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Universidad del País Vasco Euskal Herriko Unibertsitatea

CFM

Electron Transport Simulations of 4-Terminal Crossed Graphene Nanoribbons Devices

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Aran Garcia-Lekue[3,4], Thomas Frederiksen[3,4], Daniel Sánchez-Portal[1,3]

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3 *Donostia International Physics Center, Spain*
4 *IKERBASQUE, Basque Foundation for Science, Spain*

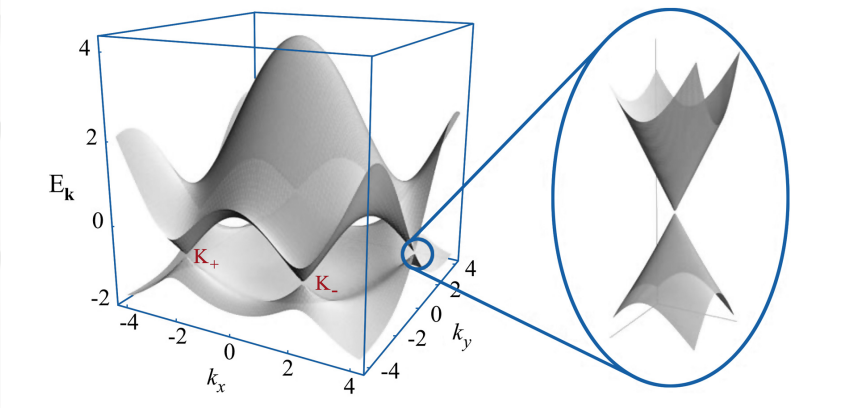
March 14, 2016

Graphene

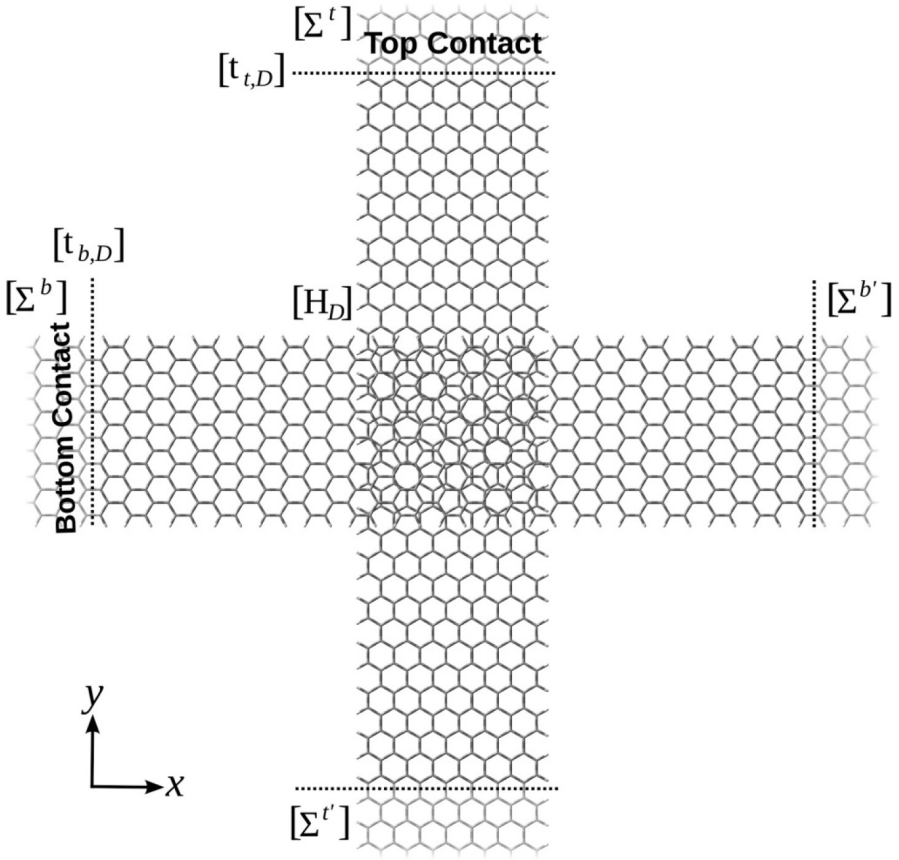
- High mobility ⟶ 10^5 $cm^2V^{-1}s^{-1}$

K. Novoselov *et al*. *Science* **306**, 666-669 (2004).

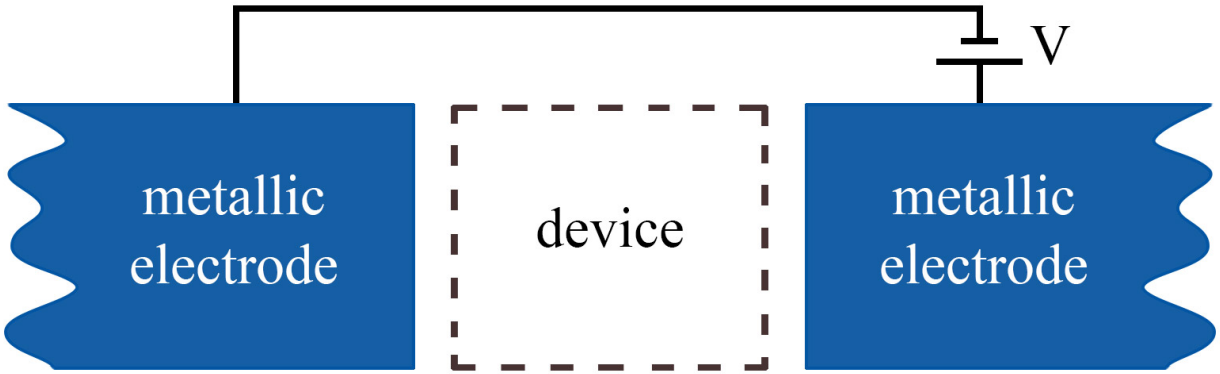
- Gap absence:



A. Castro Neto *et al*. *Rev. of Mod. Phys.* **81**, 109-162 (2009).



M. Masum Habib and Roger K. Lake. *Phys. Rev. B* **86**, 045418 (2012).



Density-Functional Theory (DFT) **SIESTA**

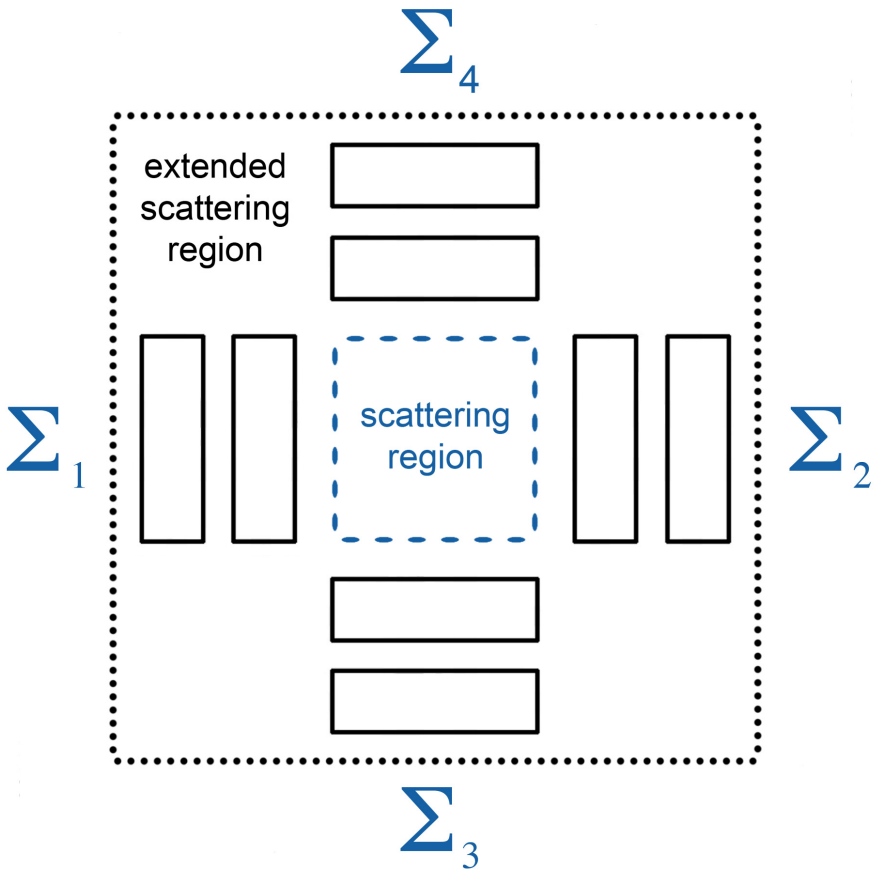
+

Non-Equilibrium Green's Function Formalism (NEGF)

TranSIESTA

E. Artacho *et al*. *Phys. Stat. Sol. (b)* **215**, 809-817 (1999).
Mads Brandbyge *et al*. *Phys. Rev. B* **65**, 165401 (2002).

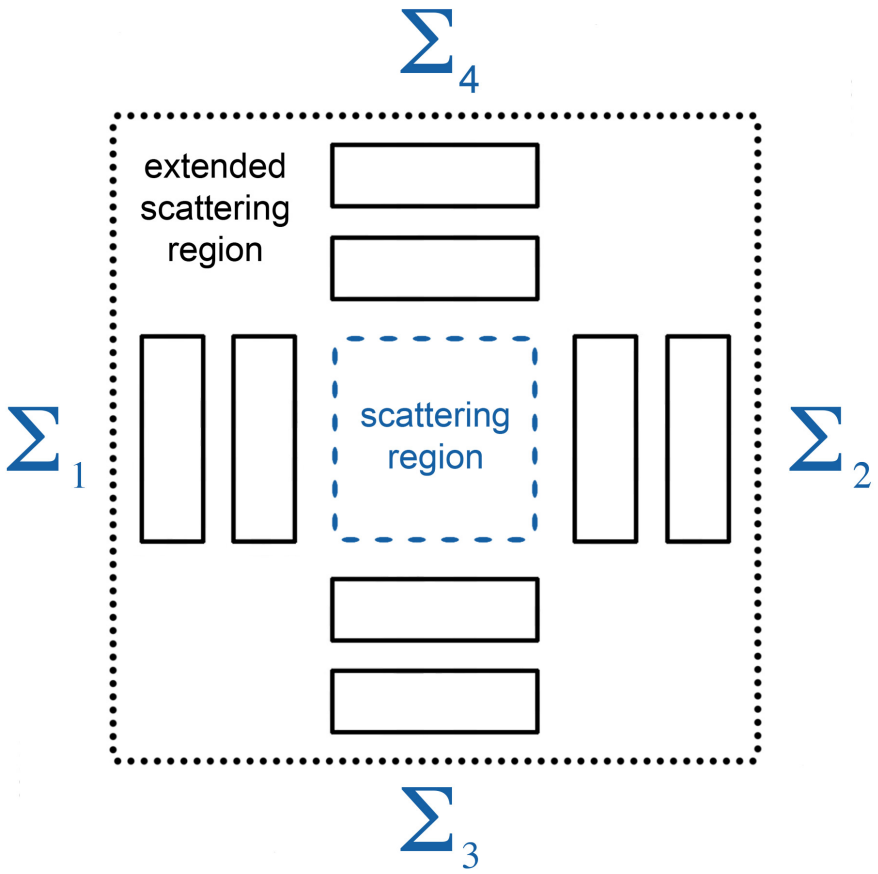
Multi-terminal TranSIESTA



N≥1 arbitrarily distributed electrodes at finite bias

Kamal K. Saha *et al. J. Chem. Phys.* **131**, 164105 (2009).
Nick R. Papior. *In preparation* (2016).

