

Characterization of two- and three-terminal graphene diodes by fully-ballistic or semi-classical methods

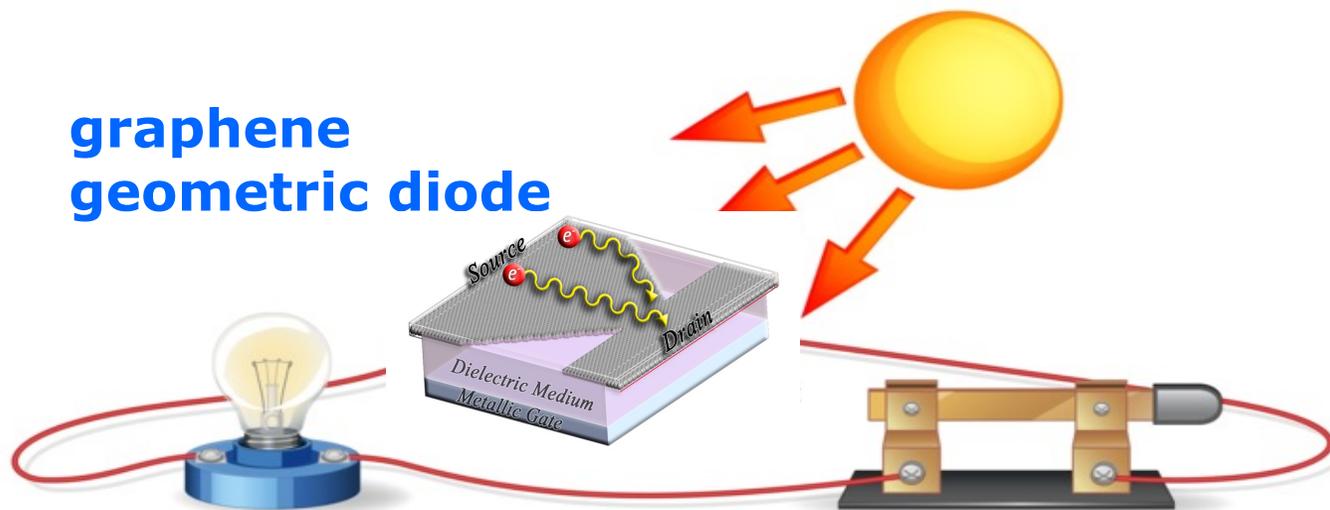
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9 September 2024

Research objectives of GREENERGY

[H2020-LC-SC3-2018-2019-2020](#)



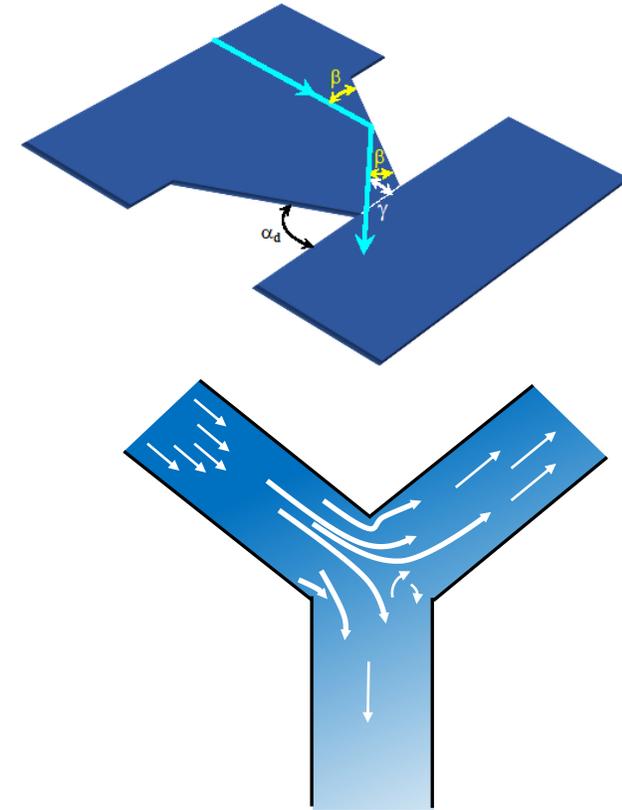
1. Optical nanoantennas:

wide bandwidth, dual polarization, angle independent

2. **Nano-rectifiers** based on **graphene geometric diodes** to optical frequencies

3. **On-chip** integration of antenna rectifier with **energy storage** components

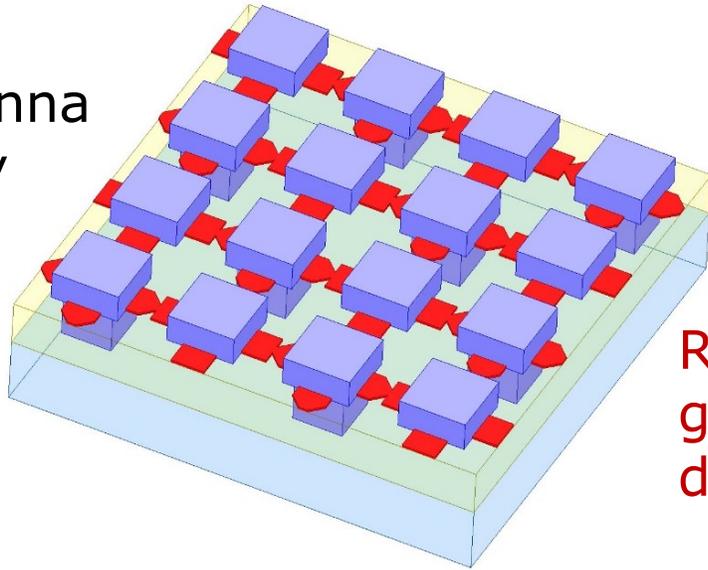
1. DFT based approach
2. MonteCarlo
3. Scattering Matrix (Landauer)
4. Drift-diffusion



Very different approaches with completely different assumptions

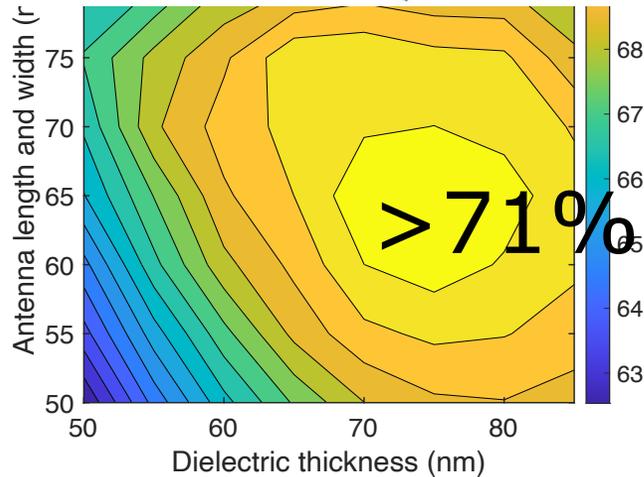
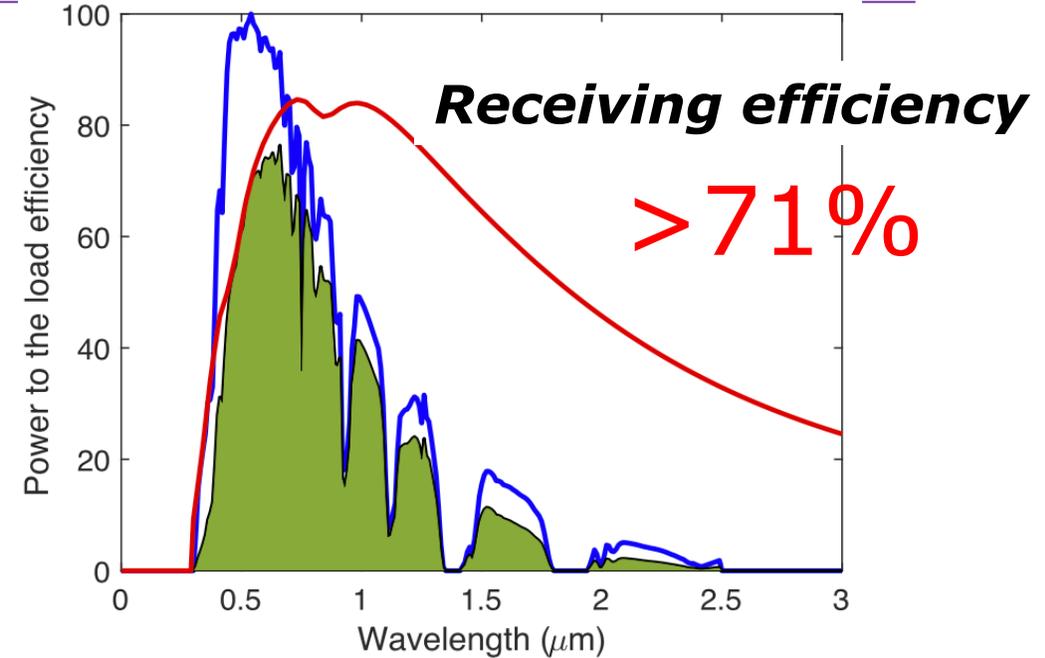
Optical simulation of the proposed architecture

