Please find the Video Tutorial at
https://nanohub.org/resources/22447

# PhotonicVASEfit
# extracting optical constants of new materials by ellipsometry

- FAQ
- INTRO
- TUTORIAL
- DEMO
- USING RESULTS

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Materials Research Science and Engineering Center

# nanoHUB FAQ
# How do I … ?

# FAQ: How do I … ?

## How do I launch simulation tools?

**All you need is to open an account - it's free!**

**Go to tool page and press 'Launch Tool' button**

https://nanohub.org/tools/photonicvasefit

**PhotonicVASEfit: VASE fitting tool**

By Ludmila Prokopeva[1], You-Chia Chang[2], Alexander V. Kildishev (editor)[3]

*1. Novosibirsk State University 2. University of Michigan 3. Purdue University*

Retrieves optical constants of a material by fitting it to VASE (Variable Angle Spectroscopic Ellipsometry) data

Launch Tool

Version 1.3.1 - published on 11 Jun 2015

doi:10.4231/D39Z90C98 cite this

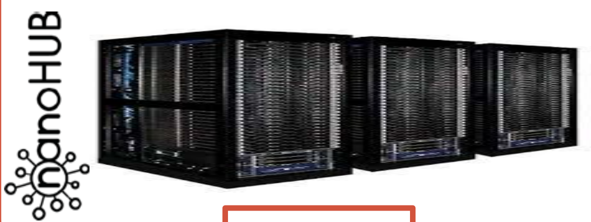
This tool is closed source.

View All Supporting Documents

## How do I upload (ellipsometry data) file to use it with the tool?

**Understand file systems locations and directories**

Physical machines (running virtual machines)




**local files**

internet

You


**remote files**

+ ☐ remote files

+ ☑ remote files

```
% simulation tool directory, auto cleaned
/home/nanohub/userName/data/sessions/852606
```

(examples)

tool running

nanoHUB.org ONLINE SIMULATION AND MORE FOR NANOTECHNOLOGY

an NCN project

**Upload**

Use this form to upload data. If you don't specify a file for a particular input, that input won't be modified by the *Upload* operation.

```
% your home directory ("Storage"), fixed
/home/nanohub/userName
```

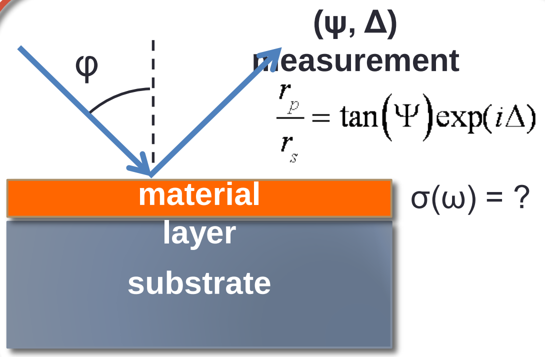
webdav ssh, scp

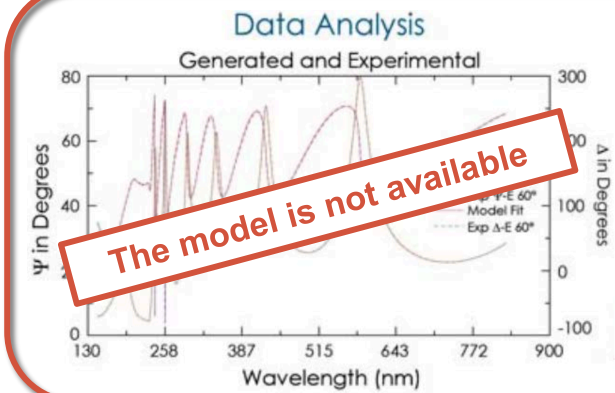
```
% webdav (native support for most OS)
https://webdav.nanohub.org/webdav

% ssh, scp (natively or client, e.g. WinSCP)
nanohub.org (nanoHUB username & password)
```

# INTRODUCTION

# INTRO: WHY ANOTHER TOOL?




- 2D (graphene)
- custom physical models (RPA for graphene)
- custom mathematical models (splines, Padé approximation)

Variable Angle Spectroscopic Ellipsometer

Sounds familiar?