Multi-terminal TranSIESTA

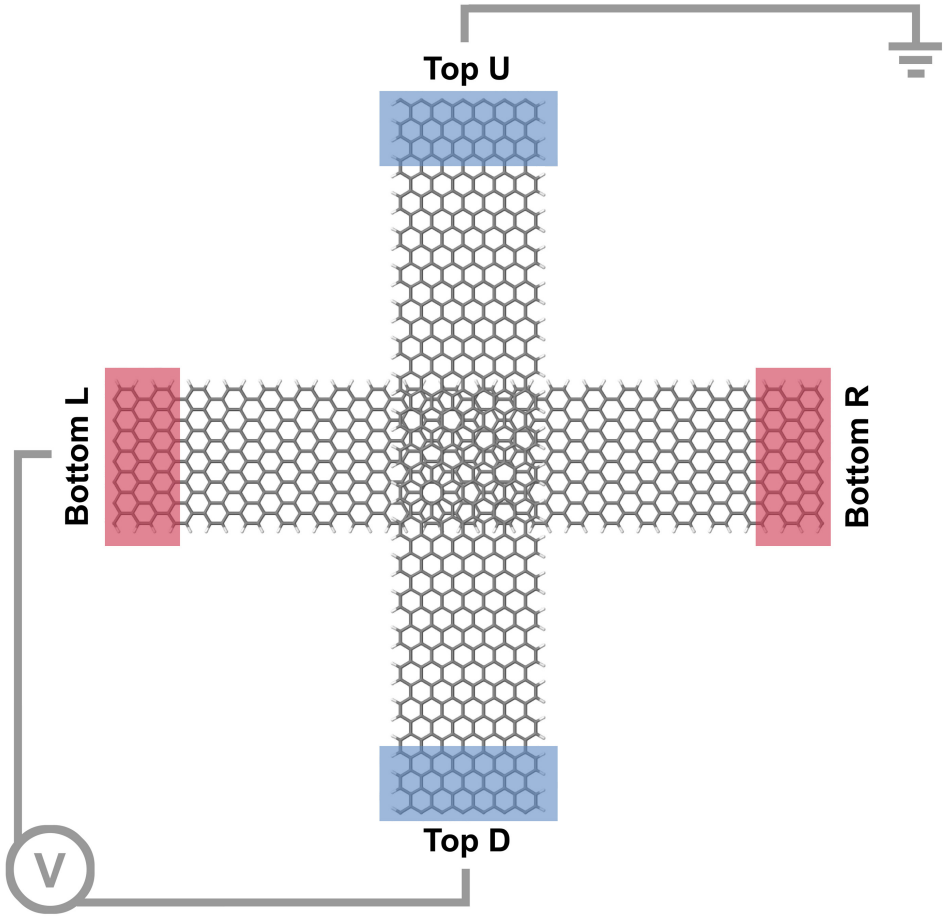


N≥1 arbitrarily distributed electrodes at finite bias

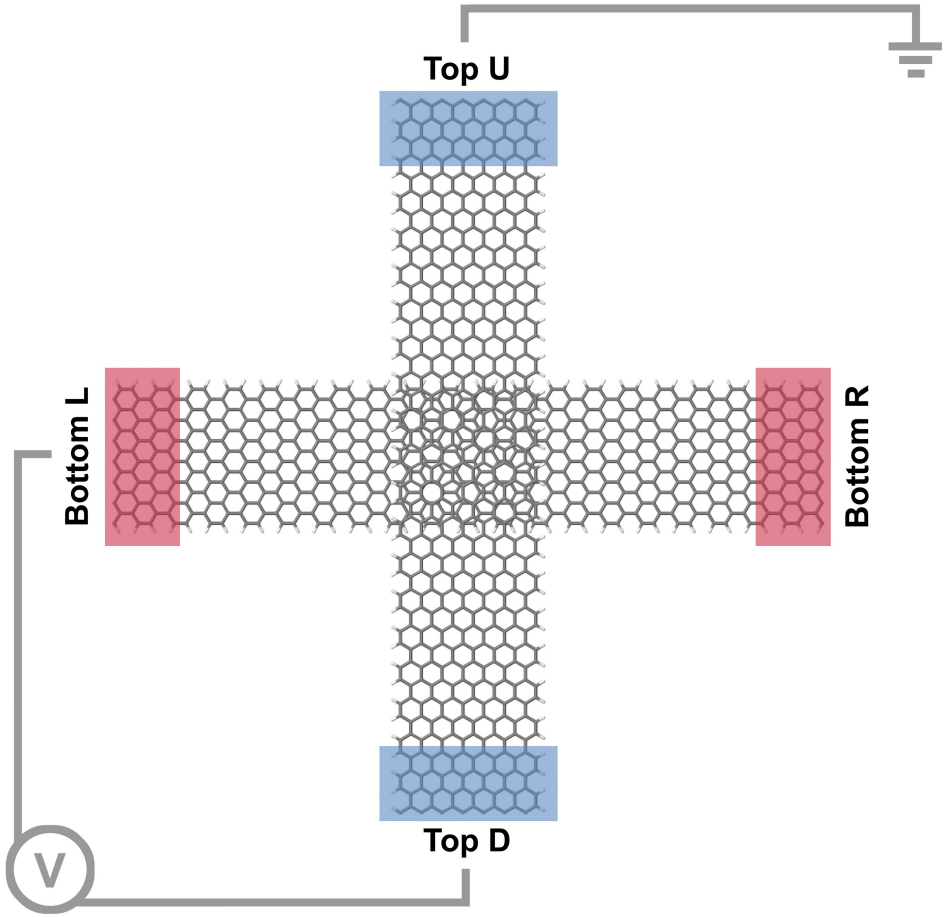
$$V_H(\mathbf{r}) = \tilde{\phi}(\mathbf{r}) + \begin{cases} \mu_j\,, & \text{for } \mathbf{r} \in \mathbf{r}_j \\ 0\,, & \text{for } \mathbf{r} \notin \mathbf{r}_j \end{cases}$$

Kamal K. Saha *et al. J. Chem. Phys.* **131**, 164105 (2009).
Nick R. Papior. *In preparation* (2016).

Crossed 14-AGNR



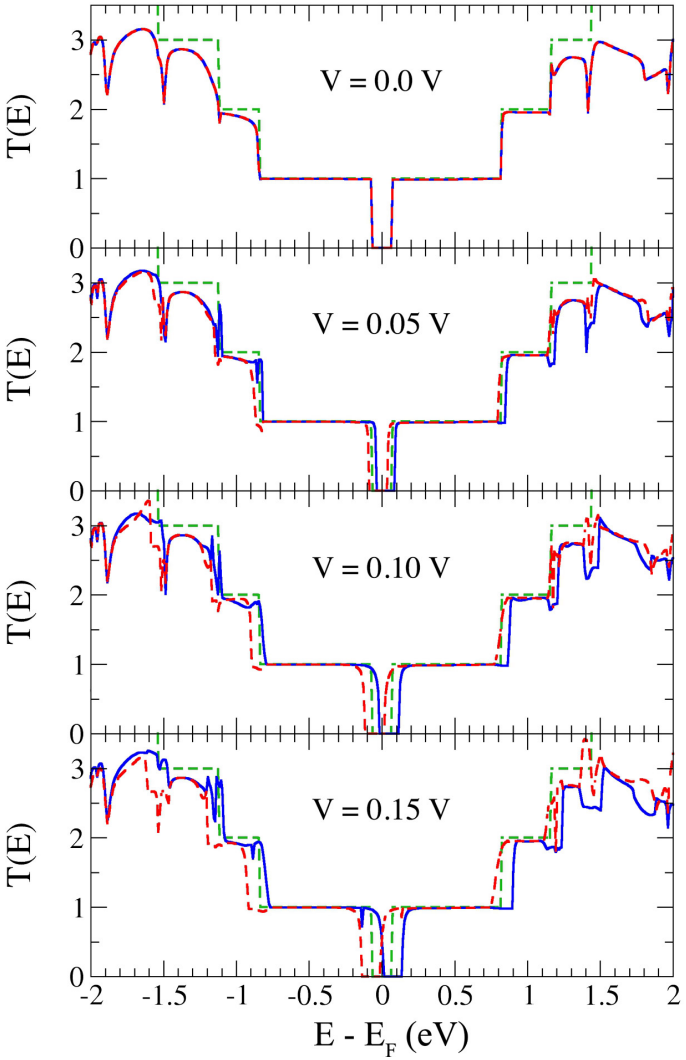
Crossed 14-AGNR

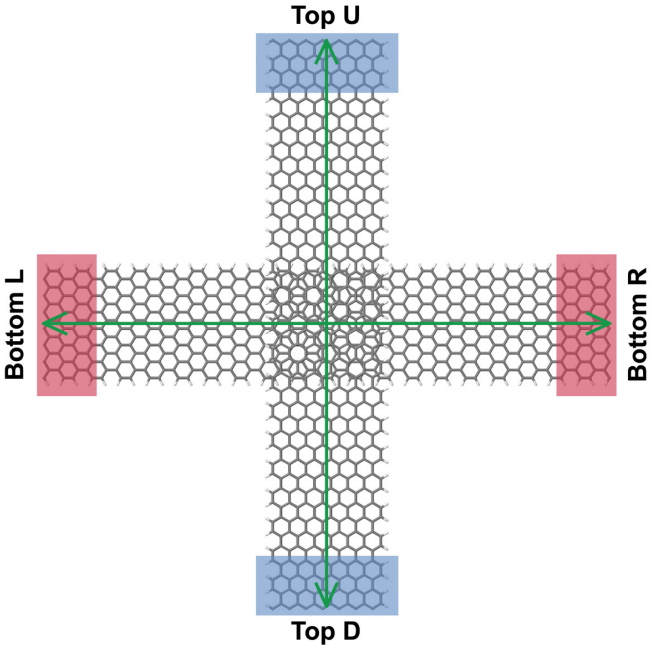


Simulation characteristics:

- 1280 atoms;
- double-ζ (9280 orbitals);
- vdW (optB88);
- real space grid cutoff: 350 Ry;
- forces < 5 meV/Å;
- interlayer distance: 3.34 Å.

Direct transmission





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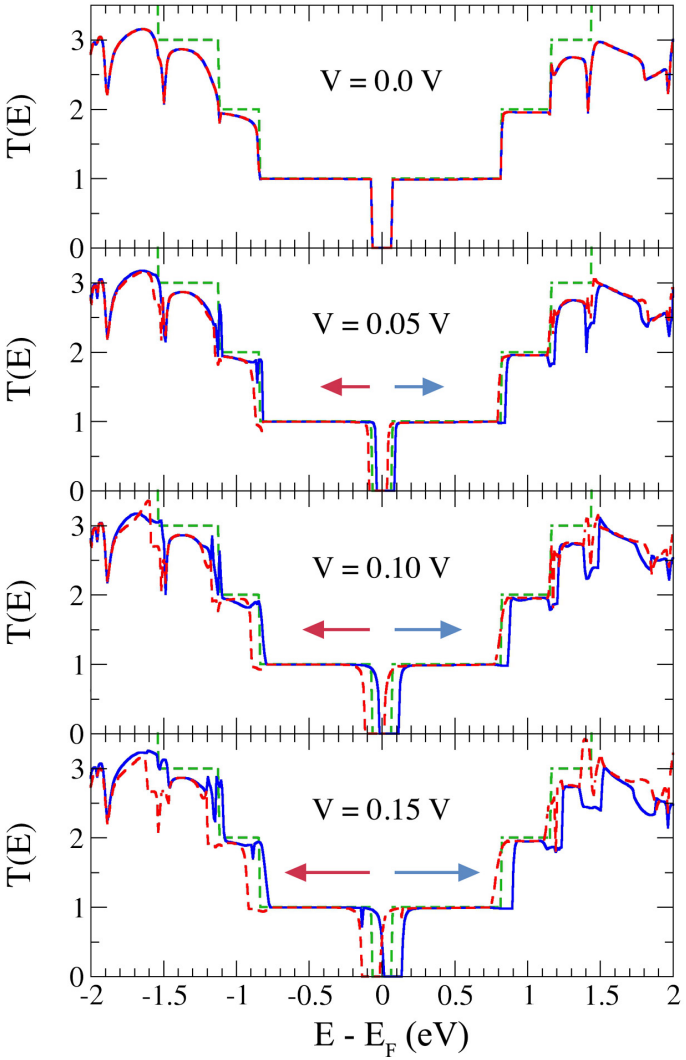
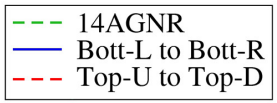
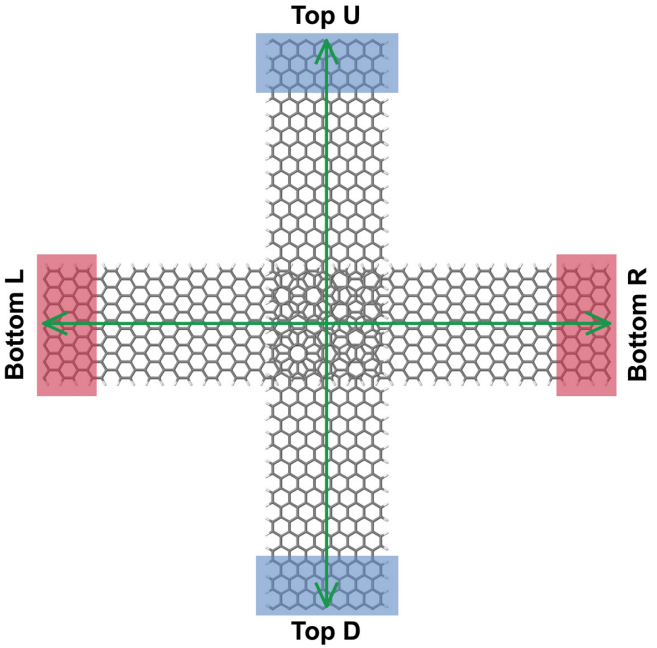
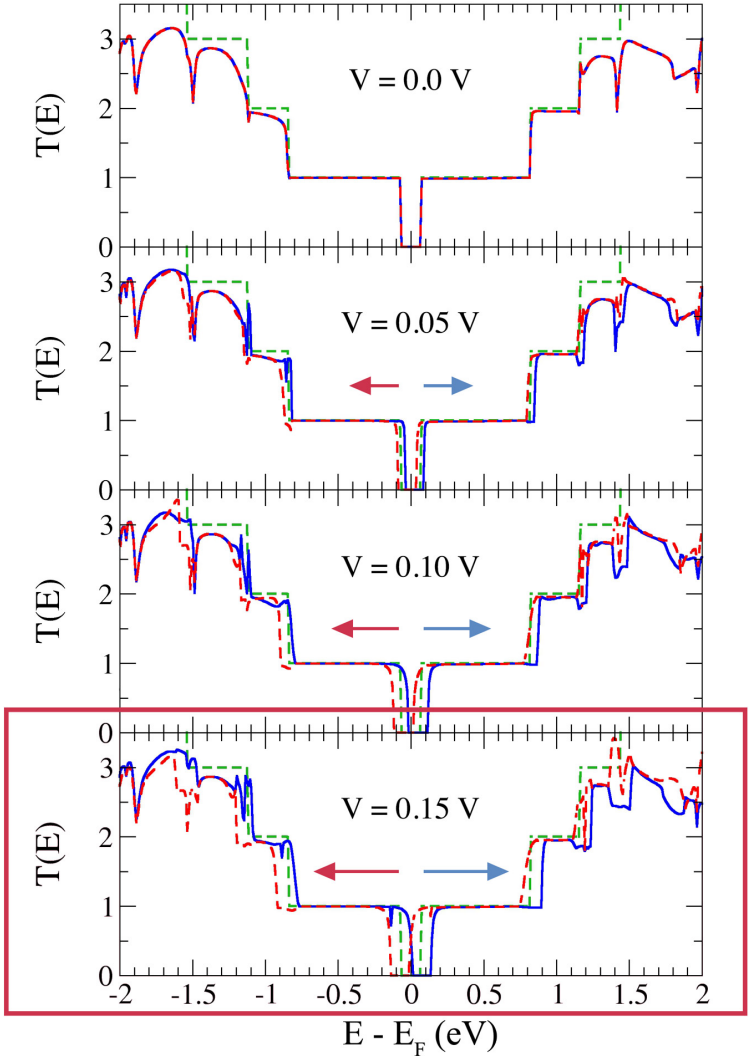
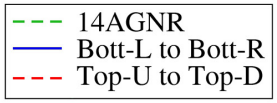