Antenna array

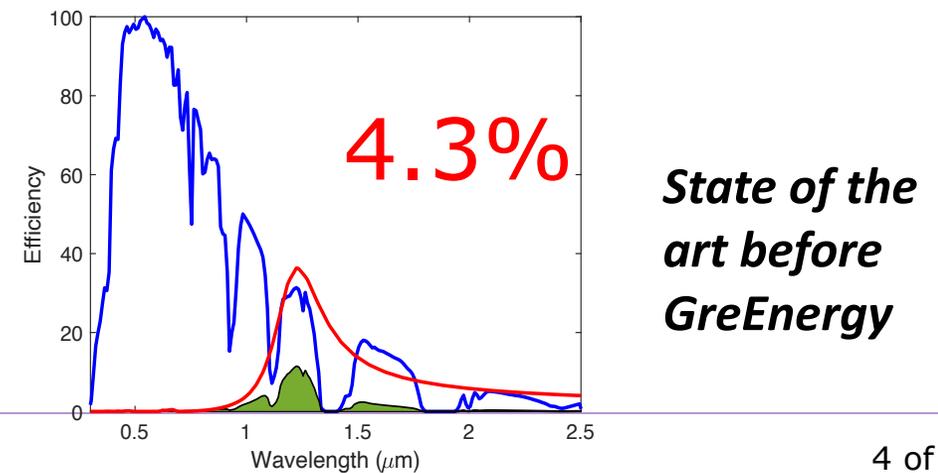


Blue squares:
metal patches

Red squares:
graphene ballistic diodes

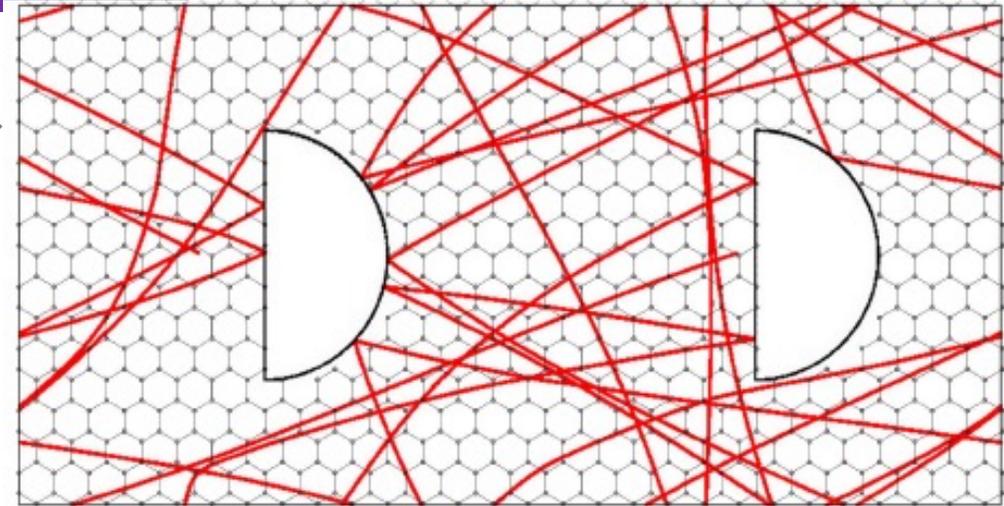
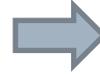


< 30% is
dissipated
or reflected



The ratchet effect is a **collective motion** of particles in a preferential direction, **due to spatially-asymmetric perturbations**

An external action is needed, to have the 2nd Law of thermodynamics preserved



Semi-disk holes

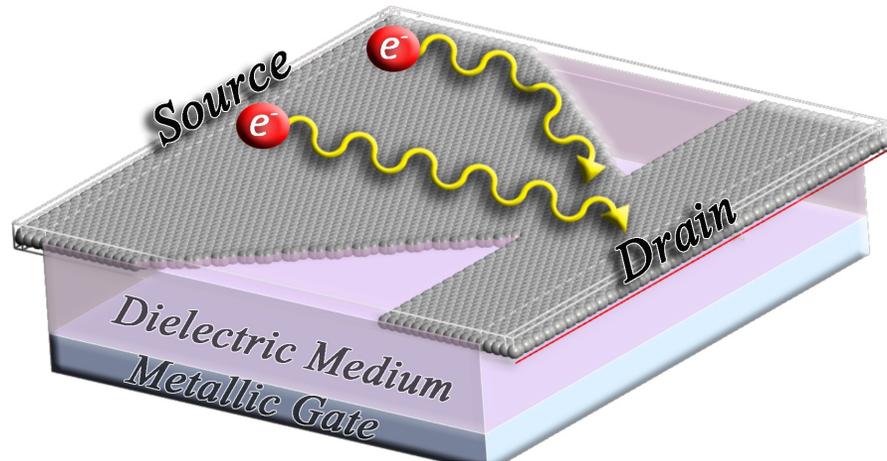
L. Ermann and D. L. Shepelyansky: Relativistic graphene ratchet



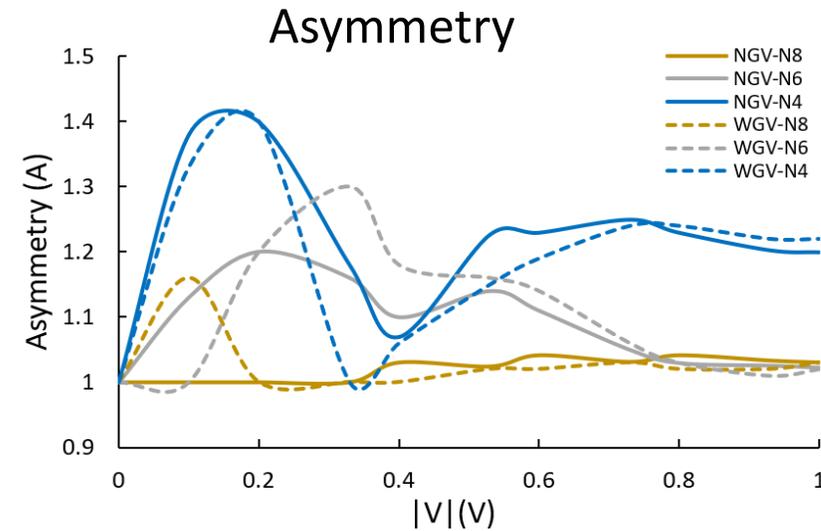
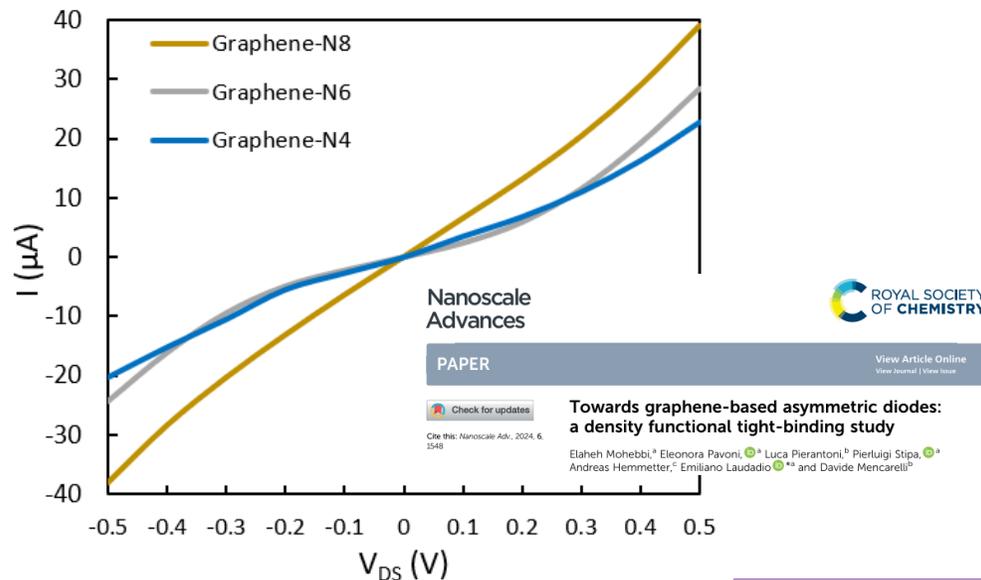
In our case, EM fields at optical frequencies

