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PAMS

CFM

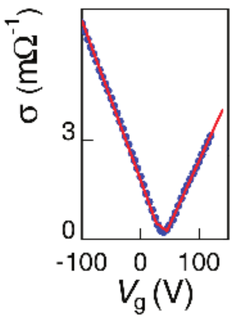
Aspects of Graphene Nanoribbons Devices Simulations

Pedro Brandimarte

June 13, 2016

Graphene

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



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

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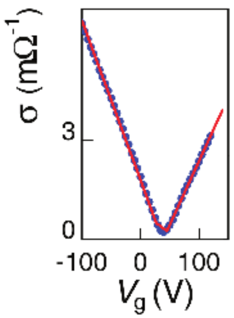
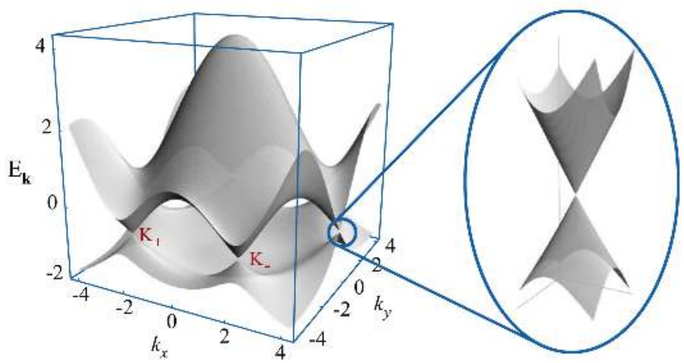


K. Novoselov *et al*. *Science* **306**, 666-669 (2004).

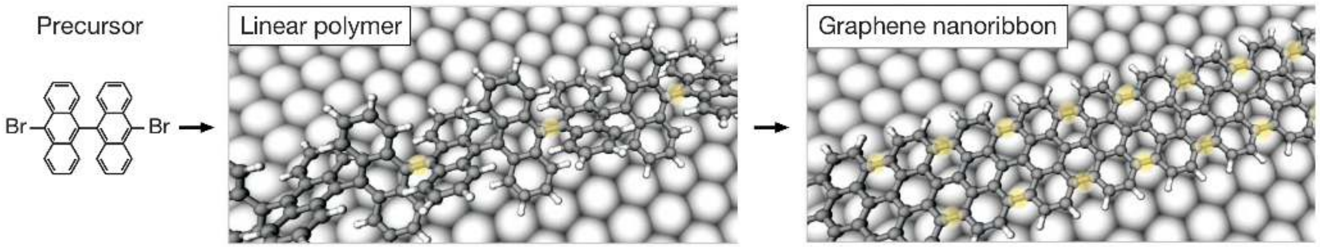
- Gap absence:



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

Graphene Nanoribbons (GNRs)

- Bottom-up fabrication of both AGNR and ZGNR by on-surface reaction of molecular precursors.



J. Cai *et al*. *Nature* **466**, 470 (2010).

L. Talirz, P. Ruffieux, and R. Fasel. *Advanced Materials* (2016).

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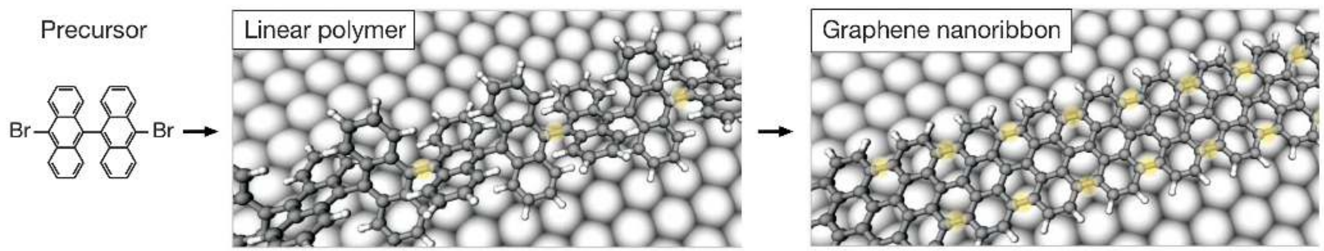
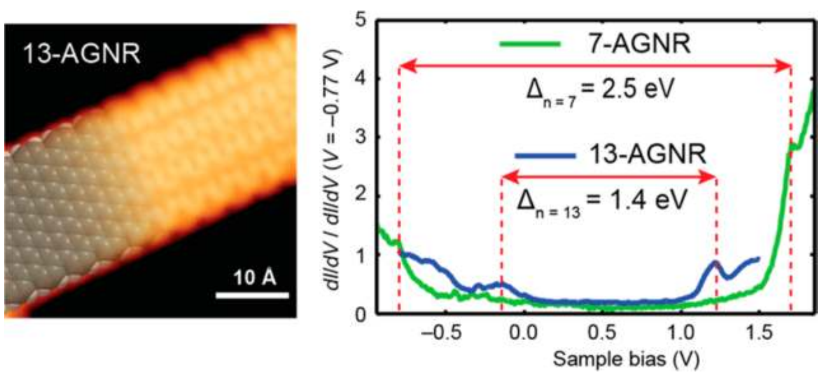


