GreEnergy
Power from optical antennas

Multiphysics Simulation of Nanodevices

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UNIVERSITÀ POLITECNICA DELLE MARCHE

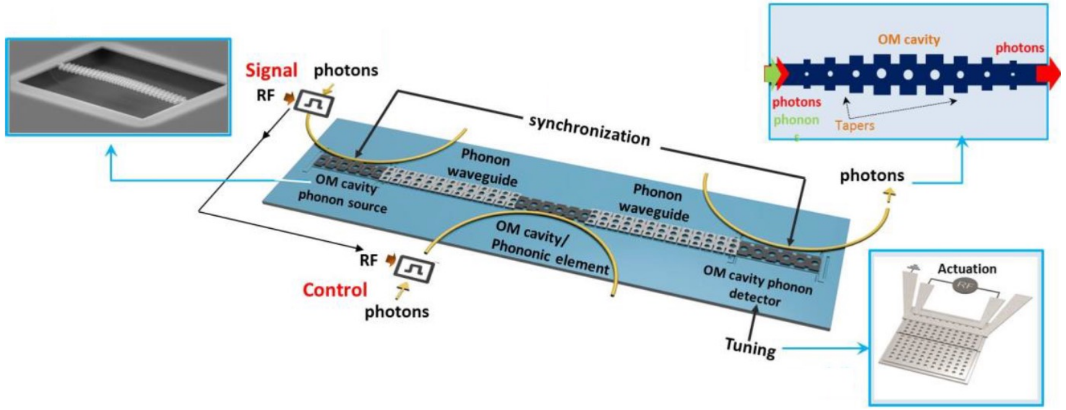
OUTLINE

- Research Areas and Activities
- Nano- /smart material in devices/systems
- The computational platform for the multi-physics modeling
- Examples

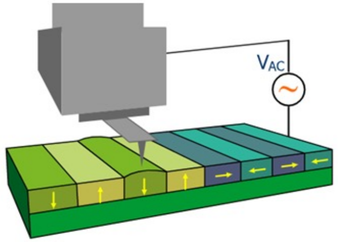
Electromagnetics – Nanotechnology group :
Research Areas and Activities

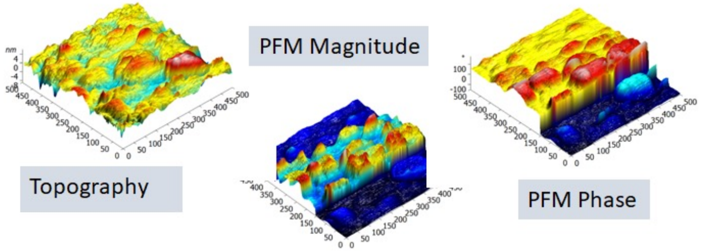
- Analysis **EM + Quantum** / thermal **transport** in nano-structures
- **Computational platform** for the multi-physics modeling of **nano-to-meso-scale systems**
- **Atomistic** (*ab-Initio*) simulations
- **Molecular Dynamics** (MD) simulations

- Modeling/design of **opto-mechanical systems**



- Opto-electronics and **microscopy**





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Electromagnetics – Nanotechnology group : Research Areas and Activities

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- Atomistic (*ab-Initio*) simulations
- Molecular Dynamics (MD) simulations

GOAL → Combining (coupling) electromagnetics, quantum transport, thermal effects …

KEY DEVELOPMENT →
- Bridging from atomistic to continuum level
- Interfacing mathematical models (PDEs)

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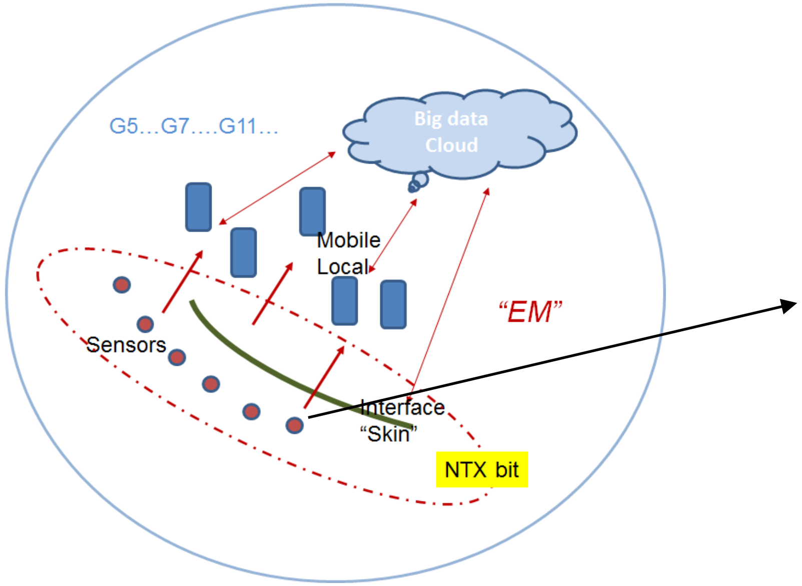
... a typical scenario where the mutiphysics modeling becomes necessary a technological platform incorporating nano- / smart-materials

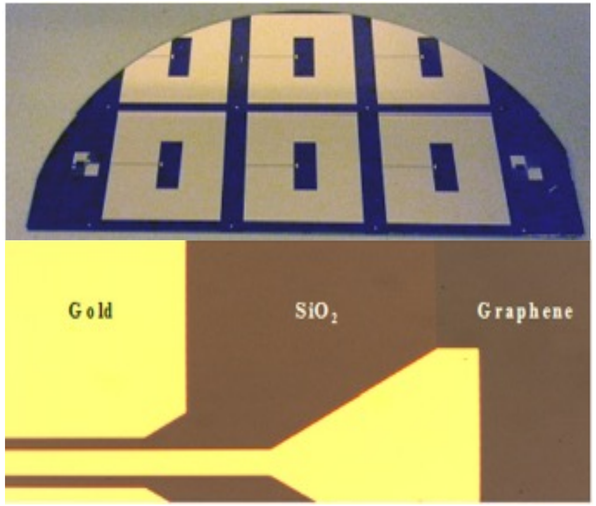
- nano-structured material regions (CNT, graphene etc…)
- embedded in micro-/mm regions
- Extreme multi-scale: geometrical/electrical aspect ratios
- Multi-physics (EM+transport+thermal+…) phenomena



Sensor Network

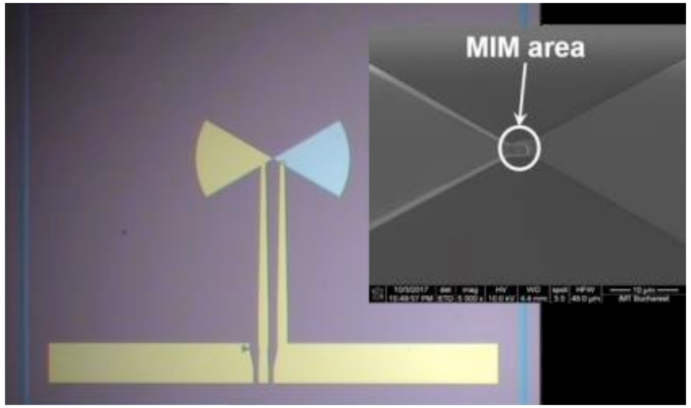
M. Dragoman, L. Pierantoni, et al.,
APPLIED PHYSICS LETTERS 106, 2015

Graphene antenna



Graphene thicknss:
< 1 nm

rectifying antenna



MIM diode based is a 6-nm-thick HfO_2

M. Aldrigo, M. Dragoman, M. Modreanu, et al., 2018,
https://doi.org/10.1109/TED.2018.2835138

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- embedded in micro-/mm regions (EM models)
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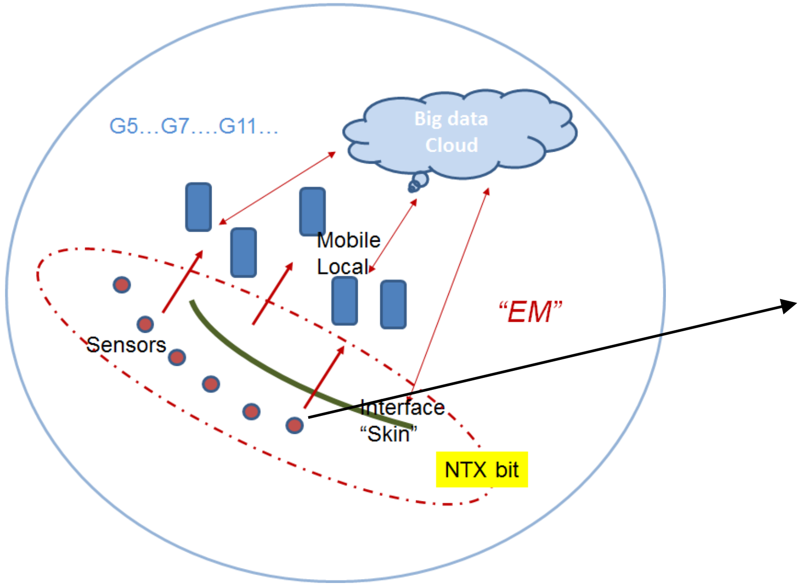

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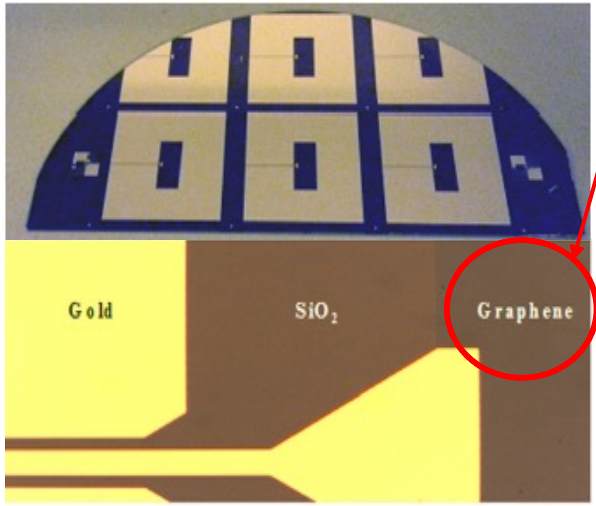
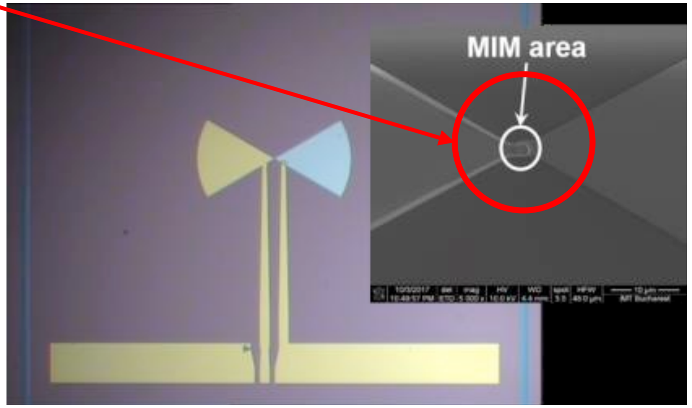


Graphene thicknss:
< 1 nm

Quantum model (Schrödinger/Dirac)

rectifying antenna



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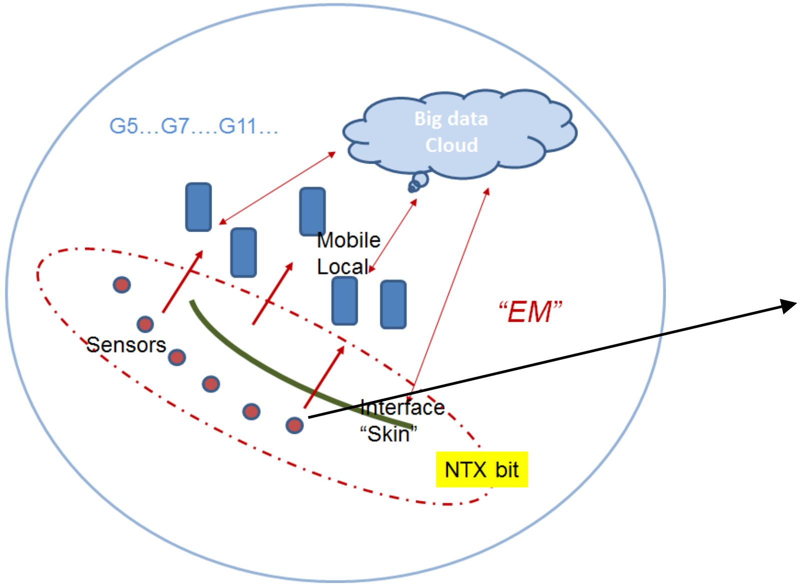

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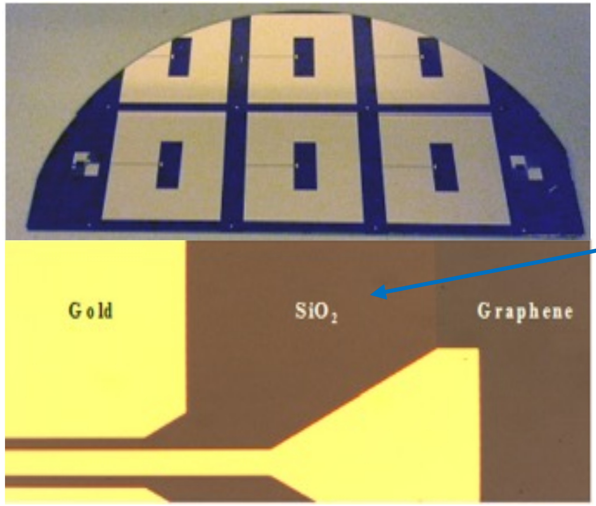
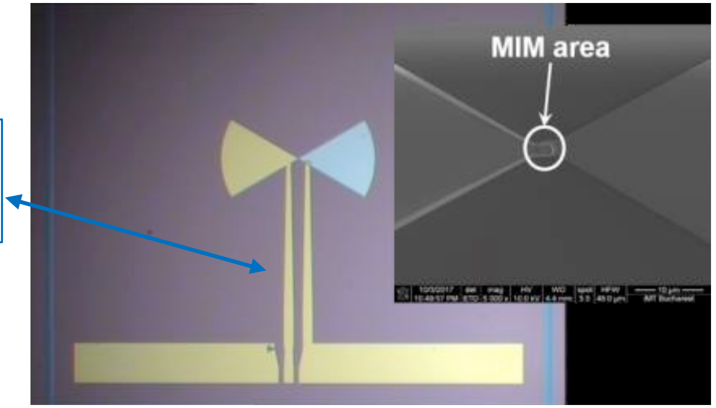


Graphene thicknss:
< 1 nm

EM model
(Maxwell)

rectifying antenna



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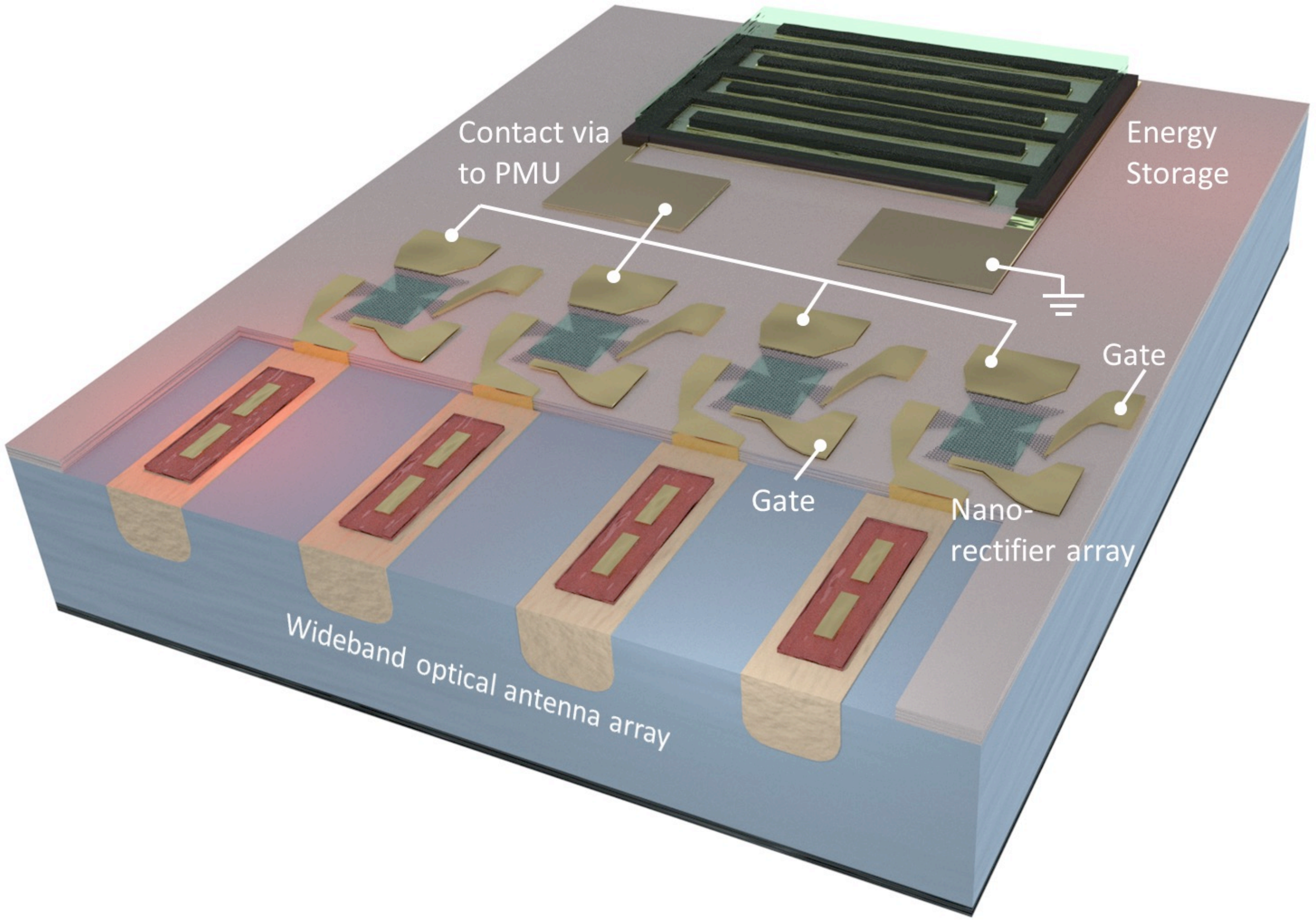
GreEnergy scenario: rectenna + diode + supercap + …



Schematic view of the future combined system architecture

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KEY DEVELOPMENT

- Bridging from atomistic to continuum level
- Interfacing mathematical models (PDEs)

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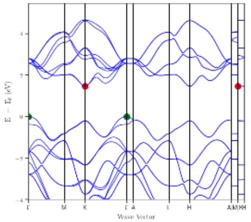
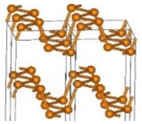
ATOMISTIC LEVEL

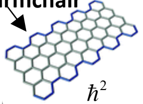


MoS2 Band-strcture



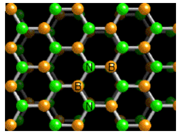
Black phosphorus

armchair GNR



$$m_{eff.} = \frac{\hbar^2}{\frac{d^2 E}{d k^2}}$$

graphene



Ab-initio Methods

Quantum Schrodinger eq.

$$H(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

Atomistic Solvers

THE BRIDGE

$$\underline{\underline{\varepsilon}}(\omega,\mathbf{k})$$

$$\underline{\underline{\mu}}(\omega,\mathbf{k})$$

$$\underline{\underline{\sigma}}(\omega,\mathbf{k})$$

$$m_{effective}$$

$$\mathbf{J}(\mathbf{r}) = \int d^2r' \sigma_{HO}(\mathbf{r}-\mathbf{r}')\cdot\mathbf{E}(\mathbf{r}')$$

$$\sigma_{HO} = \sigma_{Hafniun\ Oxide}$$

constitutive eqs./relations

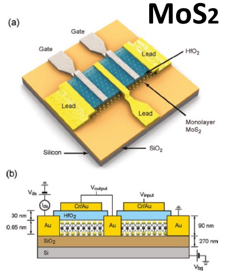
FULL-WAVE SOLVERS

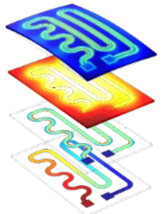
$$\nabla\times\mathbf{E}(\mathbf{r},t) = -\frac{\partial}{\partial t}\mathbf{B}(\mathbf{r},t)$$

$$\nabla\times\mathbf{H}(\mathbf{r},t) = \frac{\partial}{\partial t}\mathbf{D}(\mathbf{r},t) + \mathbf{J}(\mathbf{r},t)$$

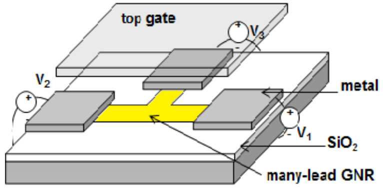
Electromagnetic: Maxwell

MoS2 FET

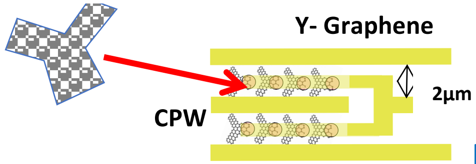




Devices Systems Interfaces



Y- Graphene



CONTINUUM LEVEL

GreEnergy Summer School 2022

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FULL-WAVE SOLVERS

Quantum: Schr./Dirac

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CONTINUUM LEVEL

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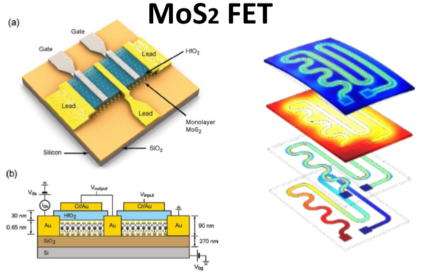

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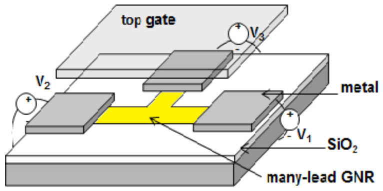

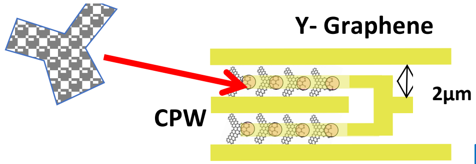

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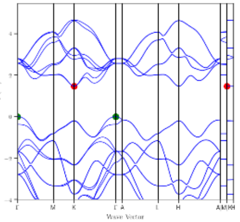
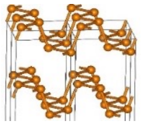
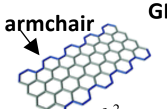


MoS2
Band-strcture



Black phosphorus



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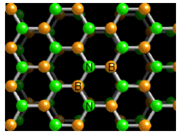
graphene



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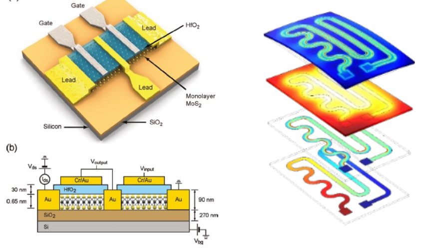
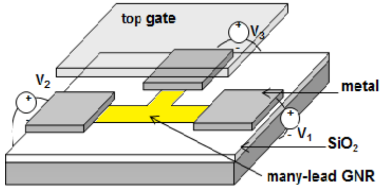
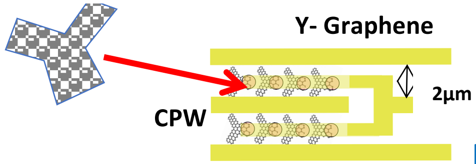


Devices
Systems
Interfaces





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The theoretical-computational platform

ATOMISTIC LEVEL

THE BRIDGE

Quantum Expresso

Quantum Wise
VNL-ATK 2016

Gromacs

Ab-initio Methods

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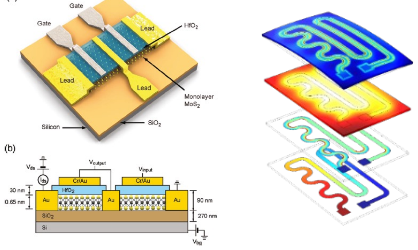


Devices Systems Interfaces

- **FDTD, TLM, FEM**
- **modal analysis**
- **hybrid methods**
- **…**

METHODS

- **COMSOL**
- **CST**
- **HFSS**
- **…**

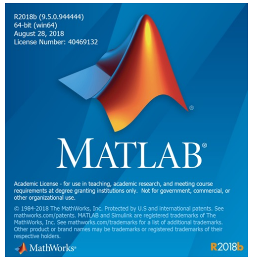
FULL-WAVE SOLVERS

Computational platform: new home-made interface COMSOL - MATLAB

- **Quantum transport, Schrödinger/Dirac**
- **SM, NEGF**
- **DFT analysis**

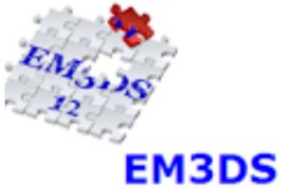
- In-house software: Fortran, Matlab, C, etc.
- Quantum W, Gromacs

Java Python PHP C++



- **DC – AC analysis**
- **Full-wave EM analysis of FET in linear regime**
- **Equivalent circuits**