Summarizing, **two conditions** required: 1) breaking of spatial or temporal inversion symmetry 2) breaking of equilibrium (thermal, electrical mechanical)

#1 Modelling of geometric diodes: DFT based approach

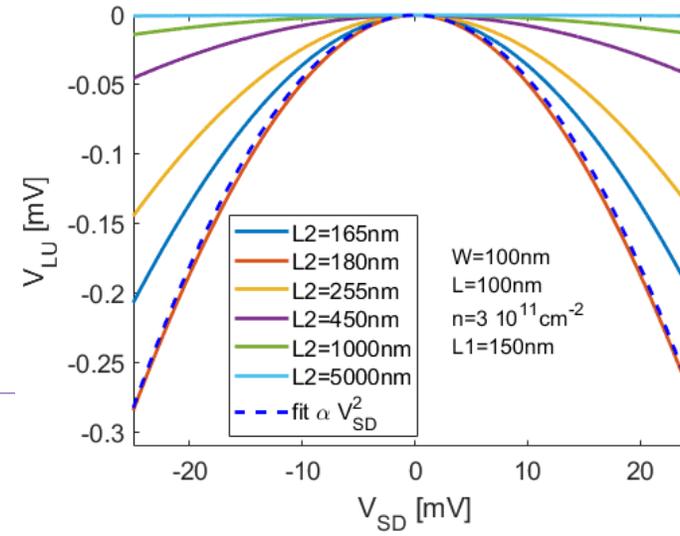
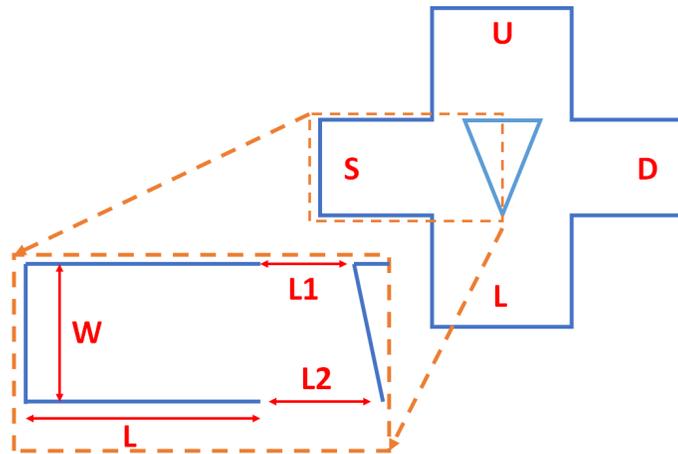
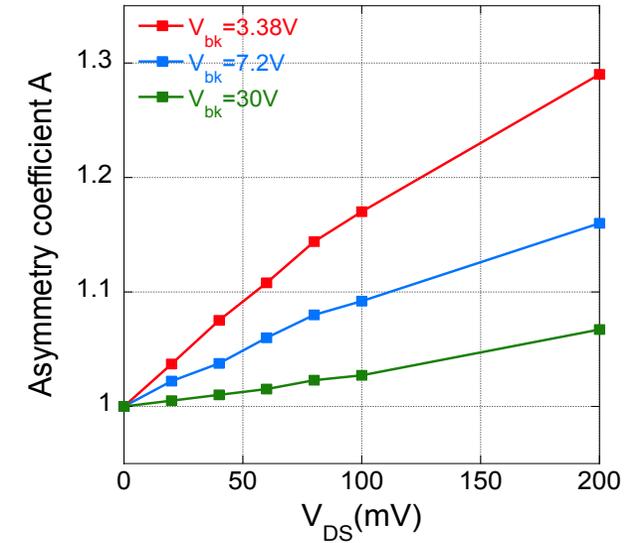
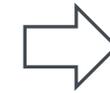
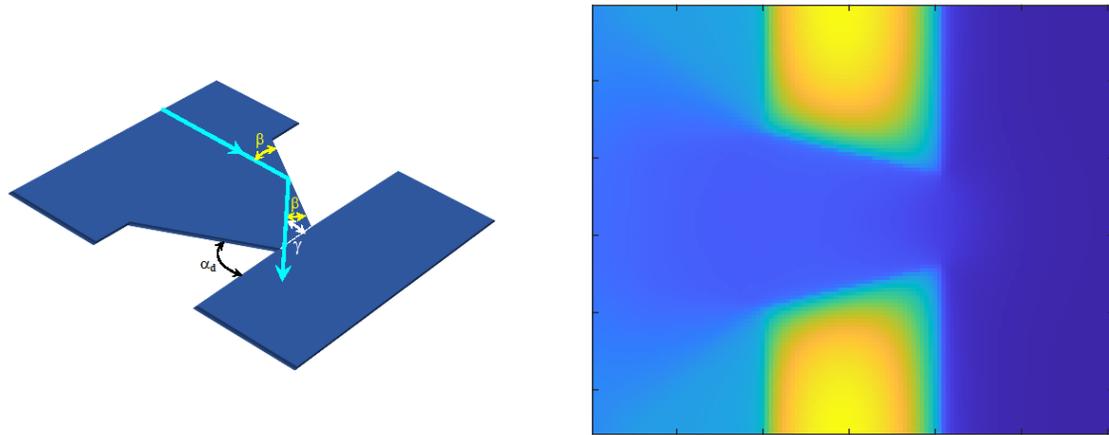


Very large asymmetric graphene diodes by Density Functional TB approach



#2 Modelling of geometric diodes: MonteCarlo

[data from D. Truccolo, M. Midrio et al., UNIUD]



Parabolic relation between input and output voltages

#3 Modelling of geometric diodes: Scatt. Matrix

Current from scattering parameters

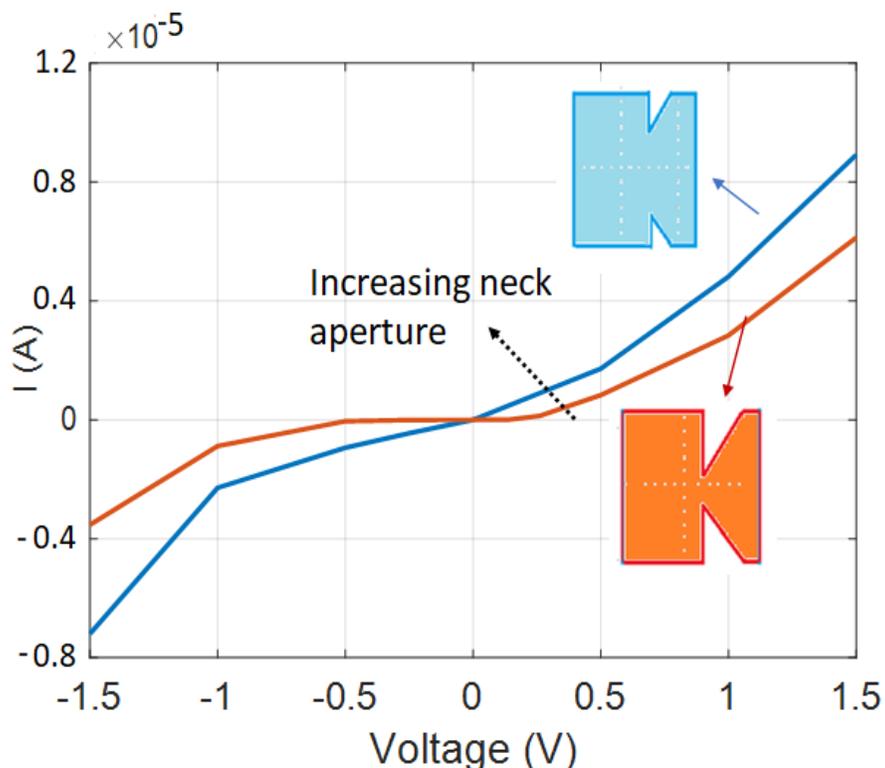
$$I_m^q = \frac{2e^2}{h} \int \left[\sum_{n=1, n \neq m}^N \sum_p T_{n,m}^{p,q}(E) \right] dE$$

