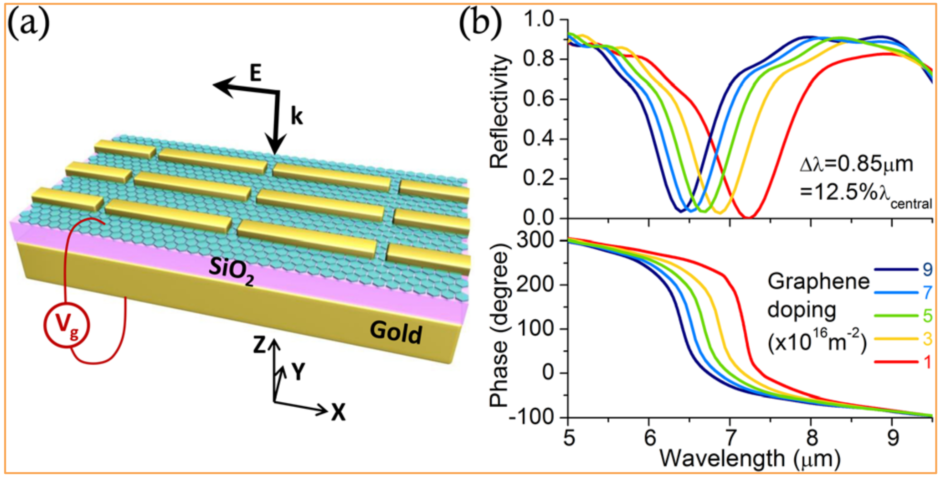
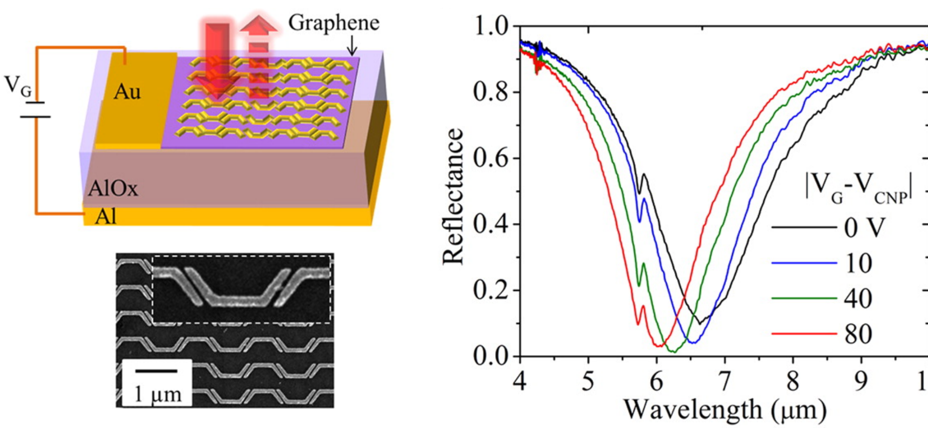
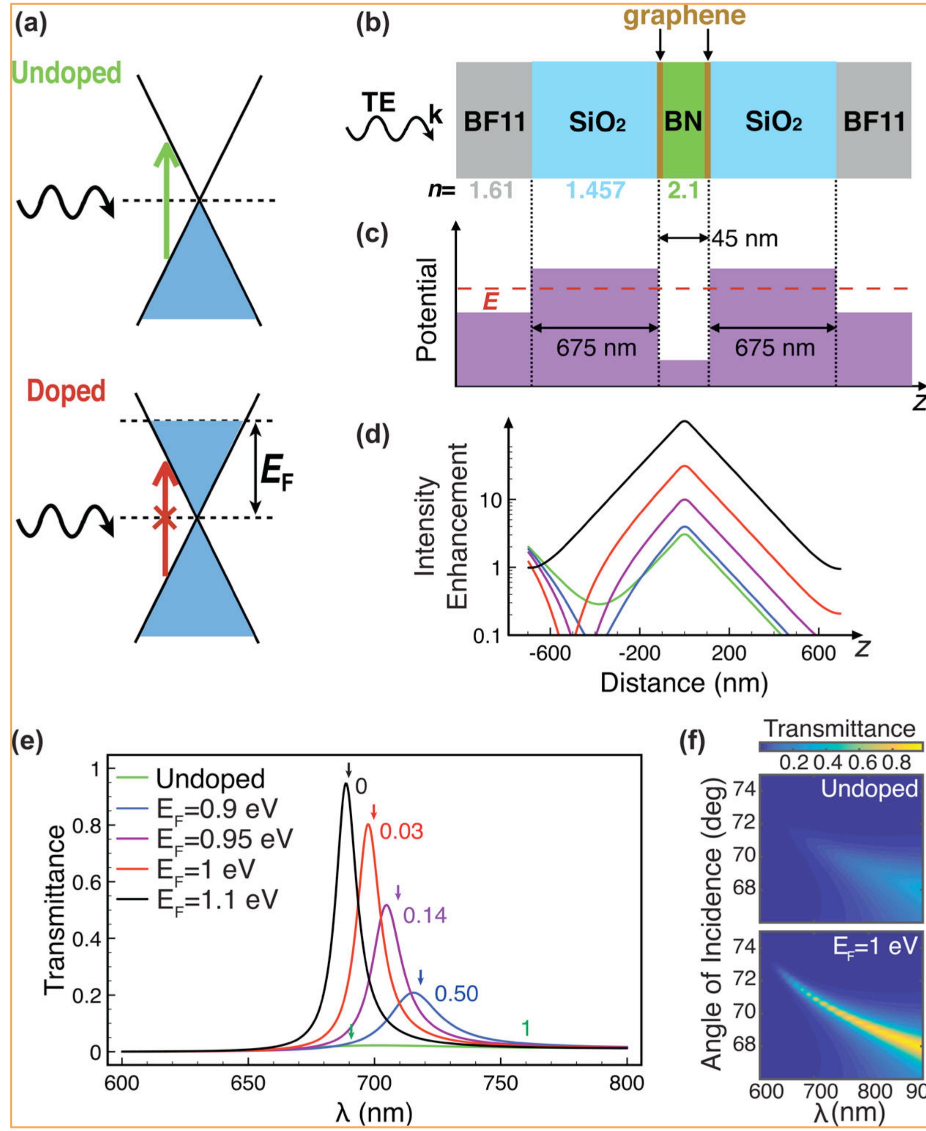
Graphene Plasmonics: Applications