J. Cai *et al*. *Nature* **466**, 470 (2010).
L. Talirz, P. Ruffieux, and R. Fasel. *Advanced Materials* (2016).

- Semiconductor character, with energy gap depending on their width and shape.



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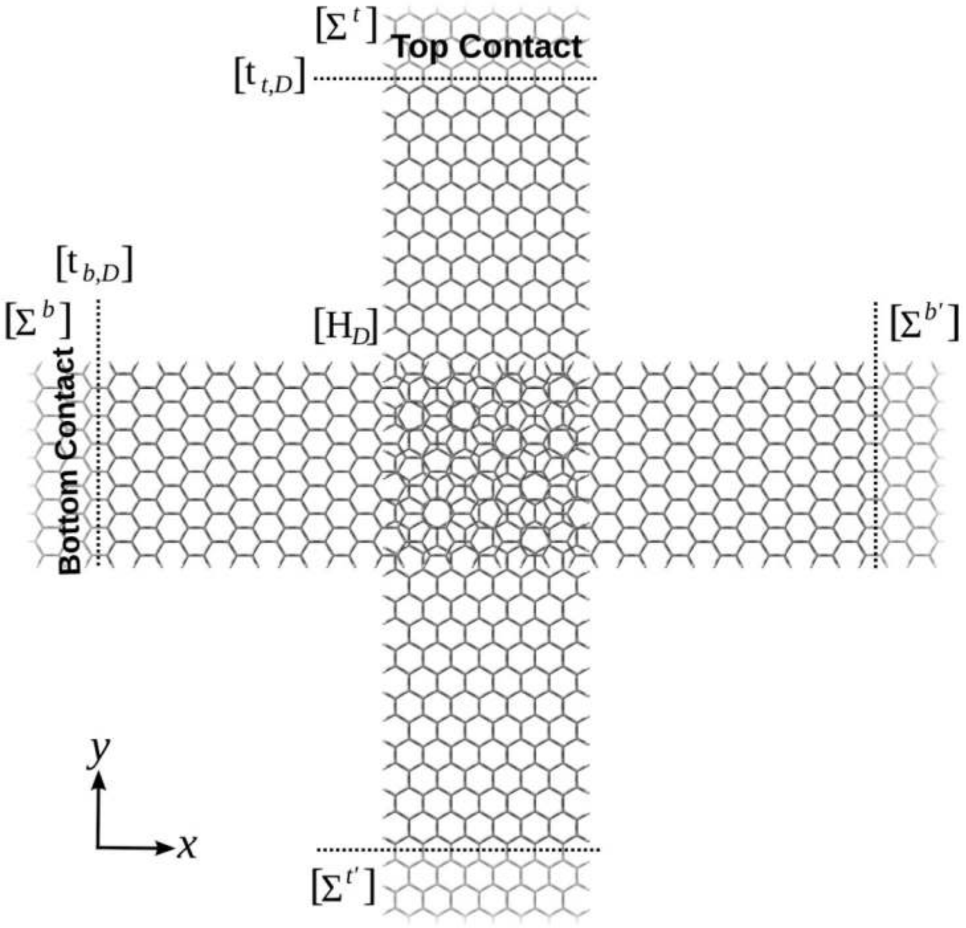
Y.-C. Chen *et al*. *ACS Nano* **7**, 6123 (2013).
A. Kimouche *et al*. *Nature Communications* **6**, 10177 (2015).