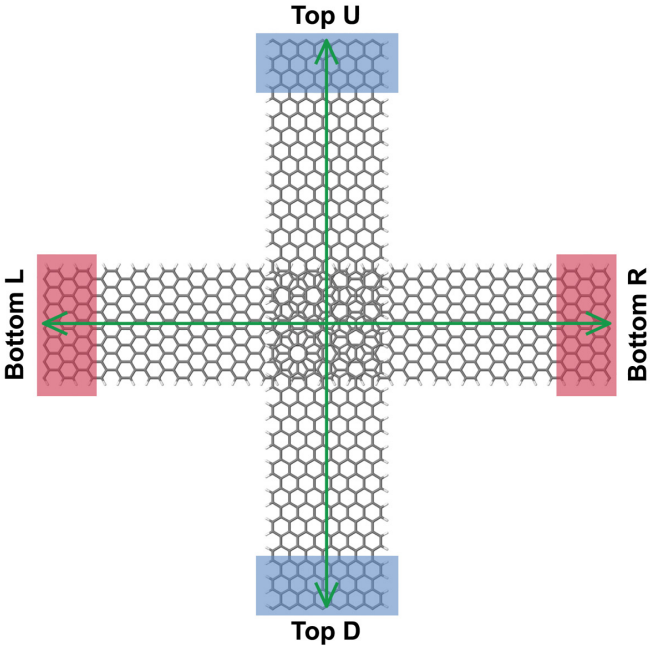




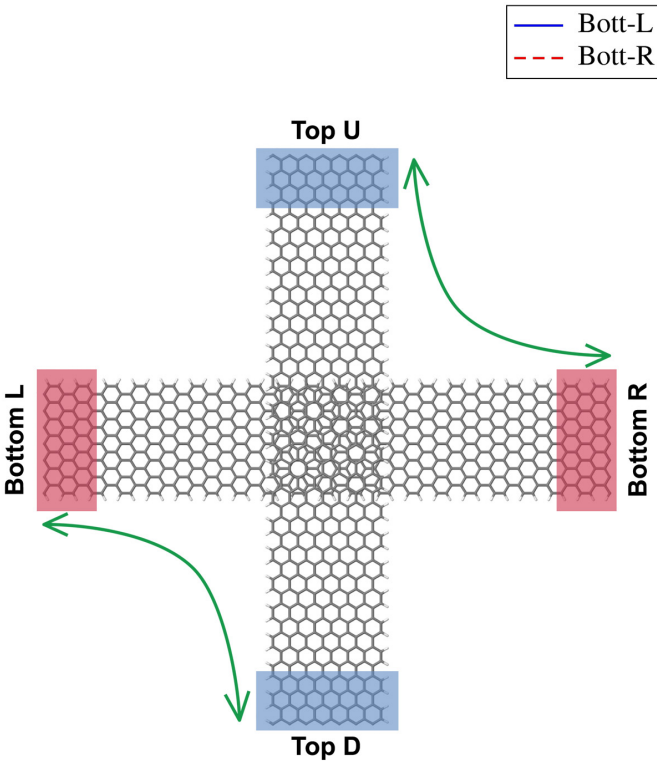
Direct transmission

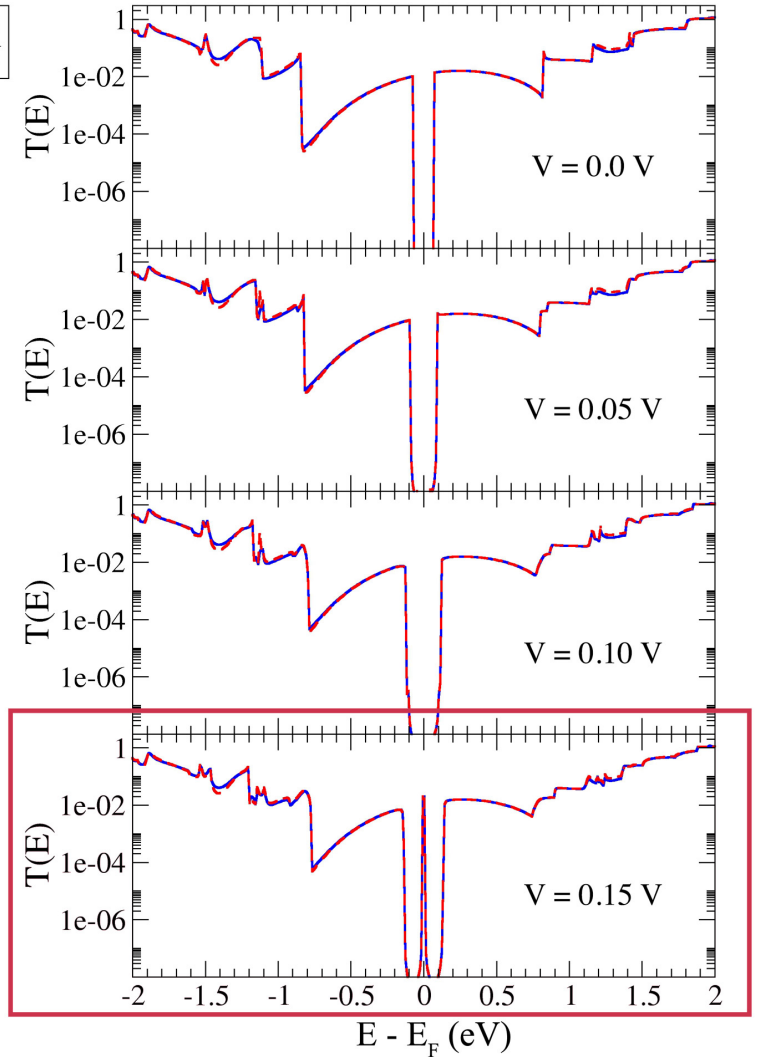




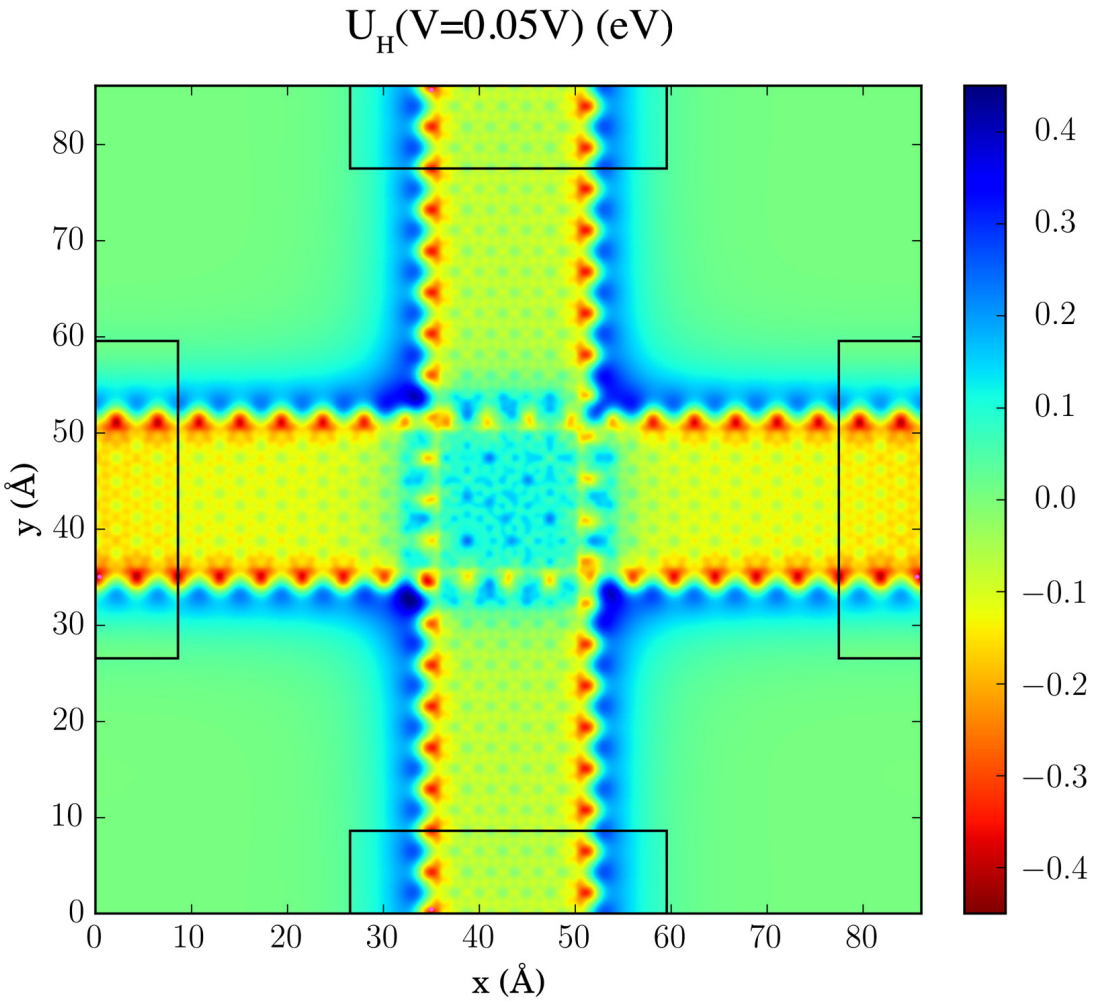


Inter-ribbon transmission



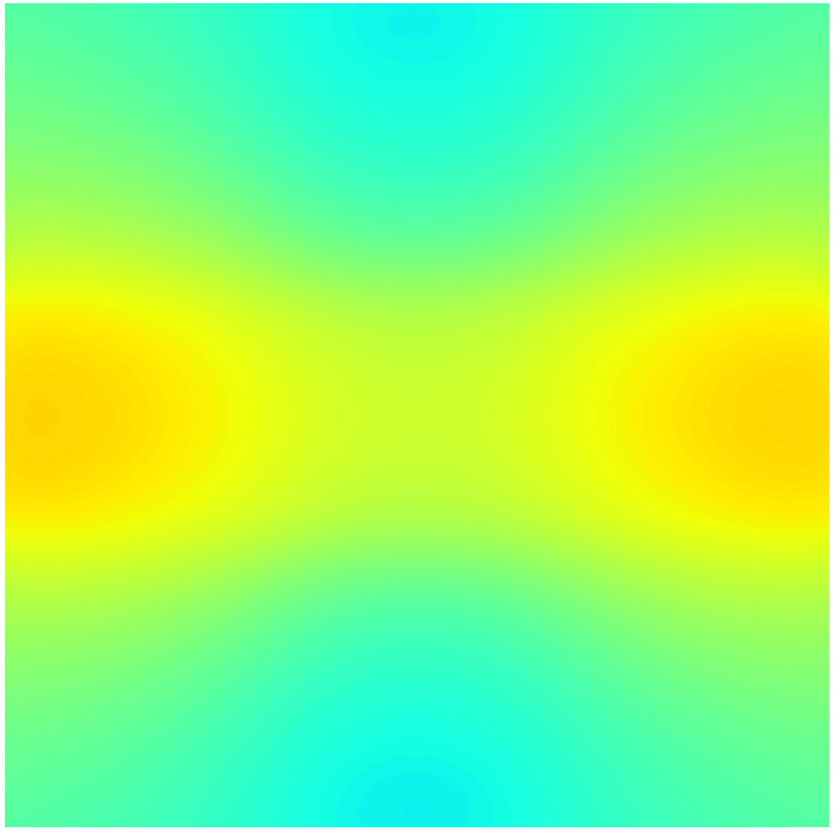


Electrostatic potential at V = 0.05 V



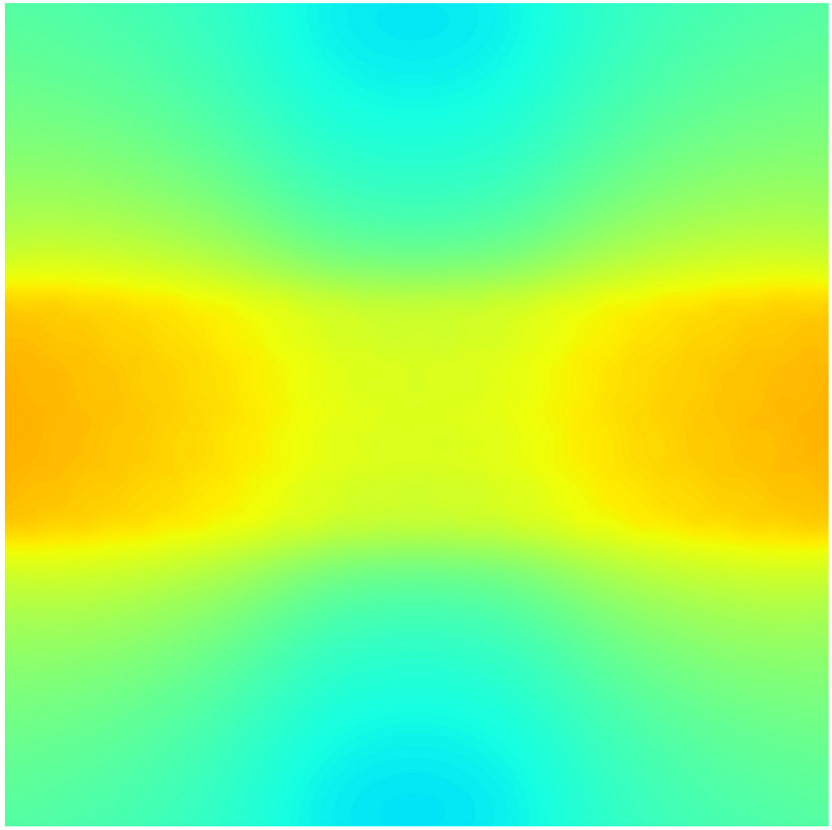
Electrostatic potential at V = 0.05 V

$U_H(V=0.05V) - U_H(V=0.0V)$ (eV)



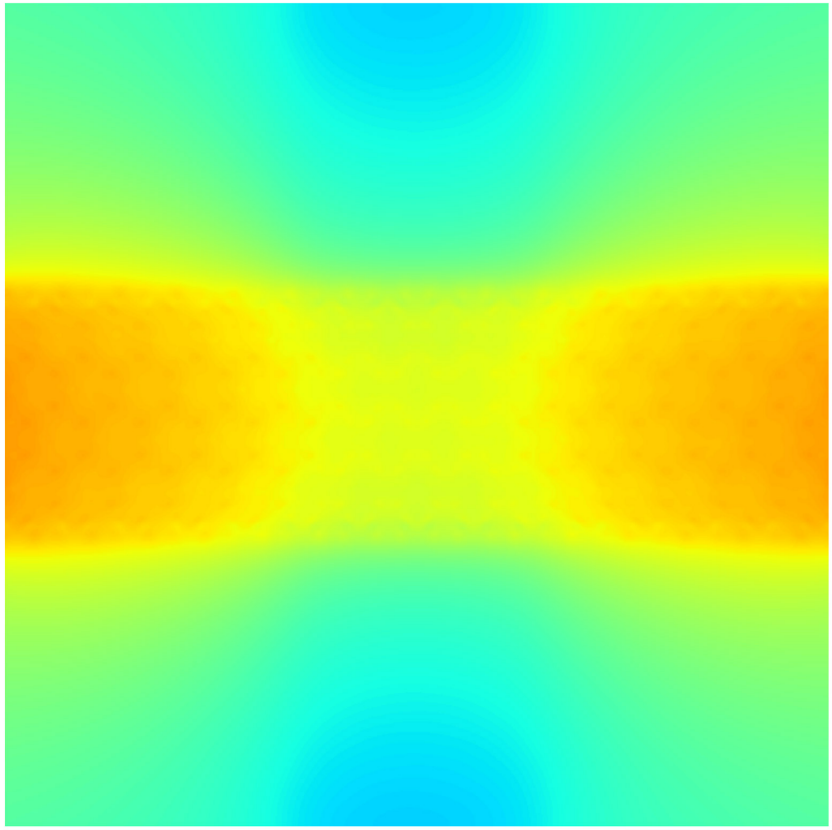
Electrostatic potential at V = 0.05 V

$U_H(V=0.05V) - U_H(V=0.0V)$ (eV)