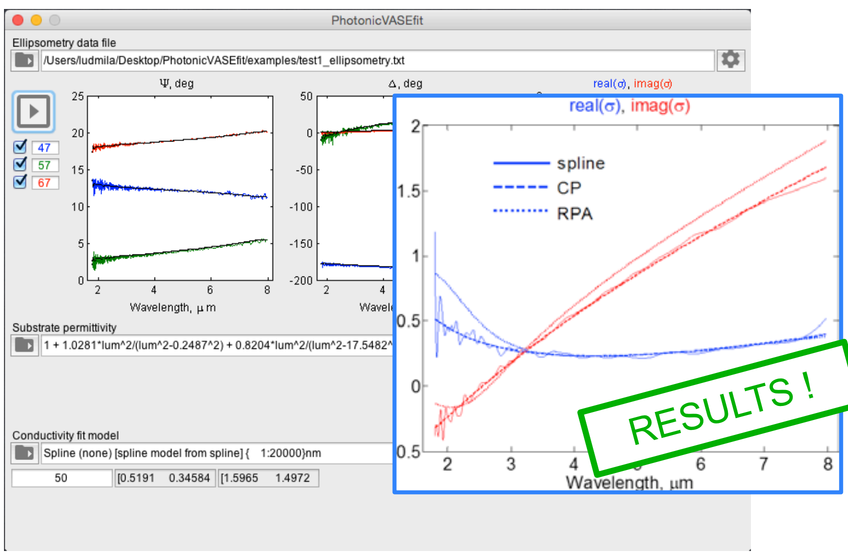
**Try PhotonicVASEfit**

A light fitting companion for ellipsometry measurements

- 2D
- custom physical models
- custom mathematical models

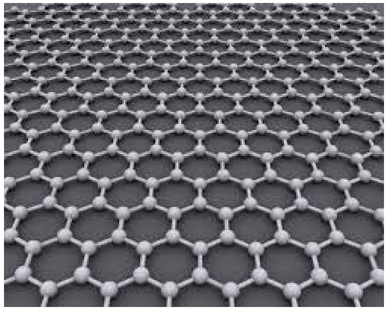
new materials

Powered by




- Current functionality is limited to a 2D-layer on a substrate. More is under development: we've just started!

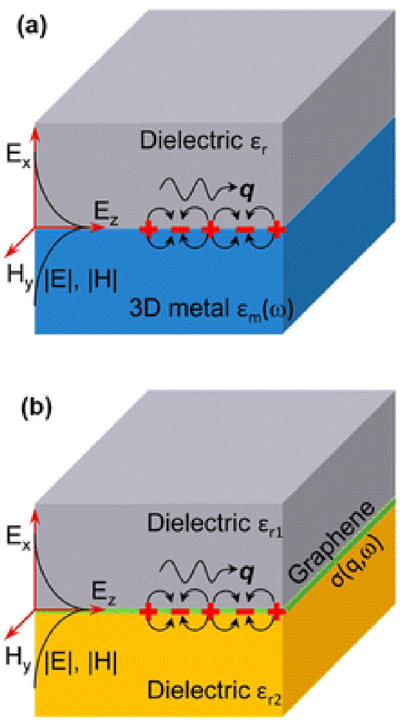
# INTRO: GRAPHENE MODELS



Graphene, a new optical material

- 2D material (atomic thickness)
- plasmonics
- tunable optical response, controlled by applied bias voltage

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




Fundamental model for relative surface conductivity ($\sigma_r = \sigma/\sigma_0$) of graphene

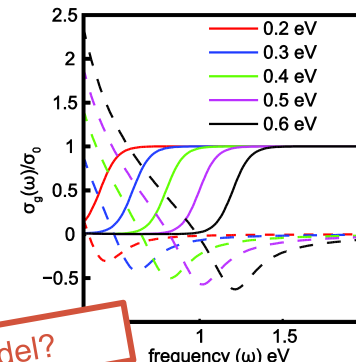
$$\sigma_{\mathrm{RPA}}(\omega) = \frac{8\iota}{\pi}\frac{\omega_T}{\omega + \iota\Gamma}\log\left[2\cosh\left(\frac{\omega_F}{2\omega_T}\right)\right]$$

Intraband term (Drude model)

$$+\frac{4}{\iota\pi}(\omega + \iota\gamma)\int_0^{\infty}\frac{f(\omega')}{4\omega'^2 - (\omega + \iota\gamma)^2}d\omega'$$

Interband term (not TD-friendly)

Random Phase Approximation (RPA)




Ellipsometric characterization? 2D? RPA model?

$$f(\omega) = \sinh(\omega/\omega_T)/[\cosh(\omega_F/\omega_T) + \cosh(\omega/\omega_T)]$$ from Fermi-Dirac distribution

| | | | |
|---|---|---|---|
| $\omega$ | frequency of incident light, [eV] | $\hbar$ | the reduced Planck constant, [eV·s] |
| $\omega_T = k_B T$ | temperature, converted to [eV] | $k_B$ | the Boltzmann constant, [eV/K] |
| $\omega_F$ | chemical potential, [eV] | $\sigma_0 = \dfrac{e^2}{4\hbar}$ | universal conductivity, [S] |
| $\Gamma, \gamma$ | scattering rates, [eV] | $e$ | electron charge |

# INTRO: GRAPHENE MODELS

PhotonicVASEfit started as a Matlab script for ellipsometric characterization of graphene

- Modified Fresnel's formulas for arbitrary stacks with any number of 2D layers
- Levenberg-Marquardt algorithm, GUI in Matlab
- Models: RPA, Spline, Critical points (Padé approximation)