$$I_m = \sum_q I_m^q$$

Charge density

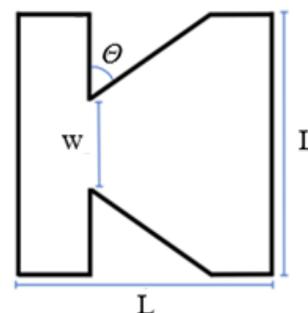
$$n = \int f(E, E_F) \frac{E}{\pi(\hbar v_F)^2}$$

where $E_F \in [0.2 \text{ eV} - 0.3 \text{ eV}]$



L	≈ 15 nm
w	≈ 8 nm
θ	60°

L	≈ 15 nm
w	≈ 4 nm
θ	60°



Example : increasing neck size

- a. the I-V asymmetry decreases
- b. the amount of current increases (diode impedance decreases)
- c. the reverse-bias current increases

#3 Modelling of geometric diodes: Scatt. Matrix

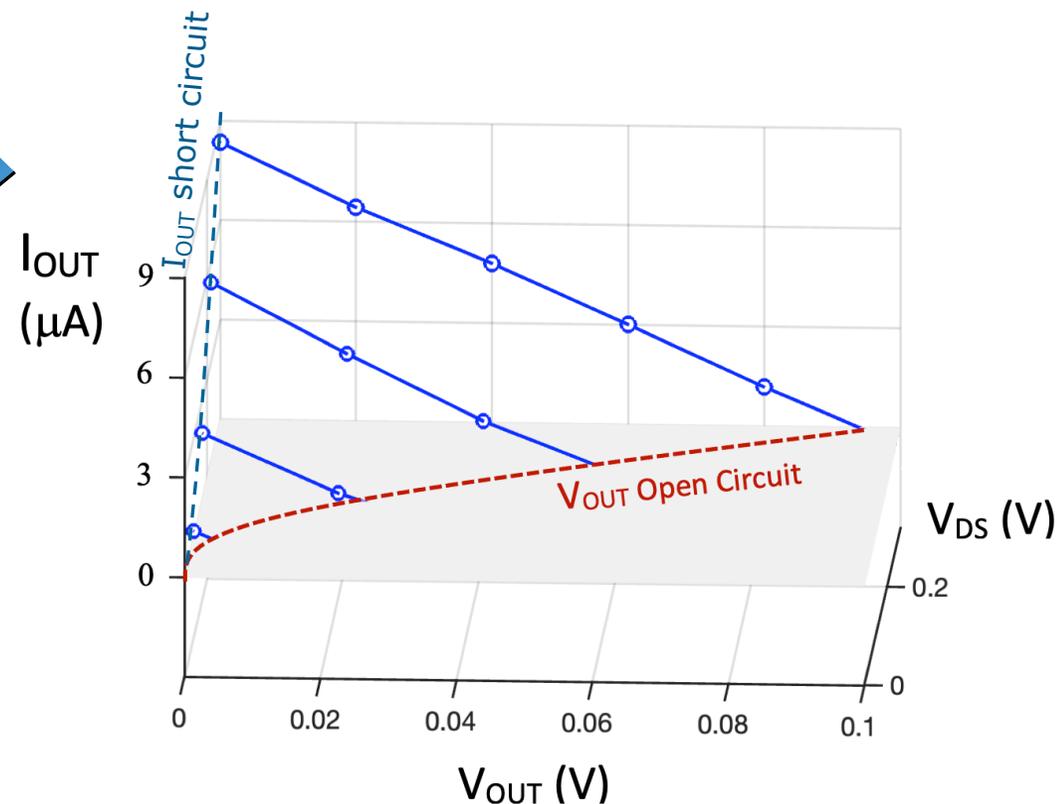
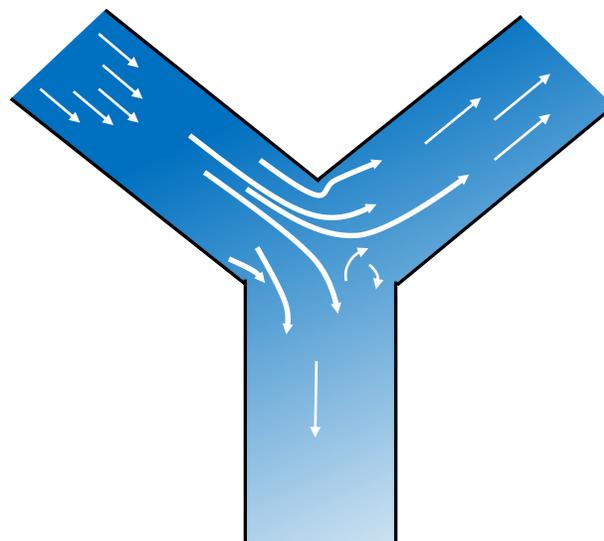
From 2-terminal devices to 3-
(or more) terminal devices

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 **RESEARCH ARTICLE**

**Current-Voltage Characterization of Multi-Port
Graphene Based Geometric Diodes for
High-Frequency Electromagnetic Harvesting**