Zhaoyi Li et al., Appl. Phys. Lett. **102** , 131108 (2013)
(Nanfang Yu Group, Columbia)

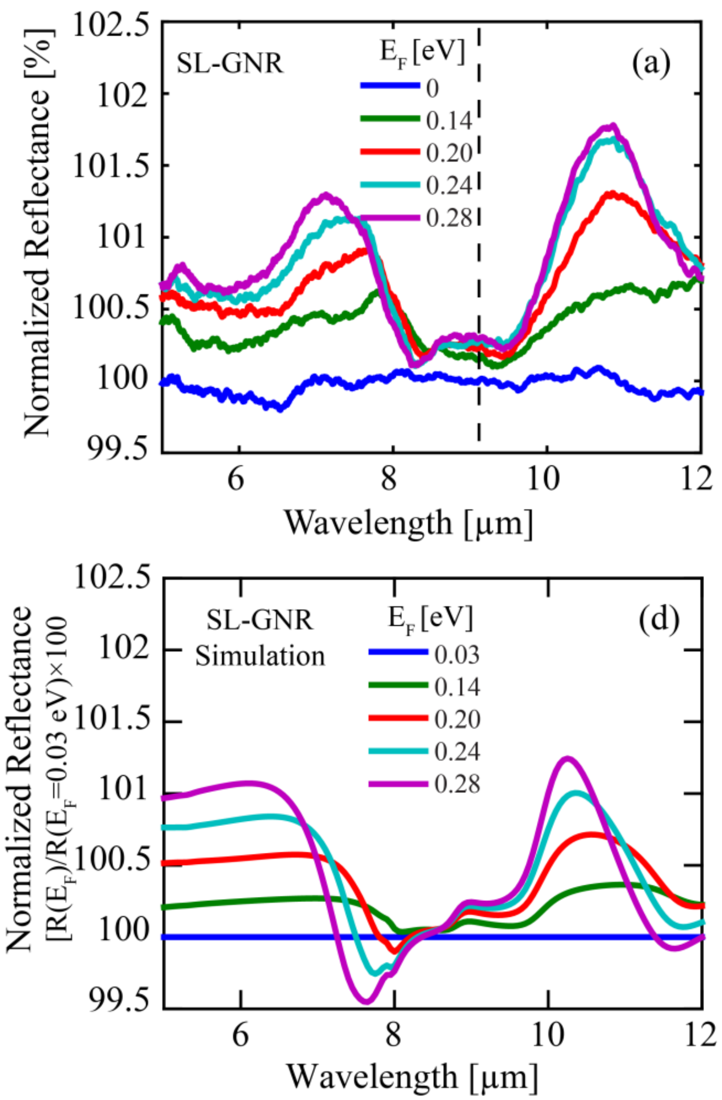


Y. Yao, et al., Nano Letters 14, 6526, (2014)
(Loncar and Capasso Groups, Harvard)