Electron Transport Simulations of 4-Terminal Crossed Graphene Nanoribbons Devices

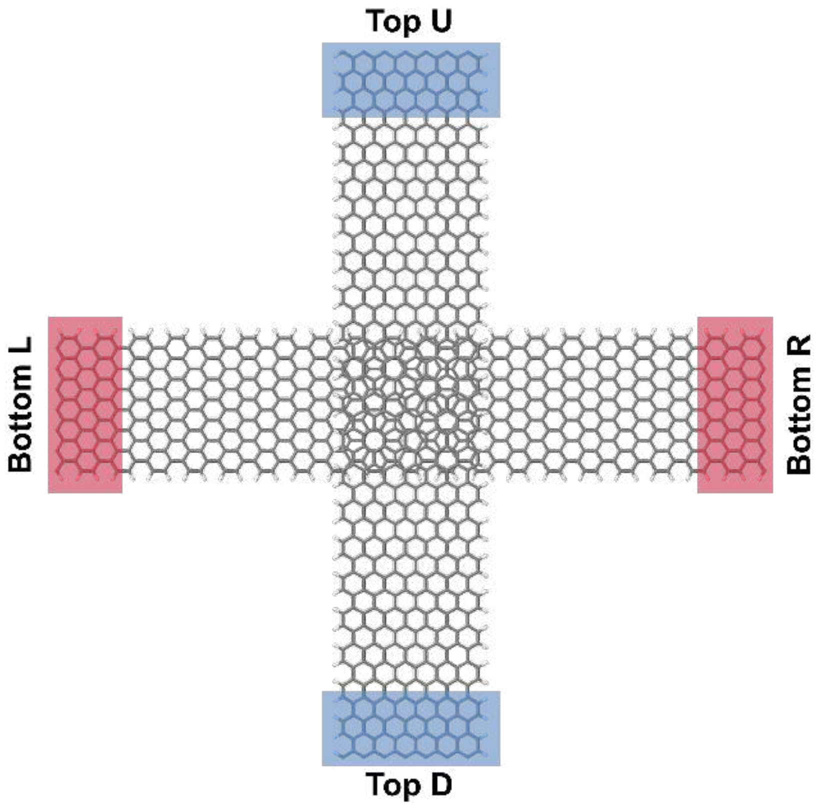
Pedro Brandimarte, Nick R. Papior, Mads Engelund,
Aran Garcia-Lekue, Thomas Frederiksen, and Daniel Sánchez-Portal

June 13, 2016



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

Crossed 14-AGNR



Density-Functional Theory (DFT)

+

Non-Equilibrium Green's Function (NEGF)

TranSIESTA

J. M. Soler *et al*. *J. Phys. Condens. Matter.* **14**, 2745 (2002).
Mads Brandbyge *et al*. *Phys. Rev. B* **65**, 165401 (2002).

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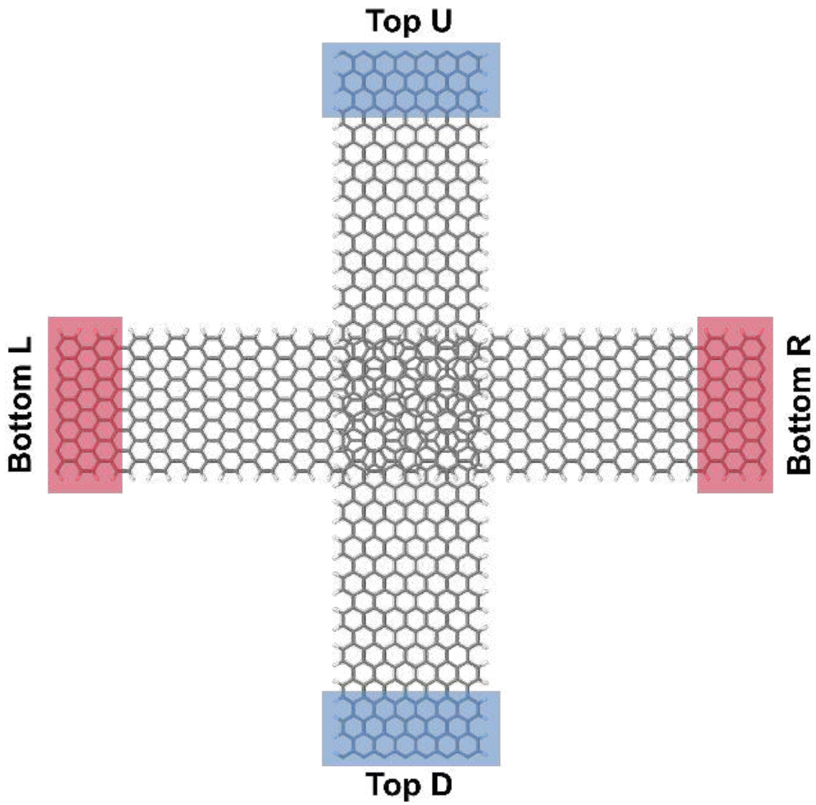