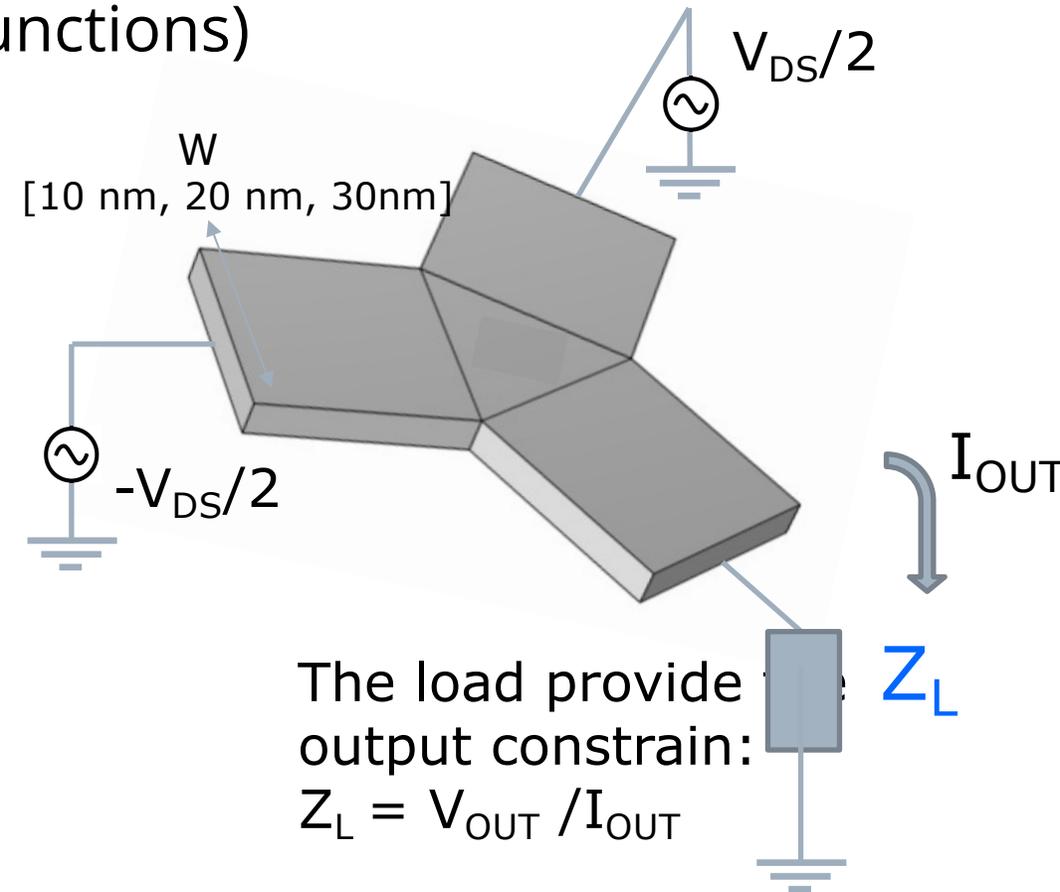
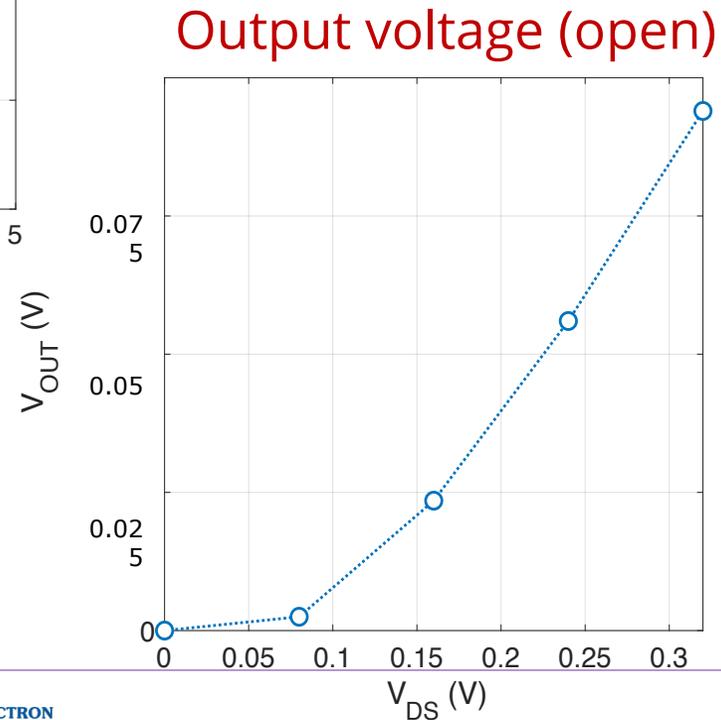
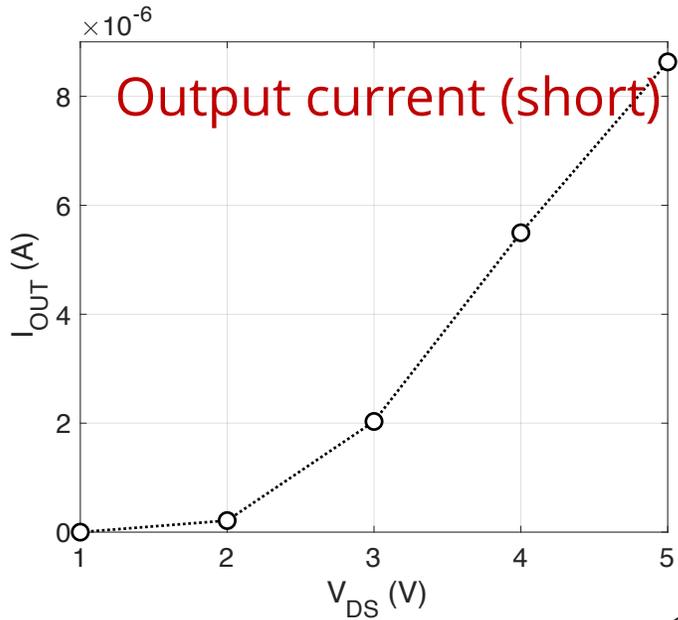
DAVIDE MENCARELLI^{1,2}, GIAN MARCO ZAMPA¹, (Graduate Student Member, IEEE),
AND LUCA PIERANTONI^{1,2}



$V_{DS} = 0.16$ V			
Width	V_{OC}	I_{SC}	I_{DS}
10 nm	25 mV	$\approx 9 \mu A$	$\approx 18 \mu A$
20 nm	18 mV	$\approx 24 \mu A$	$\approx 50 \mu A$

#3 Modelling of geometric diodes: Scatt. Matrix

Quantum coherent transport
(Tight-Binding wave-functions)



#4 Modelling of geometric diodes: Drift-Diffusion

..the above methods require
very long simulation time!

Can drift-diffusion of charges explain rectification from geometric diodes?

Electric potential

$$\nabla \cdot (\epsilon \nabla V) = \rho = p - n$$

Electron current

$$\nabla \circ (-D_n \cdot \nabla n - \alpha_n \cdot n + \gamma_n) = 0$$

Hole current

$$\nabla \circ (-D_p \cdot \nabla p - \alpha_p \cdot p + \gamma_p) = 0$$

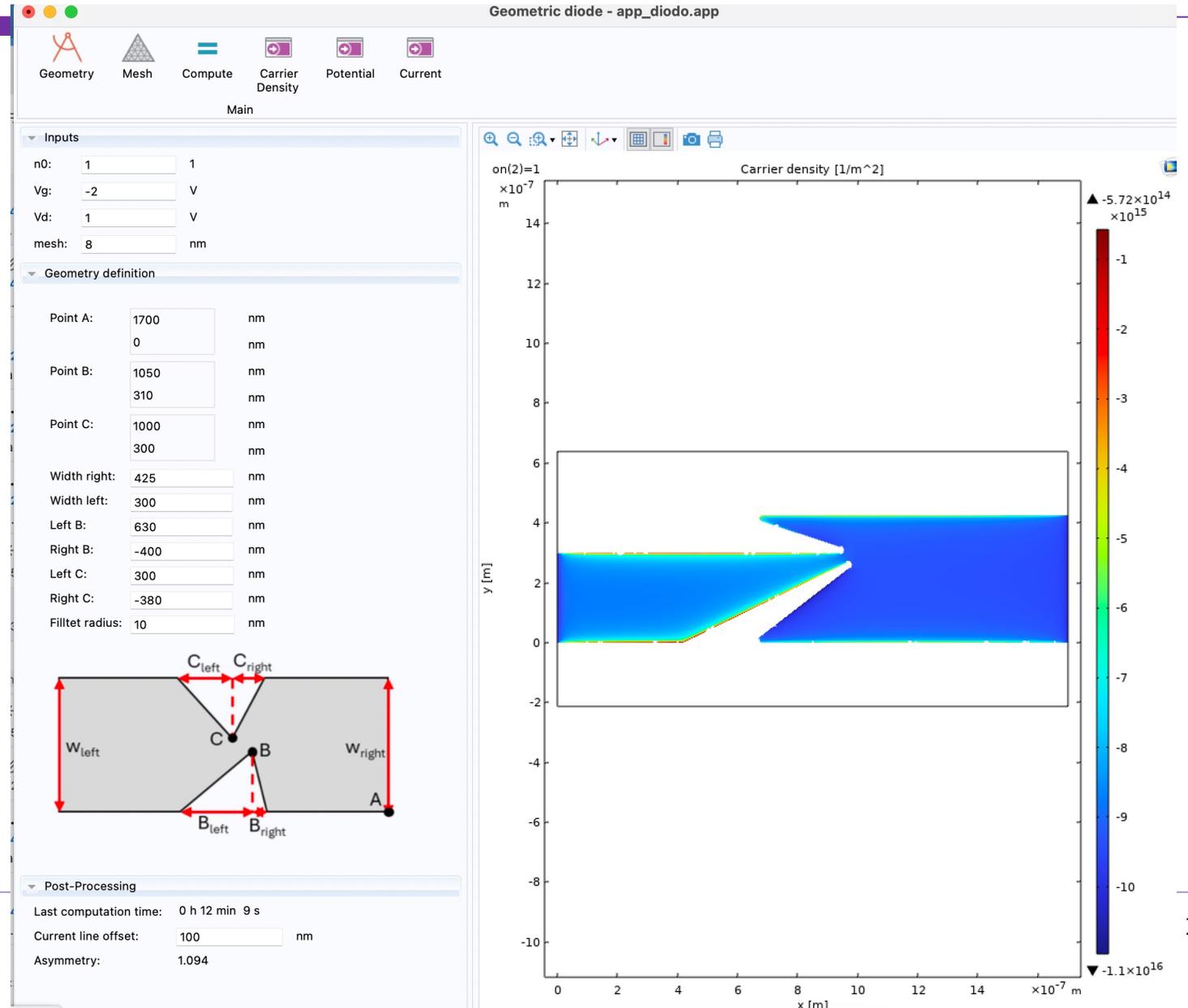
$D_{n,p}$: diffusion coefficient

The interplay between (1) asymmetric potential and (2) diffusion in an asymmetric geometry provides an asymmetric response