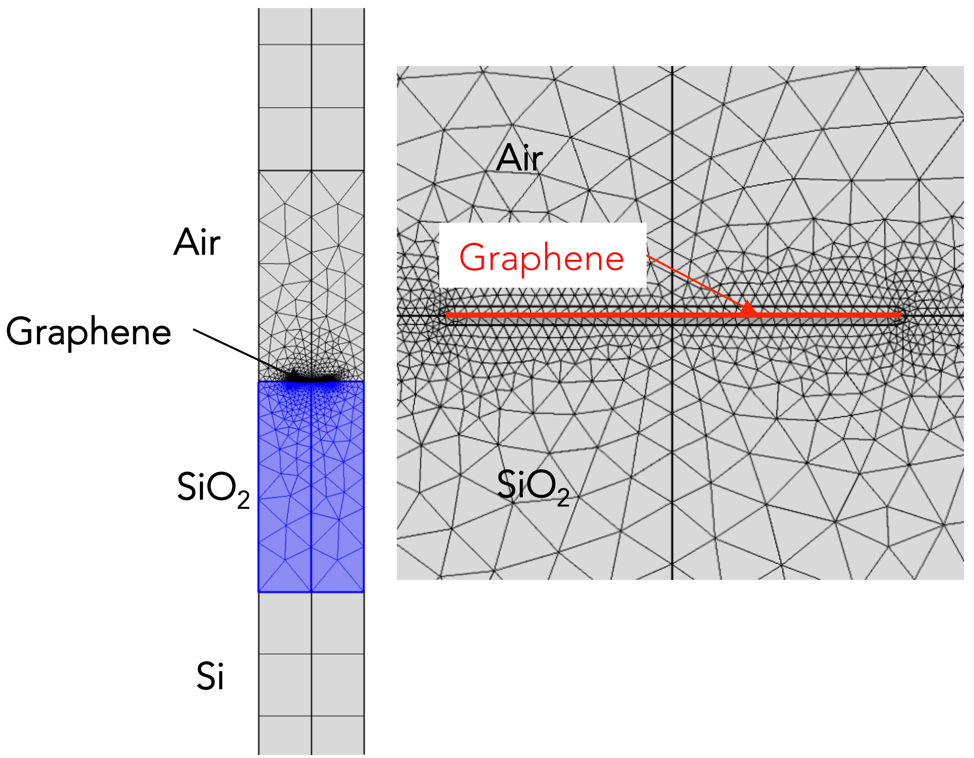
Renwen Yu et al., ACS Photonics **2**, 550–558 (2015)
(de Abajo Group, Institut de Ciencies Fotoniques)

FD Modeling: SLG nanoribbons



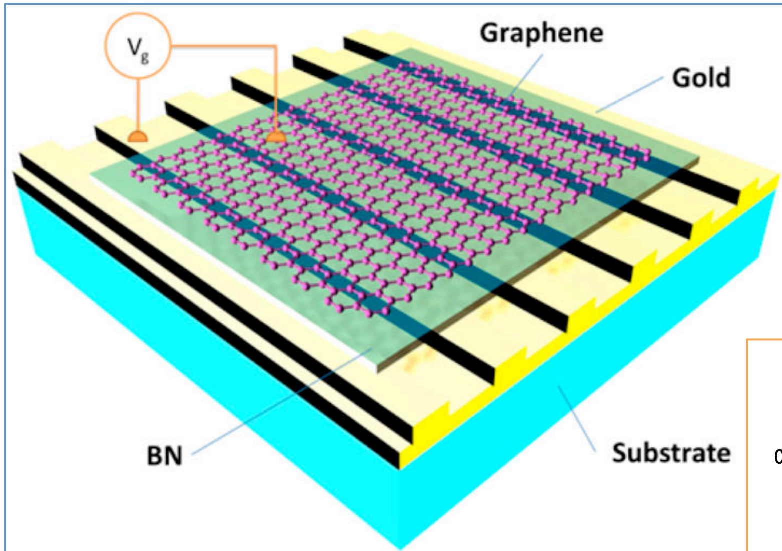
Numerical simulation with COMSOL:

- Graphene modeled as surface current
- Qualitative agreement with experiment
- Quantitative agreement for bare graphene
- Less expensive computationally
- Better convergence and stability

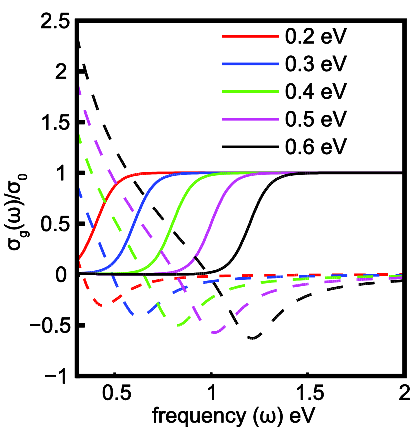


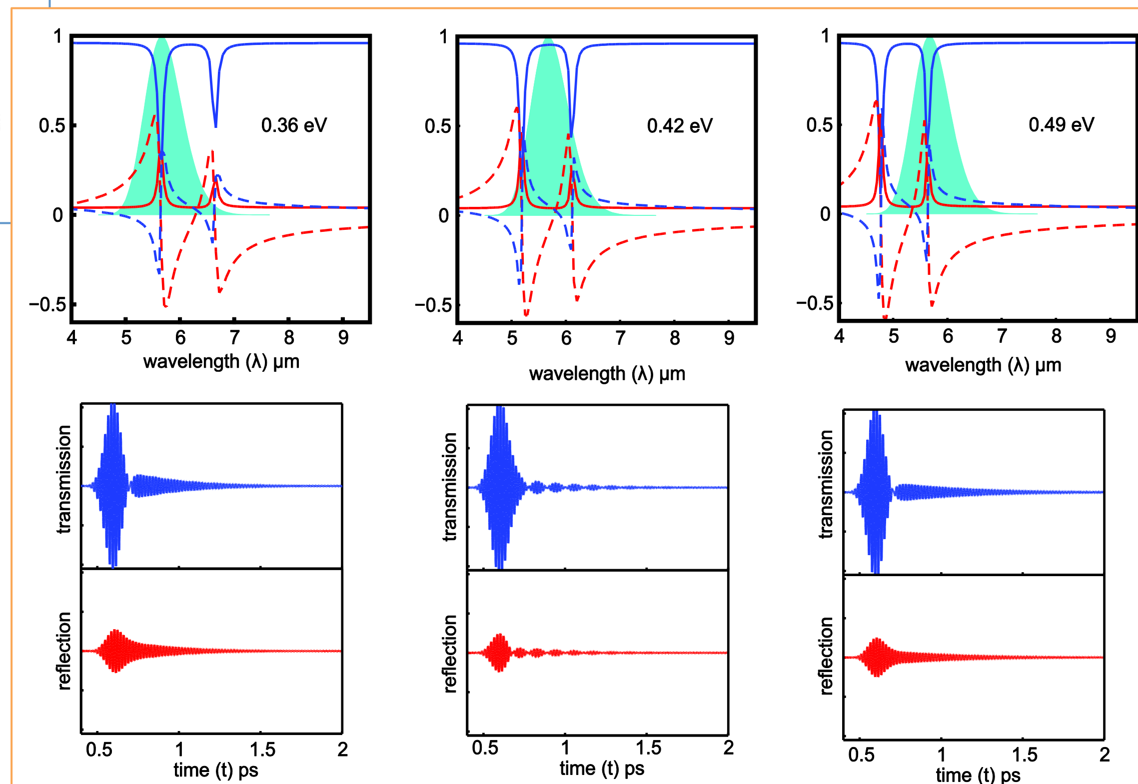
Wang, et al., in CLEO: 2015, OSA Technical Digest, paper FTu1E.3.
Emani et al., Plasmon Resonance in Multilayer Graphene Nanoribbons (submitted)