- COMSOL multiphys
- CST Microwave S.
- HFSS Ansoft
- EM3DS Univpm



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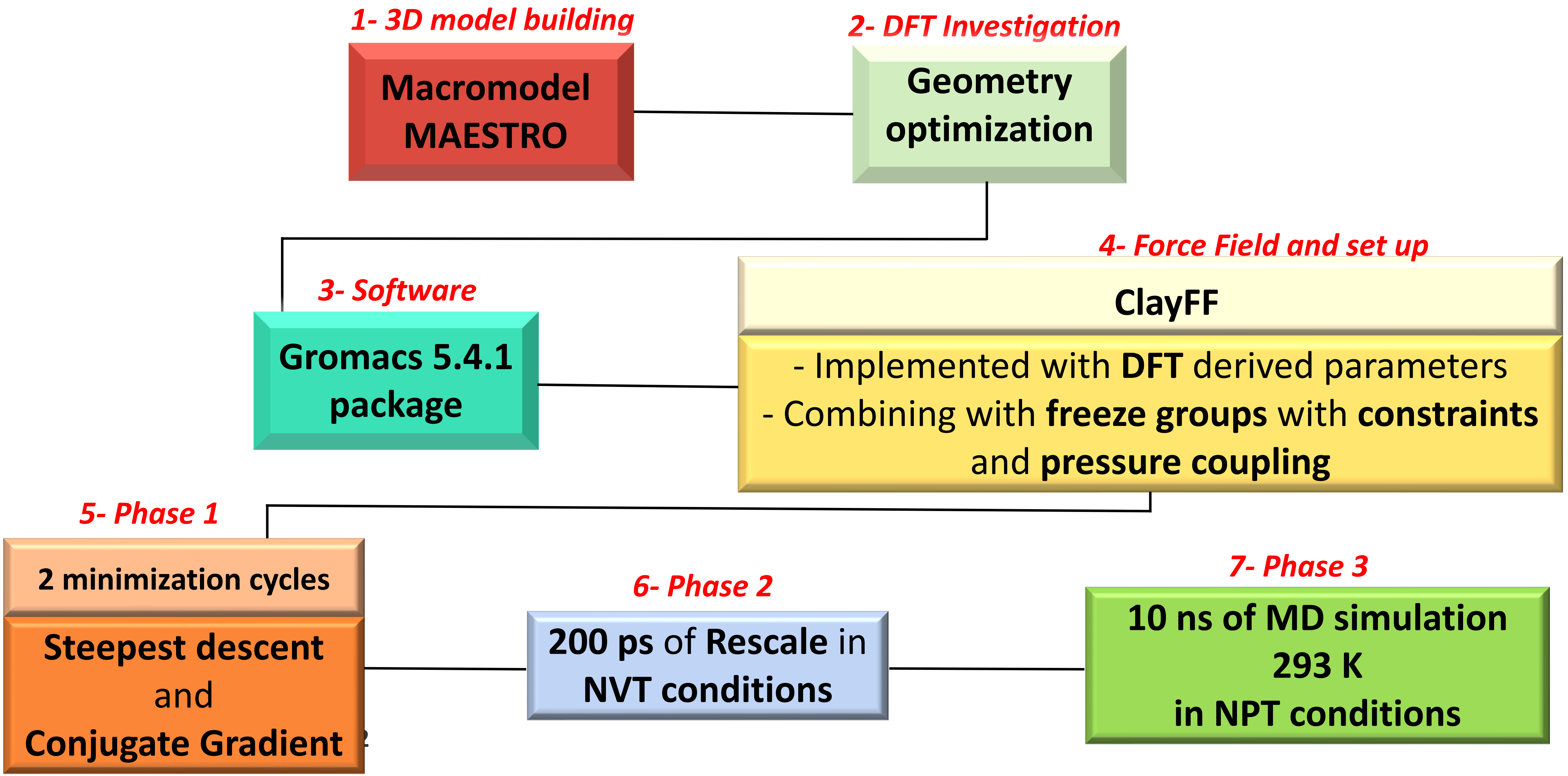
Block scheme of the Atomistic Simulations Method

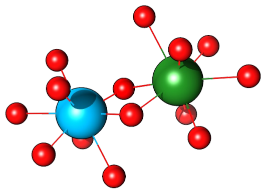


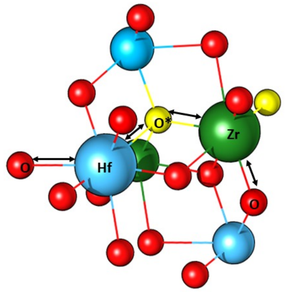
DFT and Molecular Dynamics simulations

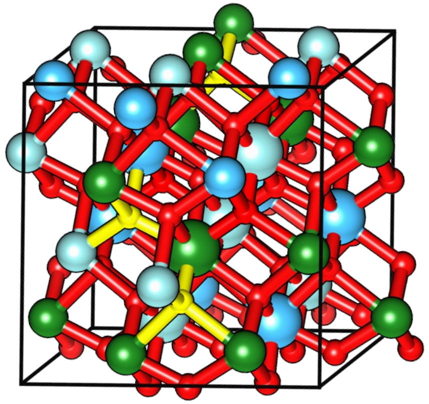
In silico methods based on combined DFT-MD simulation

Atomistic 3D System setup → *Geometry optimization of 3D reticulum* → **DFT solver** → *Implementation of new DFT derived parameters in GROMACS FFs* → **Molecular Dynamics simulation** → *Use of GROMACS tools* → **Extrapolation of electrical properties from MD trajectories**

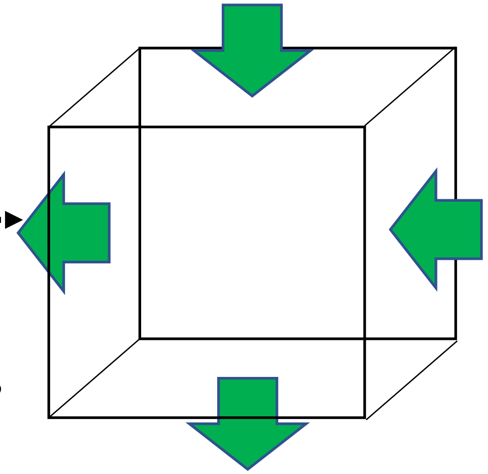
Number of explicit atoms







Periodic Boundary Conditions



Quantum and EM Models at continuum level (ii)

1) Quantum models are coupled to Maxwell eqs. in time- and/or freq. domain
2) combined electromagnetic-transport phenomena
3) Multi-scale numerical techniques (FEM, FDTD, …)

$$\nabla \times \mathbf{E}(\mathbf{r},t) = -\frac{\partial}{\partial t}\mathbf{B}(\mathbf{r},t)$$

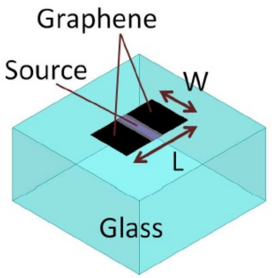
$$\nabla \times \mathbf{H}(\mathbf{r},t) = \frac{\partial}{\partial t}\mathbf{D}(\mathbf{r},t) + \mathbf{J}(\mathbf{r},t)$$

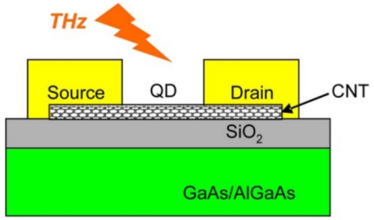
Electromagnetic: Maxwell

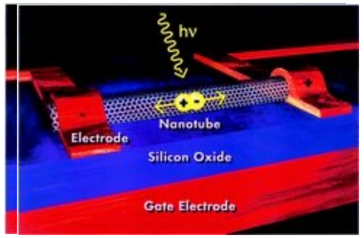
$$H(\mathbf{r},t)\psi(\mathbf{r},t) = i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}$$

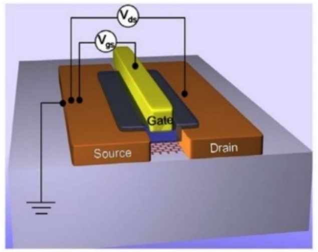
Quantum: Schrödinger/Dirac

- interaction particles-EM field - transient
- Quantum dots, quantum wells
- Ballistic electronics
- non linear devices
- Spintronics
- photodetectors
- …









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Examples

- Graphene Antenna
- MoS_2 FET
- Schrödinger – Poisson eqs.: CNT FET
- Dirac – Maxwell eqs.: Ballistic Ratchet effect on graphene

Examples

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- MoS_2 FET
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Tunable Graphene-based Antenna

M. Dragoman, L. Pierantoni, et al.,
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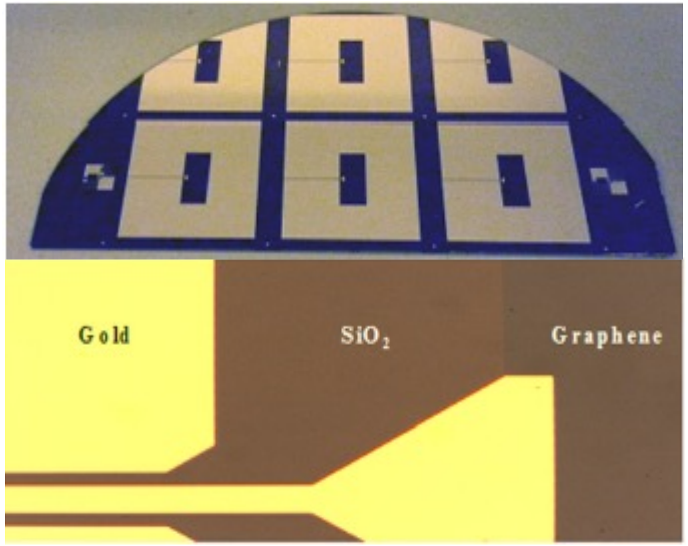
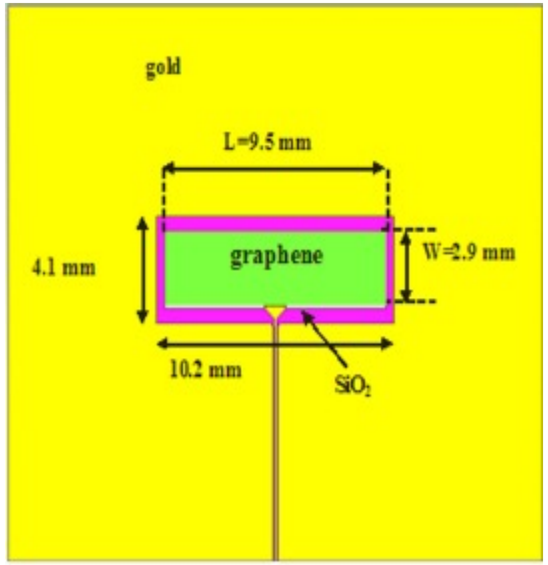
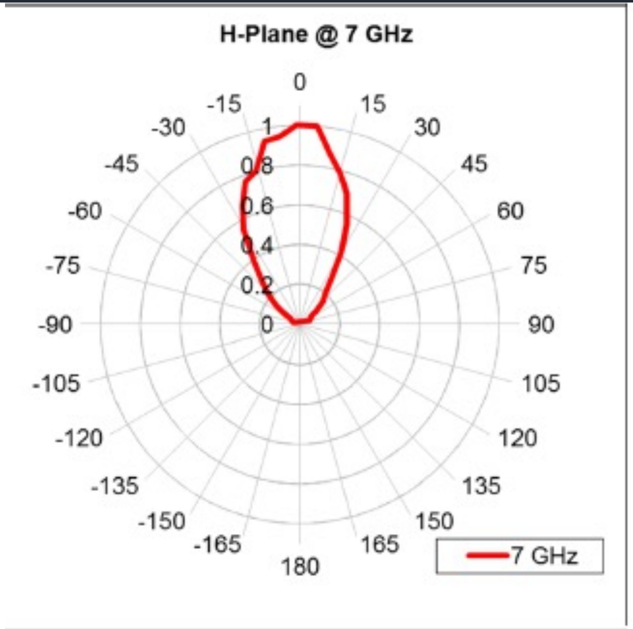
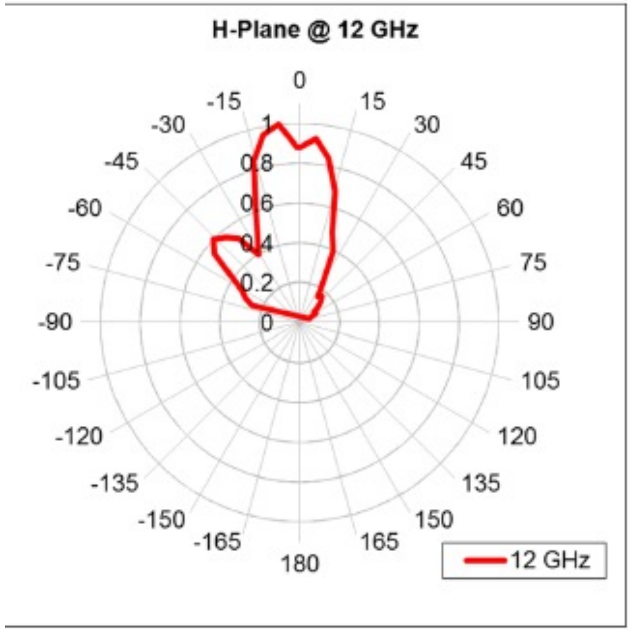


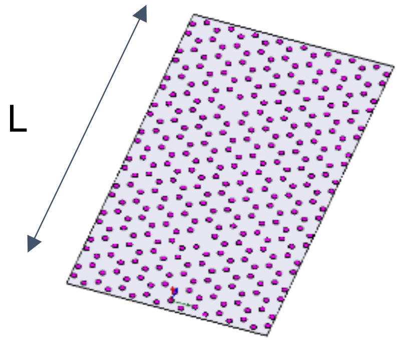






- microwave slot antenna in a CPW based on graphene
- Antennas fabricated on a high-resistivity Si wafer
- 300 nm SiO_2 layer
- A CVD grown graphene layer is transferred on the SiO_2
- Reflection parameter can be tuned by a DC voltage
- 2D radiation patterns in the X band (8–12 GHz)

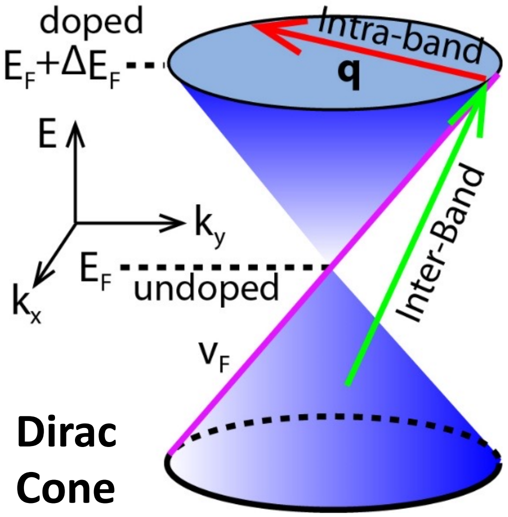
Graphene: the constitutive relation is based on the Kubo-Drude model (strictly valid for monolayer/on air)



Graphene can be described by a surface conductivity tensor tobe inserted in a EM computation

$$\underline{\underline{\sigma}}_{graphene} = \underline{\underline{\sigma}}' + j\underline{\underline{\sigma}}''$$

$$\underline{J} = \underline{\underline{\sigma}}_G \underline{E}$$



Kubo-Drude Formulation (monolayer/on air)

$$\sigma_{\pm} = \frac{i\,e^2}{\pi\hbar}\frac{1}{\hbar\omega \pm i\gamma}\int_0^{\infty} d\varepsilon\varepsilon\left(\frac{\partial f_D(\varepsilon)}{\partial\varepsilon} - \frac{\partial f_D(-\varepsilon)}{\partial\varepsilon}\right) \quad \text{intraband}$$

$$-\frac{i\,e^2}{\pi\hbar}\frac{1}{\hbar\omega \pm i\gamma}\int_0^{\infty} d\varepsilon\left[\frac{f_D(\varepsilon) - f_D(-\varepsilon)}{1 - \left(\frac{2\varepsilon}{\hbar\omega \pm i\gamma}\right)^2}\right] \quad \text{interband}$$

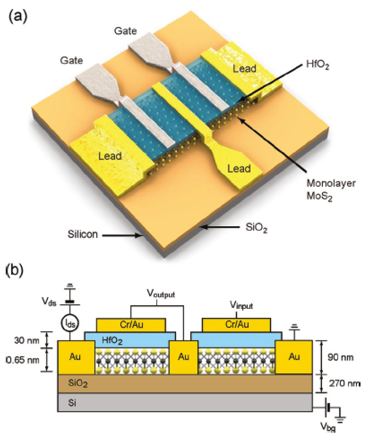
$$f_D(\varepsilon) = \frac{1}{1 + e^{\frac{\varepsilon-\mu}{k\,T}}}$$ Fermi –Dirac Distribution $\gamma = 2\pi/\tau$

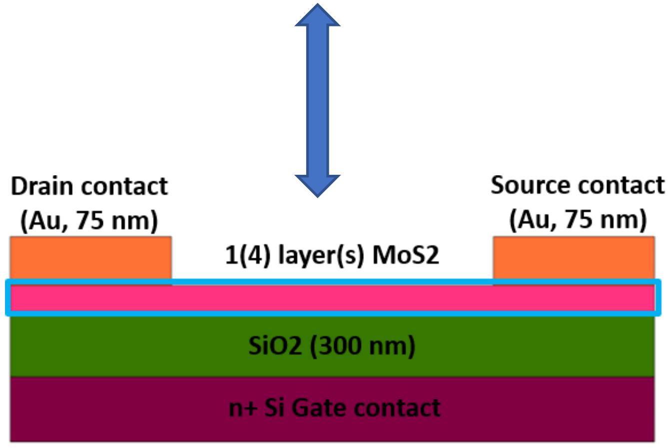
Examples

- Graphene Antenna
- MoS_2 FET
- Schrödinger – Poisson eqs.: CNT FET
- Dirac – Maxwell eqs.: Ballistic Ratchet effect on graphene

MoS2 – based Field Effect Transisitor (FET)

- **GOAL: derivation of the MoS_2 channel permittivity (conductivity)**





The device: 3.5 m. Out-of-plane thickness (width): 6.8 um
Gold contacts (orange) are 75 nm thick,
Active region (magenta): --- > number of layers
Thickness SiO_2 gate insulator (green) is 300 nm,
The n+ Si gate (plum) has a thickness of 2 um

MoS_2

- Very HIGH ON/OFF ratios >10^7 (vs 10^6 of CMOS)
- Lower mobility (many defects) vs. graphene/
- Eg = 1.8 eV

Theoretical-computational route

1. study of the material (MoS2) at the atomistic level
2. derivation of constitutive relations (CR)
3. insertion of the CR in the full-wave solver (COMSOL)
4. Coupling of Poisson and transport (drift) eqs. using the semiconductor physics module by COMSOL

- **Hafnium-Zirconium Oxide ($Hf_xZr_{(1-x)}O_2$, x = 0.3**
- **as a substrate ferroelectric material**
- **high tunability**
- **CMOS technology compatibility**

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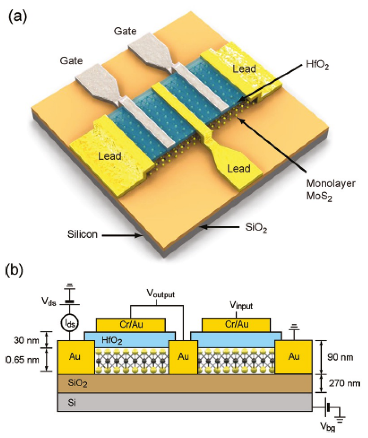
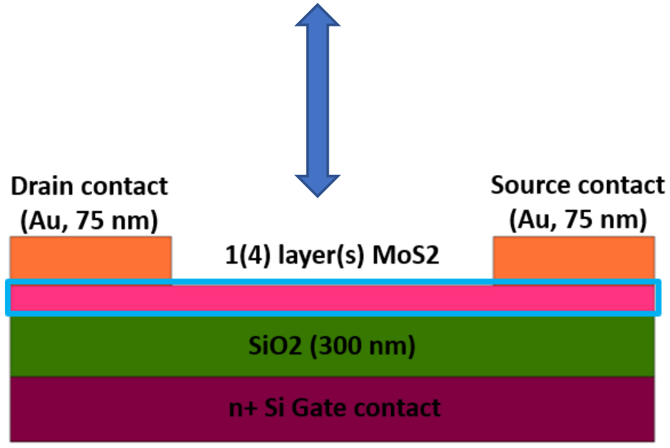
MoS2 – based Field Effect Transisitor (FET)

- **GOAL: derivation of the MoS2 channel permittivity (conductivity)**





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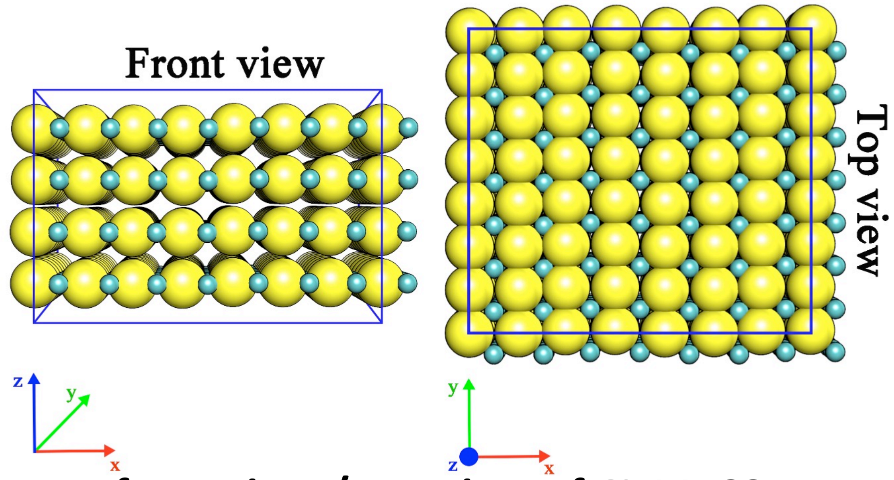
MoS2

- Very HIGH ON/OFF ratios $>10^7$ (vs 10^6 of CMOS)
- Lower mobility (many defects) vs. graphene/
- Eg = 1.8 eV
- Electron affinity: 4.7 eV
- Electron (hole) mobility: 10 $cm^2\ V^{-1}\ s^{-1}$ (10 $cm^2\ V^{-1}\ s^{-1}$)
- Electron (hole)effective mass: $0.5 \times m_e$ ($0.5 \times m_e$)
- Defect n-type doping: $1.5 \times 10^{18}\ cm^{-3}$

Atomistic Simulations



- front view / top view of 4L MoS2
- Mo atoms in green sticks
- S atoms in yellow

possibility of simulating defects and particular contacts with the substrate

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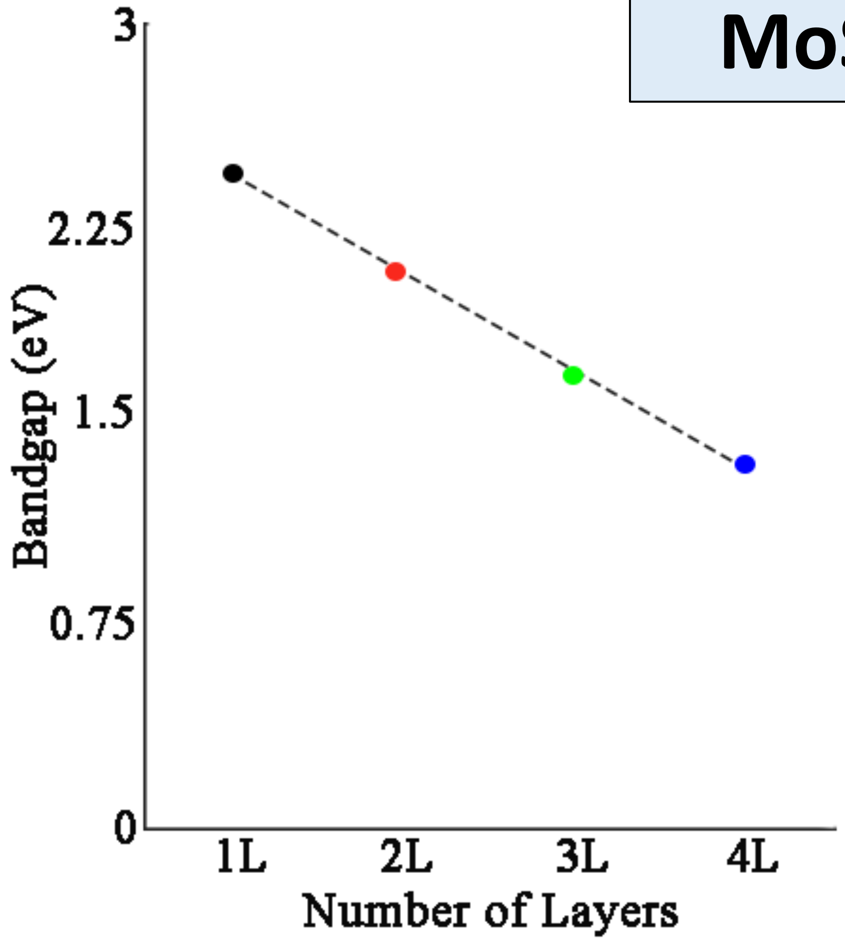
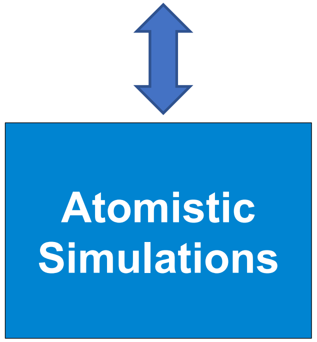
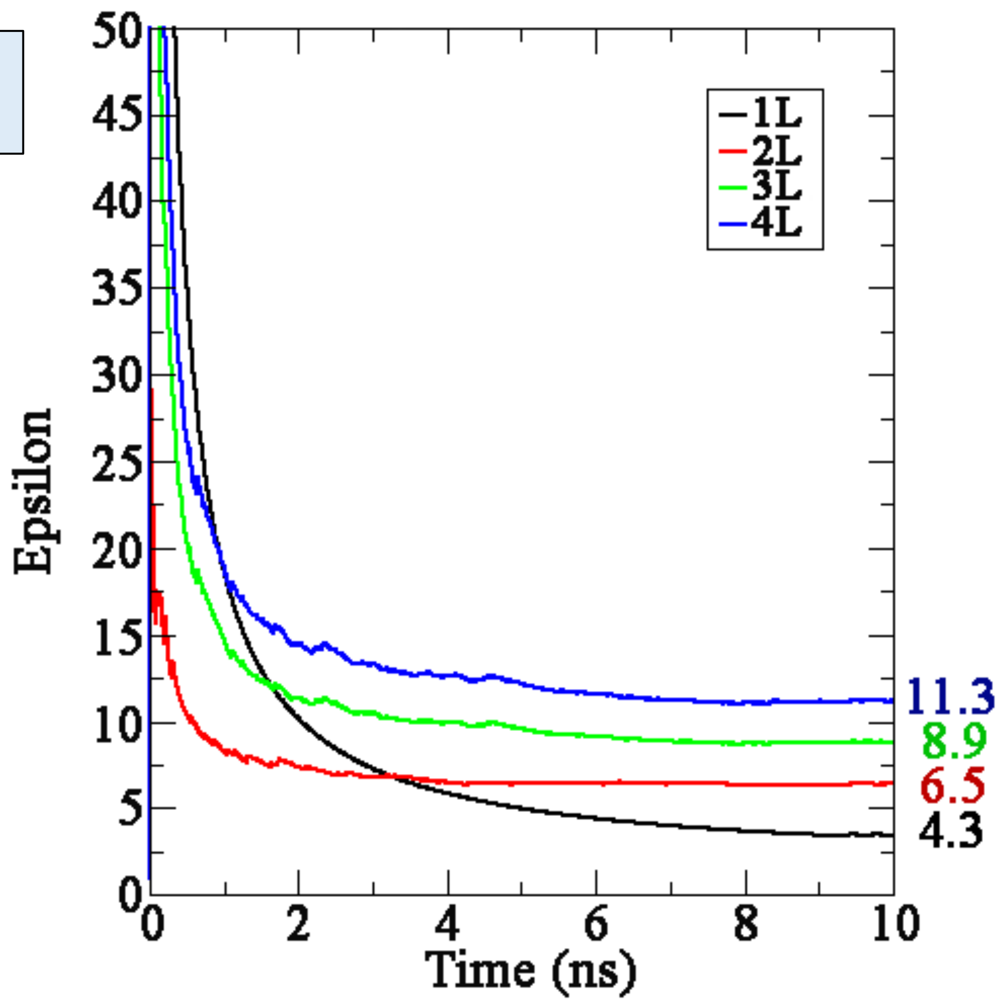
MoS2 permittivity



Bandgaps decreased with increasing MoS2 layers' number [Zhao, C M Wei, L Yang, M Y Chou. Phys Rev Lett. 2004;92(23):236805]



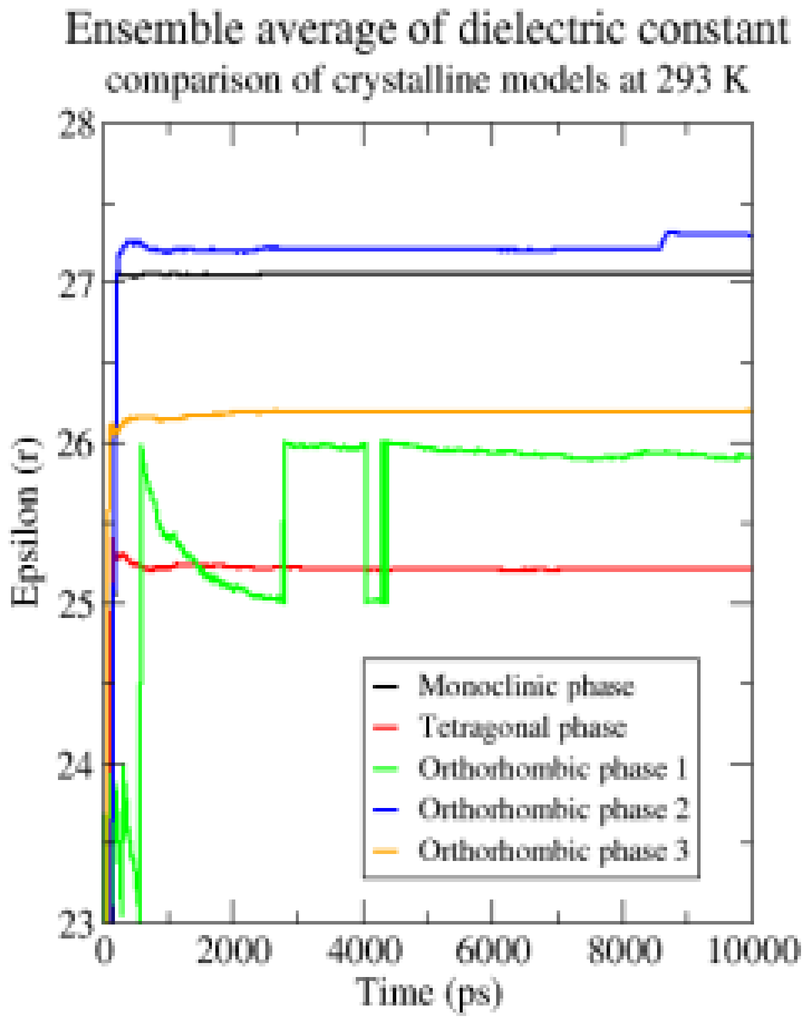


A direct correlation between the number of layers and the dielectric constant value was observed

Pelagalli N, Laudadio E, Stipa P, Mencarelli D, Pierantoni L., Electronics, Aug. 2020

rantoni

HfO_2 : Comparison of DFT simulations vs. data reported in the literature



27.242 → ***Orthorhombic phase 2*** (bandgap= **3.393 eV**; from lit.)