**RPA**

$$\sigma_{\mathrm{RPA}}(\omega) = \frac{8\iota}{\pi}\frac{\omega_T}{\omega+\iota\Gamma}\log\left[2\cosh\left(\frac{\omega_F}{2\omega_T}\right)\right] + \frac{4}{\iota\pi}(\omega+\iota\gamma)\int_0^\infty \frac{f(\omega')}{4\omega'^2-(\omega+\iota\gamma)^2}d\omega'$$

Not TD friendly

**Spline**

```
% w - frequency range from ellipsometry
% w0 - spline points, fixed parameter
Sigma_spline = spline(w0, sigma_re_fit + sigma_im_fit, w)
```

Not TD friendly

**Critical points model**

$$\sigma(\omega) = \sigma_1 + \sum_{i\in I_1}\frac{a_{0,i}}{b_{0,i}-\iota\omega} + \sum_{i\in I_2}\frac{a_{0,i}-\iota\omega a_{1,i}}{b_{0,i}-\iota\omega b_{1,i}-\omega^2}$$

(Drude term) — critical points term

FT

$$\sigma(t) = \sigma_1\delta(t) + \sum_{i\in I_1}A_i e^{-\gamma_i t}U(t) + \sum_{i\in I_2}A_i e^{-\gamma_i t}\sin(\omega_i t-\varphi_i)U(t)$$

single pole — damped oscillator, phase-relaxed

$$\mathbf{J}_i' + b_{0,i}\mathbf{J}_i = a_{0,i}\mathbf{E}$$

$$\mathbf{J}_i'' + b_{1,i}\mathbf{J}_i' + b_{0,i}\mathbf{J}_i = \sigma_0\left(a_{0,i}\mathbf{E} + a_{1,i}\mathbf{E}'\right)$$

$$\sigma(\omega) \approx \frac{a_0-\iota\omega a_1+\ldots+(-\iota\omega)^m a_m}{b_0-\iota\omega b_1+\ldots+(-\iota\omega)^n}$$

[m/n] Padé approximant, **m≤n**

SBC

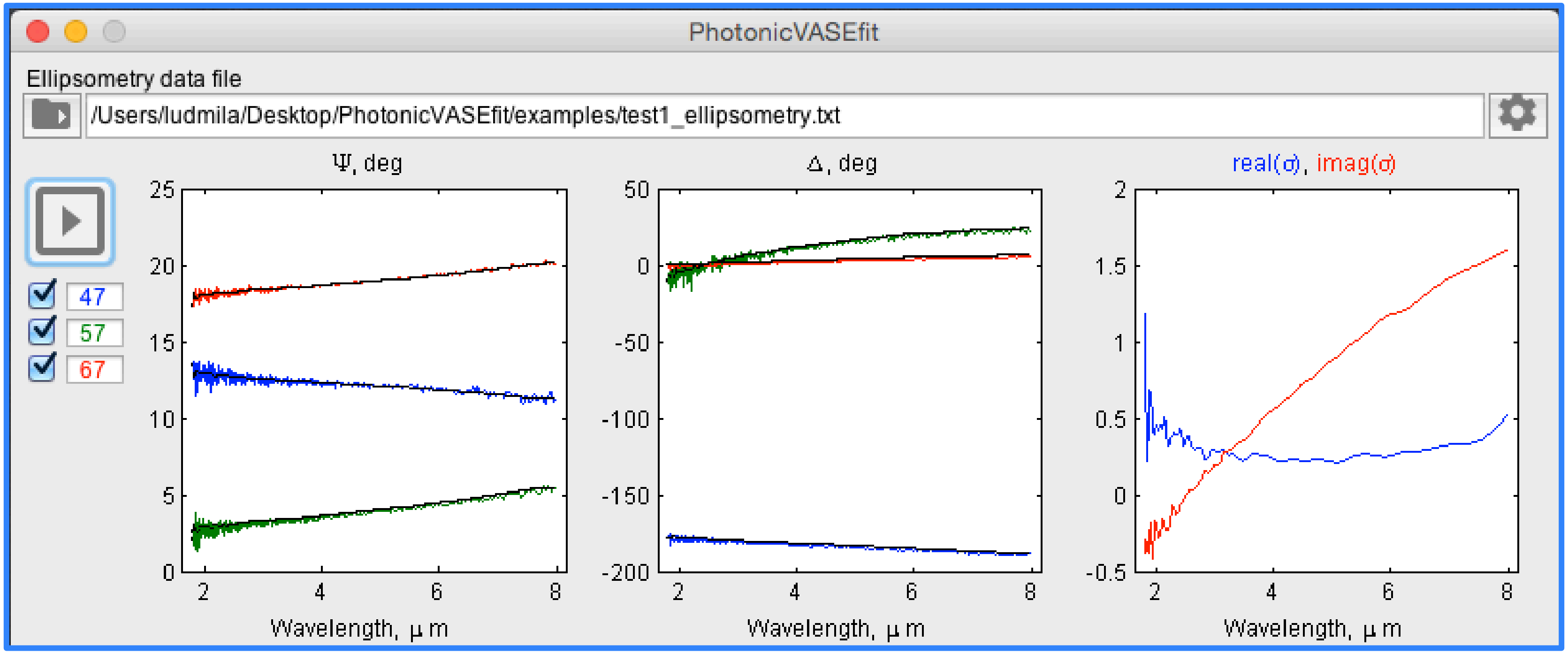
$$\begin{cases}\mathbf{J}_s = \sigma_0\sigma_1\mathbf{E}_\mathbf{x} + \sum_i \mathbf{J}_i \\ \mathbf{n}\times(\mathbf{H}_1-\mathbf{H}_2) = \mathbf{J}_s\end{cases}$$