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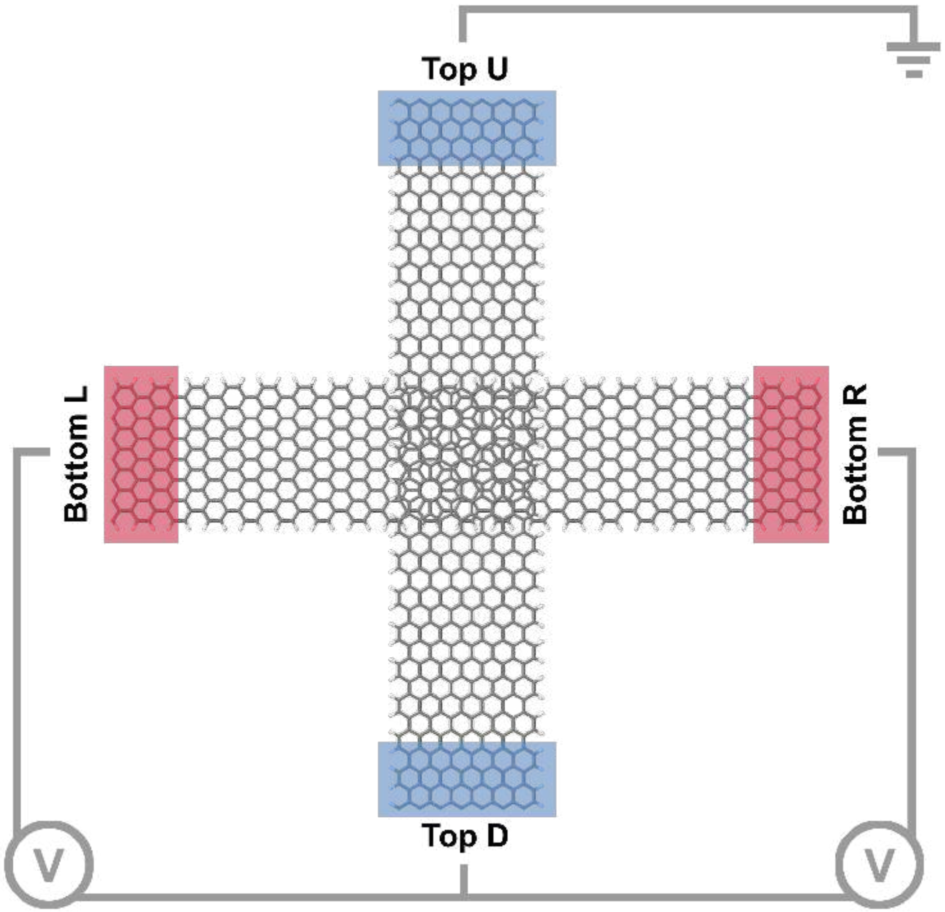
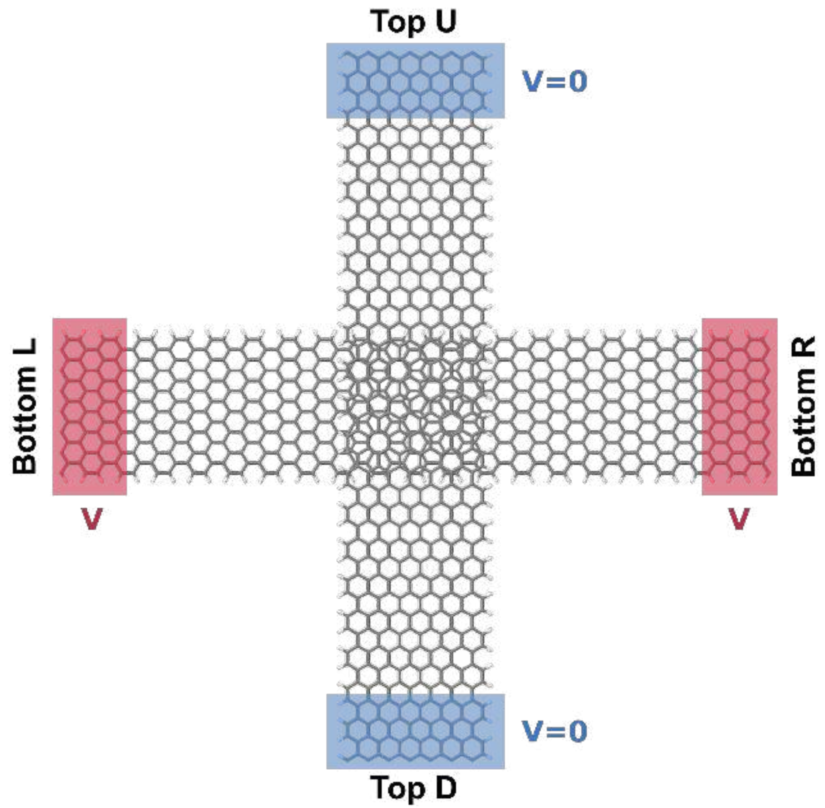
Nick R. Papior. *In preparation* (2016).