27.083 → ***Monoclinic phase*** (bandgap= **4.017 eV**; from lit.)

26.236 → ***Orthorhombic phase 3*** (bandgap= **4.227 eV**; from lit.)

25.907 → ***Orthorhombic phase 1*** (bandgap= **4.413 eV**; from lit.)

25.244 → ***Tetragonal phase*** (bandgap= **4.668 eV**; from lit.)

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Comparison to experimental results

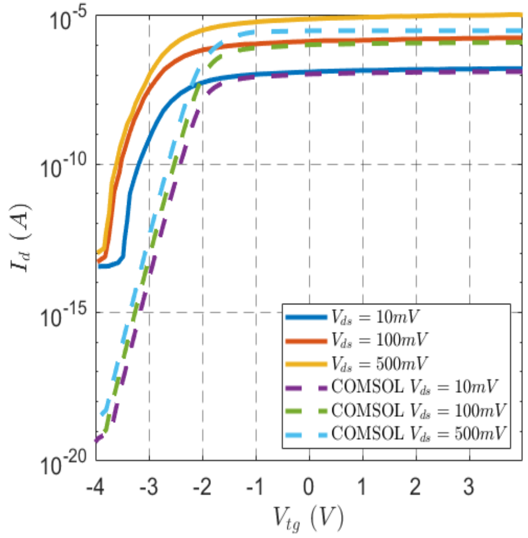
Atomistic Simulations

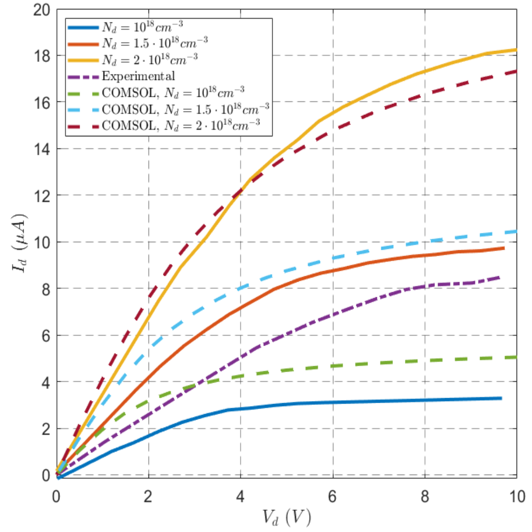
↓

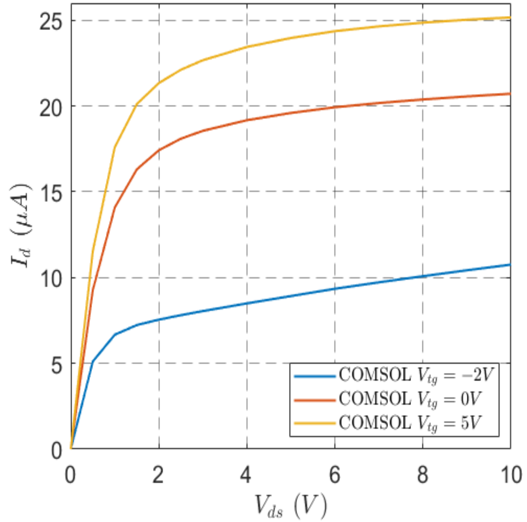
Derivation of constitutive relations

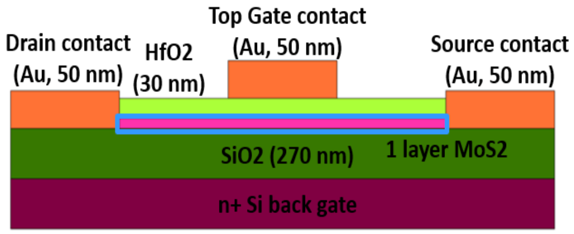
↓

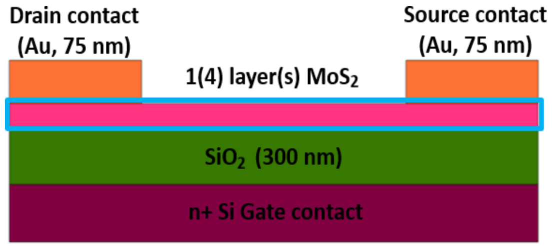
FEM **Full-Wave** Modeling

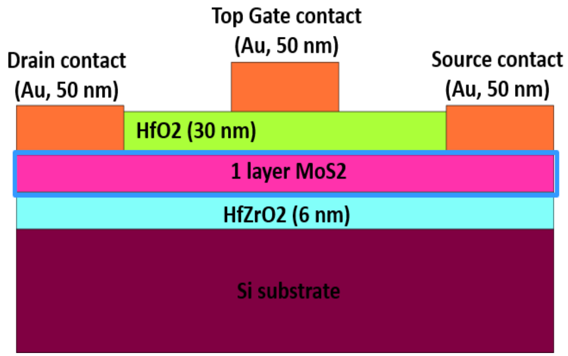












Examples

- Graphene Antenna
- MoS_2 FET
- Schrödinger – Poisson eqs.: CNT FET
- Dirac – Maxwell eqs.: Ballistic Ratchet effect on graphene

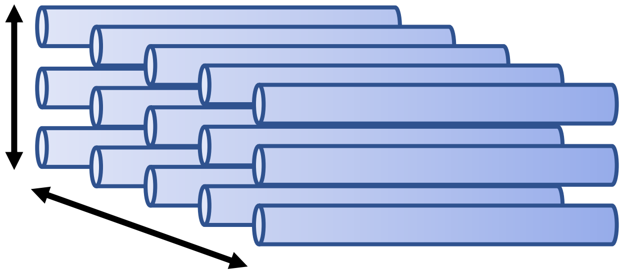
Schrödinger – Poisson eqs. coupling

Modeling of sensors, FETs, quantum dots, ...

Quantum capacitance, effective transconductance, etc....

Schrödinger – Poisson eqs. coupling

- **Possibility to evaluate multiwall/multichannel structures**
- **Rigorous analysis (no equivalent circuit approximations)**



CNT Matrix

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Simulation method

3D FEM
full-wave
solver

Poisson

$\nabla^2 V = \rho/\varepsilon$

Schrödinger

$H\psi = E\psi$

Transmission
line matrix
cascade

Coupling

$U \pm eV$

$\rho = e|\psi|^2$

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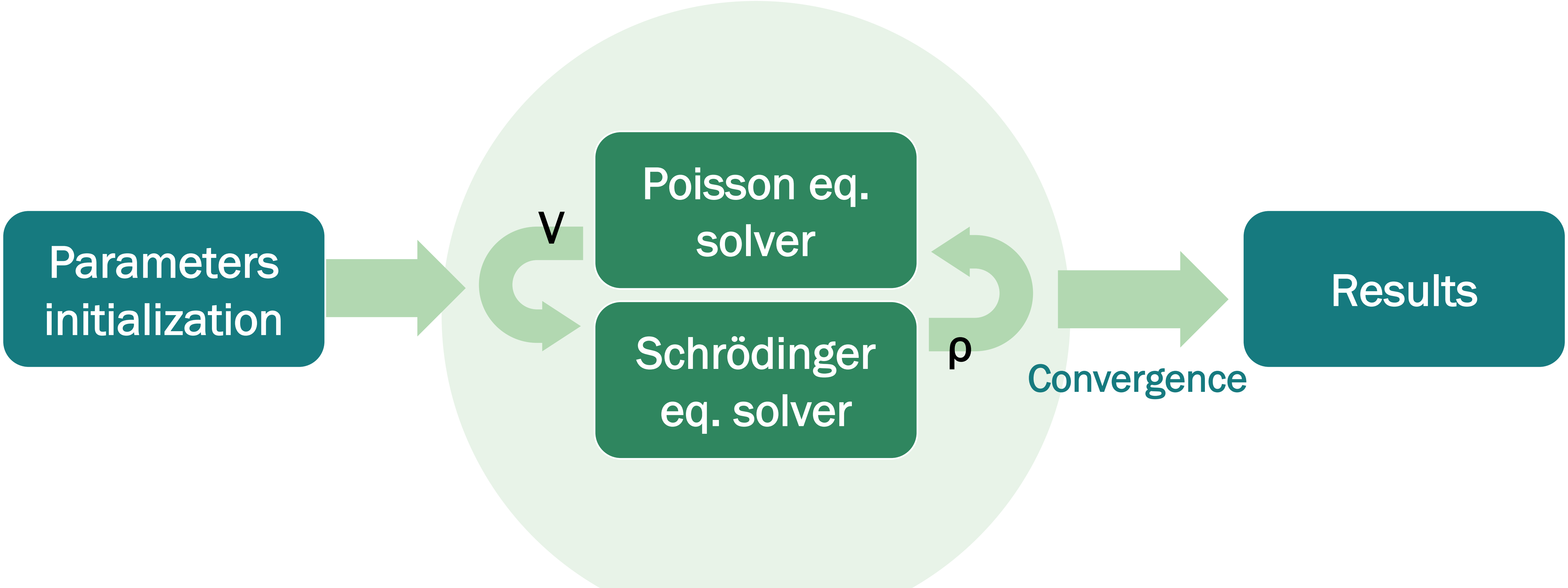
Simulation workflow



STEP 1 STEP 2⟶N STEP N

Schrödinger Equation model for CNT

describes the quantum mechanical behaviour of a charge carrier

wave function $\psi(\mathbf{r},t)$

$$i\hbar \frac{\partial \psi(\mathbf{r},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\psi(\mathbf{r},t) = \left(\frac{1}{2m}\hat{\mathbf{p}}^2 + V(\mathbf{r})\right)\psi(\mathbf{r},t)$$

$$\hbar = \frac{h}{2\pi}$$

$h=6.26*10^{-34}$ [J*sec]
Plank's constant

V(r) is the potential barrier

$$\int_{-\infty}^{+\infty} \left|\psi(\mathbf{r},t)\right|^2 d\mathbf{r} = 1$$

$q=-e=1.602*10^{-19}$ [C]
electron charge

m is the "effective mass" of the particle

$\hat{\mathbf{p}} = -i\hbar\nabla$ is the kinematic momentum

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CNT-based Devices: self-consistent solution of the combined Poisson- Schrödinger eqs.

Schrödinger equation

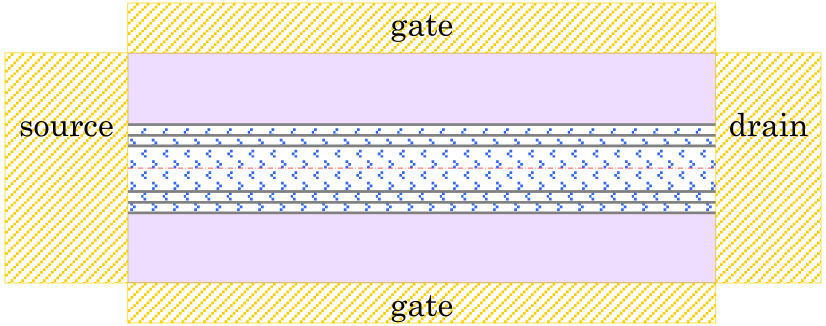
$$\nabla^2 \psi = -\frac{2m_0}{\hbar^2}[E+V]\psi$$

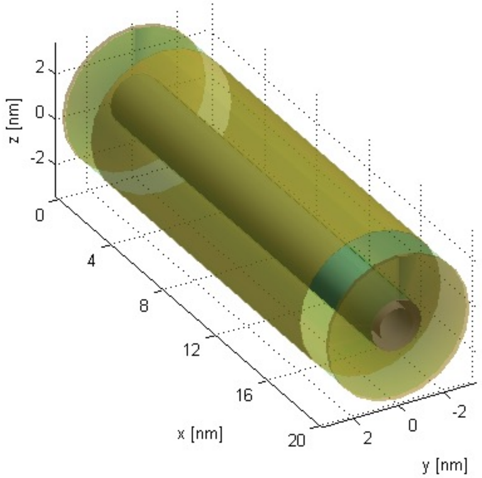
$$q\int \left|\psi(\mathbf{r},E)\right|^2 dE = \rho_T$$

normalization condition

$$\nabla^2 V = \frac{\rho_T}{\varepsilon}$$

Poisson equation

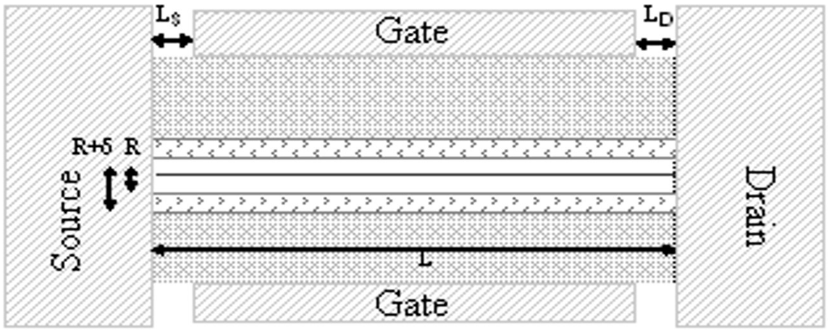




- Schrödinger equation for all the transport channels (modes)
- multi-wall and multi-band coherent carrier transport
- *V* is the electrostatic potential satisfying the Poisson equation

D. Mencarelli, T. Rozzi, L. Pierantoni “Modelling of multi-wall CNT devices by self-consistent analysis multichannel transport” IOP Science Nanotechnology,

…we developed an home-made solver

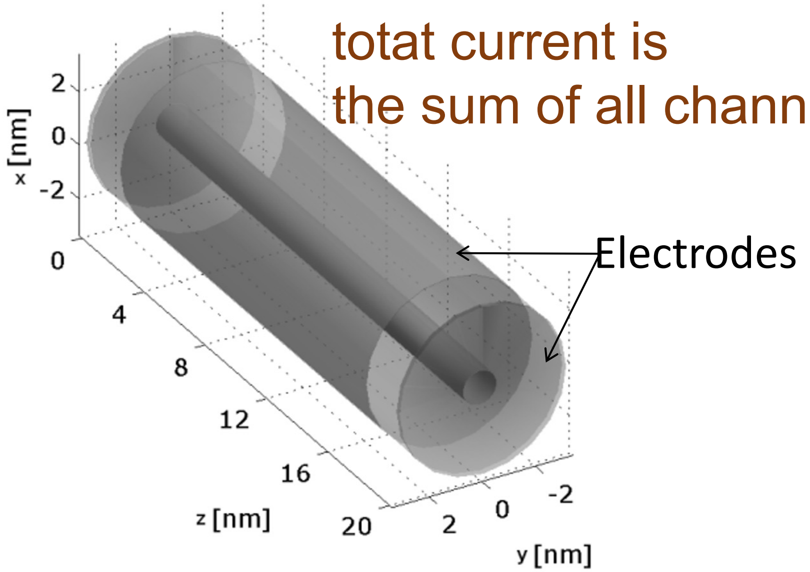


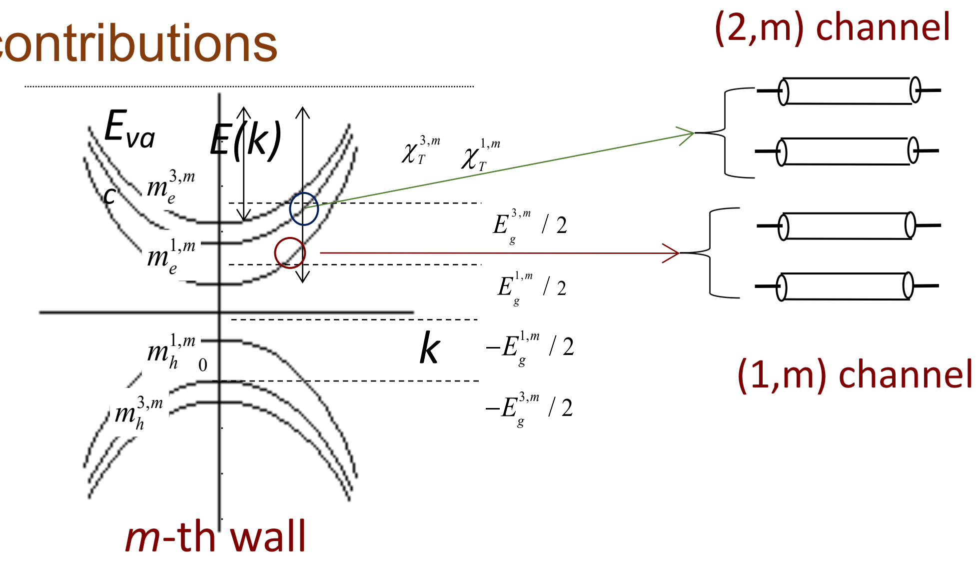
The current is computed by the Landauer-Büttiker formula

$$I_{h,e}^{n,m} = \frac{4e}{h}\int (f_{h,e}^{S} - f_{h,e}^{D}) T_{h,e}^{n,m}\, dE$$

$$I = \sum_{n,m} \left(I_h^{n,m} + I_e^{n,m} \right)$$

totat current is
the sum of all channel contributions





D. Mencarelli, L. Pierantoni,
Modeling of Multi-wall CNT Devices by Self-consistent Analysis of Multi-channel Transport, Nanotechnology, vol. 19, Number 16, 2008

Analysis of CNT Transistors

multi-wall and multi-band coherent carrier transport

$$\frac{d^2\Psi_{h,e}^{n,m}}{dz^2} = -\frac{2m_{h,e}^{n,m}}{\hbar^2}\left(E - U_{h,e}^{n,m}(z)\right)\Psi_{h,e}^{n,m}$$

m-th wall *n*-th sub-band

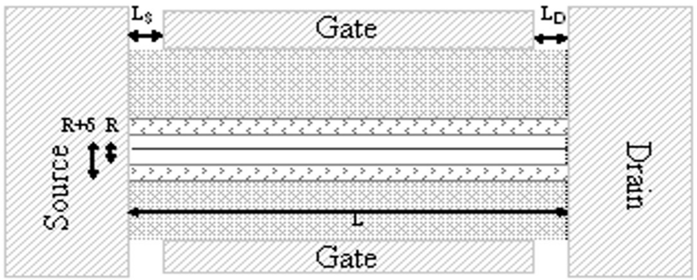
$$\frac{d^2V}{d\rho^2} + \frac{1}{\rho}\frac{dV}{d\rho} + \frac{dV}{dz^2} = -\frac{Q}{\varepsilon}$$

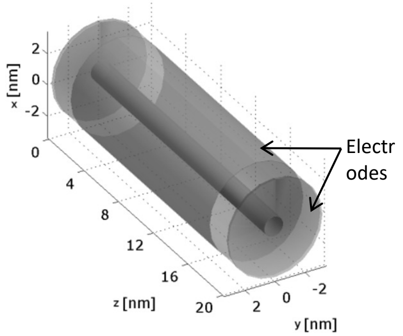
Schrödinger equations

Transmission Line approach

Poisson equation

FEM approach





The Schrödinger equation is written for each individual transport channel

V is the electrostatic potential satisfying the Poisson equation

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$\chi_T^{n,m}$

iterative solution

potential energy of the (n-m) channel

$$\frac{d^2\Psi_{h,e}^{n,m}}{dz^2} = -\frac{2m_{h,e}^{n,m}}{\hbar^2}\left(E - U_{h,e}^{n,m}(z)\right)\Psi_{h,e}^{n,m}$$

$$Q(V) = Q \equiv \Psi_{h,e}^{n,m}$$

$$\frac{d^2V}{d\rho^2} + \frac{1}{\rho}\frac{dV}{d\rho} + \frac{dV}{dz^2} = -\frac{Q}{\varepsilon}$$

$$V(Q) = V$$

$$Q = \frac{e}{2\pi}\frac{\delta(\rho - R)}{\rho}q \qquad q = \int\left|\Psi_e^D\right|^2 + \left|\Psi_e^S\right|^2 dE - \int\left|\Psi_h^D\right|^2 + \left|\Psi_h^S\right|^2 dE$$

$$\begin{cases} U_e^{n,m}(z) = \tilde{U}_e^{n,m}(z) - eV(R+\delta_m, z) \\ U_h^{n,m}(z) = \tilde{U}_h^{n,m}(z) + eV(R+\delta_m, z) \end{cases} \qquad \begin{cases} \tilde{U}_e^{n,m}(z) = E_{vac} - e\chi_T^{n,m} \\ \tilde{U}_h^{n,m}(z) = \tilde{U}_e^{n,m}(z) - E_g^{n,m} \end{cases} \qquad \begin{cases} V(R_G, z) = V_g - \Phi_g \\ V(R+\delta_m, 0) = V_s - \Phi_s \\ V(R+\delta_m, L) = V_d - \Phi_d \end{cases}$$

E_{vac} is the vacuum energy

R_G radius of the gate electrode

Φ_g, Φ_d, Φ_s, the work functions

$E_g^{n,m}$ *n*-th energy gap of the *m*-th wall

$\chi_T^{n,m}$ is the electron affinity

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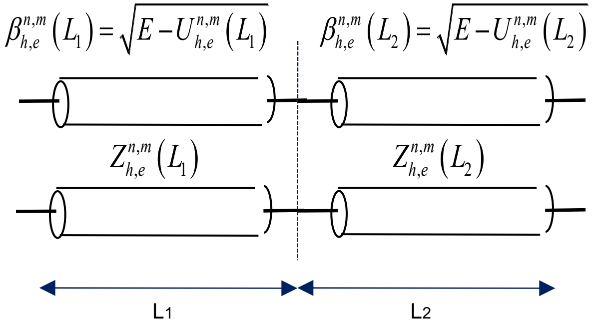
Transmission Line approach



telegrapher's equations

$$\begin{cases} \Psi_{h,e}^{n,m} = V_{h,e}^{n,m+} e^{-j\beta_{h,e}^{n,m} z} + V_{h,e}^{n,m-} e^{j\beta_{h,e}^{n,m} z} \\ \dfrac{\partial \Psi_{h,e}^{n,m}}{\partial z} = I_{h,e}^{n,m+} e^{-j\beta_{h,e}^{n,m} z} + I_{h,e}^{n,m-} e^{-j\beta_{h,e}^{n,m} z} = \dfrac{V_{h,e}^{n,m}}{jZ_{h,e}^{n,m}}^{+} e^{-j\beta_{h,e}^{n,m} z} - \dfrac{V_{h,e}^{n,m}}{jZ_{h,e}^{n,m}}^{-} e^{j\beta_{h,e}^{n,m} z} \end{cases}$$

$$\beta_{h,e}^{n,m} = \sqrt{E - U_{h,e}^{n,m}}$$ **propagation constants**

$$Z_{h,e}^{n,m} = 1/\beta_{h,e}^{n,m}$$

characteristic impedances

$$\Psi_{h,e}^{n,m} = \begin{cases} A_{h,e}^{n,m} e^{-j\beta_{h,e}^{n,m,S} z} + B_{h,e}^{n,m} e^{j\beta_{h,e}^{n,m,S} z} & z<0 \text{ (source)} \\ C_{h,e}^{n,m} e^{-j\beta_{h,e}^{n,m,D} z} + D_{h,e}^{n,m} e^{j\beta_{h,e}^{n,m,D} z} & z>L \text{ (drain)} \end{cases}$$

solutions

Normalization condition

$$\left(A_{h,e}^{n,m}\right)^2 = \frac{2m_{h,e}^{n,m}}{\pi\hbar^2}\frac{f_{h,e}^{n,m,S}}{\beta_{h,e}^{n,m,S}} \qquad D_{h,e}^{n,m2} = \frac{2m_{h,e}^{n,m}}{\pi\hbar^2}\frac{f_{h,e}^{n,m,D}}{\beta_{h,e}^{n,m,D}}$$