TD friendly !

| | |
|---|---|
| $A_i$ | amplitude |
| $\omega_i$ | oscillation frequency |
| $\gamma_i$ | damping |
| $\varphi_i$ | phase |
| $\delta(t)$ | Dirac delta function |
| $U(t)$ | Heaviside step function |

# TUTORIAL

# 1. Data Selection  (TUTORIAL)



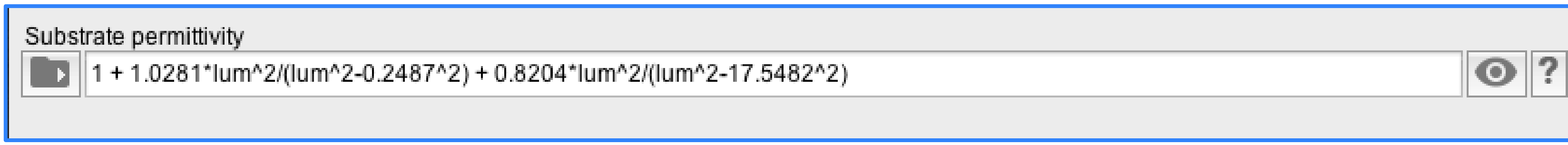

- Accepted data file formats

| Wavelength<br><br>duplicates are auto removed | 2*k columns<br>k≥0 | $\Psi_1$ | $\Delta_1$ | 2*m columns<br>m≥0 |
|---|---|---|---|---|

**...** (Zero columns are auto removed)

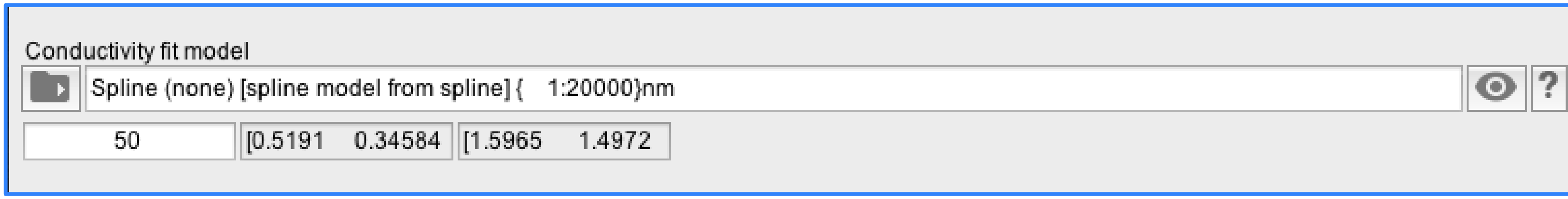
- Select ellipsometry data file
    - local files
    - remote files
- Auto scan (adjust if needed
- Fit angles selectively (checkboxes)
- Filter Data
    - visual filter (brushing tool)
    - itemized filter

# 2. Substrate (TUTORIAL)




- Interactive multi-functional “Omnibox”:
  - “as-you-type” database search
  - formula input (from file or manual)
  - file import
- Table data AND models
- Quick look AND quick compare AND quick close
- Question mark