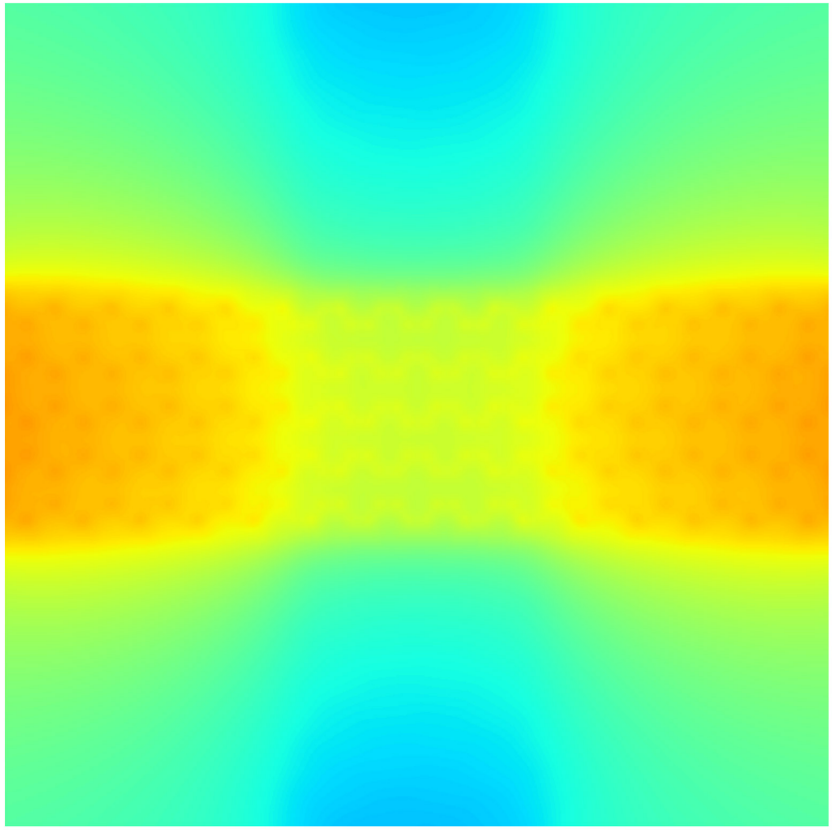
Electrostatic potential at V = 0.05 V

$$U_H(V=0.05V) - U_H(V=0.0V)\ (eV)$$



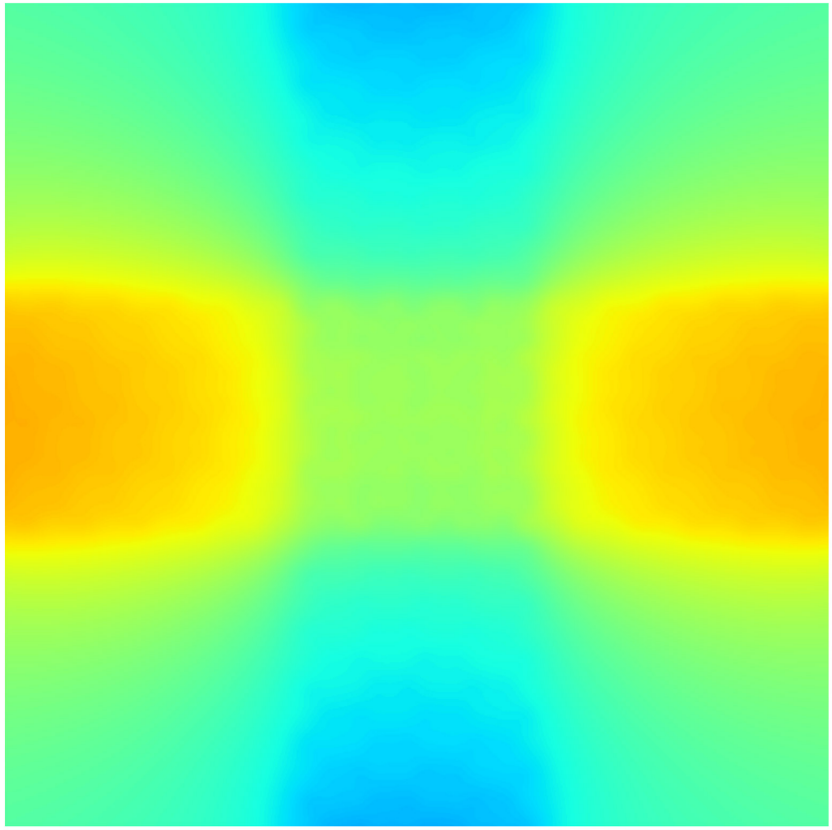
Electrostatic potential at V = 0.05 V

$$U_H(V=0.05V) - U_H(V=0.0V)\ (eV)$$



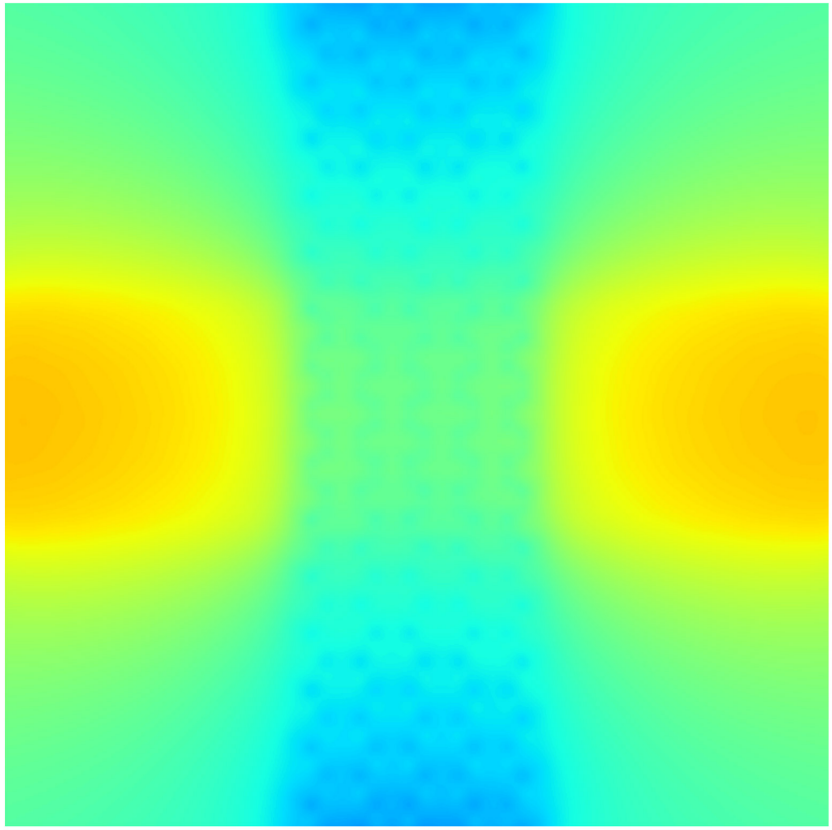
Electrostatic potential at V = 0.05 V

$$U_H(V=0.05V) - U_H(V=0.0V)\ (eV)$$



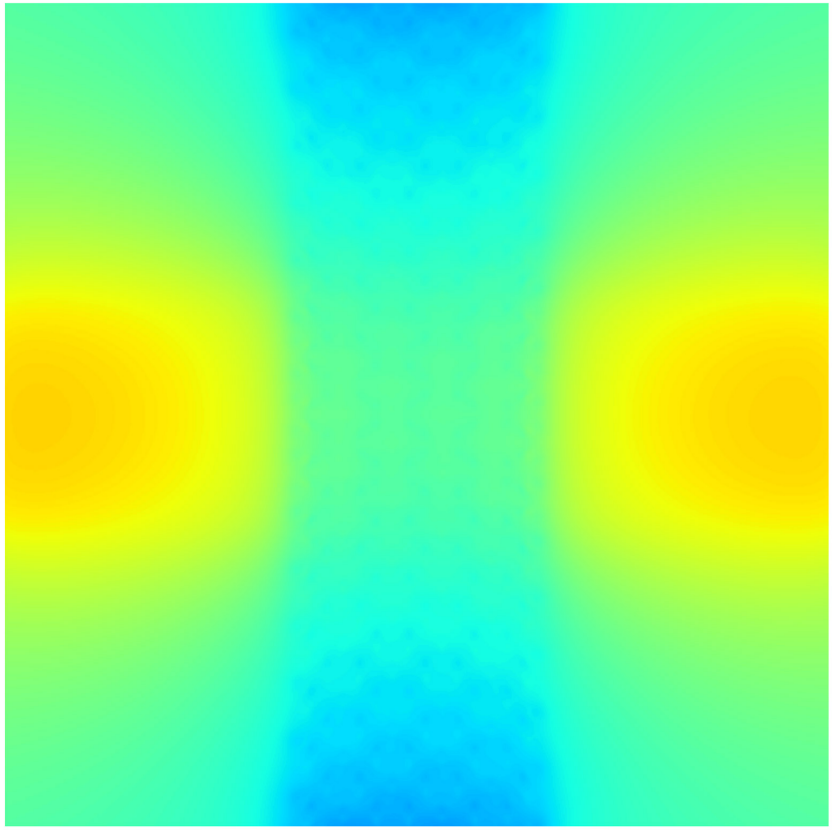
Electrostatic potential at V = 0.05 V

$$U_H(V=0.05V) - U_H(V=0.0V)\ (eV)$$



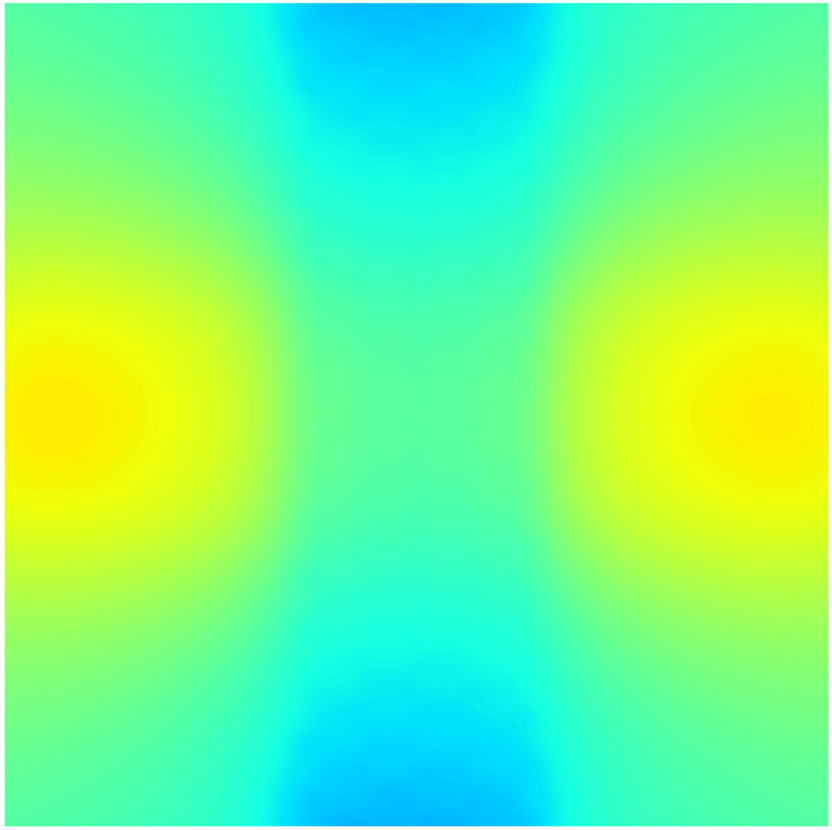
Electrostatic potential at V = 0.05 V

$$U_H(V=0.05V) - U_H(V=0.0V)\ (eV)$$



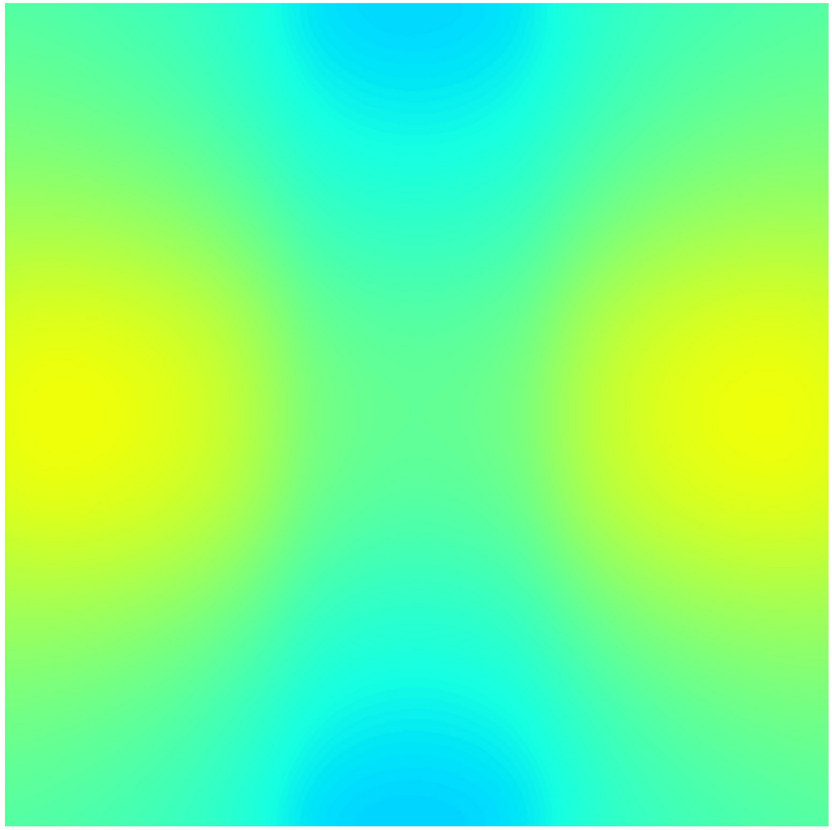
Electrostatic potential at V = 0.05 V