Analysis of CNT Transistors

multi-wall and multi-band coherent carrier transport

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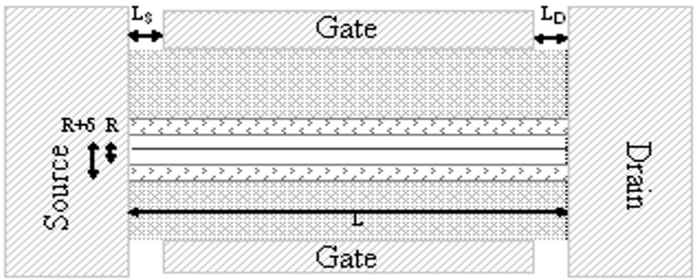

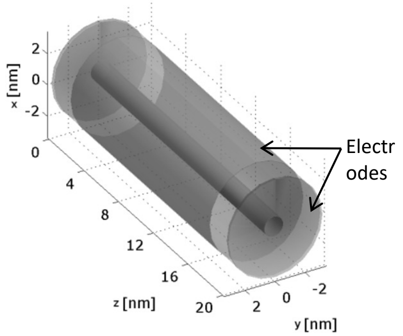

The Schrödinger equation is written for each individual transport channel

V is the electrostatic potential satisfying the Poisson equation

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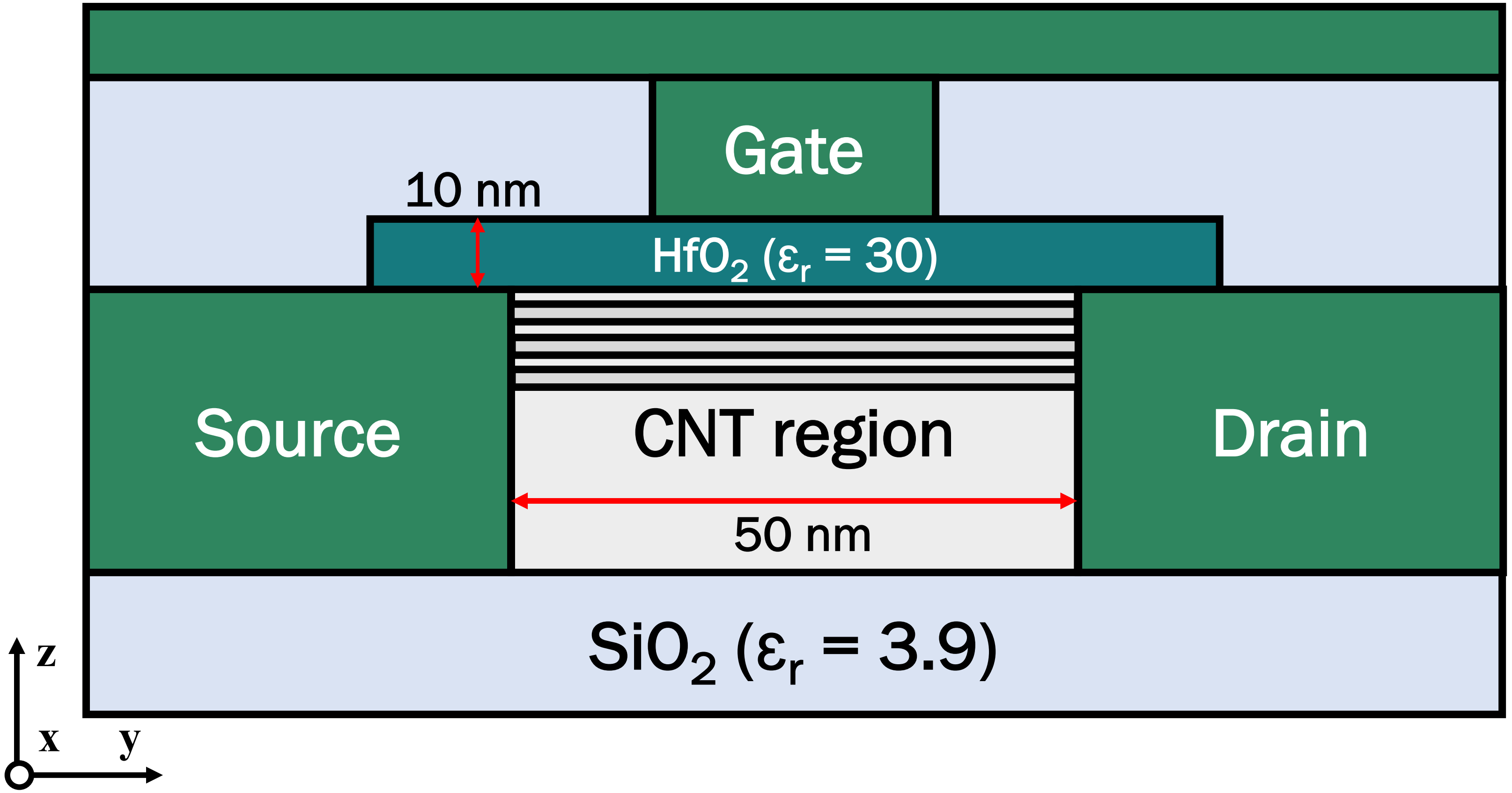
CNT-based FET: 3D Full-Wave simulation + Schrödinger – Poisson eqs. coupling

- Substrate – SiO_2
- Oxide – HfO_2
- Contacts – Gold

CNT (16,0)
- R = 0.63 nm
- L = 50 nm
- Spacing 0.50 nm



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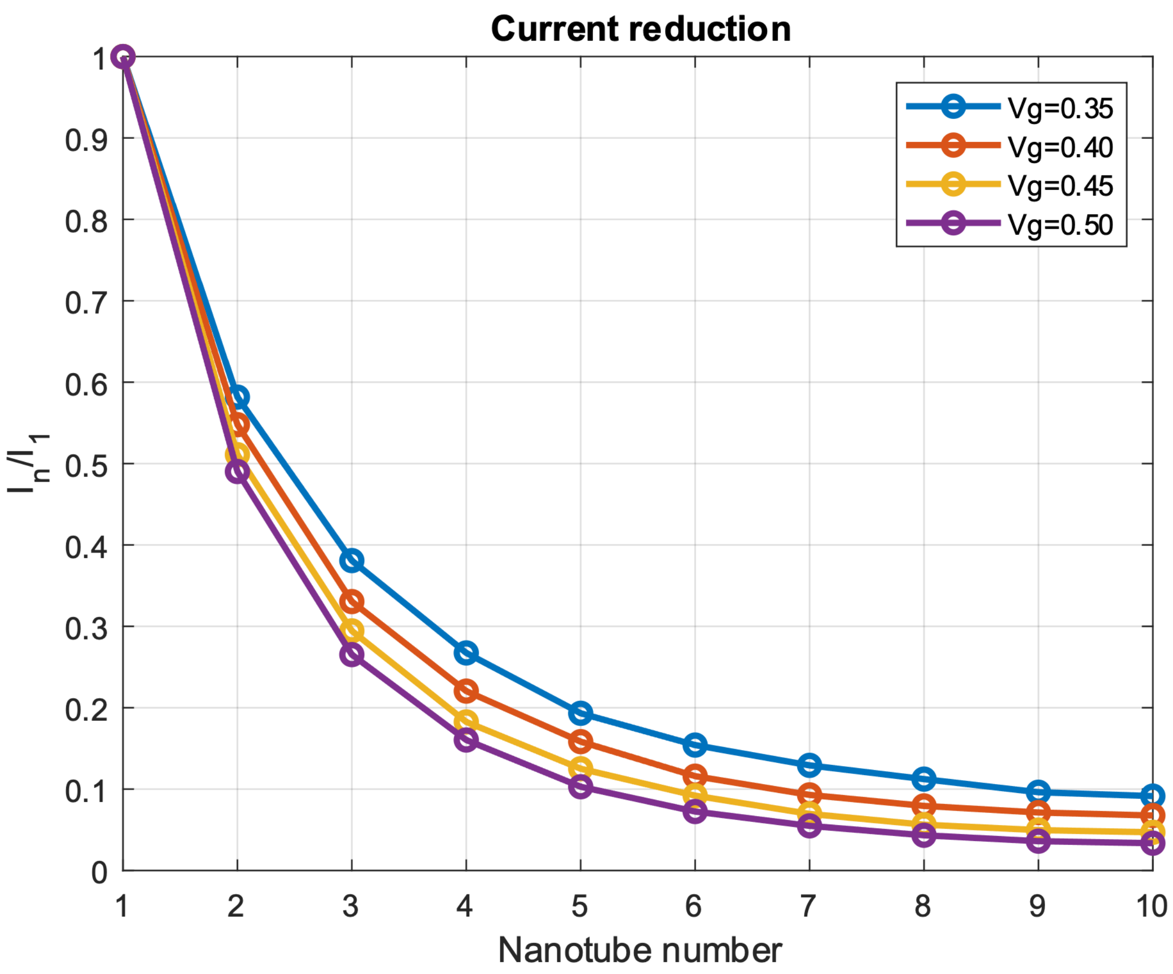
Results – Current reduction

2nd CNT 50–40% less
5th CNT 90–80% less

I_n Current in the nth CNT
I_1 Current in the 1st CNT



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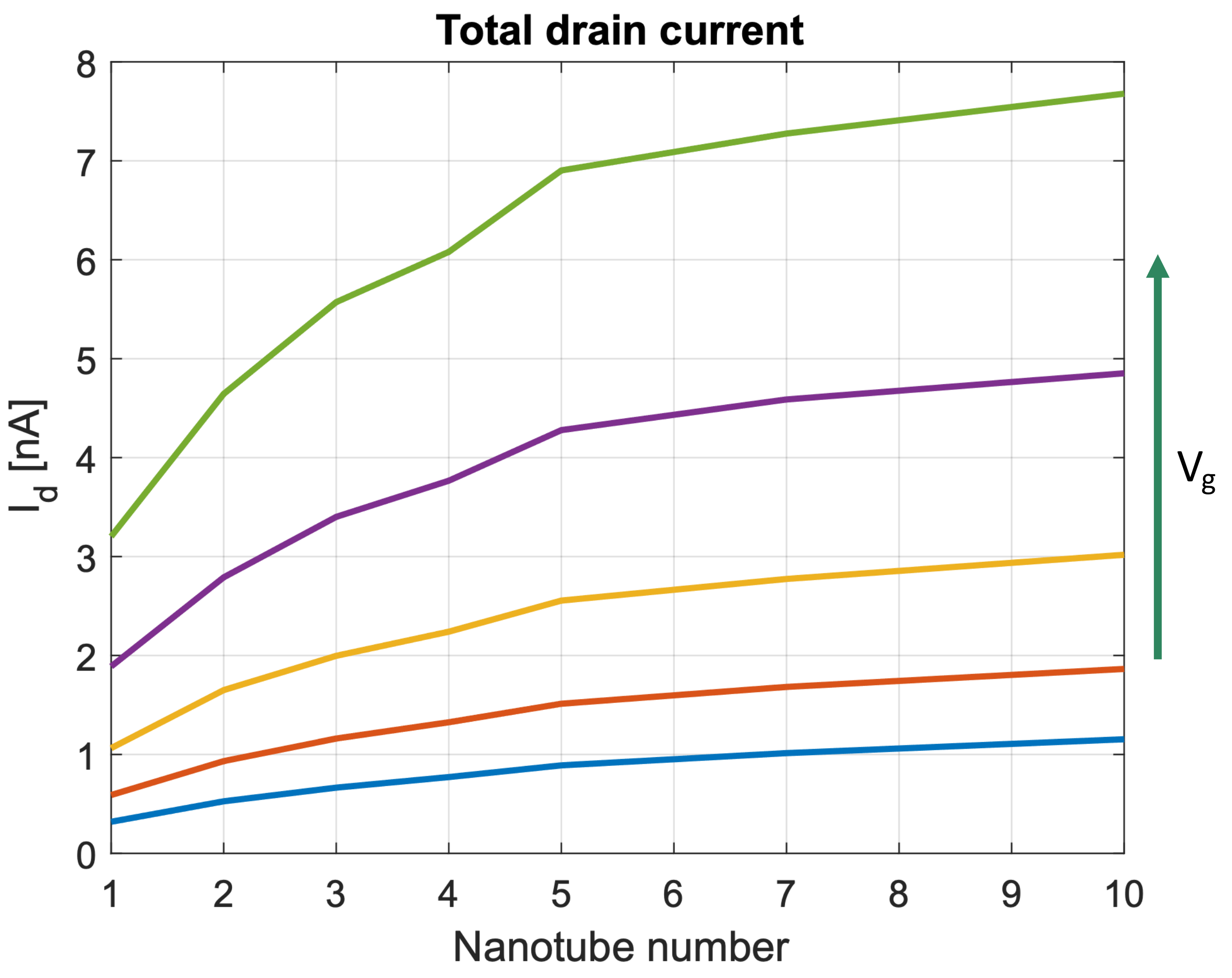
Results – Current saturation

- Distance from the gate
- Shielding from above CNTs

CNTs 1-5 more than 80% of I_{tot}



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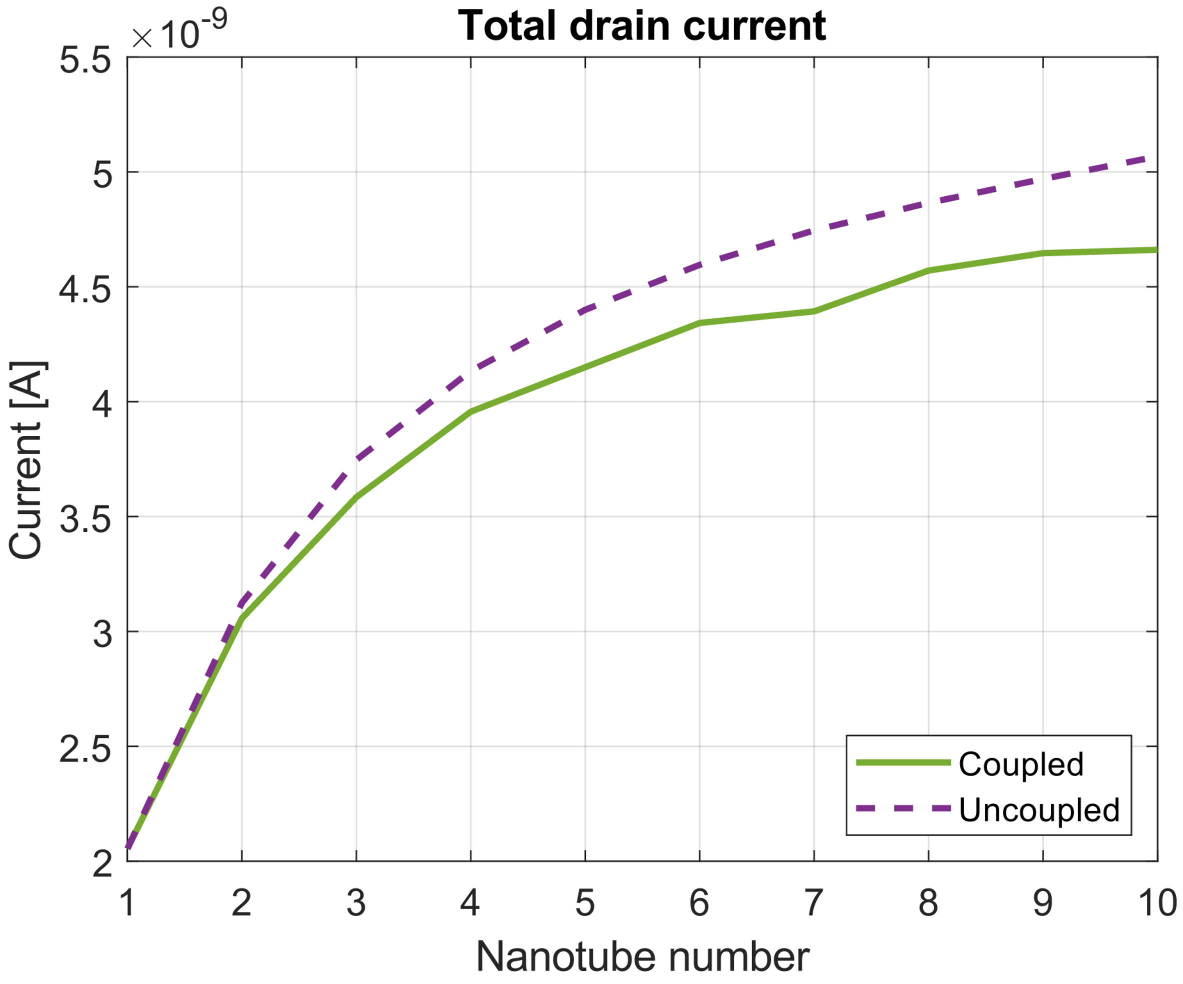
Results – Coupling

5 CNT 6% reduction
10 CNT 9% reduction



Uncoupled → One row at the time
Coupled → All rows at the same time

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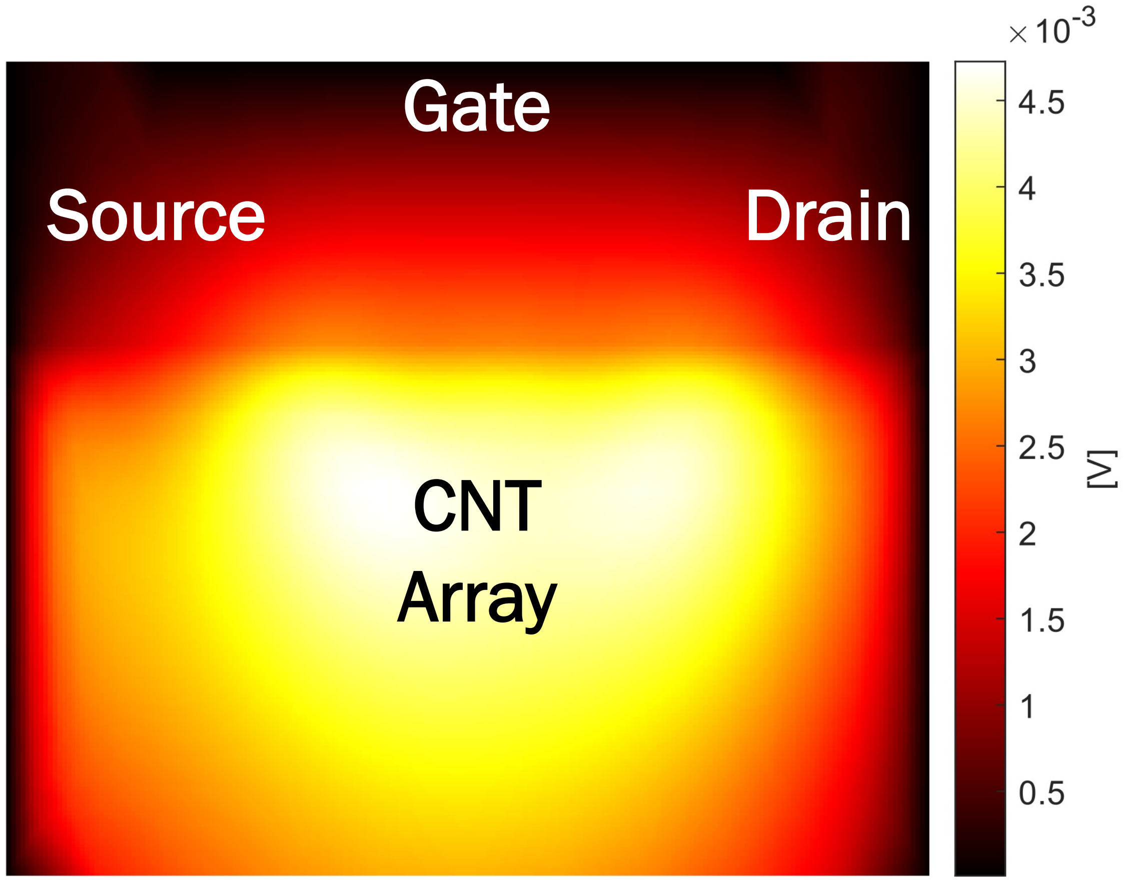
Results – Potential

Variation of the channel potential due to carriers in the CNT array

Shield Effect



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Future works

- Presence of metallic nanotubes
- Hamiltonian terms for charge correlation
- Mechanics modes analysis
- RF parameters extraction

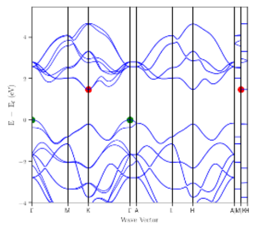
Examples

- Graphene Antenna
- MoS_2 FET
- Schrödinger – Poisson eqs.: CNT FET
- **Dirac – Maxwell eqs.: Ballistic Ratchet effect on graphene**

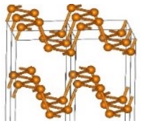
KEY DEVELOPMENT

- Bridging from atomistic to continuum level
- Interfacing mathematical models (PDEs)

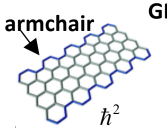
ATOMISTIC LEVEL



MoS2
Band-strcture



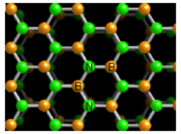
Black phosphorus



GNR

$$m_{eff.} = \frac{\hbar^2}{\frac{d^2 E}{d\,k^2}}$$

graphene



Ab-initio Methods

Quantum
Schrodinger eq.
$H(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$

Atomistic Solvers

THE BRIDGE

$$\underline{\underline{\varepsilon}}(\omega,\mathbf{k})$$
$$\underline{\underline{\mu}}(\omega,\mathbf{k})$$
$$\underline{\underline{\sigma}}(\omega,\mathbf{k})$$
$$m_{effective}$$

$$\mathbf{J}(\mathbf{r}) = \int d^2 r' \sigma_{HO}(\mathbf{r}-\mathbf{r}')\cdot\mathbf{E}(\mathbf{r}')$$
$$\sigma_{HO} = \sigma_{Hafnium\ Oxide}$$

constitutive eqs./relations

FULL-WAVE SOLVERS

Quantum: Schr./Dirac

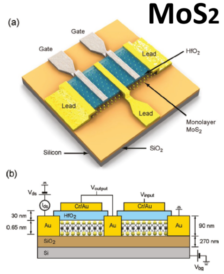
$$H(\mathbf{r},t)\psi(\mathbf{r},t) = i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}$$

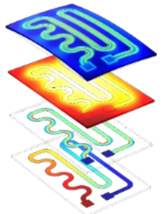
$$\nabla\times\mathbf{E}(\mathbf{r},t) = -\frac{\partial}{\partial t}\mathbf{B}(\mathbf{r},t)$$
$$\nabla\times\mathbf{H}(\mathbf{r},t) = \frac{\partial}{\partial t}\mathbf{D}(\mathbf{r},t) + \mathbf{J}(\mathbf{r},t)$$

Electromagnetic: Maxwell

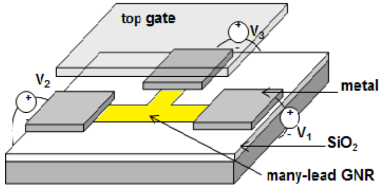
CONTINUUM LEVEL

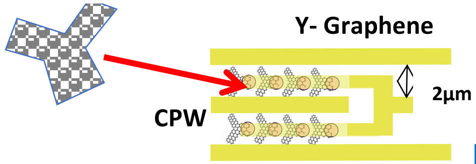
MoS2 FET





Devices
Systems
Interfaces





GreEnergy Summer School 2022

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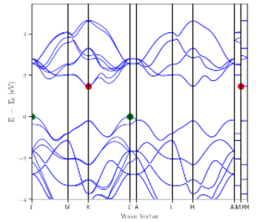
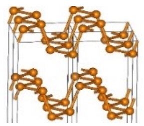
Interfacing Physics --- > PDEs equations Systems

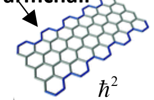
ATOMISTIC LEVEL



MoS2
Band-strcture

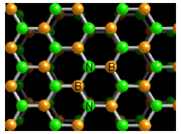


Black
phosphorus



$$m_{eff.} = \frac{\hbar^2}{\frac{d^2 E}{d\, \mathbf{k}^2}}$$

graphene



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constitutive eqs./relations

FULL-WAVE SOLVERS

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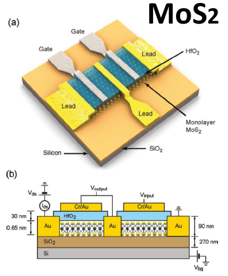
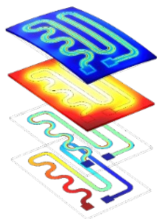
Electromagnetic: Maxwell

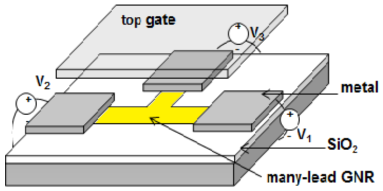
CONTINUUM LEVEL

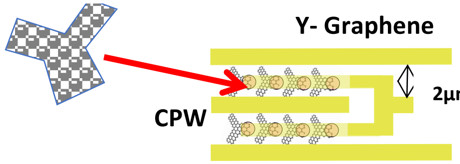
MoS2 FET





Devices Systems Interfaces





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Electrodynamics and Quantum Transport : combining Maxwell < --- > Schrödinger/Dirac

$$\nabla \times \mathbf{E}(\mathbf{r},t) = -\frac{\partial}{\partial t}\mathbf{B}(\mathbf{r},t)$$

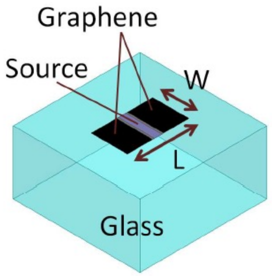
$$\nabla \times \mathbf{H}(\mathbf{r},t) = \frac{\partial}{\partial t}\mathbf{D}(\mathbf{r},t) + \mathbf{J}(\mathbf{r},t)$$

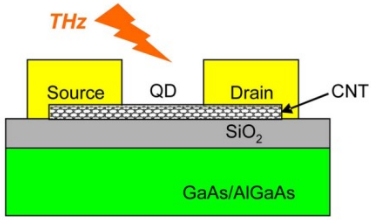
Electromagnetic: Maxwell

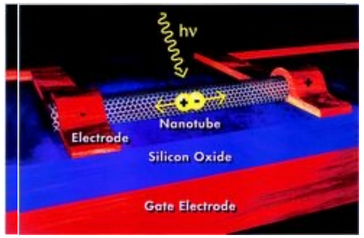
$$H(\mathbf{r},t)\psi(\mathbf{r},t) = i\hbar\frac{\partial \psi(\mathbf{r},t)}{\partial t}$$