# 3. Conductivity Fitting Model (TUTORIAL)



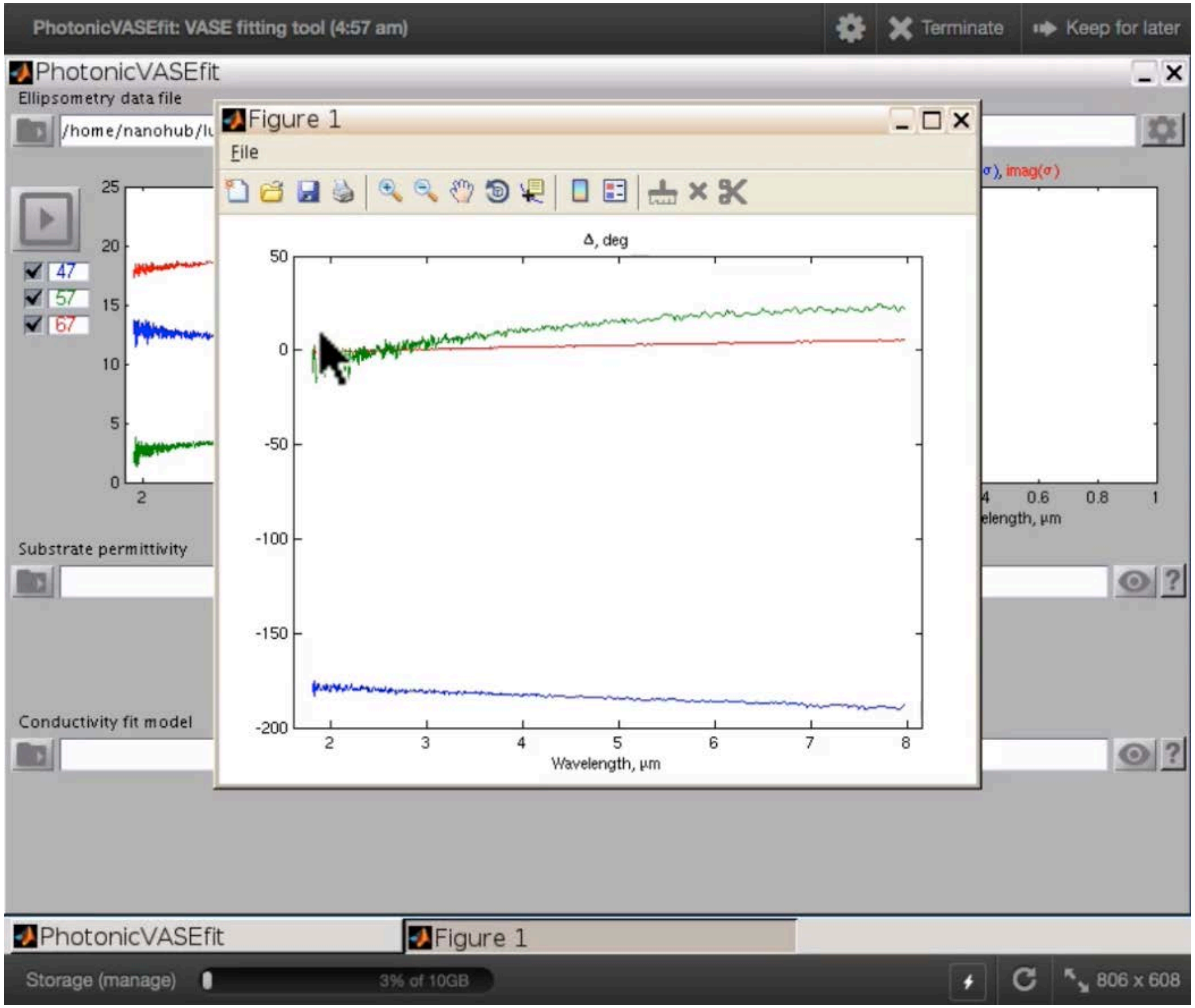

- Any model from database OR custom model
- Parameters are dynamically displayed
- Right click to include/exclude a parameter to fitting
  - white – fixed to current value
  - grayed – to be fitted using current value as initial value

- Results are not guaranteed
  - accurate substrate characterization
  - initial values
  - iteration limit