TD Multiphysics SLG Modeling: Applications



Thackray, et al., Nano Lett. 15, 3519-3523 (2015)





L. J. Prokopeva, and A. V. Kildishev "Time Domain Modeling of Tunable Graphene-Based Pulse-Shaping Device (invited)," in Computational Methods in Nanoelectromagnetics, Applied Computational Electromagnetics 2014, March 23 - 27, 2014 Jacksonville, Florida (online publication).

Graphene Plasmonics: Tunability

NANO LETTERS
Letter
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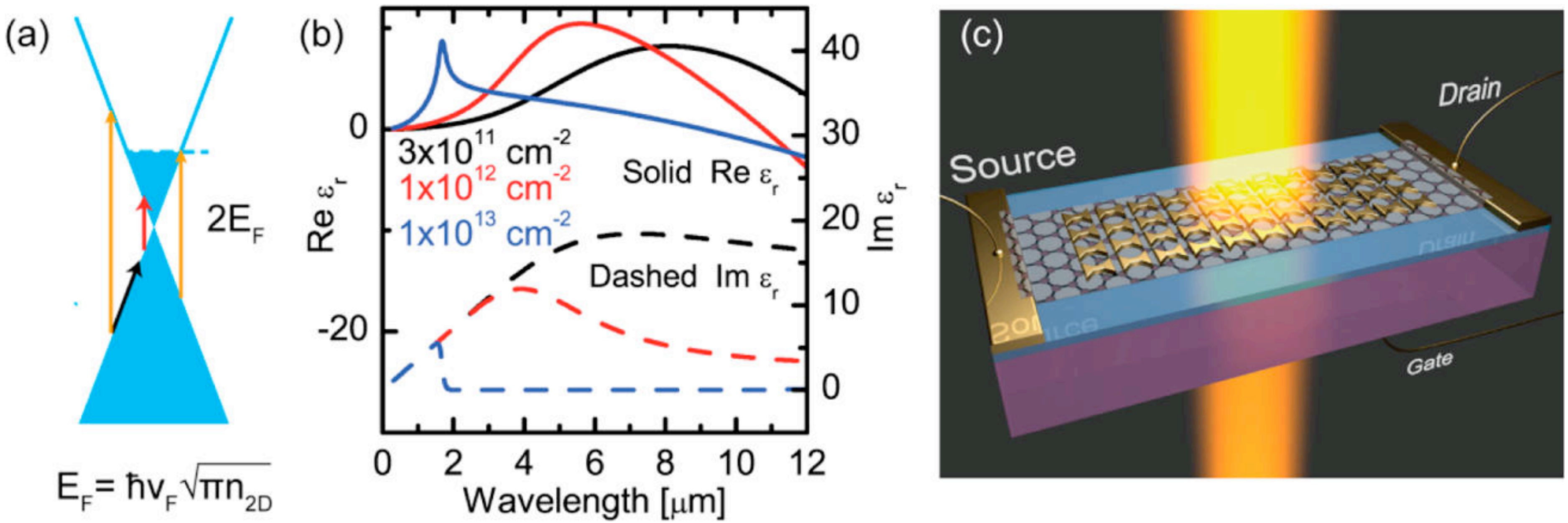
Electrically Tunable Damping of Plasmonic Resonances with Graphene

Naresh K. Emani, Ting-Fung Chung, Xingjie Ni, Alexander V. Kildishev,
Yong P. Chen, and Alexandra Boltasseva



(a) The optical response of graphene is controlled by e-h pair excitations. Photons with energies above $2E_F$ are absorbed due to transitions into the unoccupied states above the Fermi level;

(b) Calculated dielectric functions for carrier densities of 3×10^{11}, 1×10^{12}, 1×10^{13} cm^{-2} show a tunable interband threshold. Changes in the imaginary part (dashed lines) of permittivity are accompanied by corresponding changes in the real part (solid lines). The calculations were performed with $\tau = 1\times10^{-13}$ s, T = 300 K and t_g = 1 nm;

(c) schematic illustration of the experimental structure for voltage-controlled optical transmission measurements.