$$U_H(V=0.05V) - U_H(V=0.0V)\ (eV)$$



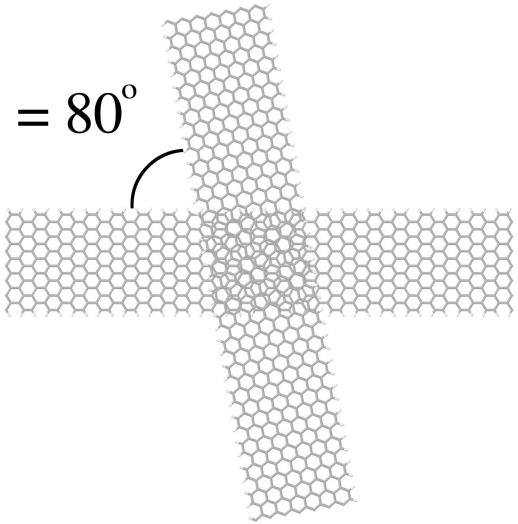
Electrostatic potential at V = 0.05 V

$$U_H(V=0.05V) - U_H(V=0.0V)\ (eV)$$

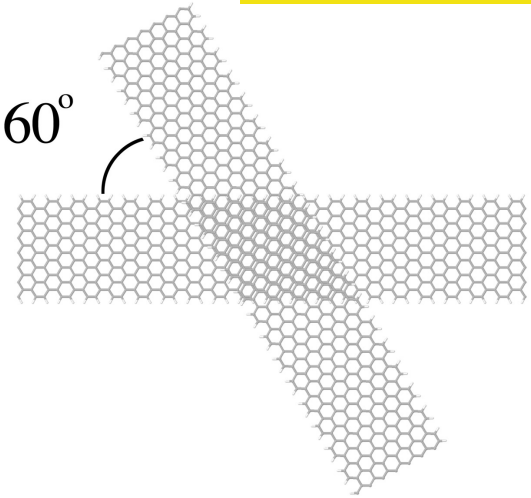


Rotated crossbar

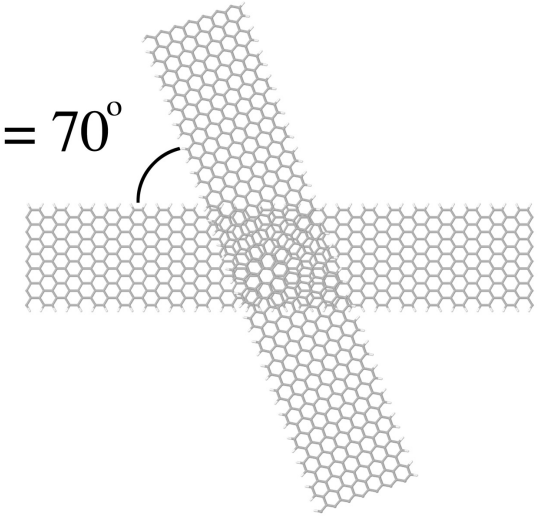
$\theta = 80^{o}$



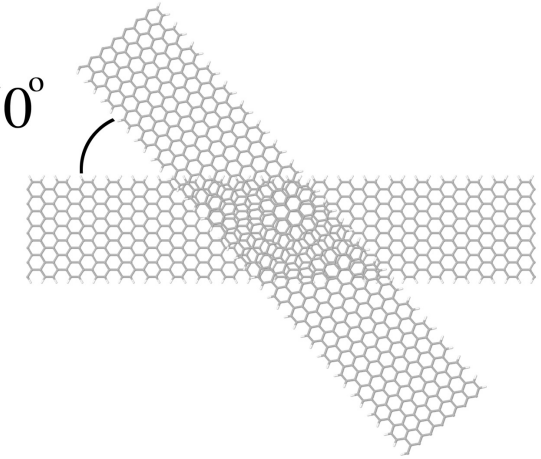
$\theta = 60^{o}$



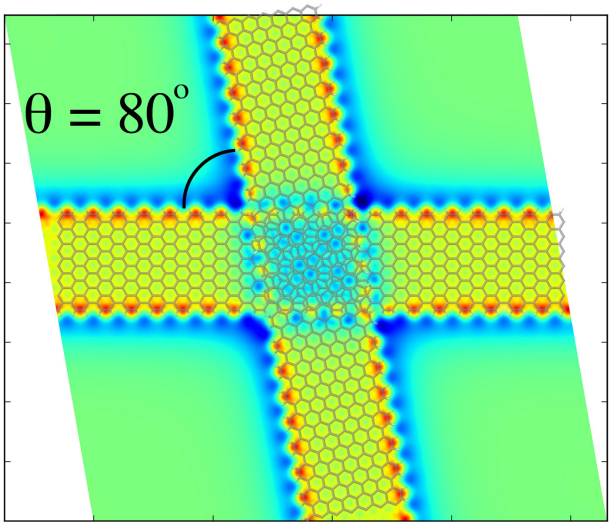
$\theta = 70^{o}$

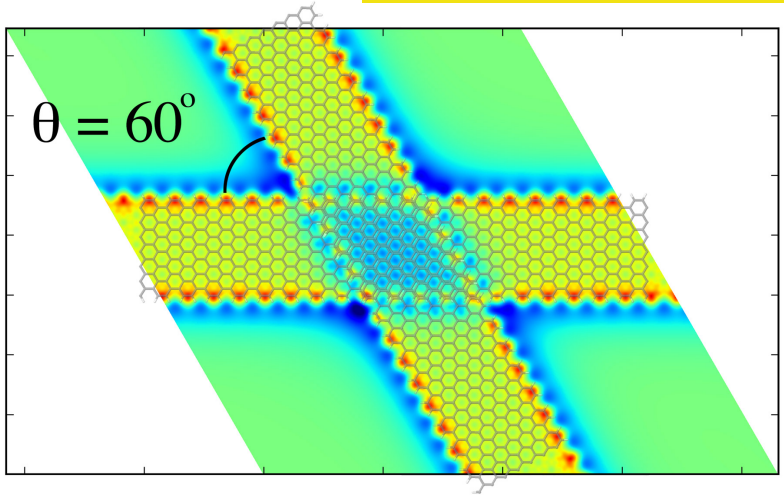


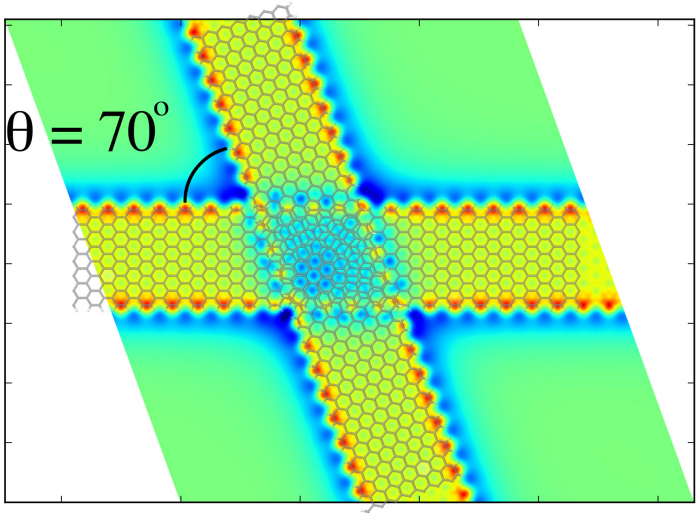
$\theta = 50^{o}$

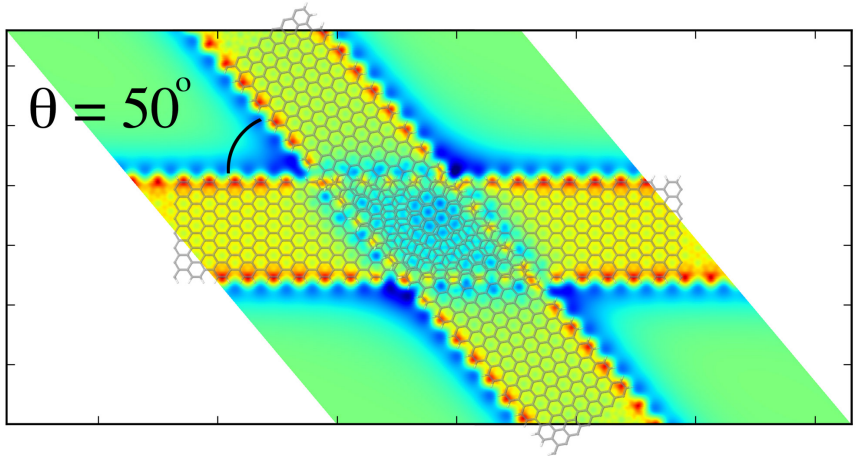


Electrostatic potential at V = 0

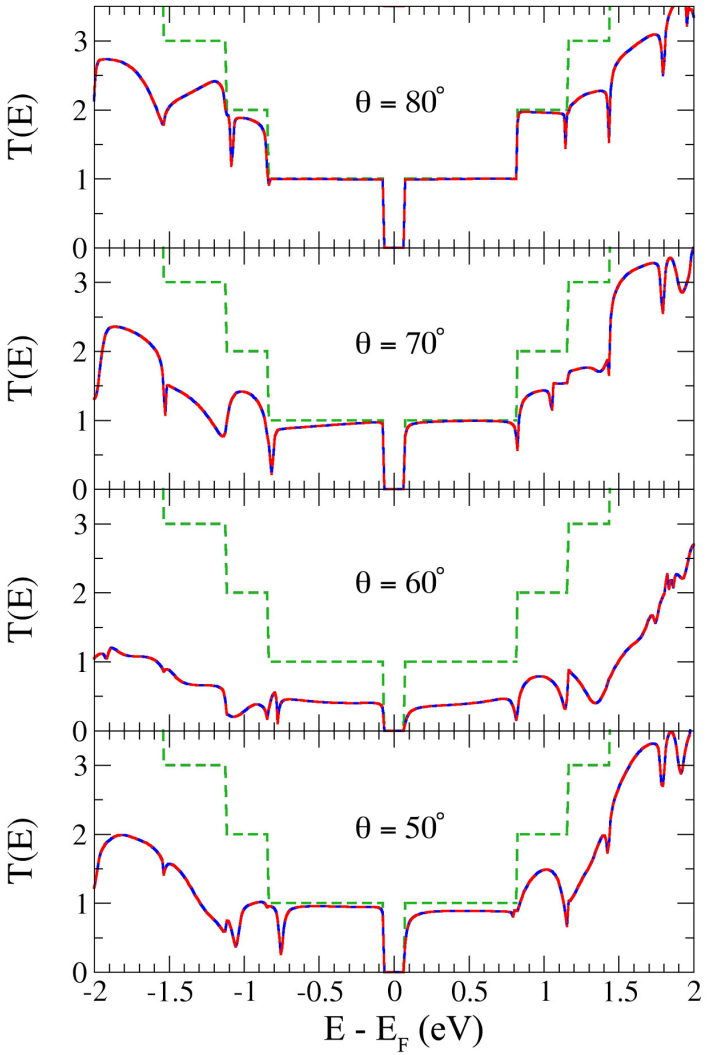