**DEMO**

**https://nanohub.org/resources/photonicvasefit**

# DEMO

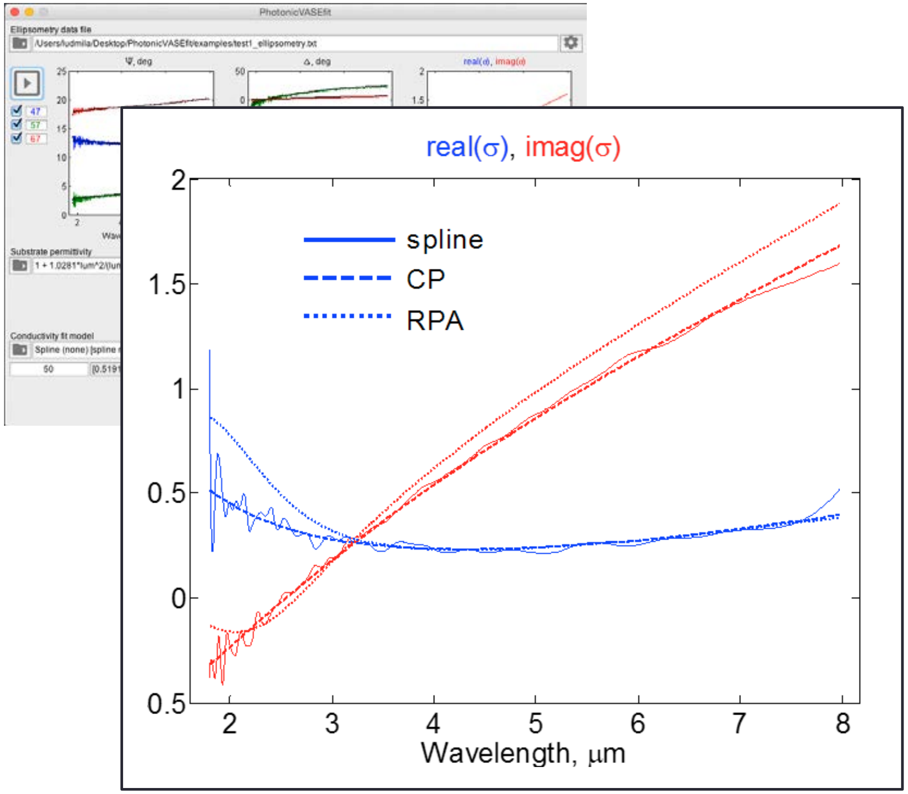


PhotonicVASEfit: VASE fitting tool (4:57 am)
Terminate
Keep for later
PhotonicVASEfit
Ellipsometry data file
/home/nanohub/l
Figure 1
File
Δ, deg
Wavelength, μm
Substrate permittivity
Conductivity fit model
Storage (manage)
3% of 10GB
806 x 608