#4 Modelling of geometric diodes: Drift-Diffusion

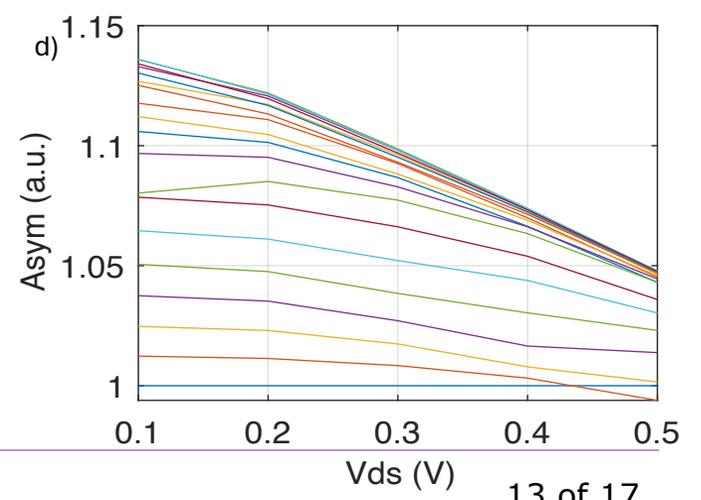
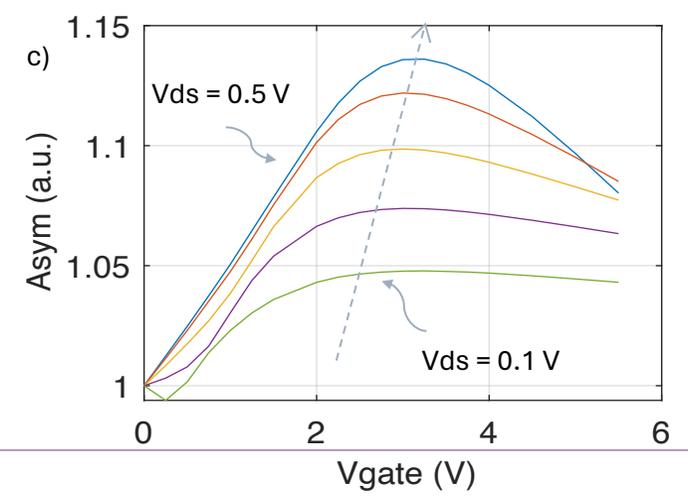
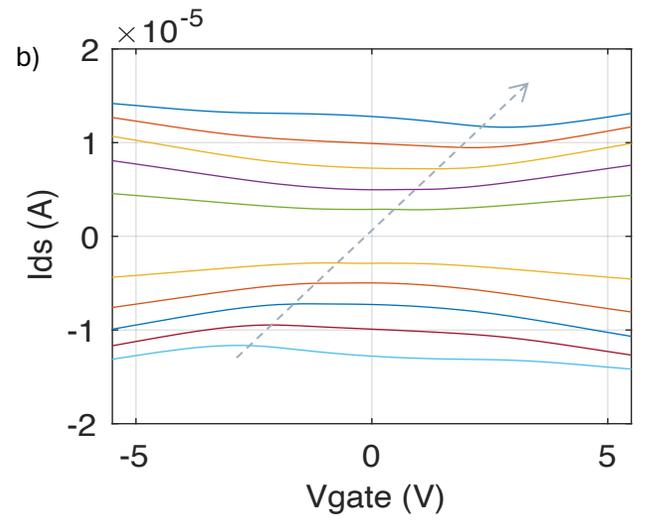
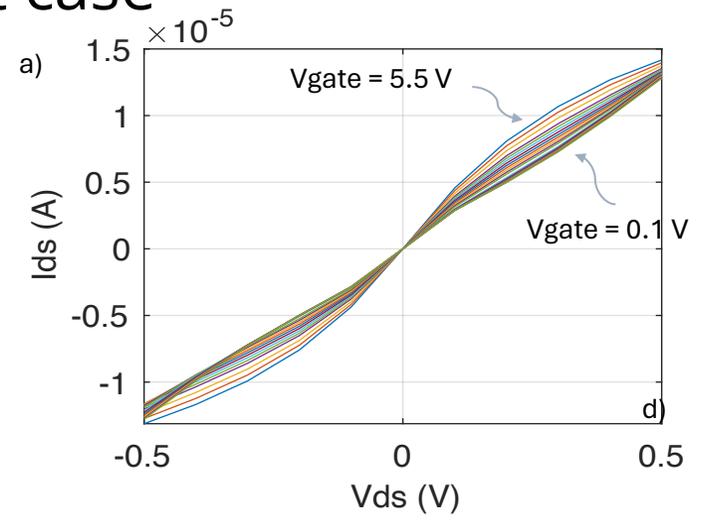
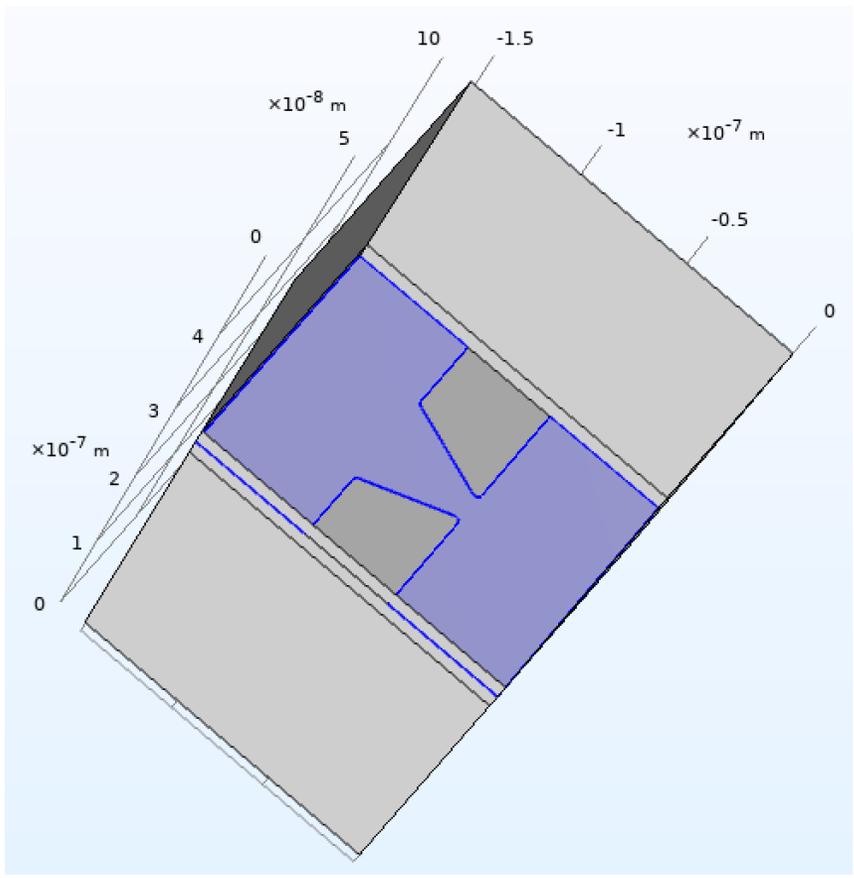
Comsol
portable
application