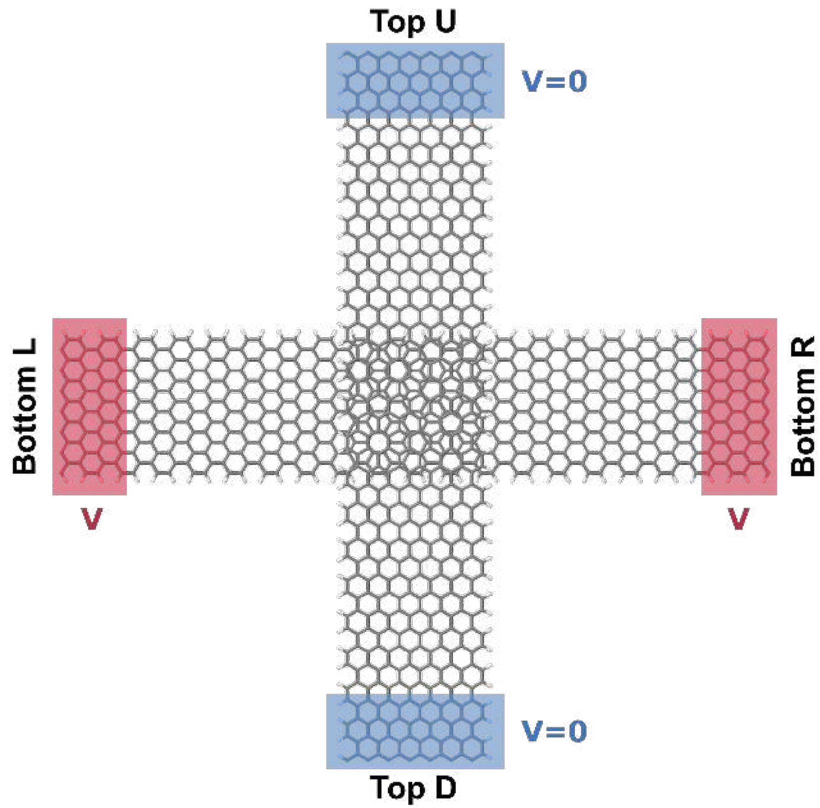
Crossed 14-AGNR



Crossed 14-AGNR



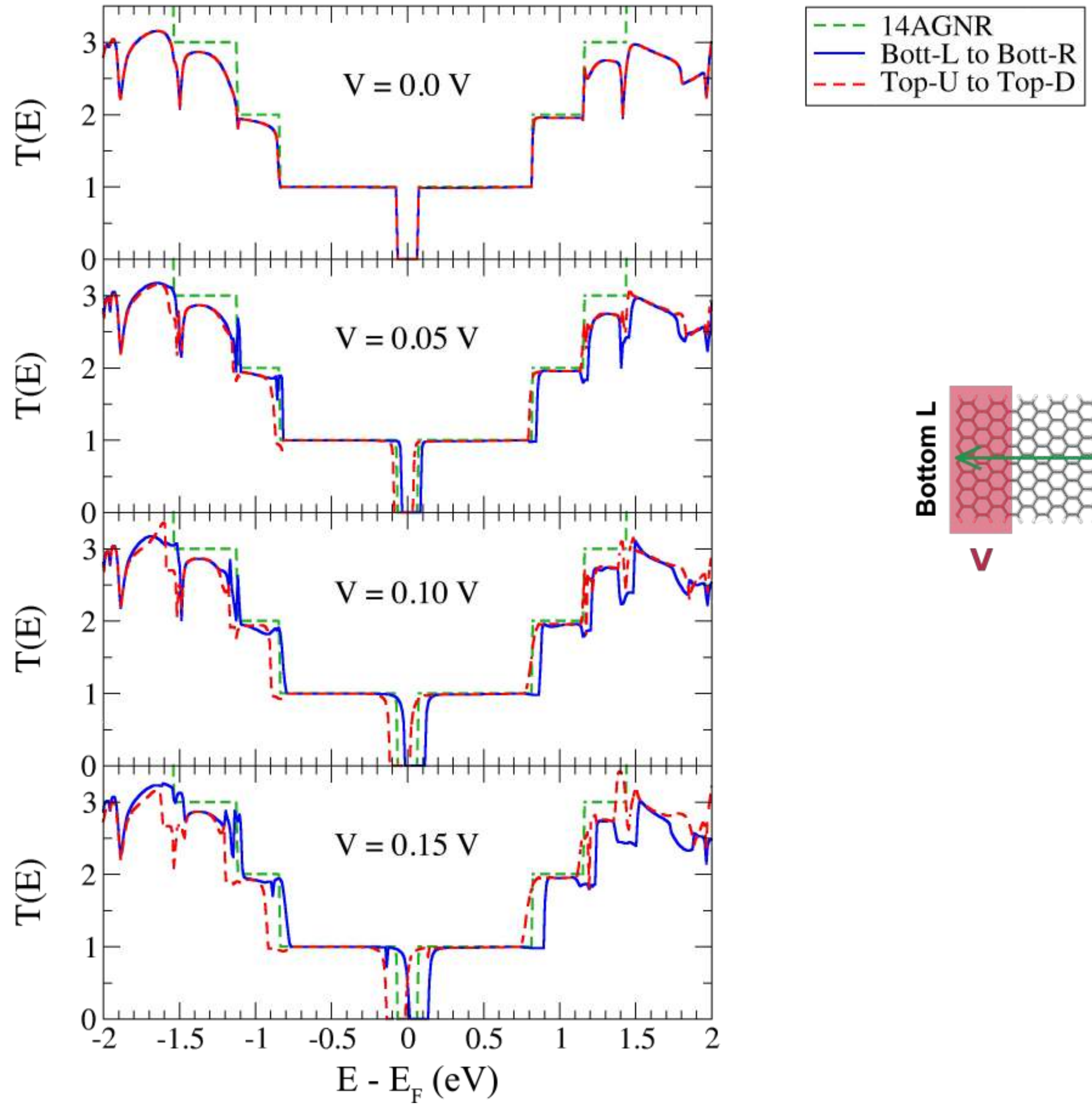