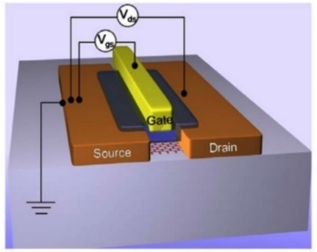
Quantum: Schrödinger/Dirac

- **interaction particles-EM field - transient**
- **Quantum dots, quantum wells**
- **Ballistic electronics**
- **non-linear devices**
- **Spintronics**
- **photodetectors**
- …









Home-made Software

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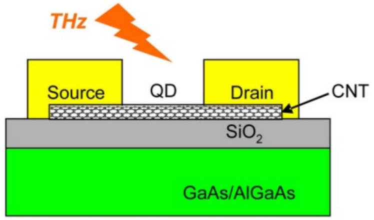
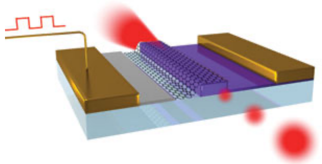
the concept





ballistic transport in the quantum device

$$\nabla \times \mathbf{E}(\mathbf{r},t) = -\frac{\partial}{\partial t}\mathbf{B}(\mathbf{r},t)$$

$$\nabla \times \mathbf{H}(\mathbf{r},t) = \frac{\partial}{\partial t}\mathbf{D}(\mathbf{r},t) + \mathbf{J}(\mathbf{r},t)$$

$$\nabla \cdot \mathbf{D}(\mathbf{r},t) = \rho(\mathbf{r},t)$$

$$\nabla \cdot \mathbf{B}(\mathbf{r},t) = 0$$

Maxwell equations

$\mathbf{J}(\mathbf{r},t)$

quantum-mechanical current

$t=t_0+1$

EM field

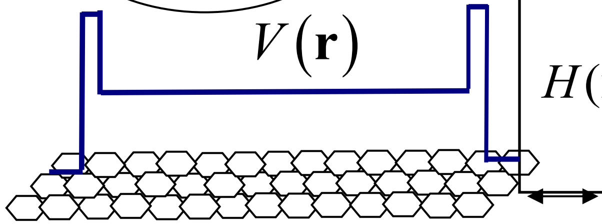
$$\mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t} \qquad \mathbf{B} = \nabla \times \mathbf{A}$$

$q\left|\underline{\psi}(\mathbf{r},t)\right|^2$

charge density

$t=t_0$

boundary conditions



$$\underline{H}(\mathbf{r},t)\underline{\psi}(\mathbf{r},t) = i\hbar\frac{\partial\underline{\psi}(\mathbf{r},t)}{\partial t}$$

$$H(\mathbf{r},t)\boldsymbol{\psi}(\mathbf{r},t) = i\hbar\left(\frac{\partial}{\partial t} + \frac{ie}{\hbar}\varphi(\mathbf{r},t)\right)\boldsymbol{\psi}(\mathbf{r},t)$$

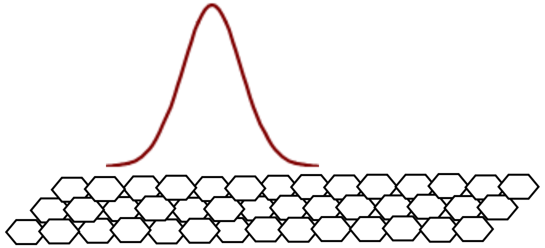
$\underline{\psi}(\mathbf{r},t)$

wave function

Dirac equation

initial conditions

$\underline{\psi}(\mathbf{r},t=0)$



Quantum-EM: Dirac Equation in the presence of an EM field

3D

$$i\hbar \frac{\partial \boldsymbol{\psi}_+}{\partial t} = v_F \boldsymbol{\sigma}\cdot\left(\hat{\mathbf{p}} + |e|\mathbf{A}\right)\boldsymbol{\psi}_- + \left(m v_F^2 - |e|\phi\right)\boldsymbol{\psi}_+$$
$$i\hbar \frac{\partial \boldsymbol{\psi}_-}{\partial t} = v_F \boldsymbol{\sigma}\cdot\left(\hat{\mathbf{p}} + |e|\mathbf{A}\right)\boldsymbol{\psi}_+ - \left(m v_F^2 + |e|\phi\right)\boldsymbol{\psi}_-$$

$$\boldsymbol{\psi} = \begin{bmatrix}\psi_0\\ \psi_1\\ \psi_2\\ \psi_3\end{bmatrix} = \begin{bmatrix}\boldsymbol{\psi}_+\\ \boldsymbol{\psi}_-\end{bmatrix} \quad with \quad \boldsymbol{\psi}_+ = \begin{bmatrix}\psi_0\\ \psi_1\end{bmatrix} \quad \boldsymbol{\psi}_- = \begin{bmatrix}\psi_2\\ \psi_3\end{bmatrix}$$

2D

$$i\hbar \frac{\partial \boldsymbol{\psi}}{\partial t} = \boldsymbol{\sigma}_{xy}\cdot\hat{\mathbf{p}}_{xy}\; v_F \boldsymbol{\psi} + m v_F^2 \sigma_z \boldsymbol{\psi}$$

$$v_F \approx \frac{c}{300}$$

$$\boldsymbol{\sigma} = \sigma_x\hat{x} + \sigma_y\hat{y} + \sigma_z\hat{z} = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\hat{x} + \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\hat{y} + \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\hat{z} = \boldsymbol{\sigma}_{xy} + \sigma_z\hat{z}$$

$$\sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \qquad \sigma_y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} \qquad \sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

$$\hat{\mathbf{p}} = p_x\hat{x} + p_y\hat{y} + p_z\hat{z} = -i\hbar\nabla = \left(-i\hbar\partial_x\right)\hat{x} + \left(-i\hbar\partial_y\right)\hat{y} + \left(-i\hbar\partial_z\right)y\hat{z} = \hat{\mathbf{p}}_{xy} + p_z\hat{z}$$

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Dirac Equation – Maxwell Equations
Graphene devices: ballistic transport, effective mass

modeling of discontinuities – absorbing boundary conditions

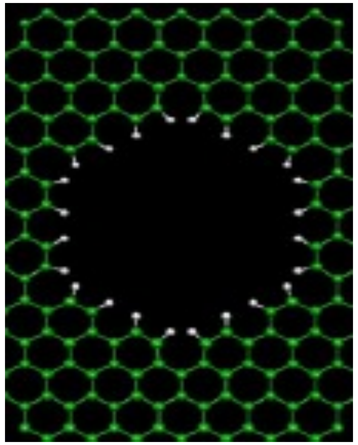
$$i\hbar \frac{\partial \psi^{+}}{\partial t} = \boldsymbol{\sigma}_{xy} \cdot \left(\hat{\mathbf{p}}_{xy} - q\mathbf{A} \right) v_F \psi^{-} + M\left(\mathbf{r}\right) v_F^2 \sigma_z \psi^{+}$$

the mass term M
may models discontinuities

$$i\hbar \frac{\partial \psi^{-}}{\partial t} = \boldsymbol{\sigma}_{xy} \cdot \left(\hat{\mathbf{p}}_{xy} - q\mathbf{A} \right) v_F \psi^{+} + M\left(\mathbf{r}\right) v_F^2 \sigma_z \psi^{-}$$

$$\boldsymbol{\sigma} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \hat{x} + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \hat{y} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \hat{z} = \boldsymbol{\sigma}_{xy} + \sigma_z \hat{z}$$

$$\psi = \begin{bmatrix} \psi^{+} \\ \psi^{-} \end{bmatrix}$$



$$\hat{\mathbf{p}} = -i\hbar\nabla = \hat{\mathbf{p}}_{xy} + p_z \hat{z}$$

$$\mathbf{J} = v_F \psi^{*} \hat{\sigma} \psi$$

$$\hat{\sigma} = \left[\sigma_x, \sigma_y \right]$$

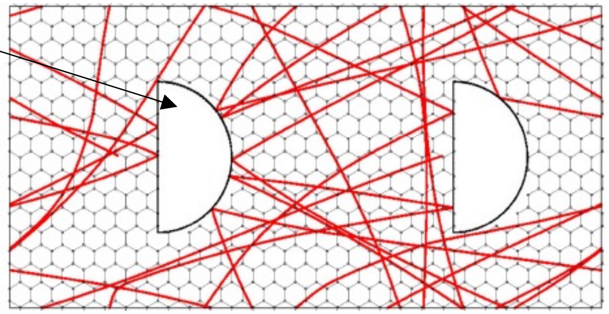
obstacles/discontinuities can be analyzed by means of the effective mass concept

L. Pierantoni, D. Mencarelli, F. Coccetti, T. Rozzi, "**Ballistic simulation of Ratchet effect in antidot lattices patterned on graphene,** 18th European Microwave Week **(EuMW),** Sept. 6 – 11, 2015, Paris, France

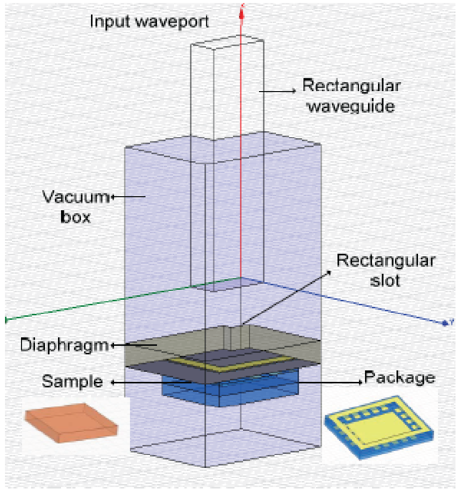
Example: Dirac + Maxwell in
Ballistic Ratchet effect in antidot patterned on graphene

… **a collective motion** of particles in a preferential direction, **due to spatially-asymmetric perturbations**

Semidisk holes



L.Ermann and D.L.Shepelyansky: Relativistic graphene ratchet



… under microwave linear polarized radiation, the effect was observed in a high mobility two-dimensional electron gas based on AlGaAs/GaAs heterojunction, with periodic array of artificial semi-discs shaped obstacles

GOAL: graphene in place of semiconductor

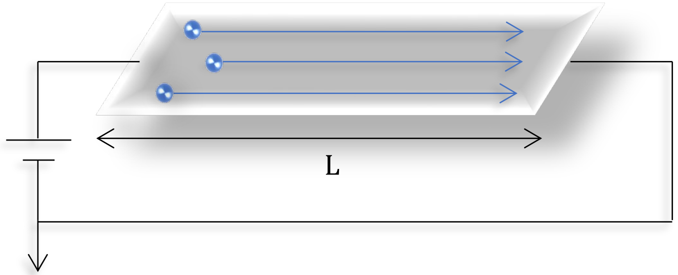
(*) D. Medhat, A. Takacs, H. Aubert, J. C. Portal, **Comparative Analysis of Different Techniques for Controlling Ratchet Effect in a Periodic Array of Asymmetric Antidots**, Micr.Conference, (2009). APMC 2009. Asia Pacific

S. Bellucci, L. Pierantoni, D. Mencarelli, **"Ballistic Ratchet effect on patterned graphene", Journal of Integrated Ferroelectrics**, Vol. 176, Issue 1, pp. 28-36, Dec. **2016**, DOI: http://dx.doi.org/10.1080/10584587.2016.1185883

Transport: Ballistic vs Diffusive

$$< l_{graphene} > \approx 10^{-6} \quad [m]$$
$$< v_{graphene} > \approx 10^{6} \quad [m/s]$$
$$< \tau_{graphene} > \approx 10^{-12} \quad [s]$$

BALLISTIC TRANSPORT

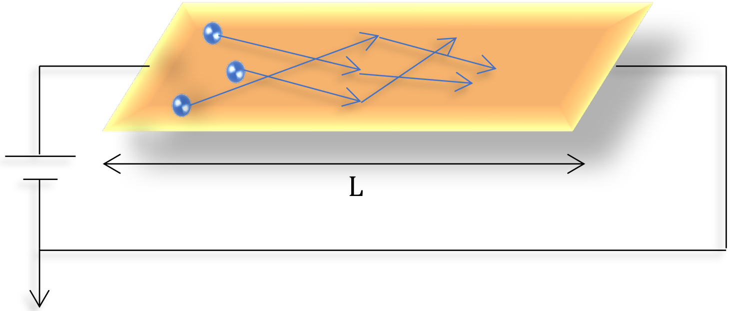


Ballistic Transport = Electrons travel **without scattering** from injected contact to absorbing contacts

weak recombination with phonons

$$< l_{cu} > \approx 10^{-10} \quad [m]$$
$$< v_{cu} > \approx 10^{5} \quad [m/s]$$
$$< \tau_{cu} > \approx 10^{-15} \quad [s]$$

NON-BALLISTIC (DIFFUSIVE) TRANSPORT



Diffusive Transport = Electrons undergo a **random walk** as they go from left to right contact

- the average distance between collisions is called the **mean free path (λ)**
- The diffusive transit time will be much longer than the ballistic transit time

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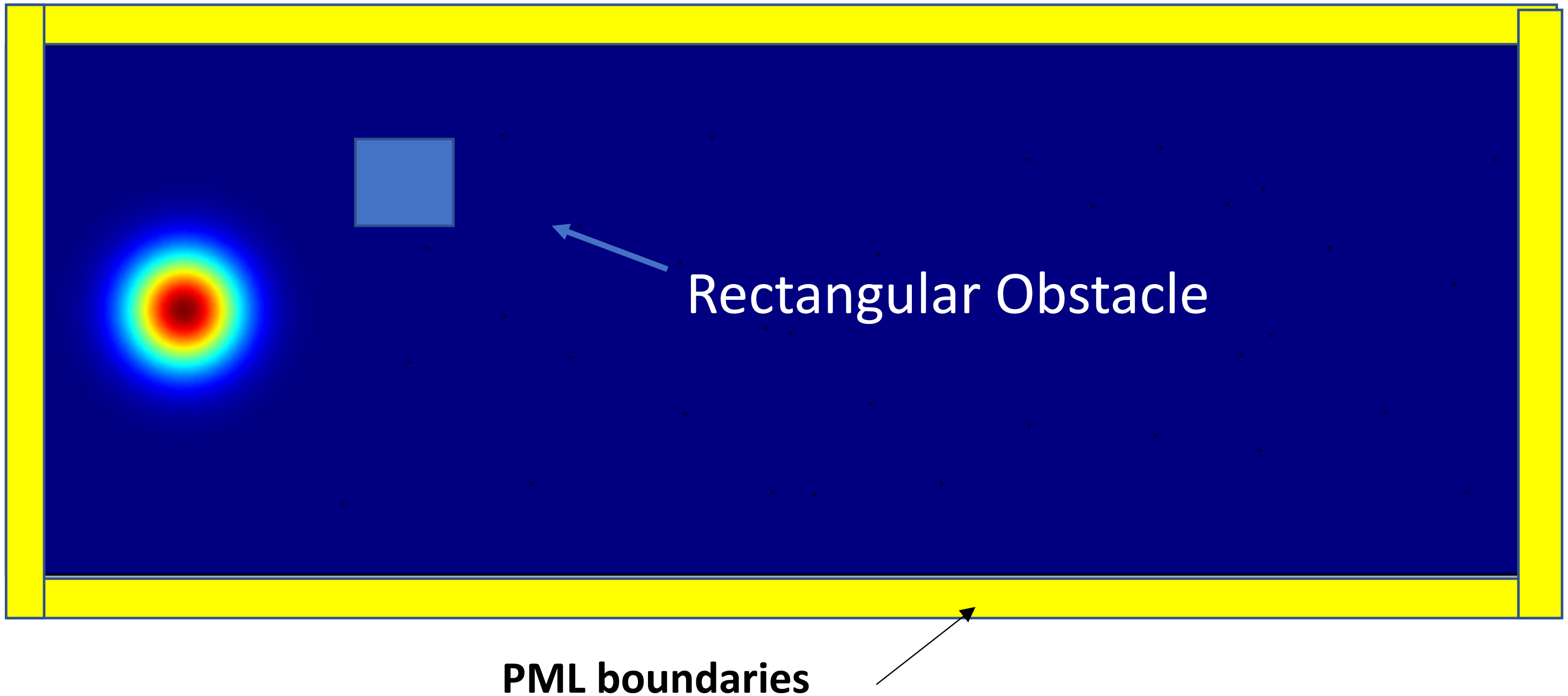
scattering/diffraction by obstacles



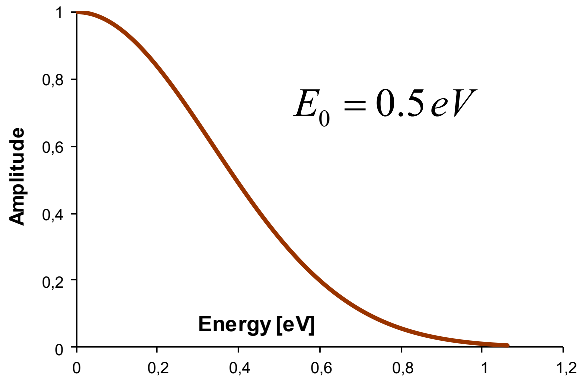
$$\Delta L_{\min} = 1\, nm$$
$$\Delta t = 0.5\ f$$
$$T_{\max} = 100\, fs$$
$$\mathrm{n_s}(t_0) = 10^{11}\, cm^{-2}$$
$$E_0 = 0.5\, eV$$
$$\Delta_{PML} = 5\, nm$$

$$\underline{\psi} = \begin{bmatrix} \psi_+ \\ \psi_- \end{bmatrix} \quad \begin{cases} \psi_+ = f(x, y; t = 0) \\ \psi_- = 0 \end{cases}$$

$$f(x, y; t = 0) = \psi_N \left\{ \exp\left(\frac{-(x - x_0)^2}{2\sigma_x^2} \right) \cdot \exp\left(\frac{-(y - y_0)^2}{2\sigma_z^2} \right) \right\}$$

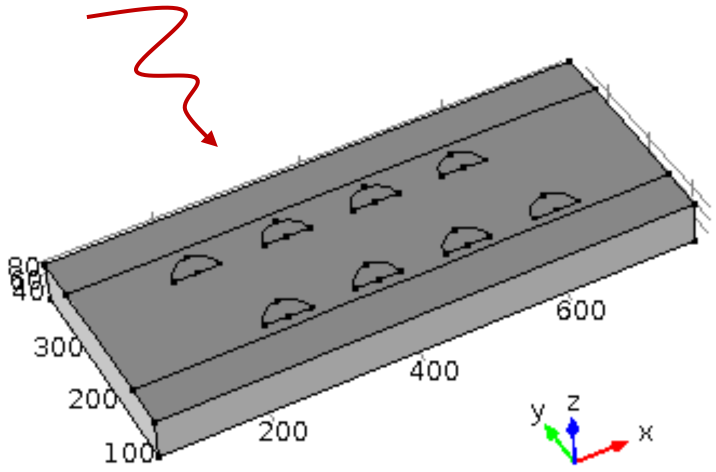
$$\int |\psi(\mathbf{r}, t)|^2 d\mathbf{r} = 1 \Rightarrow q \int |\psi(\mathbf{r}, t)|^2 d\mathbf{r} = Q_0 \quad \Rightarrow \psi_N$$

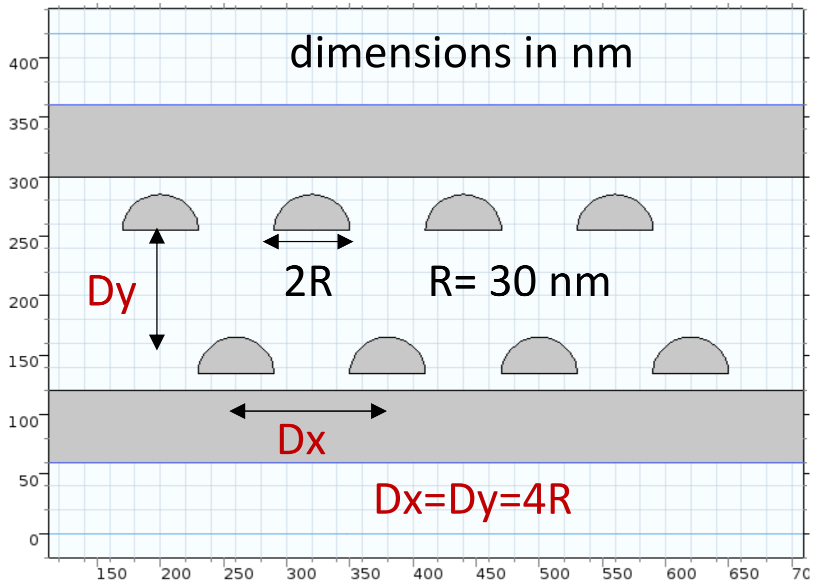
$$\mathrm{n_s}(t_0) \Leftrightarrow Q_0$$



A plane wave couples with a graphene charge wavepacket

$$E_{ext} = E_0 \cos(\omega_0 t)$$





- a uniform external time-dependent plane wave is impinging on the graphene
- EM plane wave spectrum up to THz

- a charge wavepacket is set on graphene
- corresponding Energy: up to 0.5 eV
- Q(t=0) corresponds to $n_s(t_0) = 10^{11}\ cm^{-2}$

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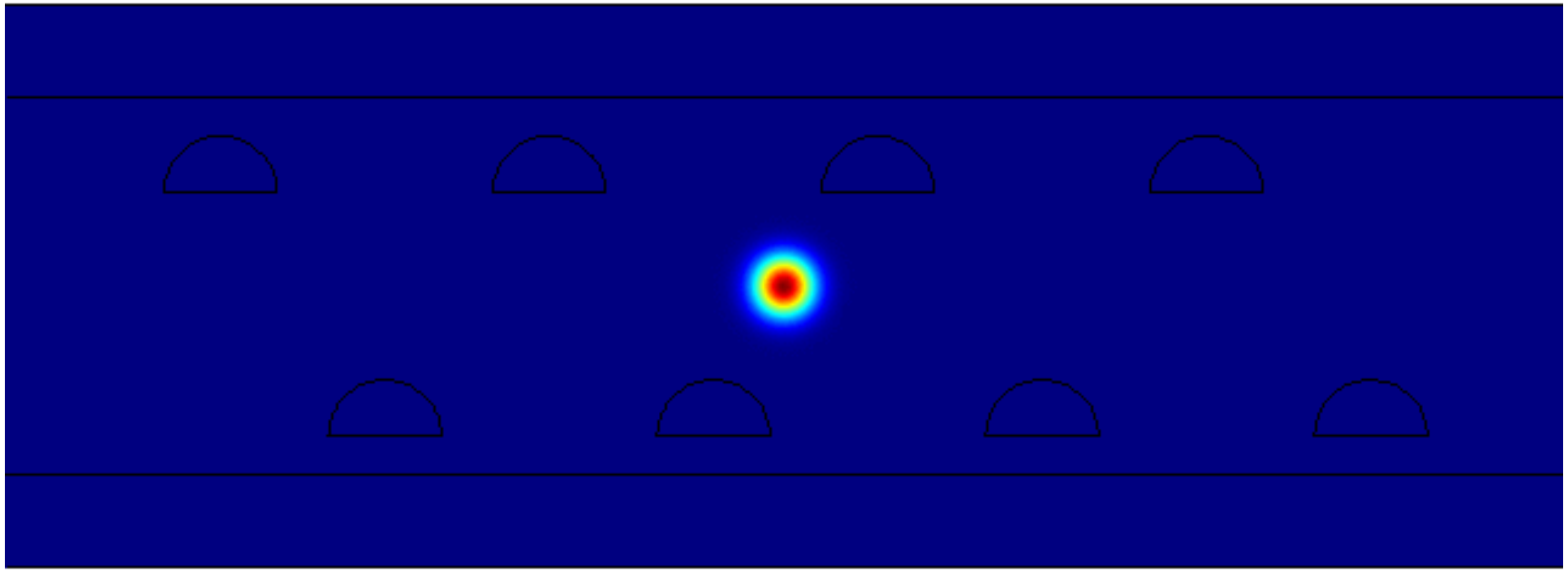
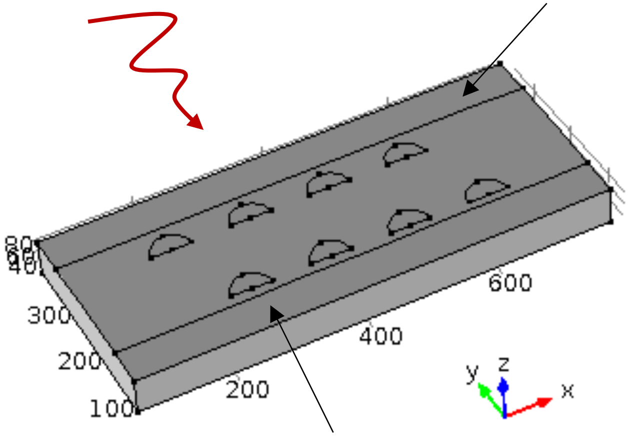
charge diffraction by ELLIPTIC obstacles