Arbitrary geometry



#4 Modelling of geometric diodes: Drift-Diffusion

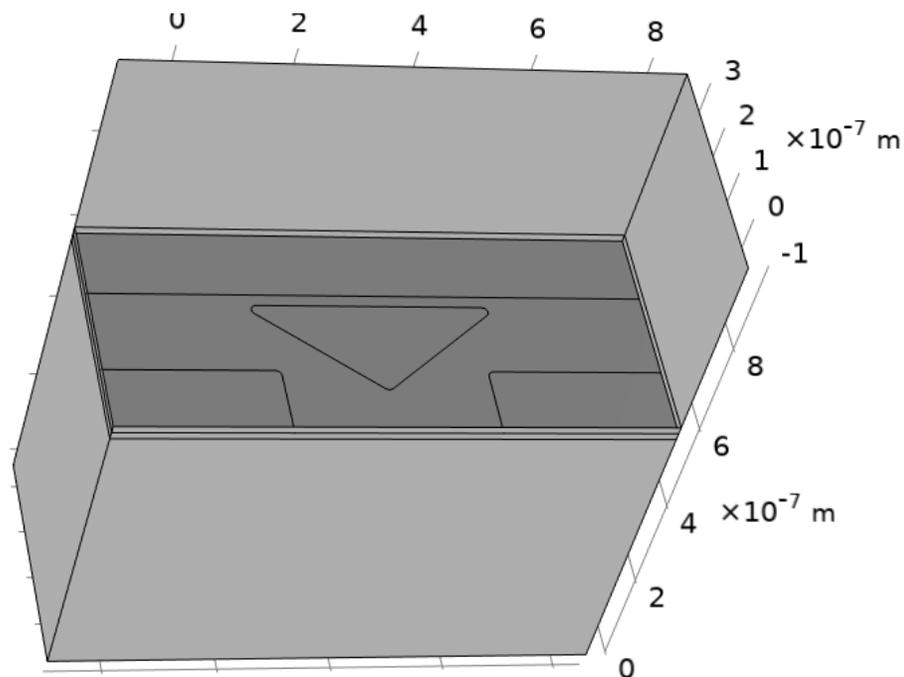
Example: 2-port bipolar transport case



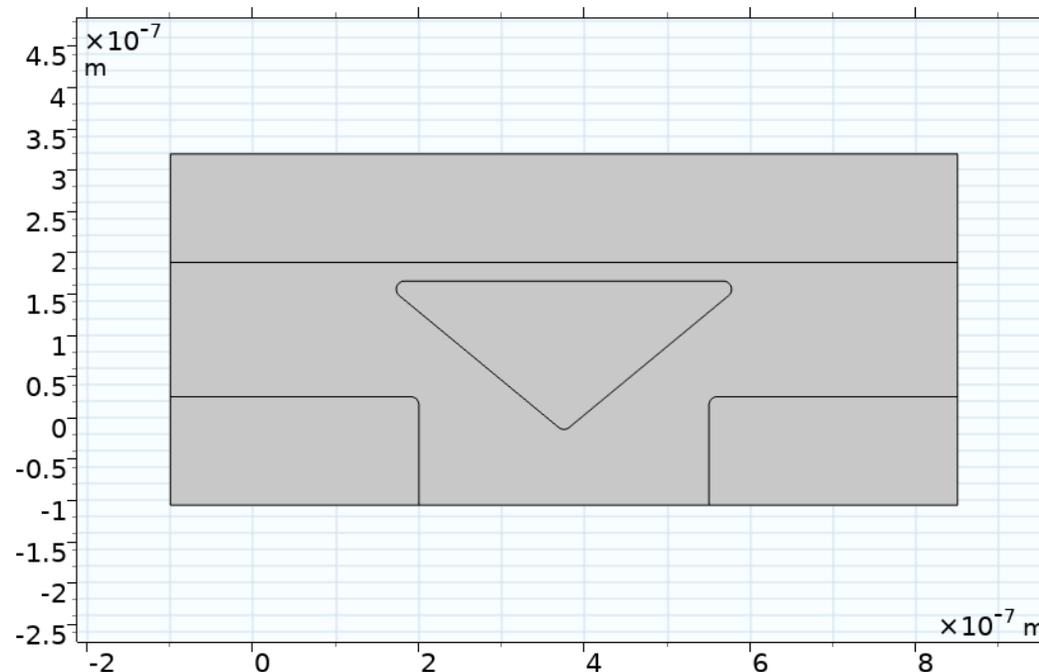
#4 Modelling of geometric diodes: Drift-Diffusion