Crossed 14-AGNR

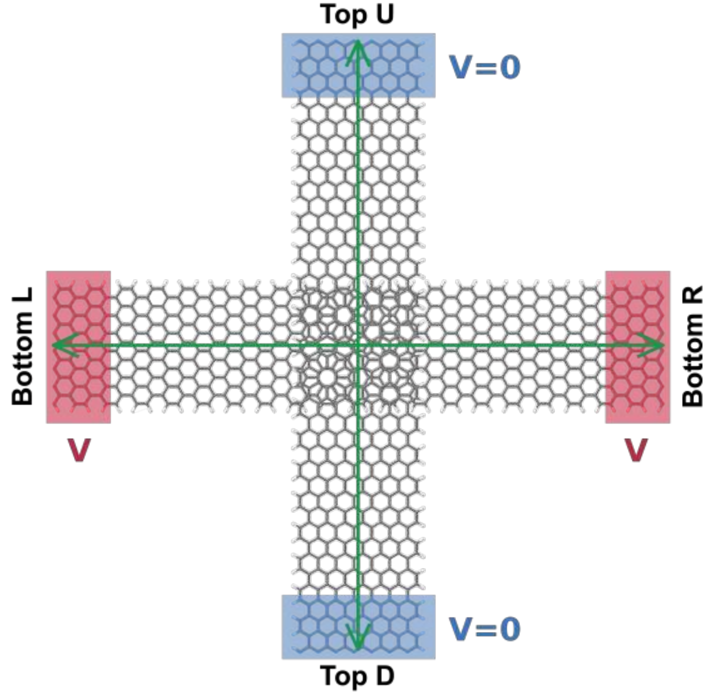


Simulation characteristics:

- 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