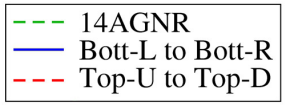


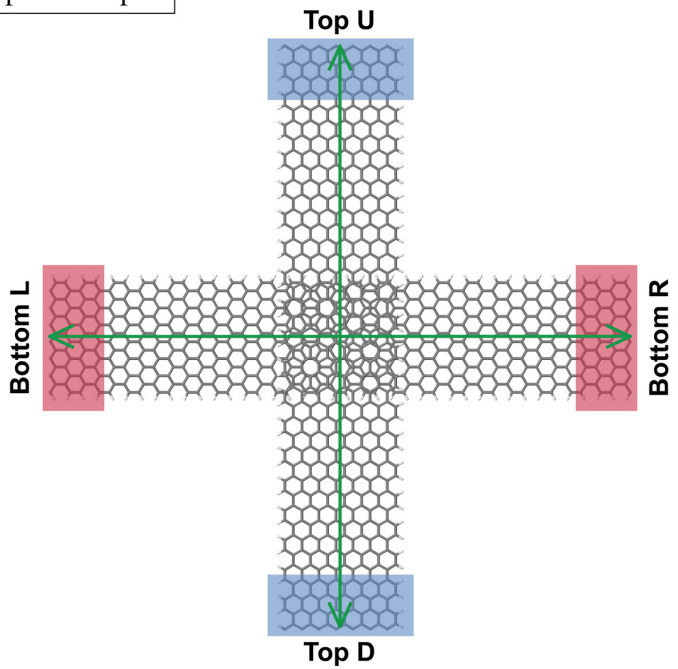




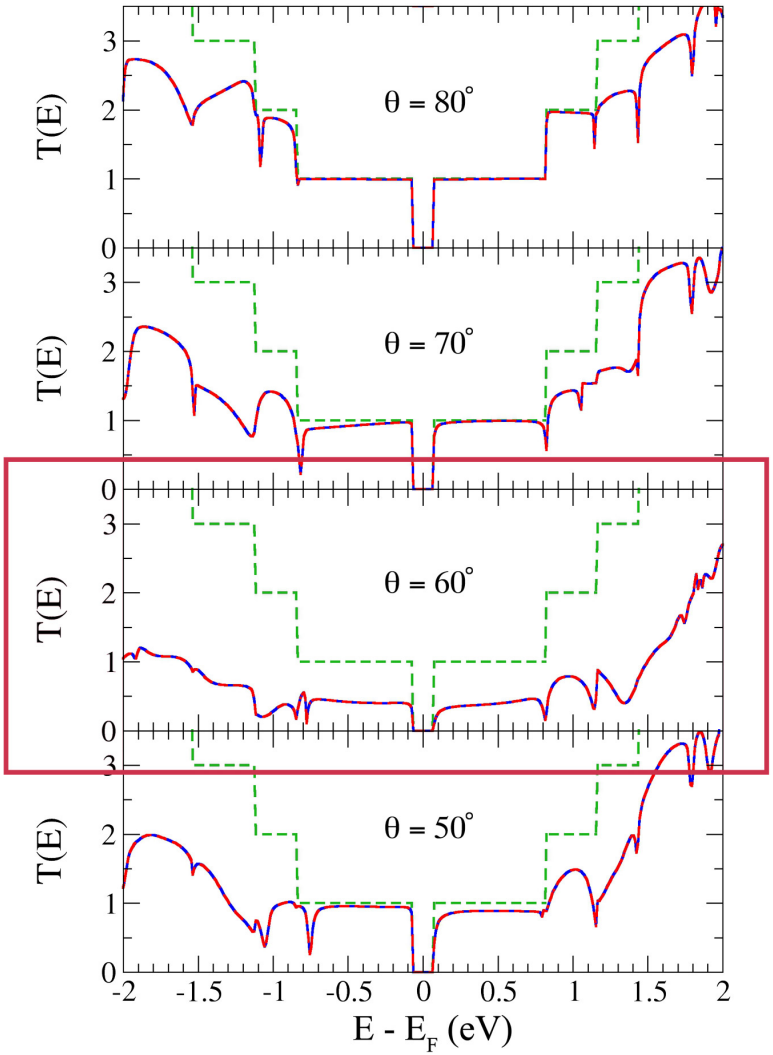
Direct transmission at V = 0

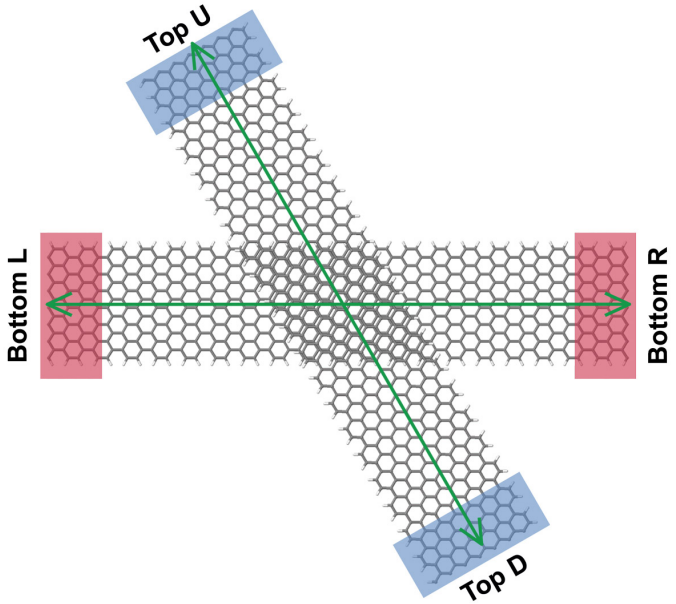




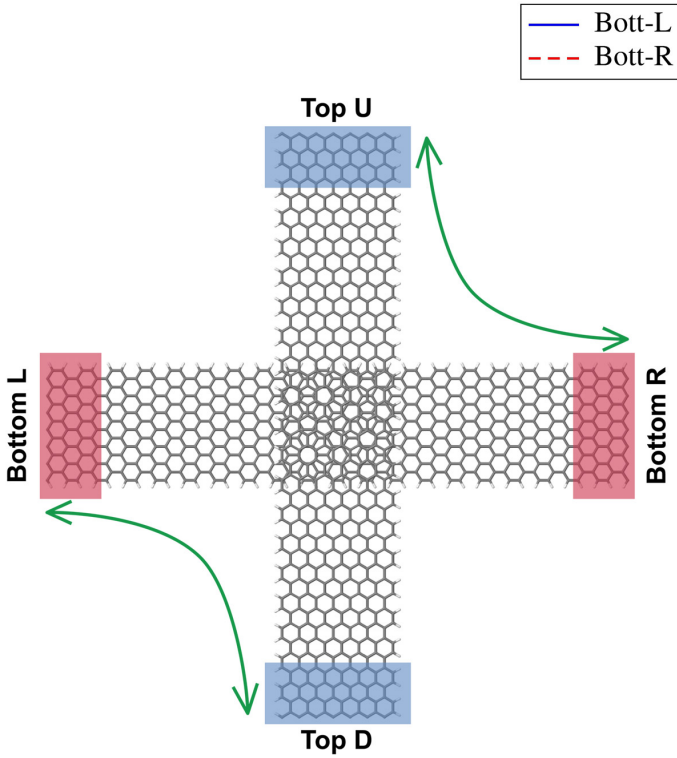


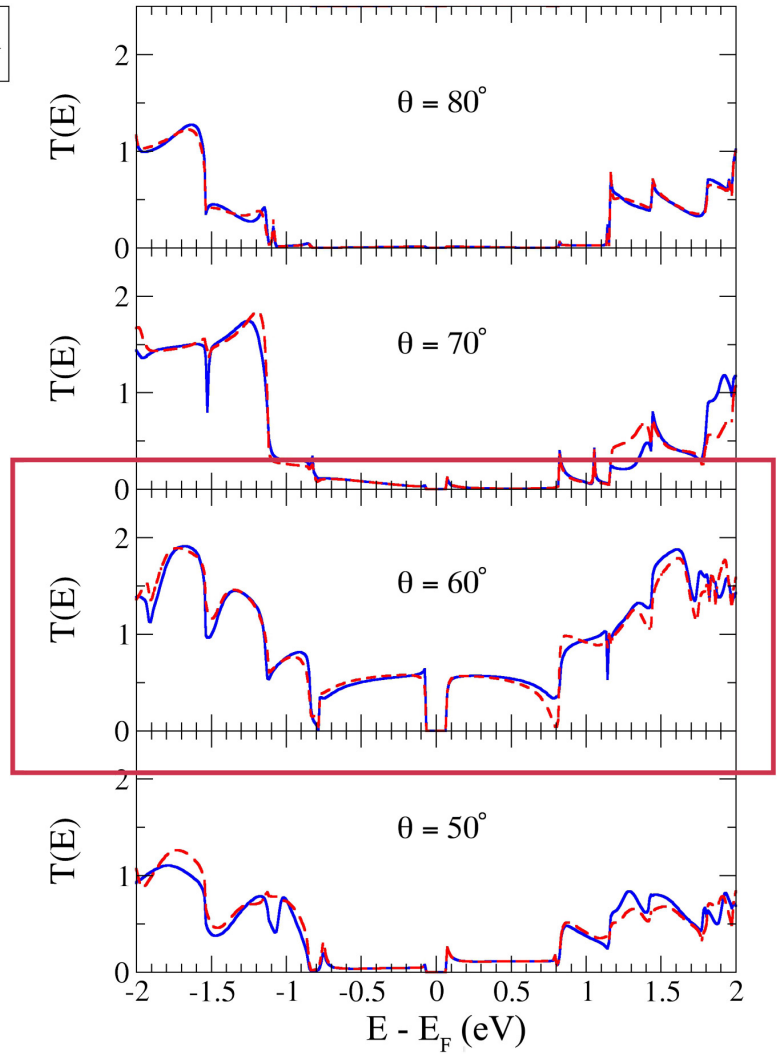
Direct transmission at V = 0



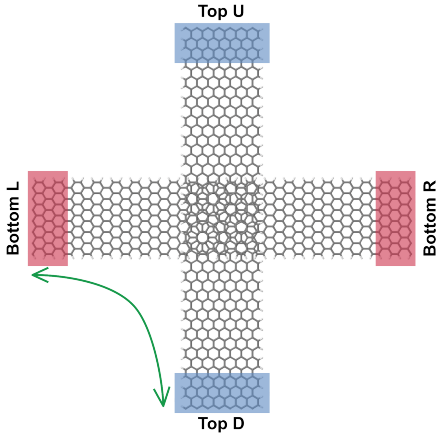


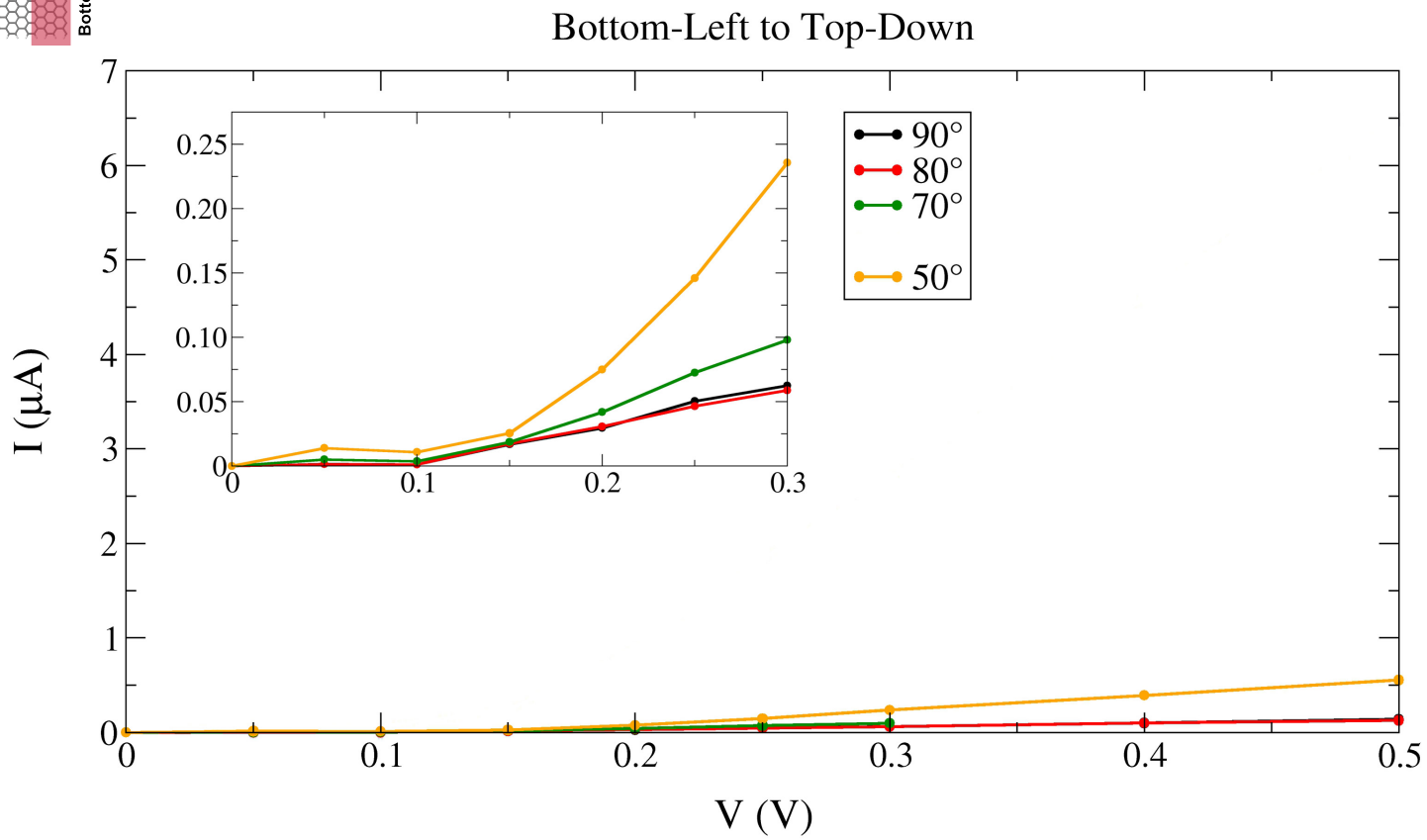
Inter-ribbon transmission at V = 0



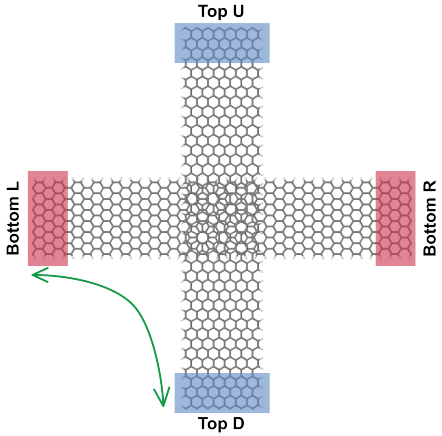


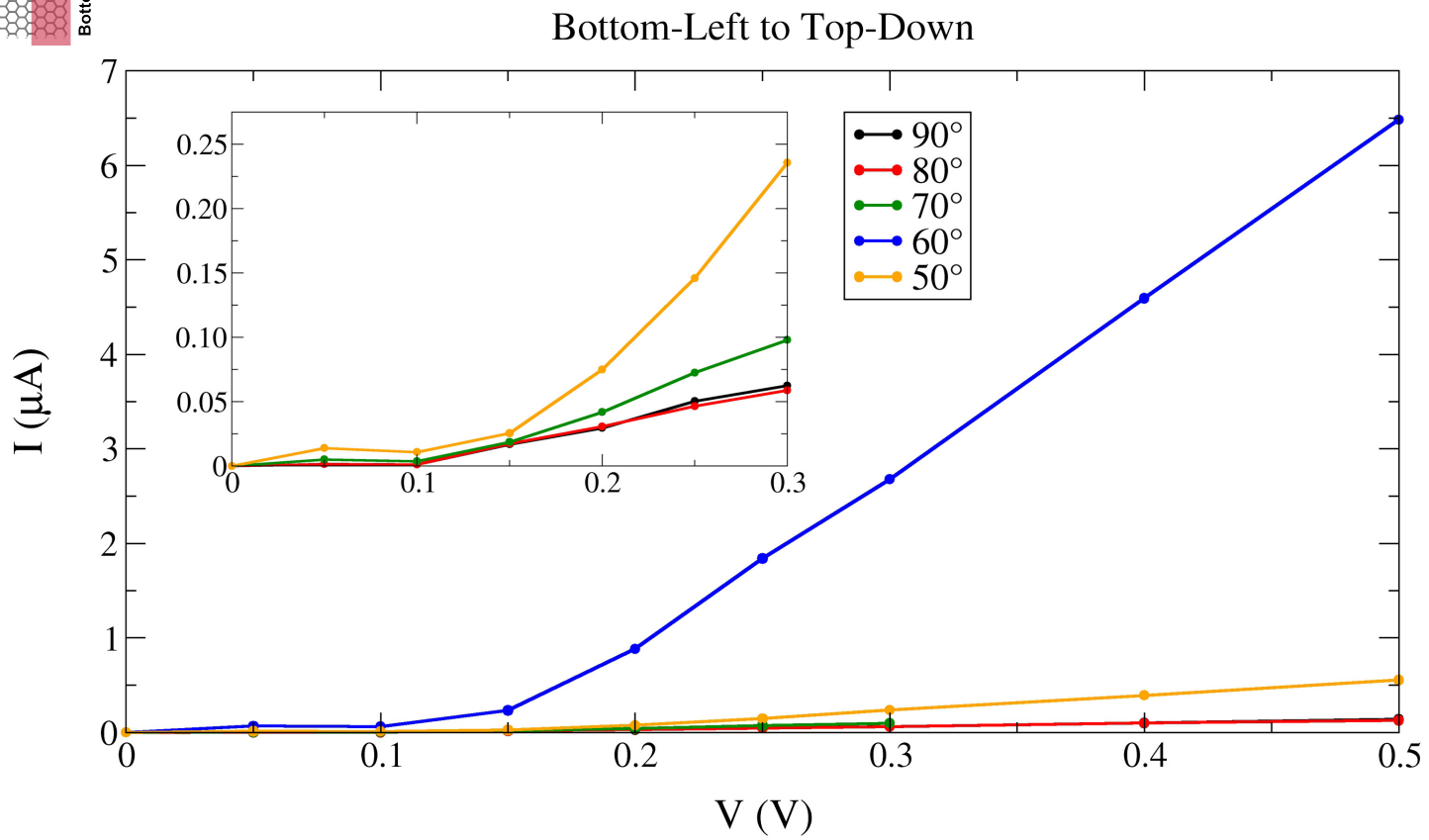
Inter-ribbon current



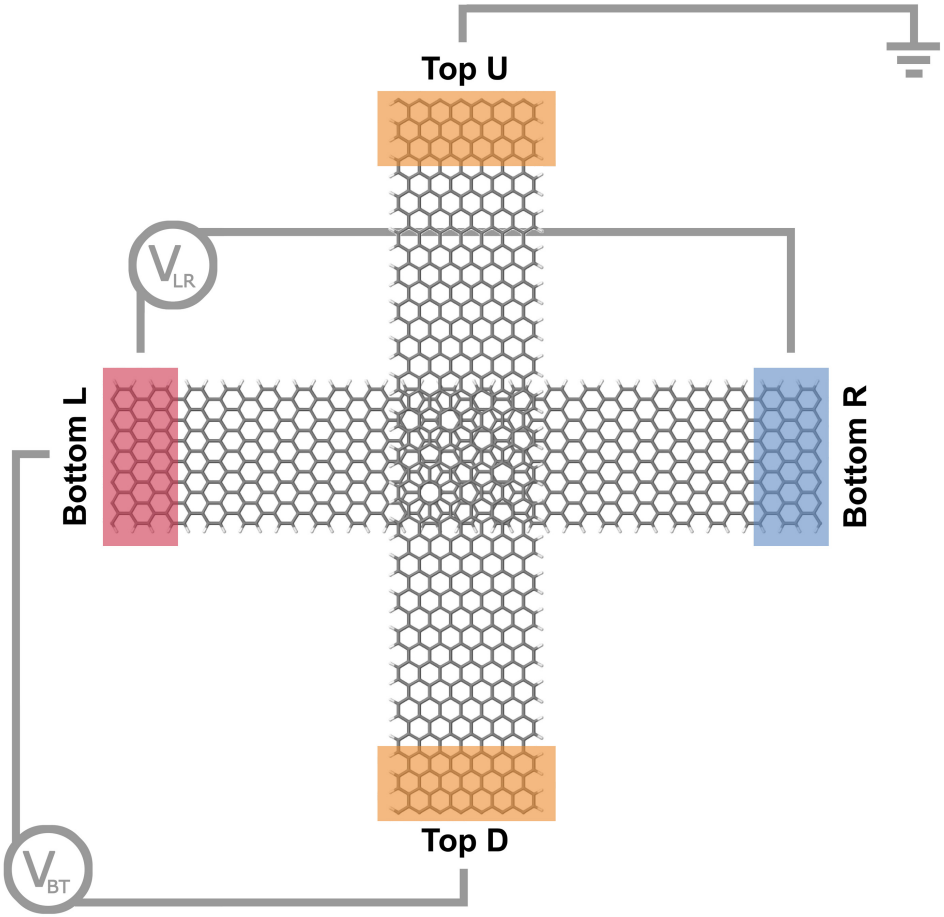


Inter-ribbon current

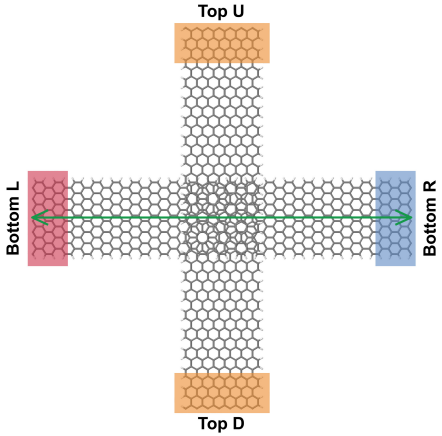


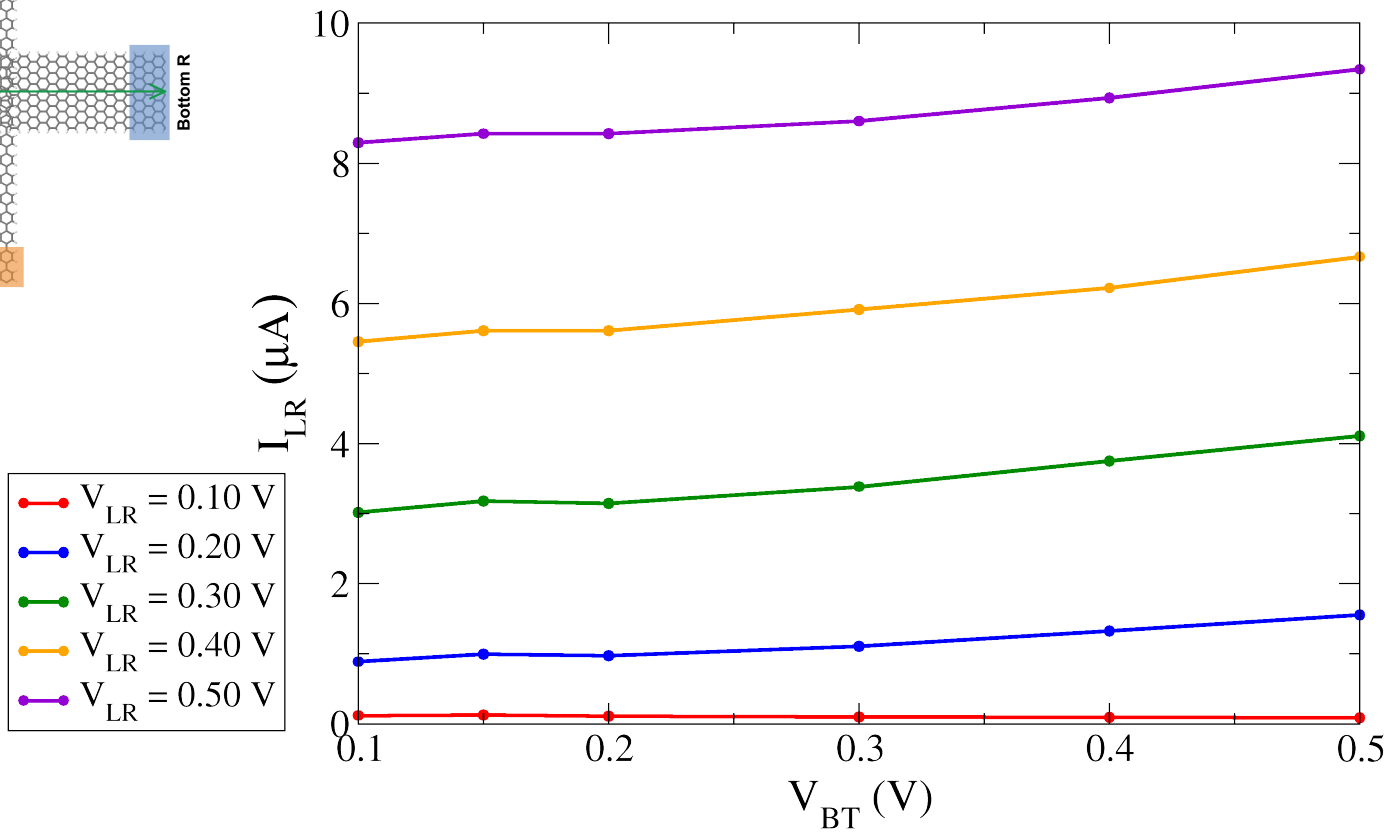