# USING RESULTS

# RESULTS: Graphene

## PhotonicVASEfit RESULTS for graphene

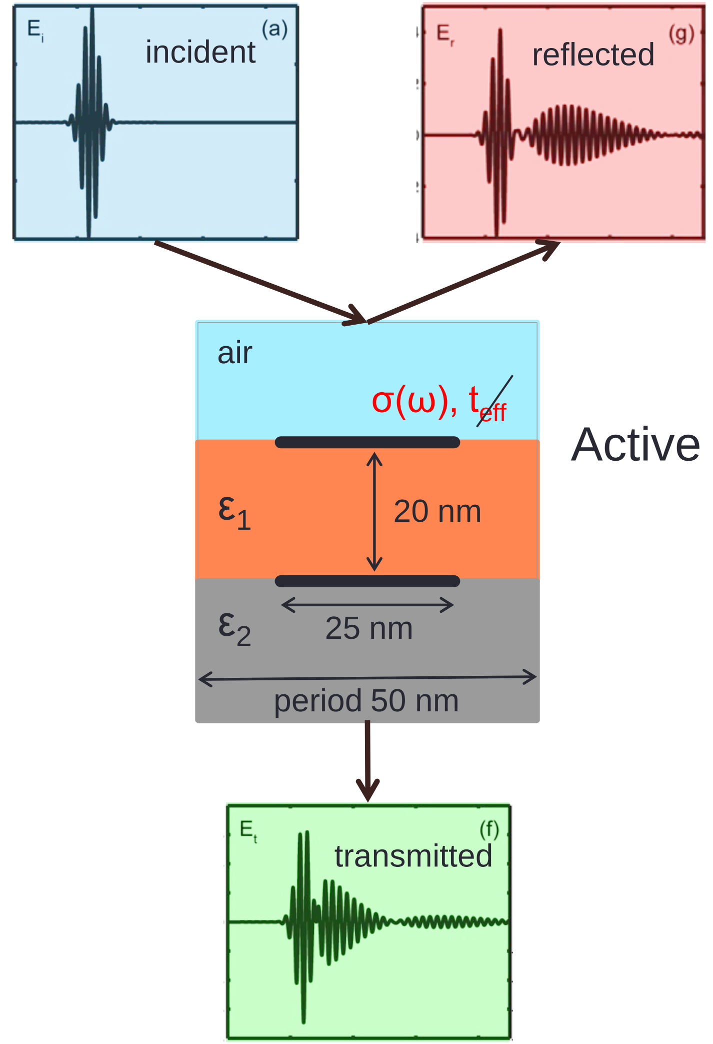



**Spline** – very good fit, slow (too many parameters ~100),
does not represent physics, fictitious oscillations

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

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

## TD: Active Pulse Shaping with graphene nanoribbons



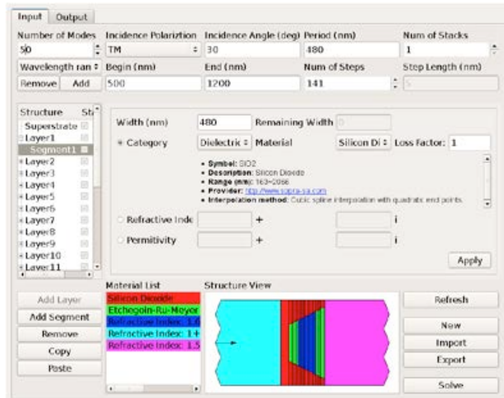

L. Prokopeva and A. Kildishev "Time Domain Modeling of Tunable Graphene-Based Pulse-Shaping Device", ACES 2014

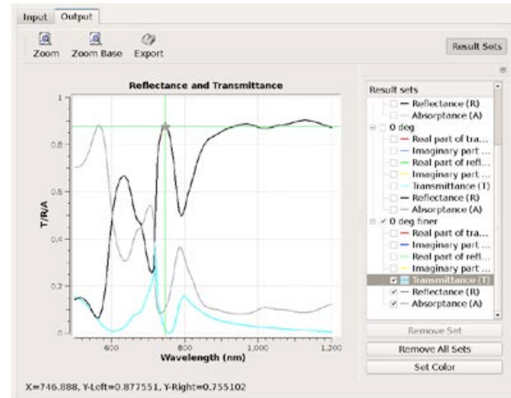
# RESULTS: FD SIMULATIONS

EXPERIMENTALLY FITTED!

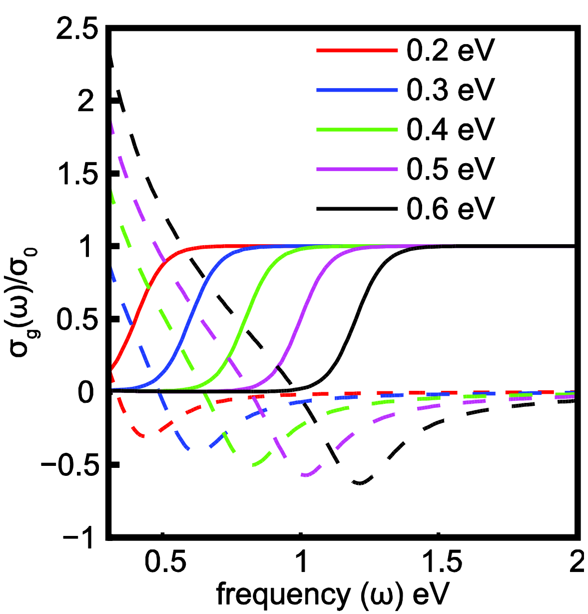
nanoHUB

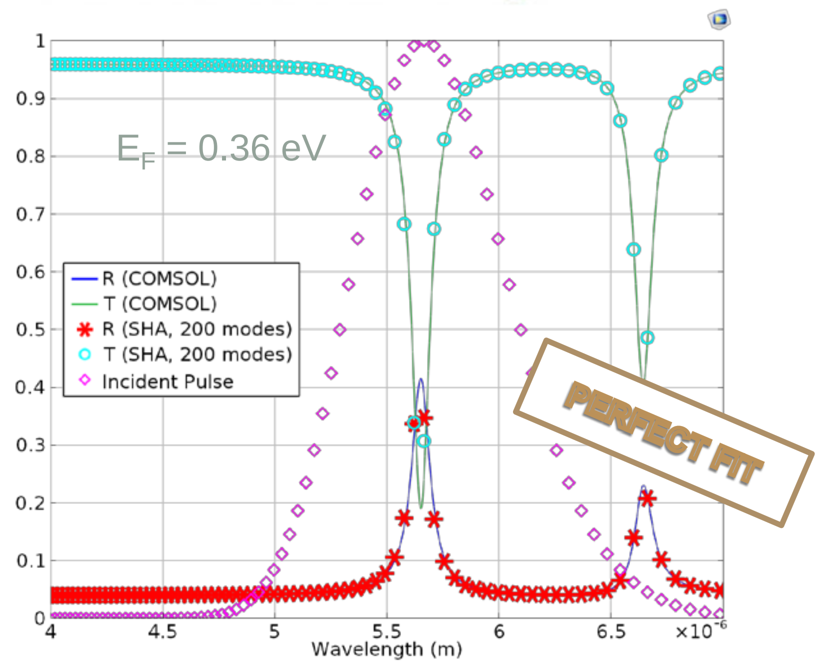
https://nanohub.org/tools/sha2d

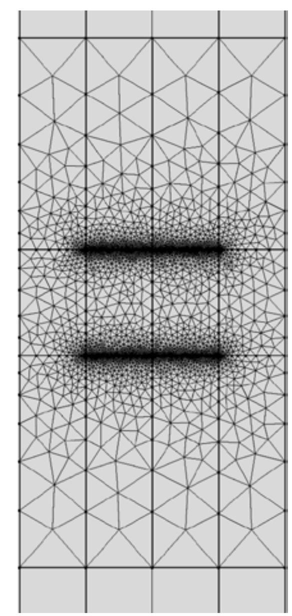



COMSOL MULTIPHYSICS



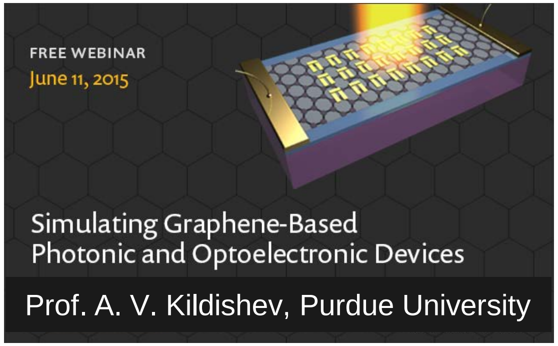



# RESULTS: TD SIMULATIONS

EXPERIMENTALLY FITTED!