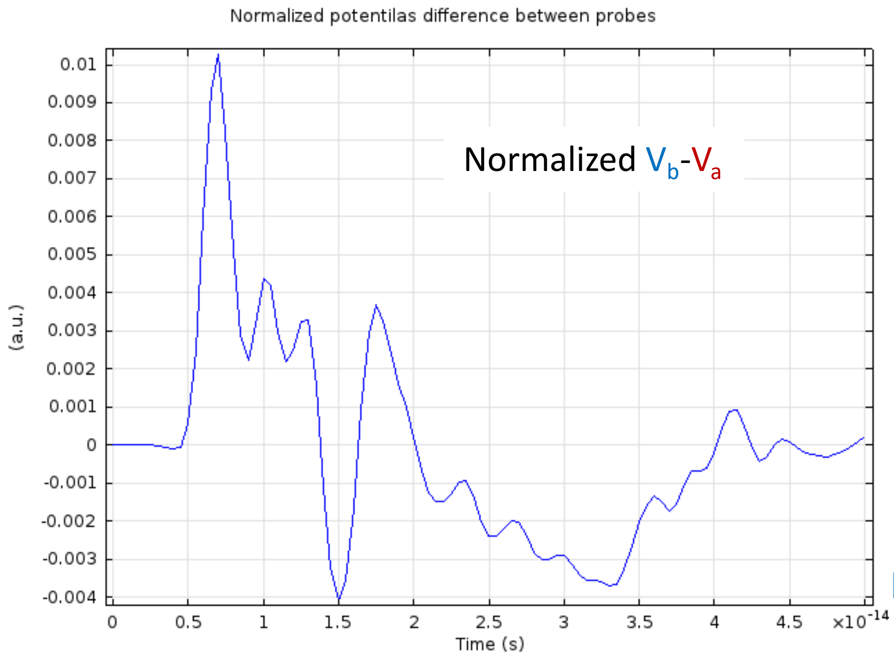
$$E_{ext} = E_0 \cos(\omega_0 t)$$

Software: originanally written in Fortran

region A



region B



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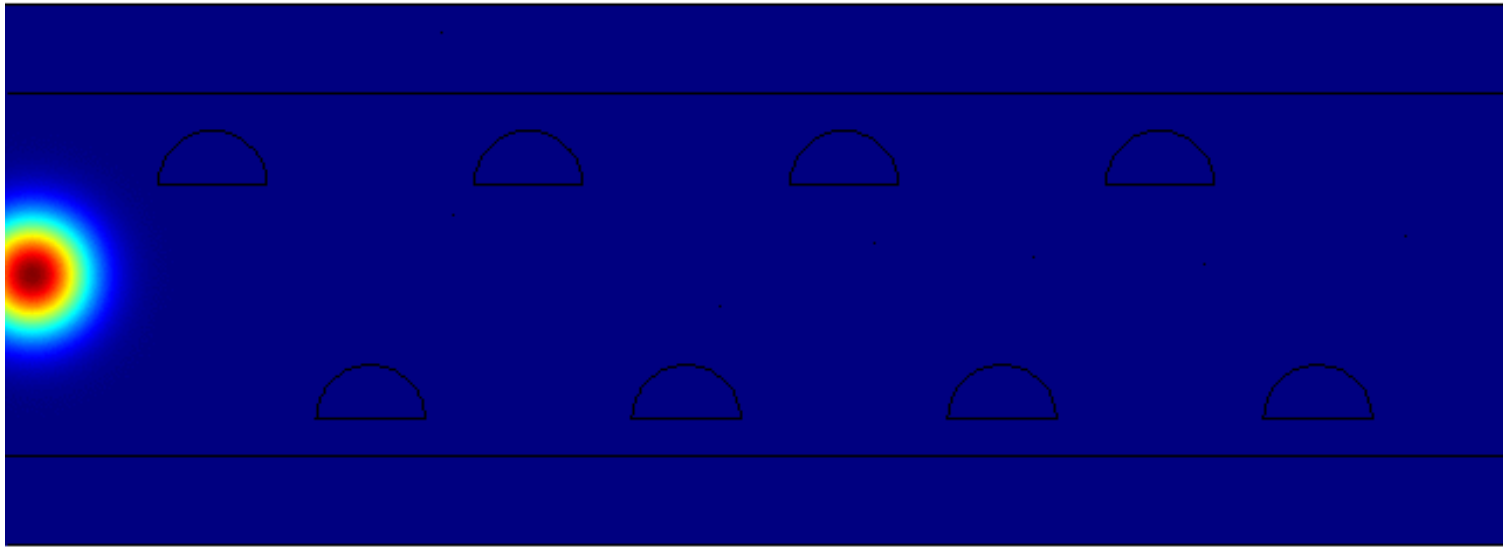
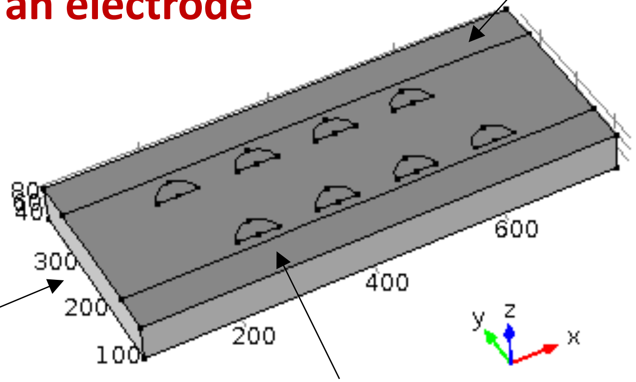
- coupling bewteen EM propagation and charge transport
- charge diffraction by obstacles

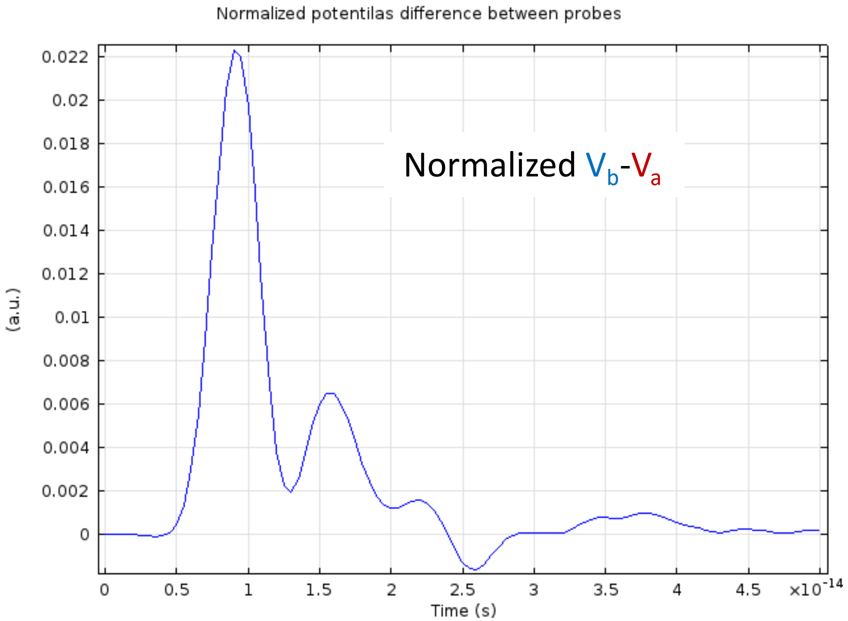


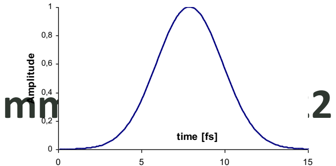
a charge wp is injected from an electrode

region A



region B





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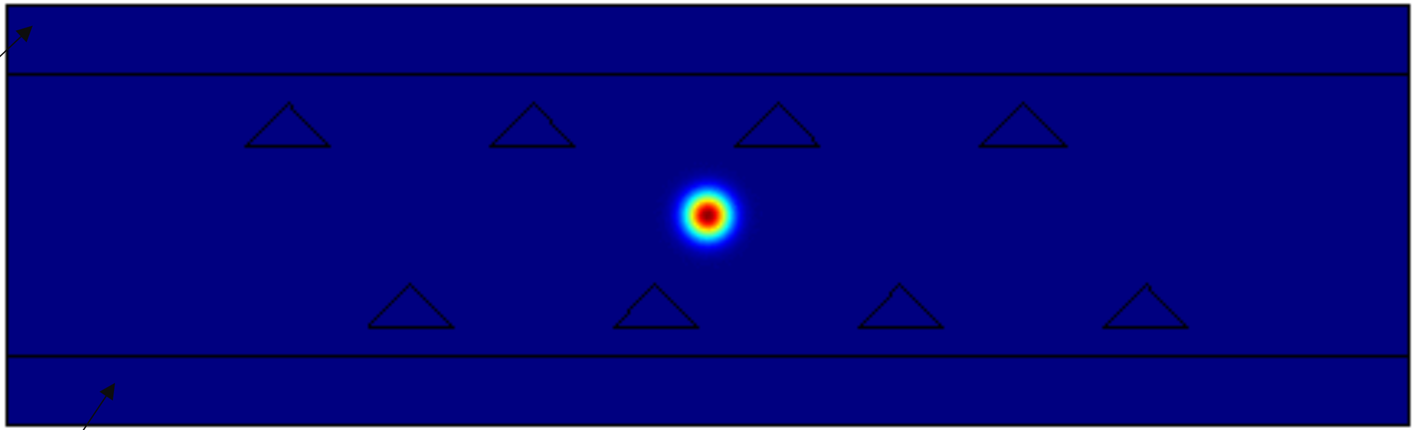
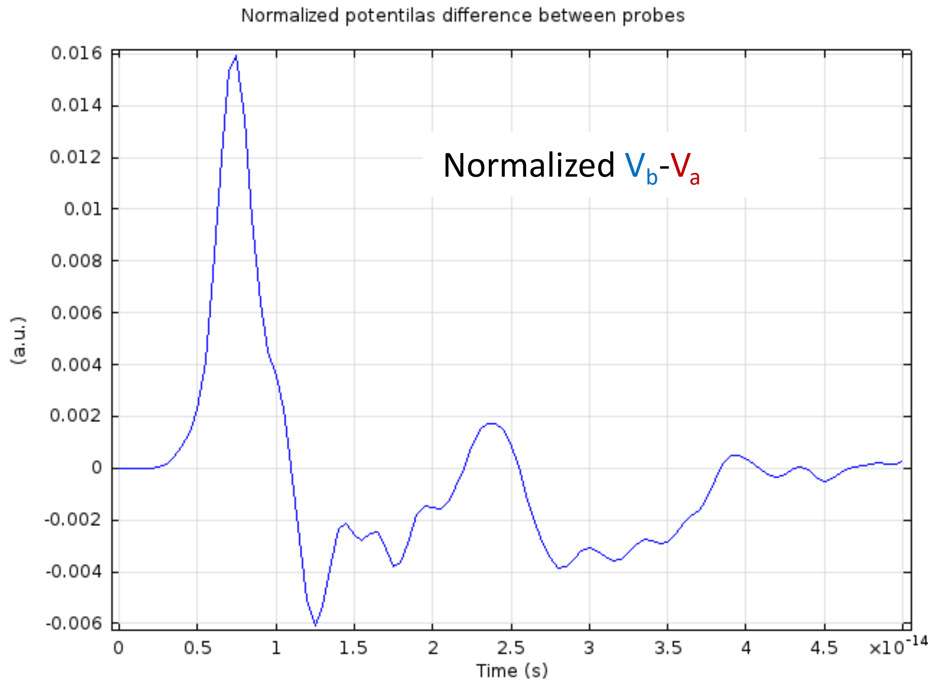
charge diffraction by TRIANGULAR obstacles

region A



region B



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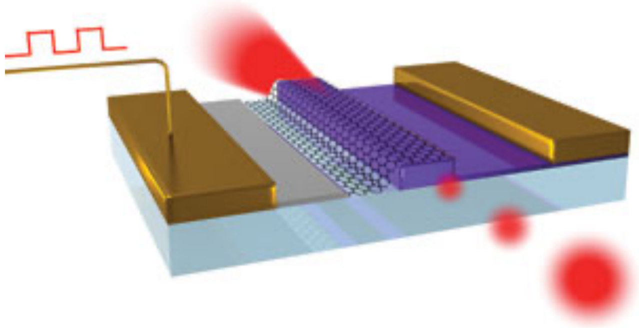
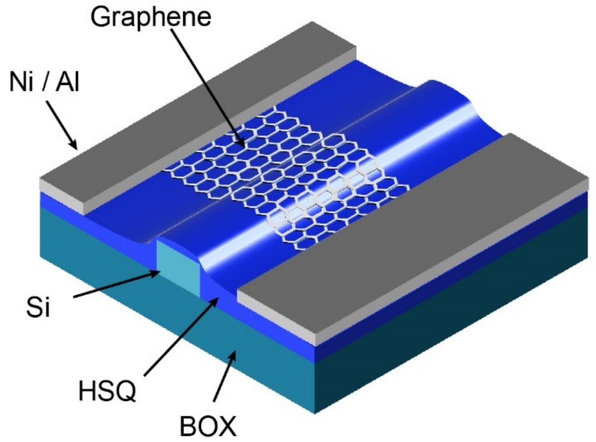
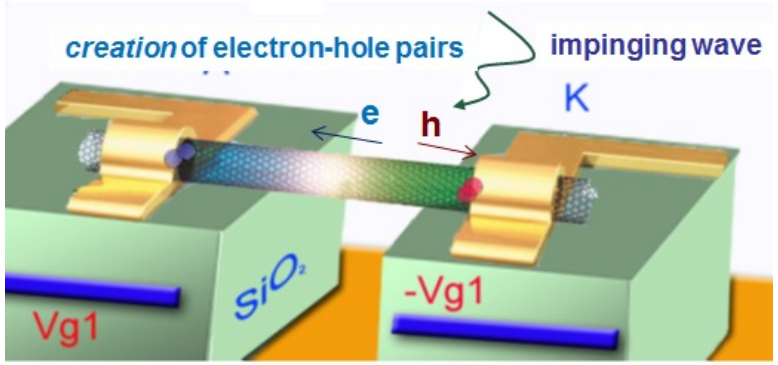
Application of the models/tools in the area of smart material-based Photonics



graphene optical modulator



graphene infrared detector



CNT photodetector

D. Mencarelli, L. Pierantoni, T. Rozzi, "Optical Absorption of Carbon Nanotube Diodes: Strength of the Electronic Transitions and Sensitivity to the Electric Field Polarization", **Journal of Applied Physics**, vol. 103, Issue 6, pp.0631-03, March 2008, DOI: 10.1063/1.2890392

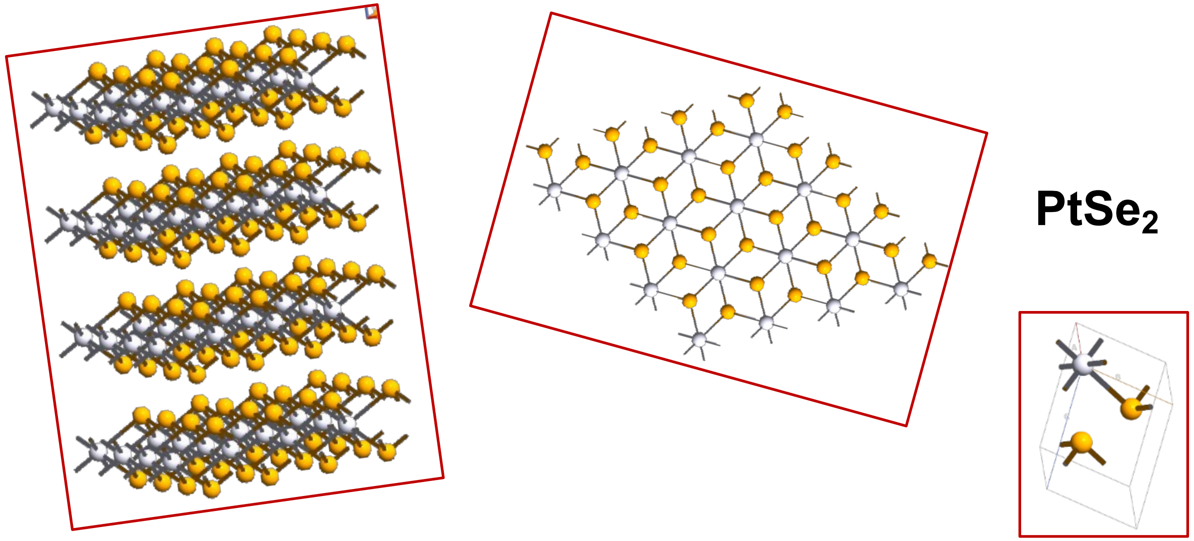
THANK YOU !!!

Back up slides

Platinum diselenide ($PtSe_2$)-based devices

- Graphene has high mobility but little bandgap
- MoS_2 has sizable bandgap but low mobility
- Black phosphorus has high mobility and sizable bandgap, but is unstable

- ❑ $PtSe_2$ has high mobility, sizable bandgap
- ❑ CMOS compatible with typical thin-film transistor processes
- ❑ is semimetallic, with low-resistance contacts–a challenge



Platinum diselenide is a transition metal dichalcogenide with a layered structure. It has an Hexagonal unit cell with a = b = 0.375 nm, c = 0.506 nm and α = β = 90°, γ = 120°.

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STEP I: ATOMISTIC SIMULATIONS

ATOMISTIC LEVEL

Ab-initio Methods

Quantum Schrodinger eq.

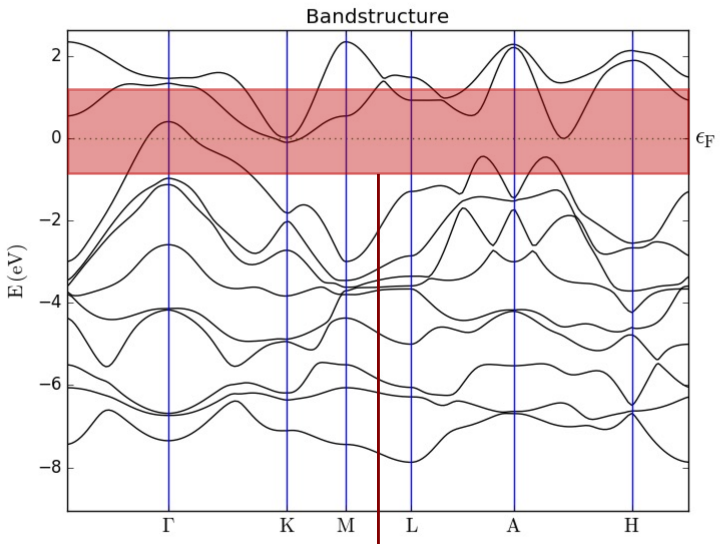
$$H(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

Atomistic Solvers

QuantumATK Synopsis Solver

MATLAB-Phyton home-made interface

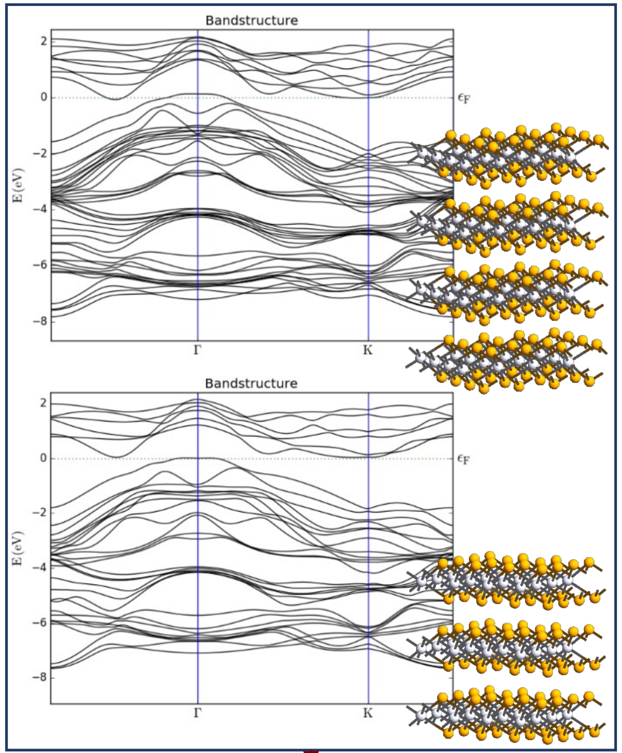
$PtSe_2$ is a metal or semiconductor depending on thickness: **bulk material** shows a metallic behaviour.

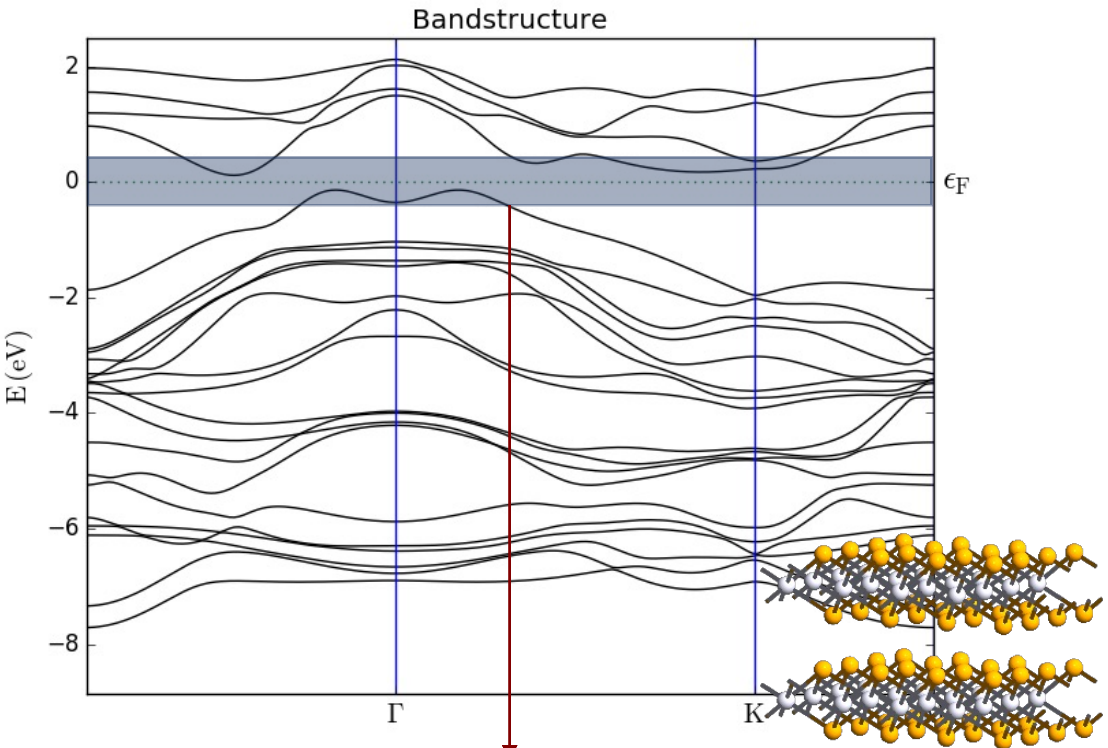


No Energy band-gap

bulk material

Band-structure vs. number of layers



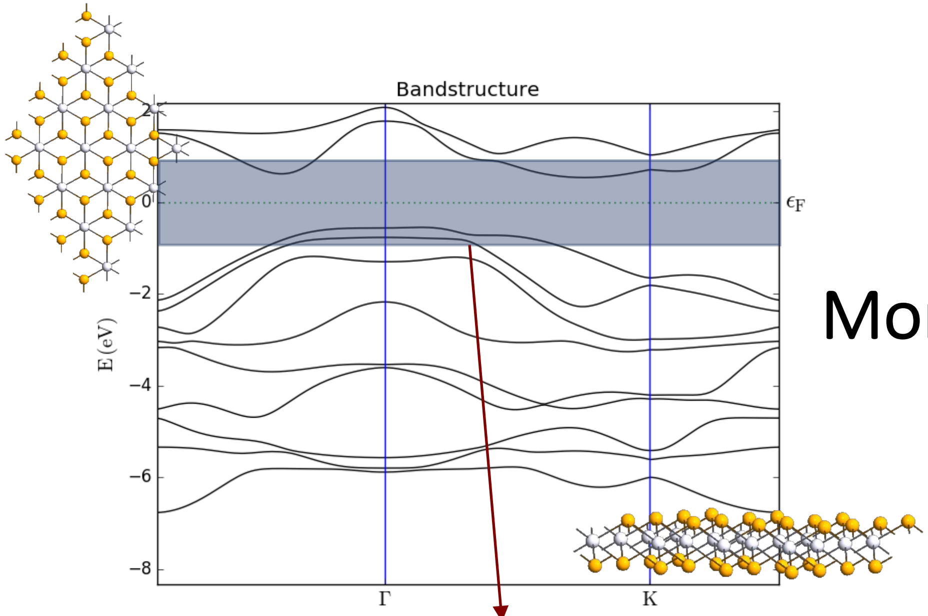


Four- and Three-Layer structure:
No Energy Band-Gap

Two-Layer structure: Energy Band-Gap of 0.31 eV, in agreement with the experimental results presented in *[1]* (0.35 eV)

[1]: **High-Electron-Mobility and Air-Stable 2D Layered $PtSe_2$ FETs**, Zhao et. al., ***Adv. Mater.*** 2017, 29, 1604230

Band-structure vs. data in literature/experimental results



Monolayer structure

Monolayer structure: Energy Band-Gap of **1.147 eV**, **in agreement with the experimental results presented in *[1]* (1.14 eV) and with the numerical calculations** done in *[2]* and *[3]* (1.2, 1.17 eV)

[1]: **Direct observation of spin-layer locking by local Rashba effect in monolayer semiconducting $PtSe_2$ film**, W. Yao, ***Nature Communications.*** 2017, 8, 14216
[2]: **Monolayer $PtSe_2$, a New Semiconducting Transition-Metal-Dichalogenide, Epitaxially Grown by Direct Selenization of Pt,** Y. Wang, ***Nano Lett.,*** 2015, 15, 4013-4018
[3]: **High-Electron-Mobility and Air-Stable 2D Layered $PtSe_2$ FETs**, Zhao et. al., ***Adv. Mater.*** 2017, 29, 1604230

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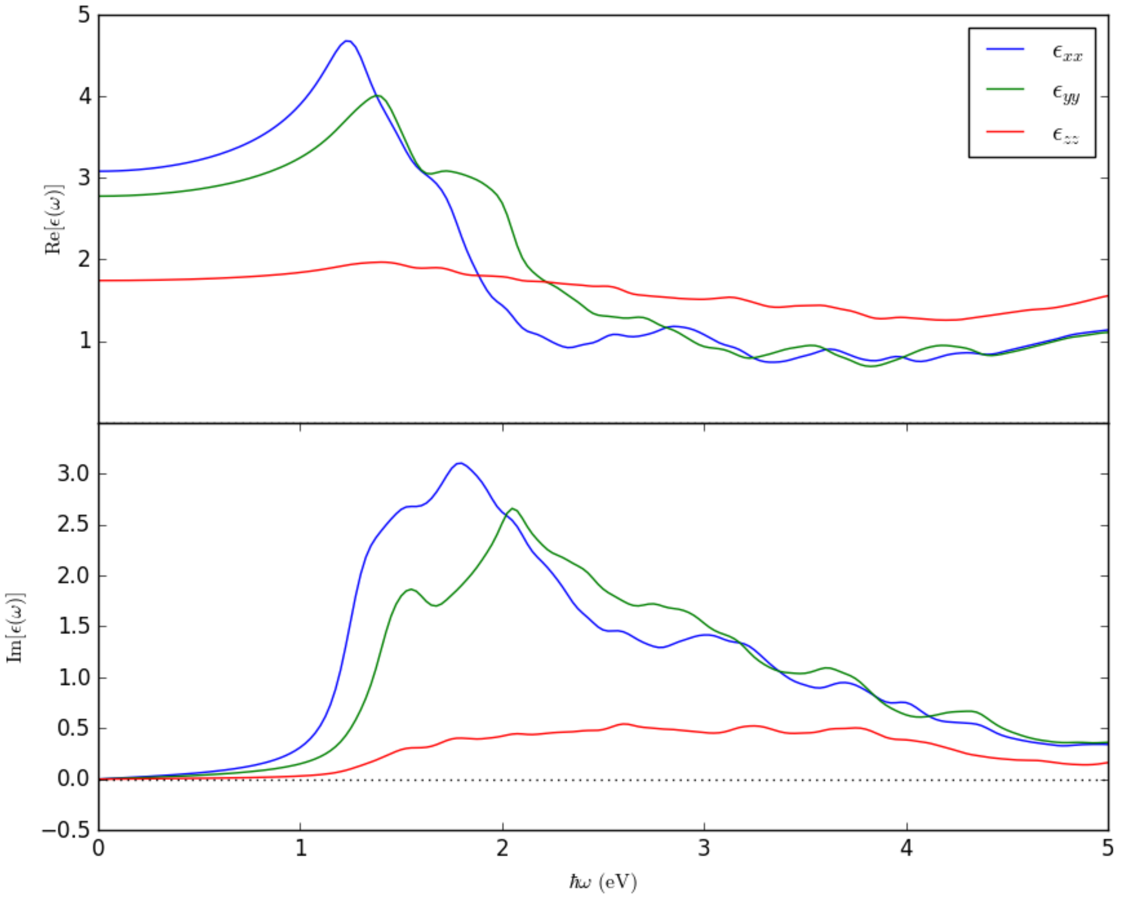
STEP II: obtaining the constitutive relations