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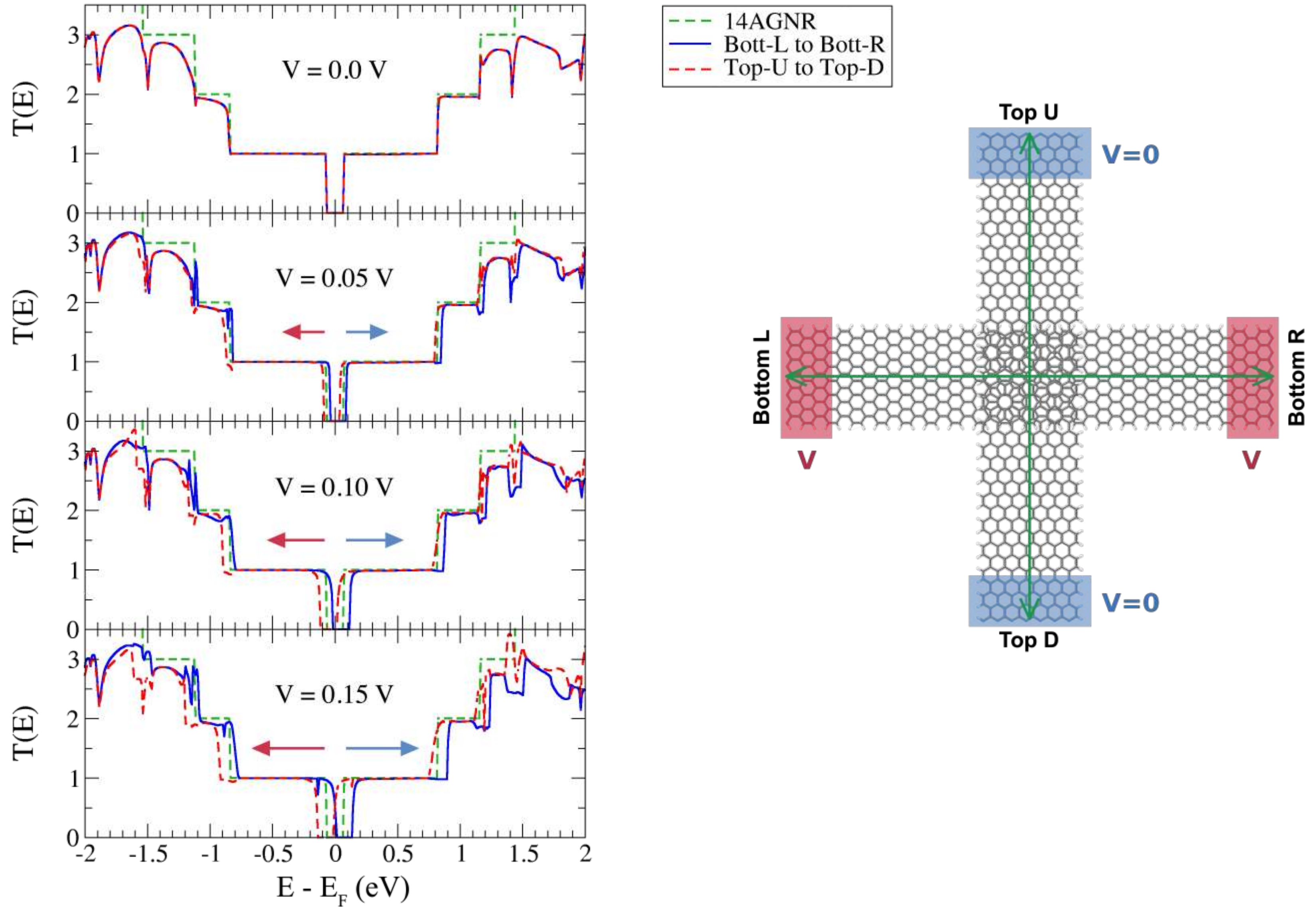