Intralayer bias

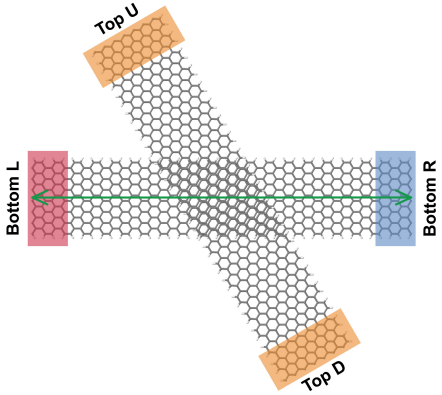


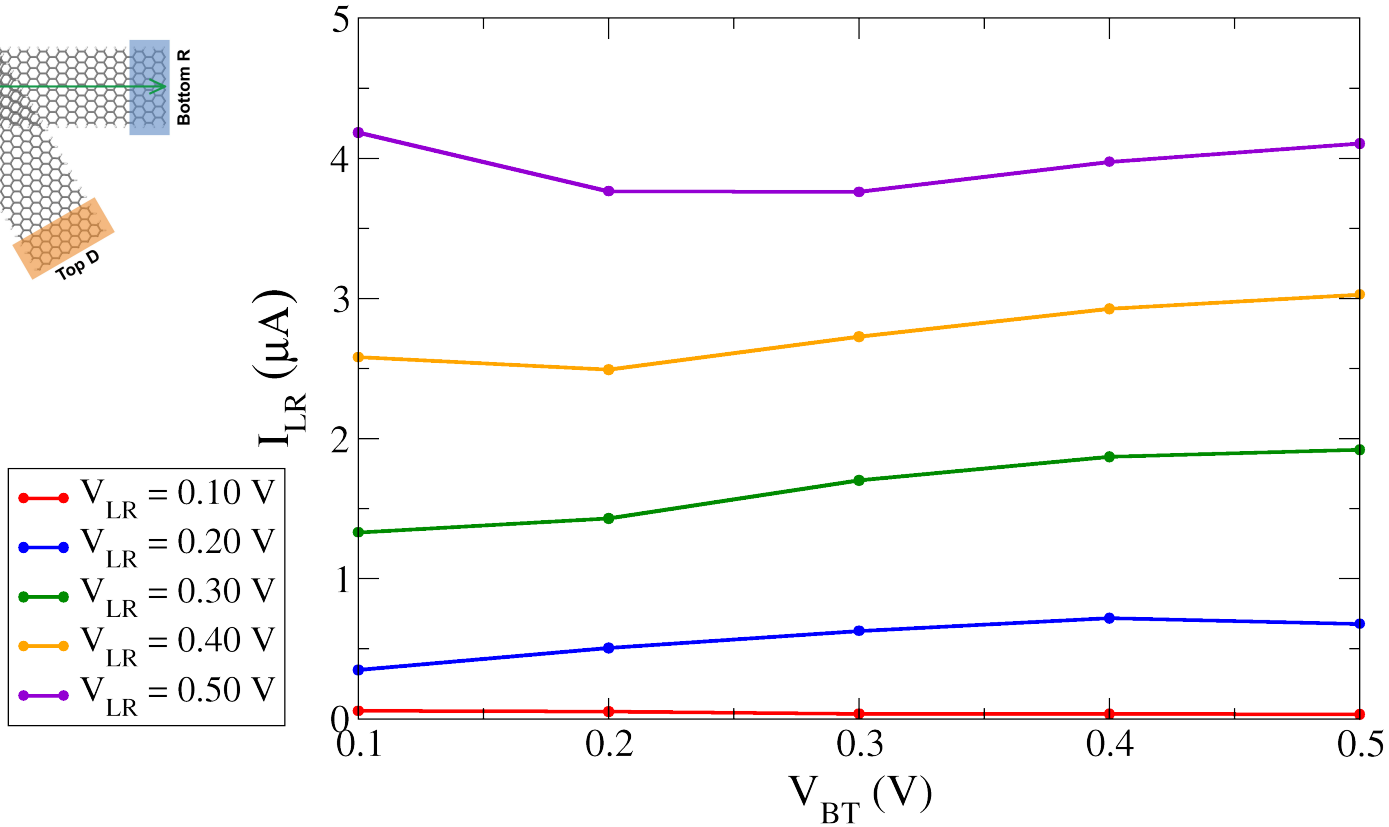
Intralayer bias





Intralayer bias





Conclusions

- TranSIESTA for **N≥1 arbitrarily distributed** electrodes at finite bias;
- Transmission **strongly depends on the stacking**;
- For a 60° rotation angle one finds a **higher inter-layer transmission**;
- In our calculations we observe a **small gating effect** due to the top ribbon.

Acknowledgements

PAMS
SEVENTH FRAMEWORK PROGRAMME
GOBIERNO DE ESPAÑA
MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD
CSIC
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

Towards reality in modelling of molecular electronics

June 13-17, 2016 · Donostia-San Sebastián, Spain

Welcome

Donostia International Physics Center (DIPC) and FET-ICT project *Planar Atomic and Molecular Scale devices* (PAMS) are organizing the international workshop **Towards Reality in Modelling of Molecular Electronics** (TRMME) that will take place in San Sebastián, Spain, on **June 13-17, 2016**.

The aim of this workshop is to bring together experienced and young researchers, as well as students, working in the field of the theory of quantum transport and the development of computational tools for transport simulations in the nanoscale.

http://trmme.dipc.org