Model extension to many port devices

$$\nabla \cdot (\epsilon \nabla V) = \rho$$

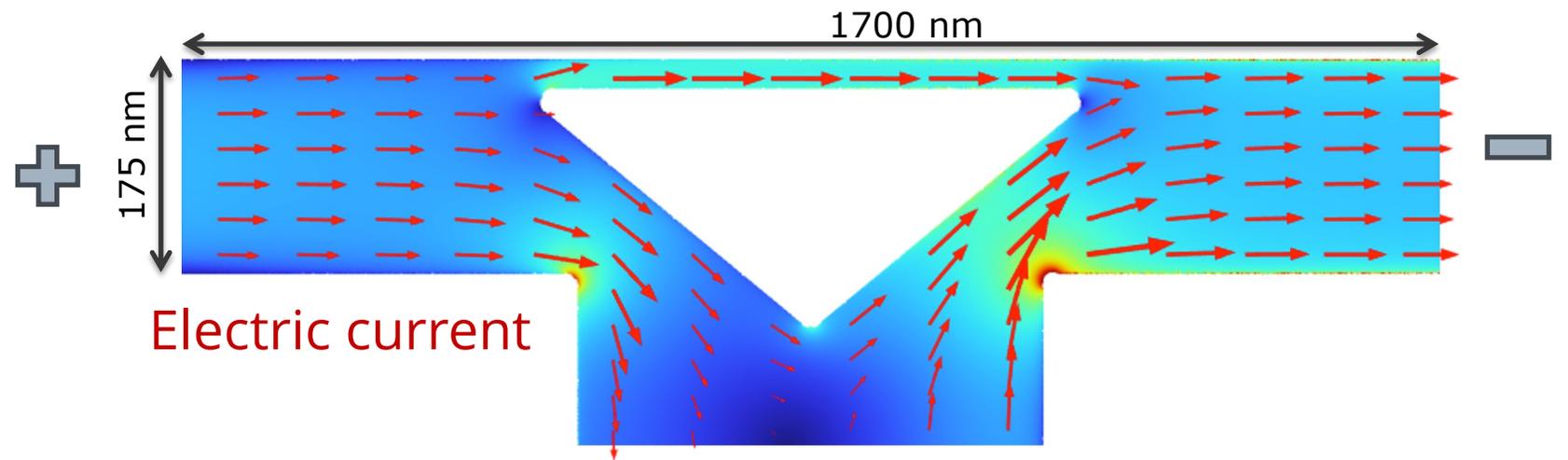


$$\nabla \cdot (-c \cdot \nabla n - \alpha \cdot n + \gamma) = 0$$

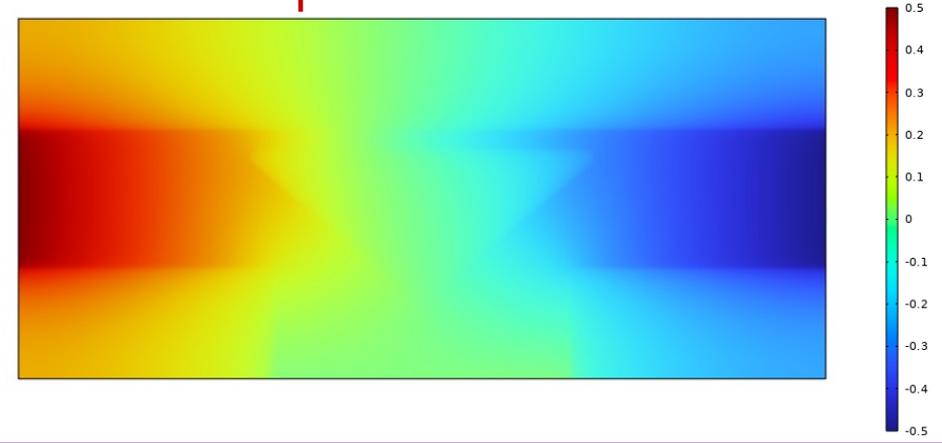


#4 Modelling of geometric diodes: Drift-Diffusion

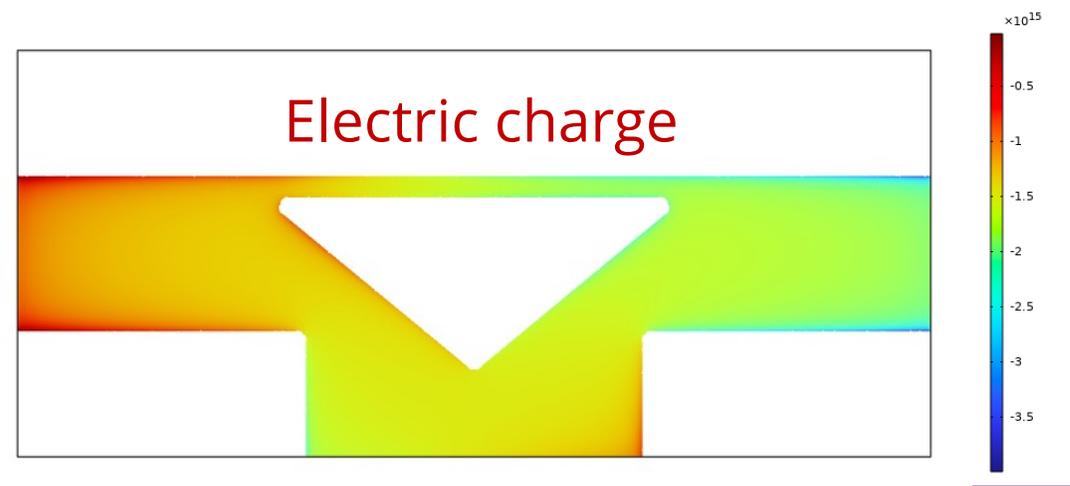
Output physical observables



Electric potential



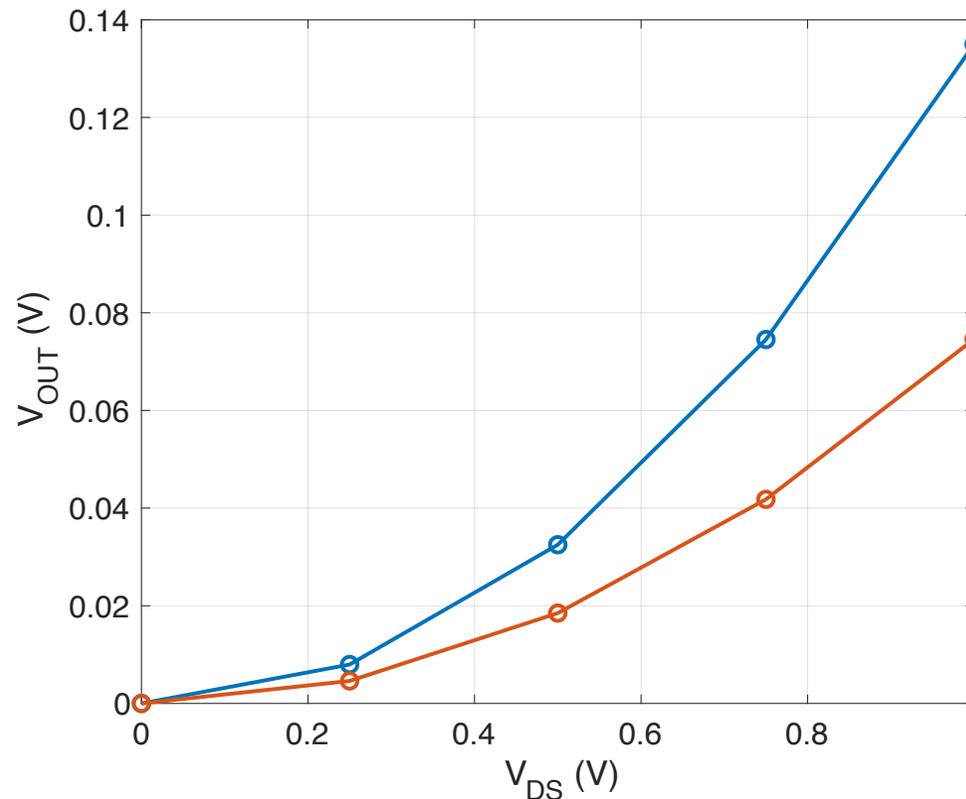
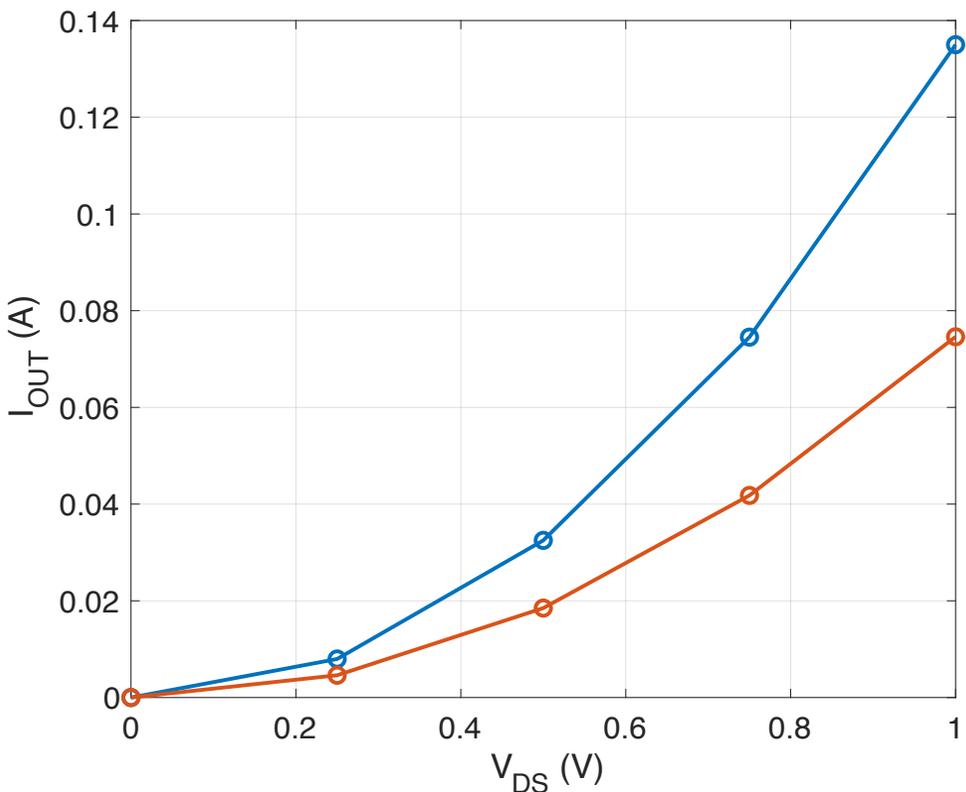
Electric charge



#4 Modelling of geometric diodes: Drift-Diffusion

Output current (short)

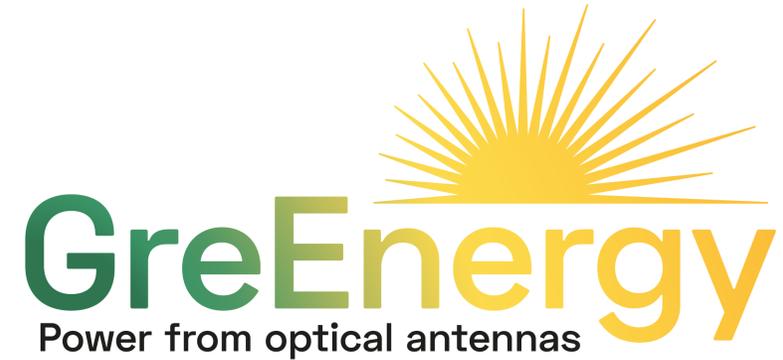
Output voltage (open)



Diode of the previous slide

Diode scaled down 50%

Thank you!



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