Tech Insiders WEBINAR SERIES

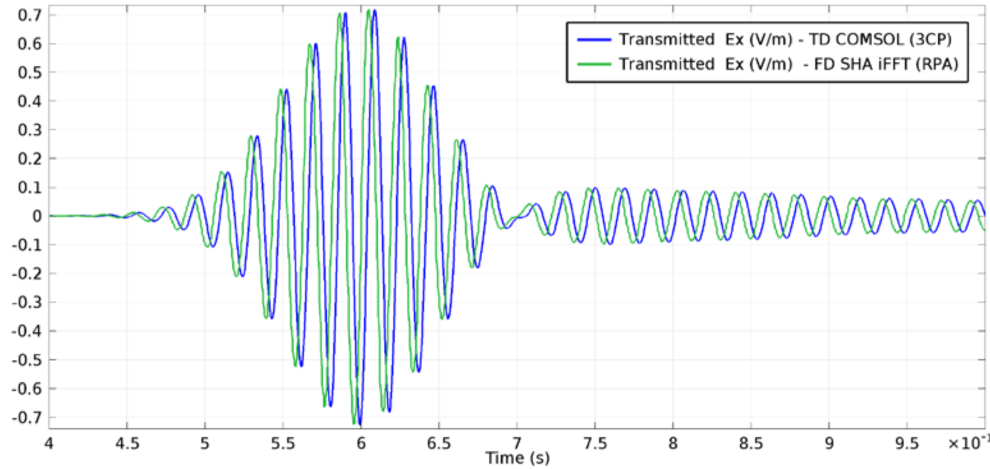
SPONSORED BY: COMSOL

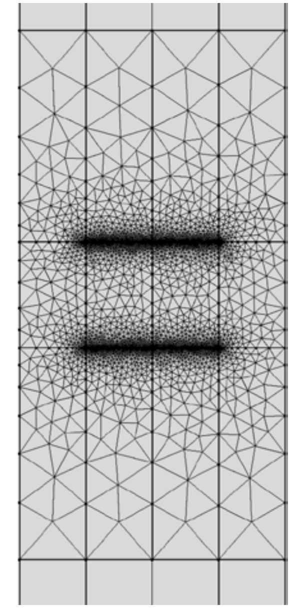



Register at:
http://www.comsol.com/events/webinars

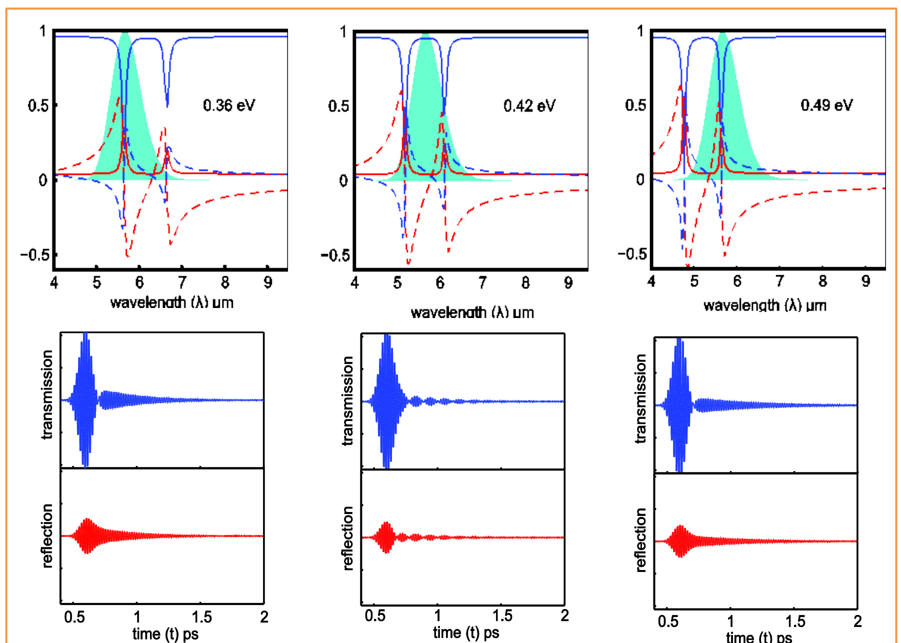
Models available at:
http://www.comsol.com/community/exchange/361/

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



FDTD with SBC
(unpublished)



# THANK YOU!

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`https://nanohub.org/tools/photonicvasefit`

**Cite this work**

Researchers should cite this work as follows:

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