Relative Permittivity $\varepsilon_r(\omega)$



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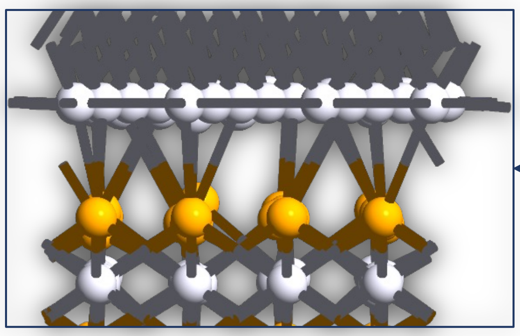
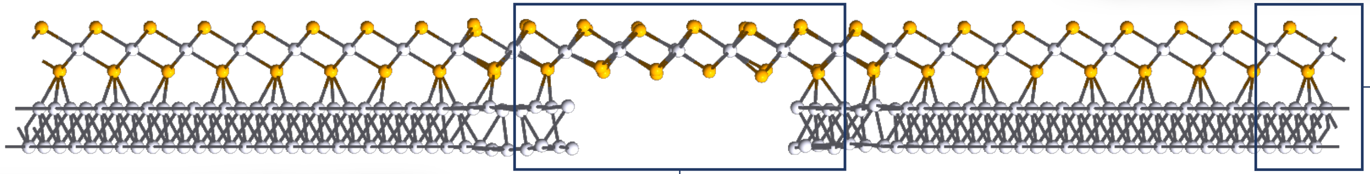
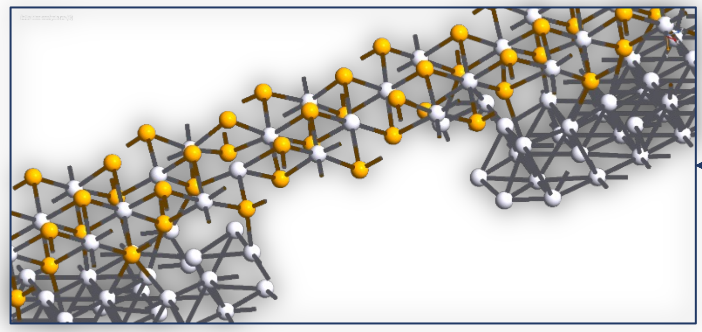
PtSe$_2$: from monolayer to bulk to metal-contact

The Selenium atoms strongly interact with the Platinum surface (i.e. the bulk material representing the substrate), which significantly decrease the losses







In the central region of the modeled device a randomly generated disorder has been introduced to produce results closer to the experimental ones

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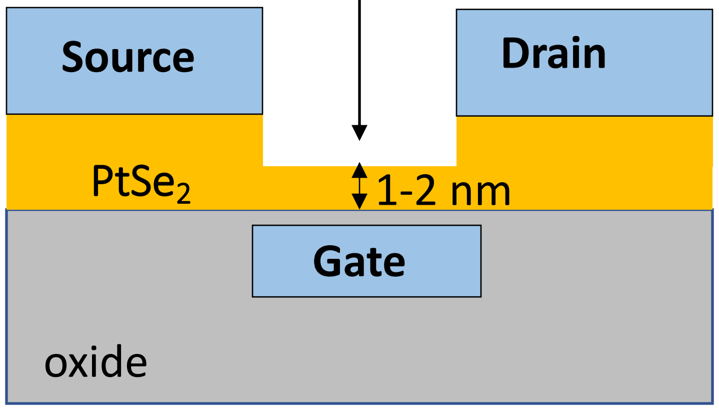
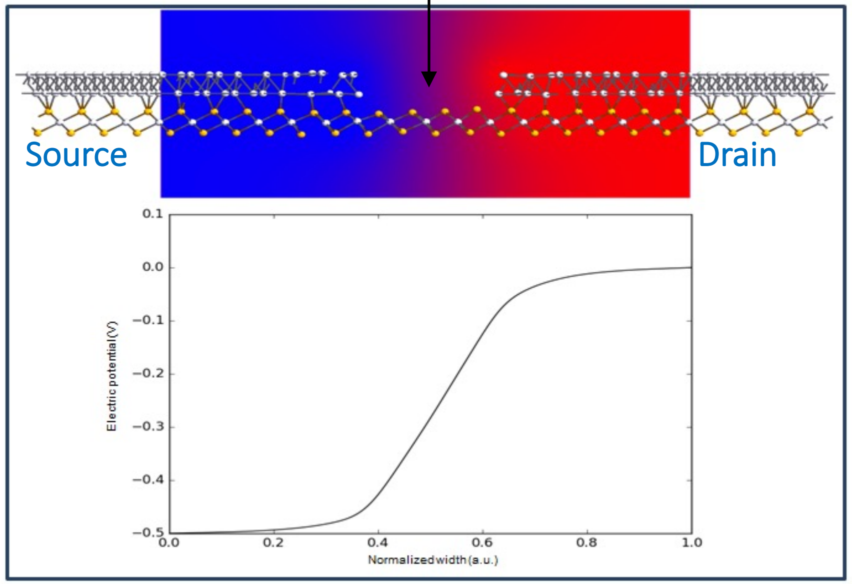
STEP III: inserting the constitutive relations into the full-wave EM simulations

- ❑ **NOTE: for the modeling of realistic $PtSe_2$ FET we are trying:**
- ▪ **A total ATOMISTIC simulation (but with a limit of 5k atoms-domain)**
- ▪ **A full-wave EM simulation (extreme scale contrast)**
- ▪ **An interfaced ATOMISTIC-EM model/simulation**





❑ Results are in the context of a International Project

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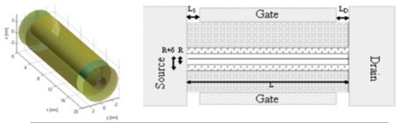
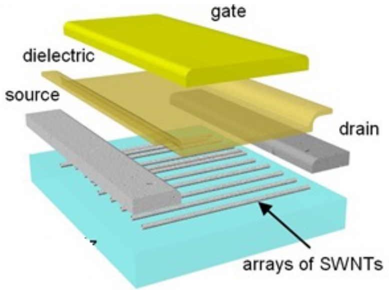
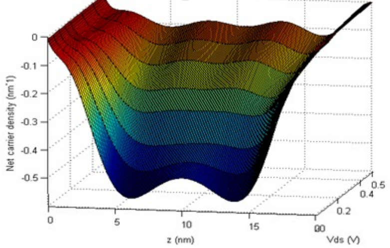


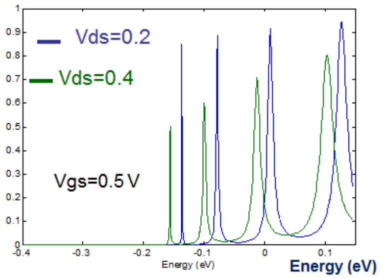


CNT DESIGN TOOLS I

Charge Distribution



Electronic Transmittivity



INPUT DATA

ELECTRICAL DATA

- geometry/shapes
- electrical bias
- external field
- dielectric const.
- **metal work function**

QUANTUM PARAMETERS

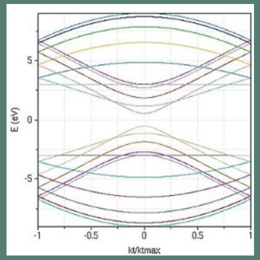
- chirality
- radius/lenght
- Fermi levels
- SW or MW-CNT
- CNT array
- CNT cascade
- energy range
- …

NUMERICAL CONSTRAINTS

- space step
- energy step
- no. iteratrions
- …

PRELIMINARY CALCULATION

- CNT electron/hole
- effective mass
- DISP. CURVES
- charge normalization



$$m_{eff.} = \frac{\hbar^2}{\frac{d^2 E}{d k^2}}$$

Schrödinger Equation

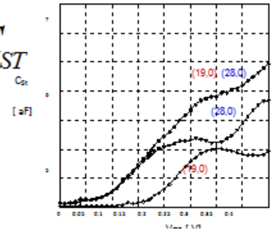
Poisson Equation

- FEM-FD based algorithms
- Iterative process
- SIMULTANEOUS SOLUTION
- optimization
- convergence control
- MATLAB code
- …

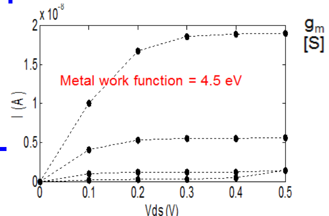
OUTPUT DATA

capacitances

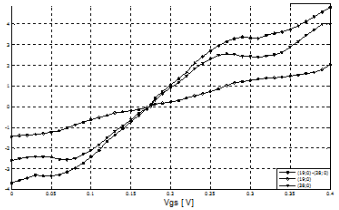
C_{ST}

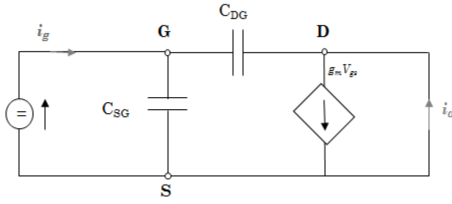


Me-Carbon contact

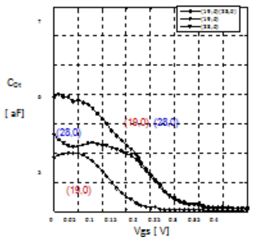


transconductance





CNT-FETequivalent circuit



C_{DT}

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CNT DESIGN TOOLS II

CNT DEVICES

ELECTRICAL DATA

- geometry/shapes
- electrical bias
- external field
- dielectric const.
- metal work function

QUANTUM PARAMETERS

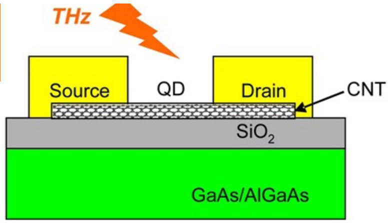
- chirality
- radius/lenght
- Fermi levels
- SW or MW-CNT
- CNT array
- CNT cascade
- energy range
- ...

NUMERICAL CONSTRAINTS

- space step
- energy step
- no. iteratrions
- ...

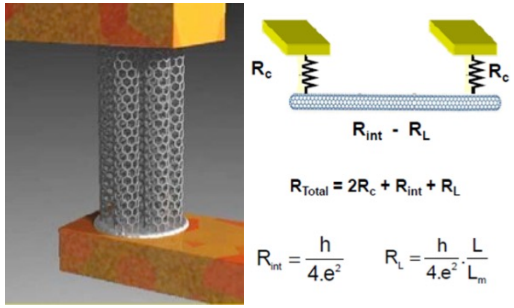
Schrödinger Equation

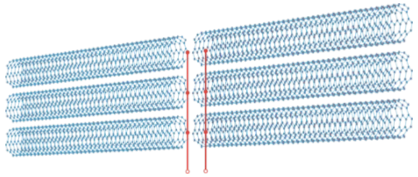
Poisson Equation



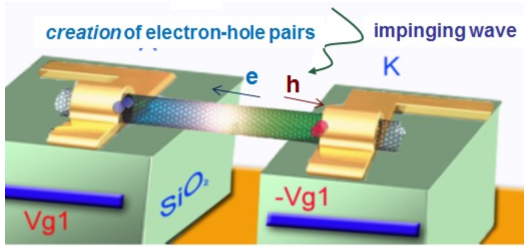
THZ DETECTOR s, PN-JUNCTIONs, QUANTUM DOTS

CNT INTERCONNECTS





CNT NANOANTENNAS



PHOTOGENERATION OF CURRENT

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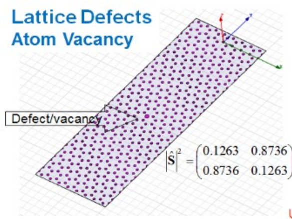
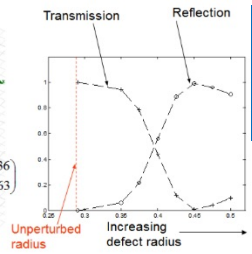
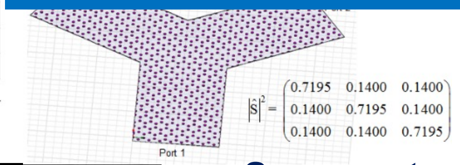
GRAPHENE DEVICES DESIGN TOOLS III

GRAPHENE/GNR CIRCUITS & FET DESIGN SOFTWARE





BALLISTIC freq. domain



ELECTRICAL DATA

- geometry/shapes
- electrical bias
- external field
- dielectric const.
- metal work function

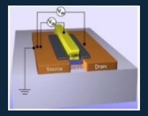
QUANTUM PARAMETERS

- width/lenght
- Fermi levels
- metallic/semimetallic/semiconductiing GNR
-

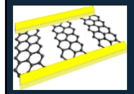
NUMERICAL CONSTRAINTS

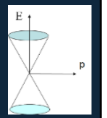
- space step
- energy step
- no. iteratrions
- adaptive energy refinement

PRELIMINARY CALCULATION



- GNR electron/hole
- effective mass
- DISP. CURVES
- charge normalization





Dirac Equation

Poisson Equation

- FEM-FD based algorithms
- Iterative process
- SIMULTANEOUS SOLUTION
- optimization
- convergence control
- MATLAB code
- …

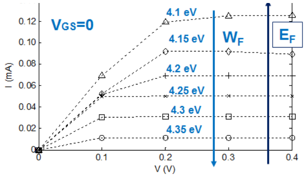
S-parameters

Graphene/GNR CIRCUITS

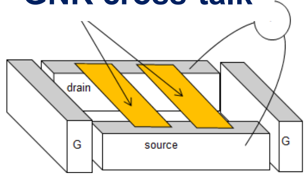
Graphene/GNR FET

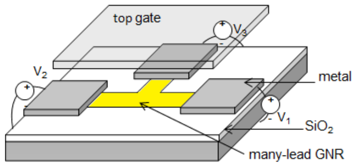
FET Analysis

Me-Carbon contact



GNR cross-talk





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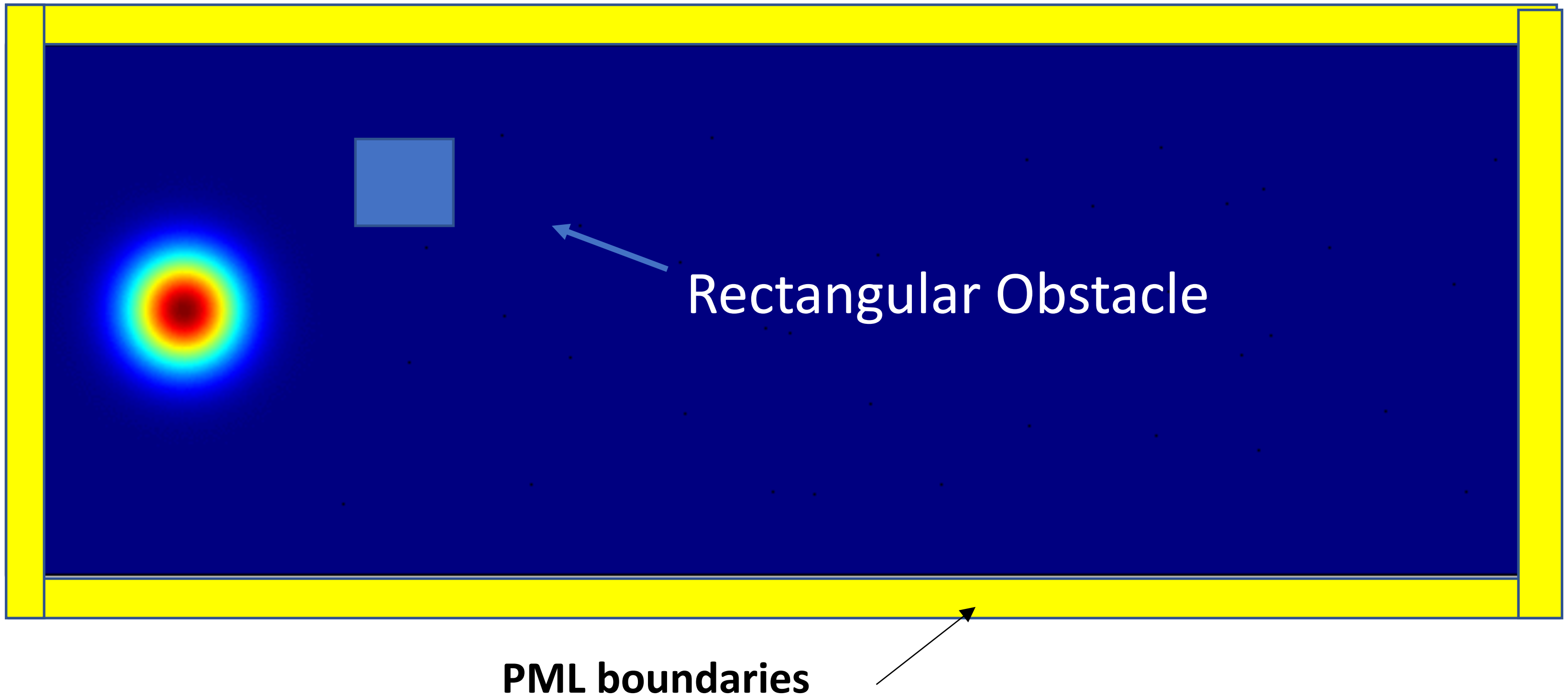
scattering/diffraction by obstacles



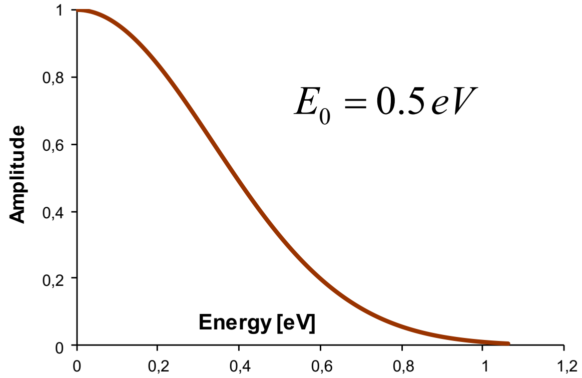
$$\Delta L_{\min} = 1\, nm$$
$$\Delta t = 0.5\ f$$
$$T_{\max} = 100\, fs$$
$$n_s(t_0) = 10^{11}\ cm^{-2}$$
$$E_0 = 0.5\, eV$$
$$\Delta_{PML} = 5\, nm$$

$$\underline{\psi} = \begin{bmatrix} \psi_+ \\ \psi_- \end{bmatrix} \quad \begin{cases} \psi_+ = f(x, y; t=0) \\ \psi_- = 0 \end{cases}$$

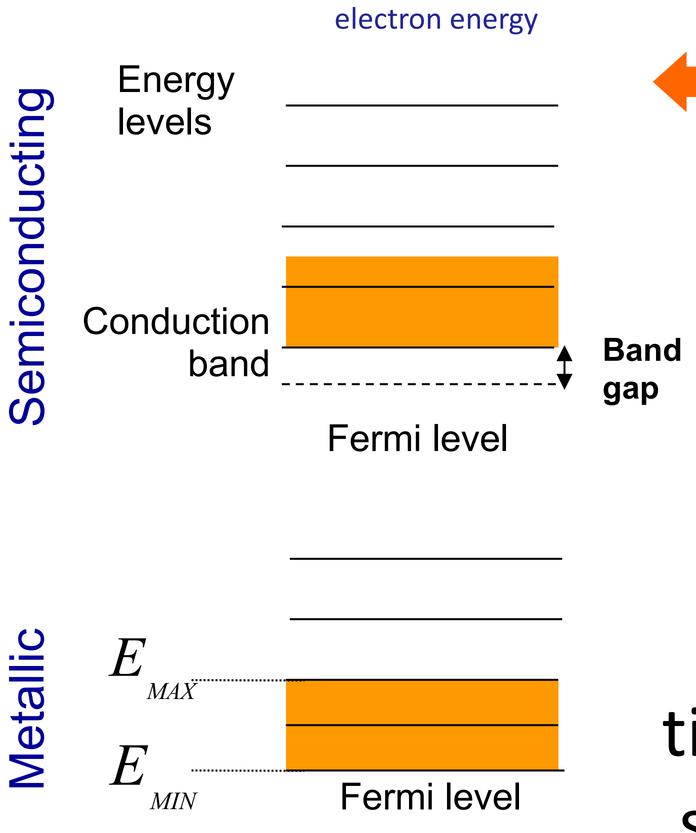
$$f(x, y; t=0) = \psi_N \left\{ \exp\left(\frac{-(x-x_0)^2}{2\sigma_x^2} \right) \cdot \exp\left(\frac{-(y-y_0)^2}{2\sigma_z^2} \right) \right\}$$

$$\int |\psi(\mathbf{r}, t)|^2 d\mathbf{r} = 1 \Rightarrow q \int |\psi(\mathbf{r}, t)|^2 d\mathbf{r} = Q_0 \quad \Rightarrow \psi_N$$

$$n_s(t_0) \Leftrightarrow Q_0$$



Physical Properties → Computational Parameters



$$E_{elec} = \omega\hbar = hf_{elec} \Rightarrow f_{elec} = \frac{E_{elec}}{h} \qquad \hbar = \frac{h}{2\pi}$$

$$E_{MAX} \Rightarrow f_{MAX} \qquad E_{MIN} \Rightarrow f_{MIN}$$

$$\lambda_{MAX} = \frac{v_F}{f_{MIN}} \qquad \lambda_{MIN} = \frac{v_F}{f_{MAX}}$$

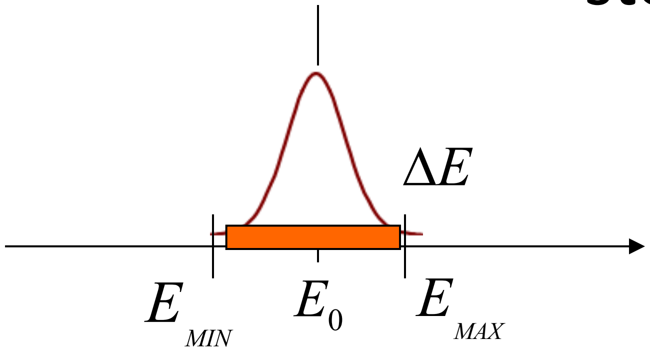
$$\Delta L_{grid} \le \frac{1}{30}\lambda_{MIN}$$ space-step

$$\Downarrow$$

time step

$$\Delta t_{EM} \le \frac{\Delta L_{grid}}{2c} \qquad c = 3\cdot 10^8 \quad m/s$$ EM grid (TLM)

$$\Delta t_{GNR} \le \frac{\Delta L_{grid}}{v_F} \qquad v_F \approx c/300 \quad m/s$$ GNR grid



Propagation of a Gaussian pulse for wide-band electron energy

$$\underline{\psi} = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} \quad \begin{cases} \psi_1 = f(x,z;t) \\ \psi_2 = -if(x,z;t) \\ \psi_3 = \psi_4 = 0 \end{cases}$$

$$\int \left|\psi(\mathbf{r},t)\right|^2 d\mathbf{r} = 1 \Rightarrow q\int \left|\psi(\mathbf{r},t)\right|^2 d\mathbf{r} = Q_T$$

$$f(x,z;t) = A_N \exp\left(\frac{-(t-t_0)^2}{2\sigma_T^2}\right)\left\{\exp\left(\frac{-(x-x_0)^2}{2\sigma_x^2}\right)\cdot\exp\left(\frac{-(z-z_0)^2}{2\sigma_z^2}\right)\right\}$$

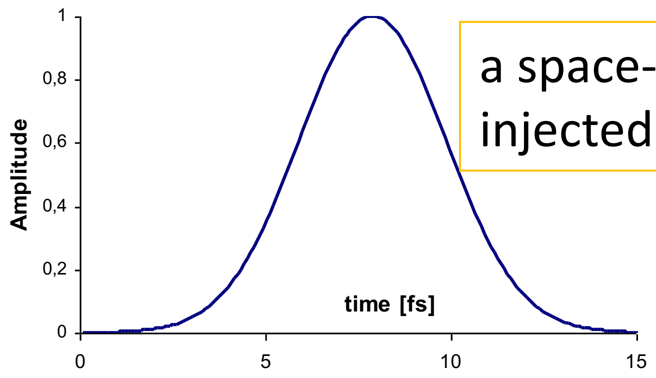
Computational Parameters

$$E_{MAX} = 1\ eV \quad f_{MAX} = 289\ THz$$

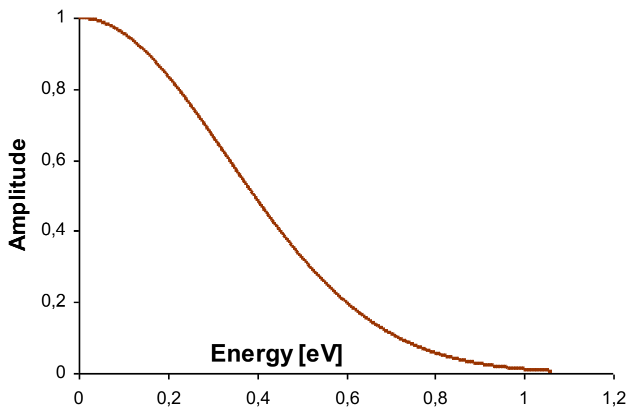
$$\sigma_T = 2 / f_{MAX}$$

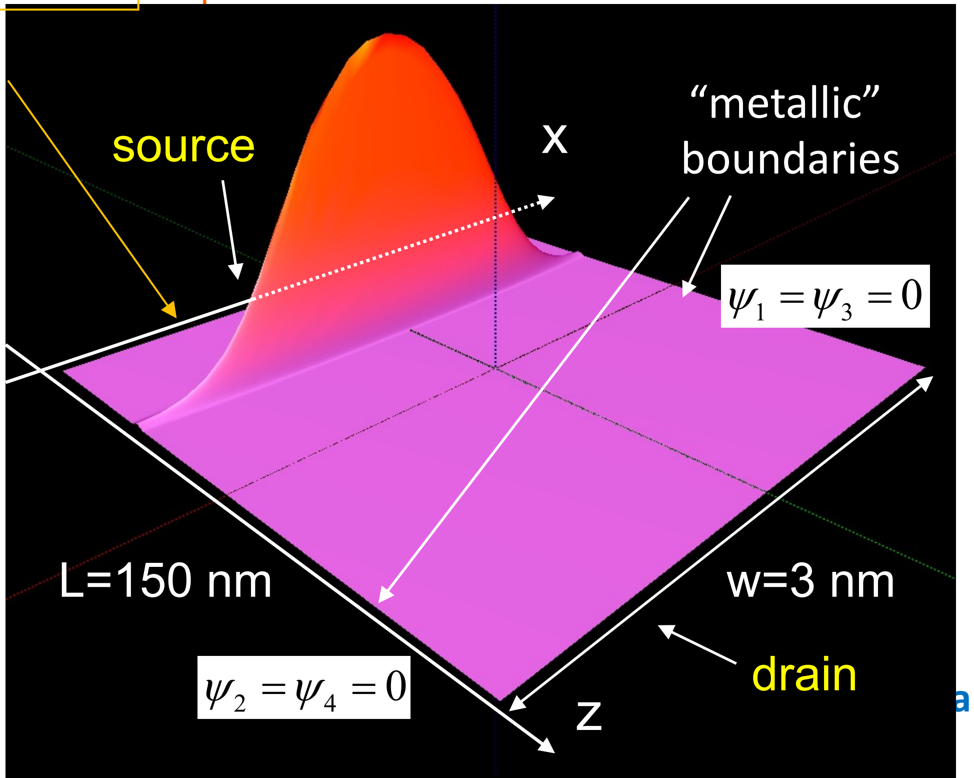
$$\lambda_{MIN} = 5\ nm \Rightarrow \Delta L_{grid} = \frac{1}{32}\lambda_{MIN} = 0.12\ nm$$

$$\Delta t_{EM} = \frac{\Delta L_{grid}}{2c_0} = 2*10^{-4}\ fs \quad \Delta t_{GNr} = \frac{\Delta L_{grid}}{v_F} = 0.12\ fs$$

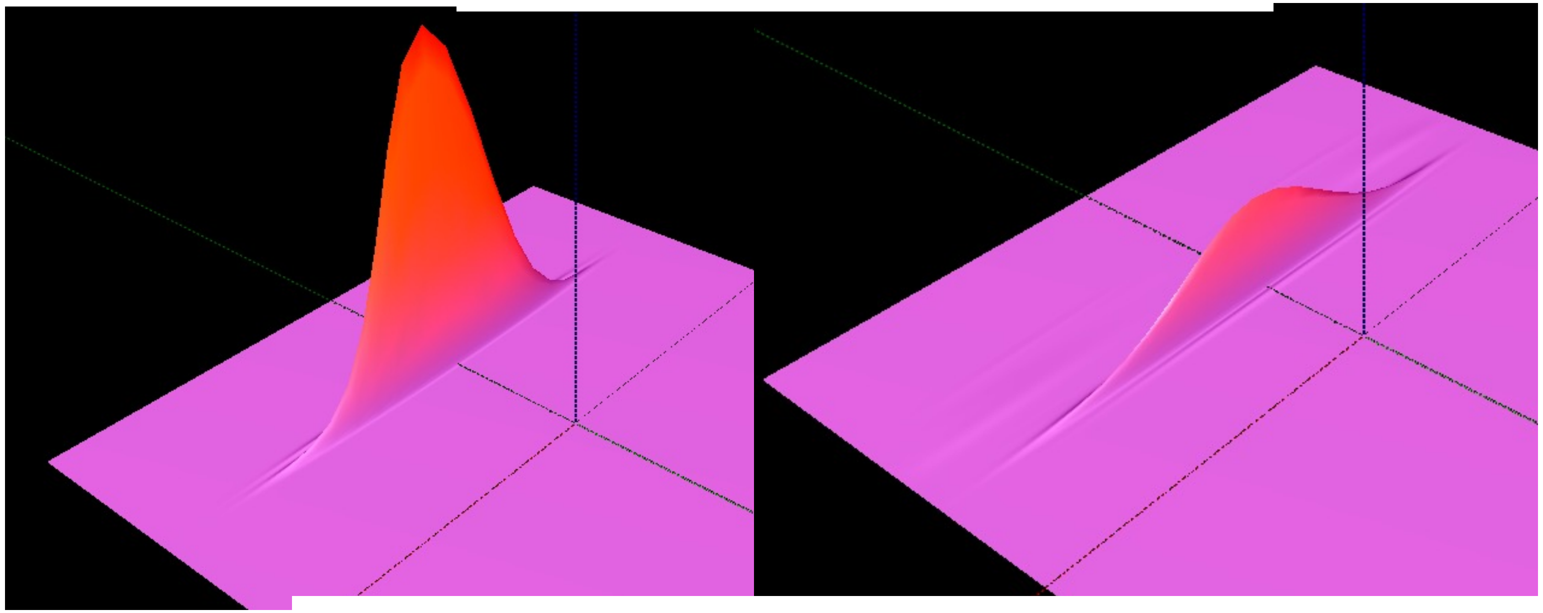


a space-time pulse is injected

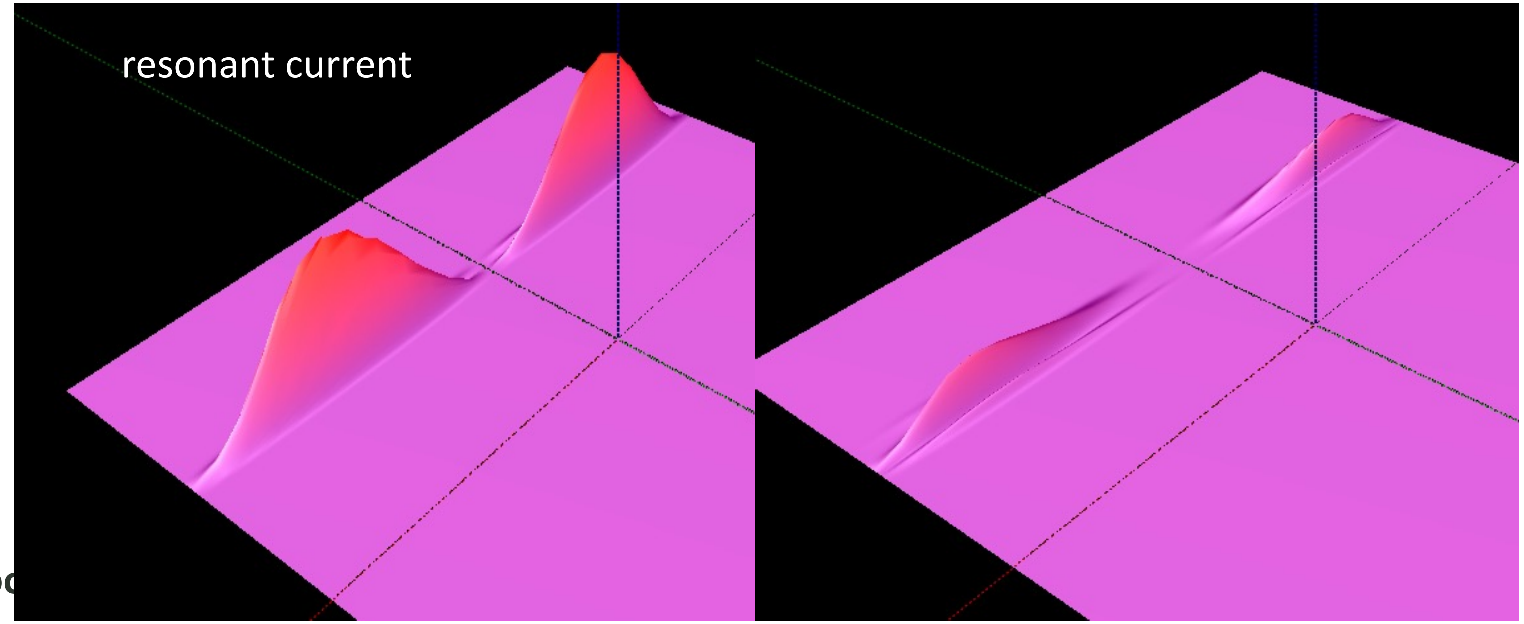




Propagation of $|J_z|$



Propagation of $|J_x|$



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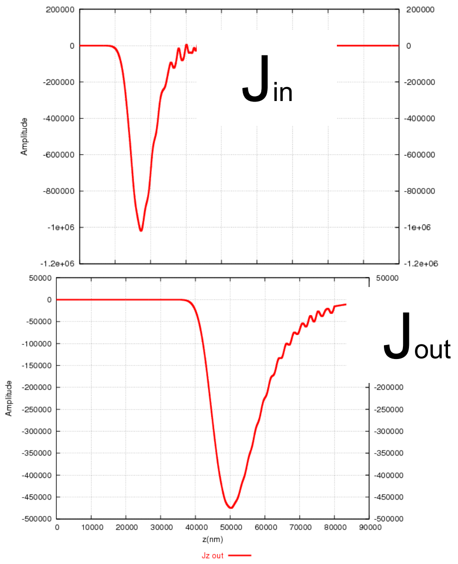
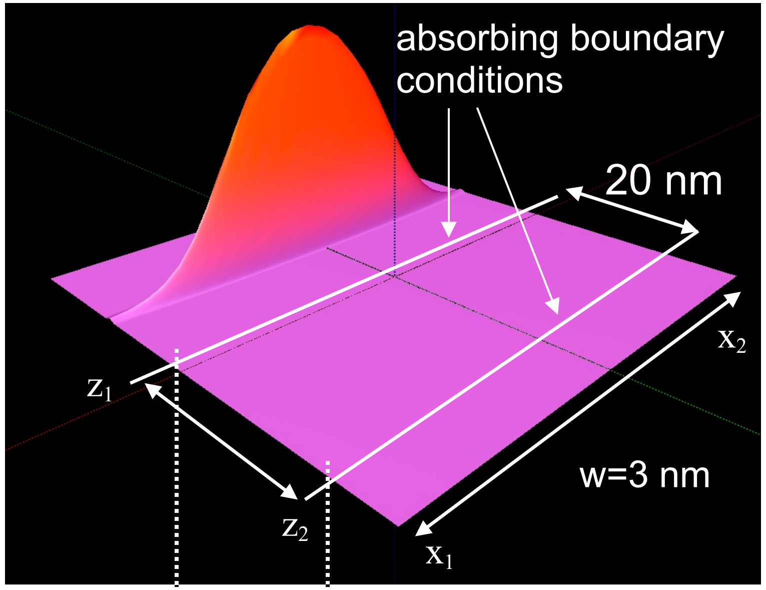
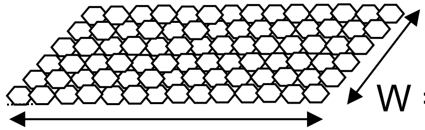
Transmittivity of a Graphene Channel

$$\mathrm{J}_z(z;t) = \int_{x_1}^{x_2} J_z(x,z;t)\,dx \quad [A]$$







$J_z(z_1,t)=u_0(t)$ → GNR channel → $J_z(z_2,t)=h_0(t)$ → FFT → $H_0(\omega)$ ↔ Transmittivity

$$H_0(\omega) = \frac{J_z(z_2,\omega)}{J_z(z_1,\omega)} = \frac{F\{J_z(z_2,t)\}}{F\{J_z(z_1,t)\}}$$

the amplitude peaks of H(ω) are eigenenergies

Transmittivity

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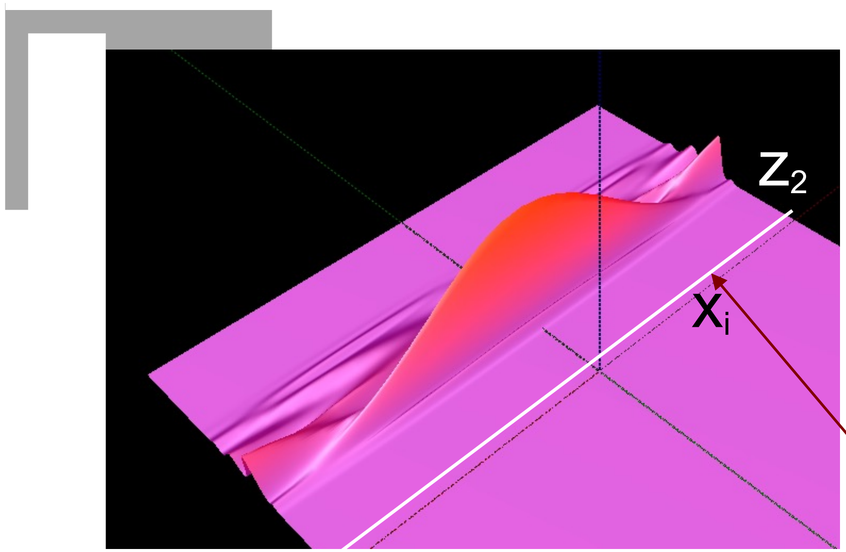
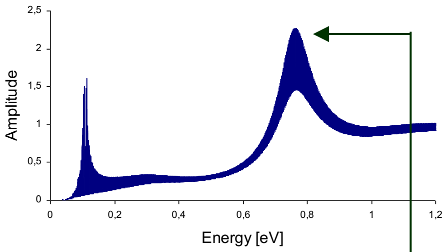
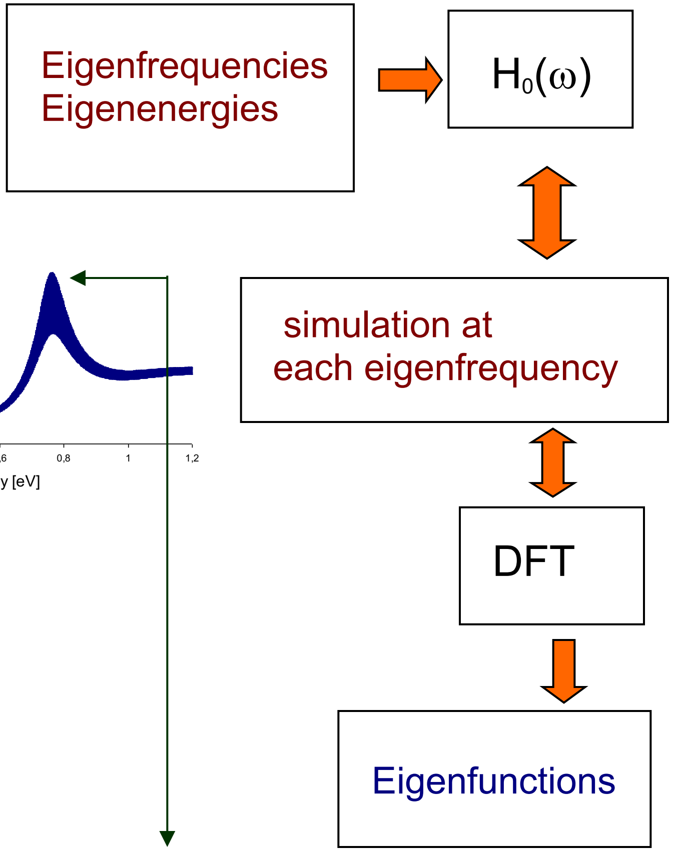
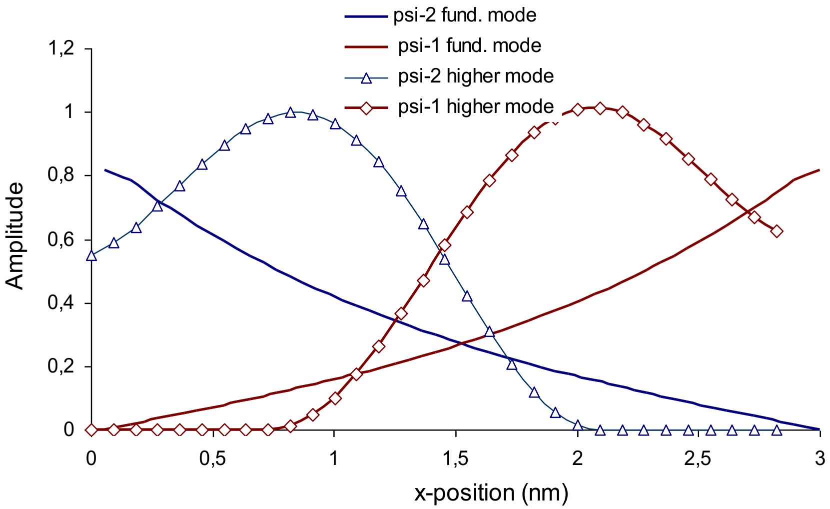
mode profile









$$\psi_k^n\left(x_{i_k}, z_2; f_0\right) = \psi_k^{n-1}\left(x_{i_k}, z_2; f_0\right) + \psi_k\left(x_{i_k}, z_2; n\Delta t\right) e^{-i2\pi f_0 n\Delta t}$$

k

a DFT at each point in the problem space at each of the eigenenergies f_0 is carried out during the simulation

Luca Pierantoni

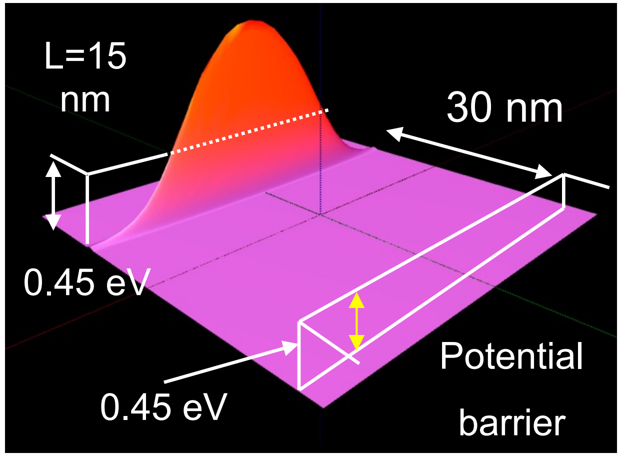
self-generated EM field in the presence of a potential barrier

$$E_{MAX} = 1 \quad eV$$

$$\Delta t_{EM} \le \frac{\Delta L_{grid}}{2c} \qquad c = 3 \cdot 10^8 \quad m/s$$

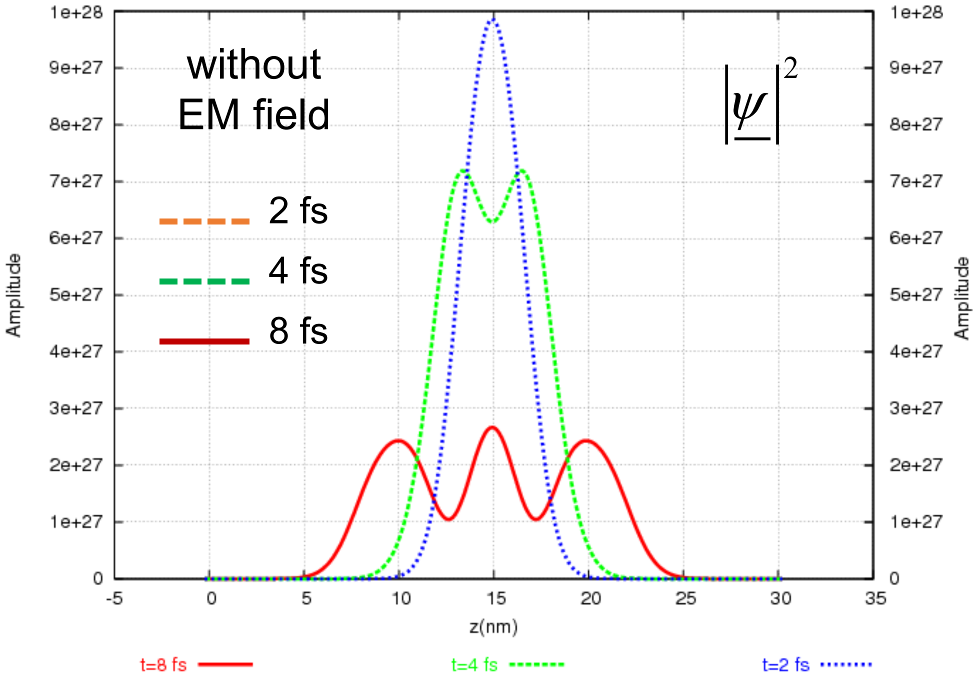
$$\Delta t_{GNR} \le \frac{\Delta L_{grid}}{v_F} \qquad v_F \approx c/300 \quad m/s$$

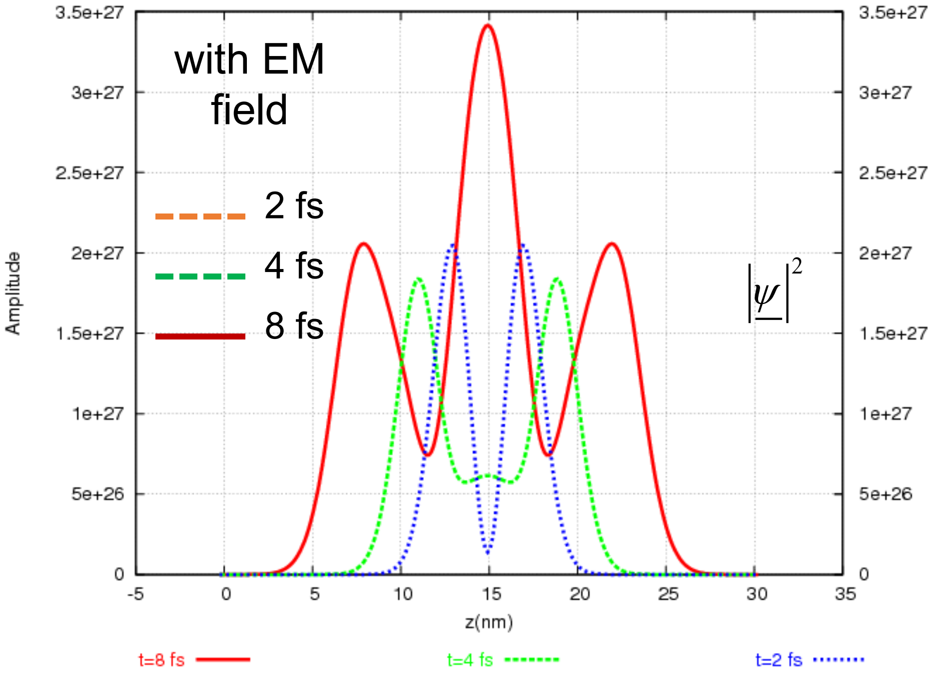
$$\Delta t_{EM} \le \frac{\Delta t_{GNR}}{600}$$



$$\mathbf{k} = \mathbf{p} - q\mathbf{A}$$

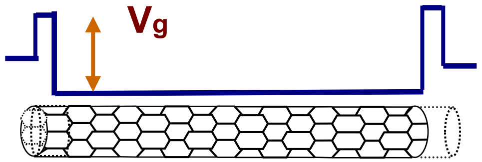
change in the dynamics

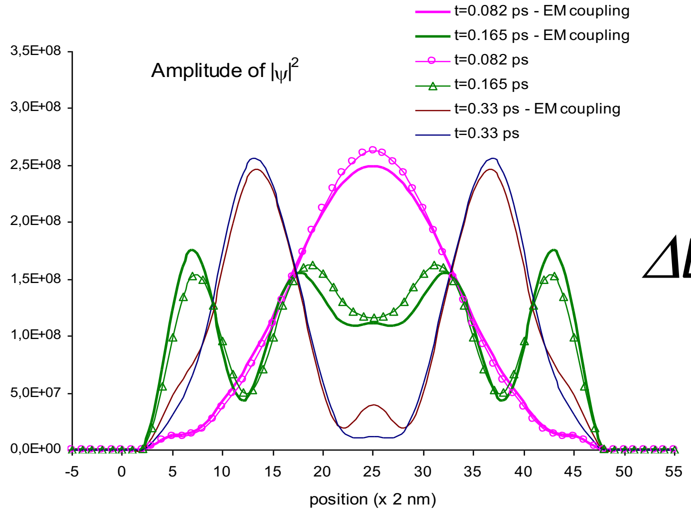




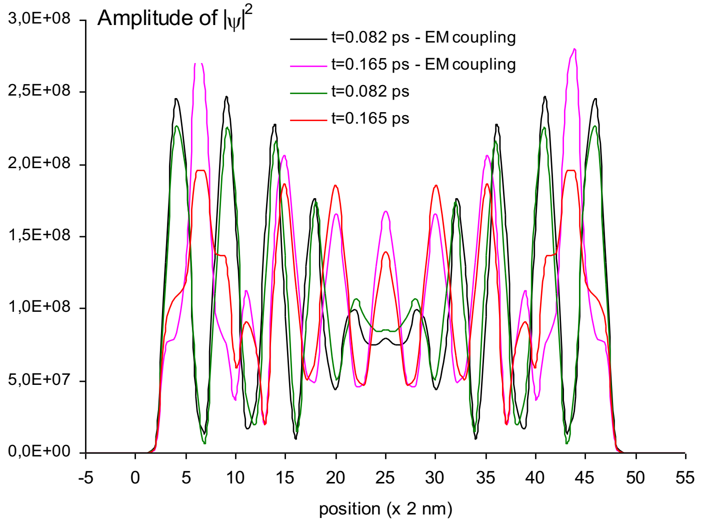
Pierantoni

CNT wavepacket dynamics with or without the self-generated EM field

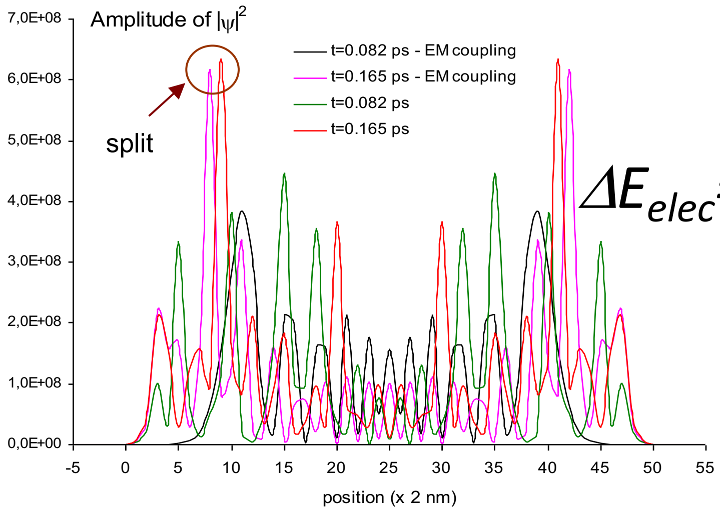




ΔE_{elec}=0.05 eV



ΔE_{elec}=0.1 eV



ΔE_{elec}=1 eV