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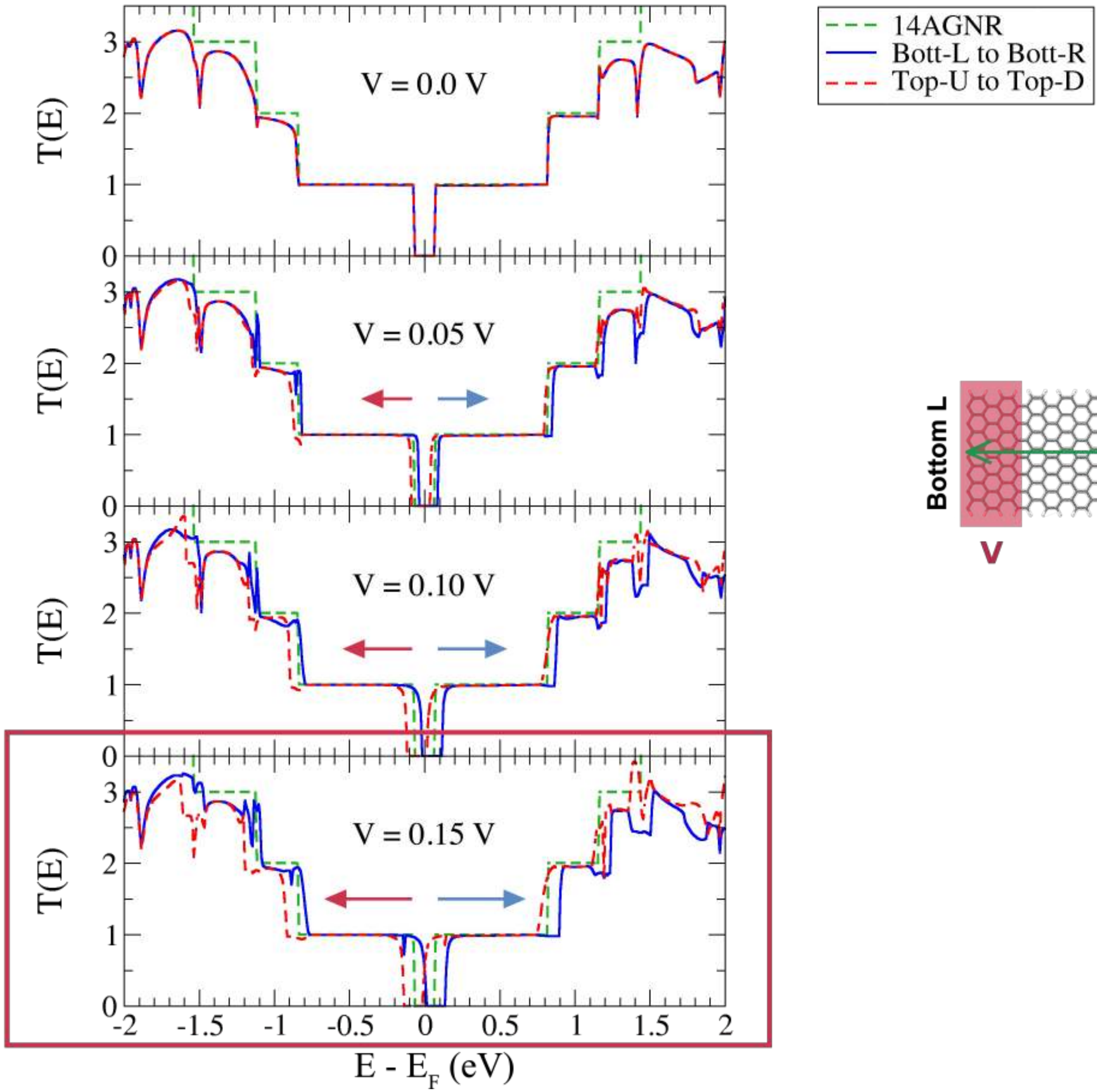
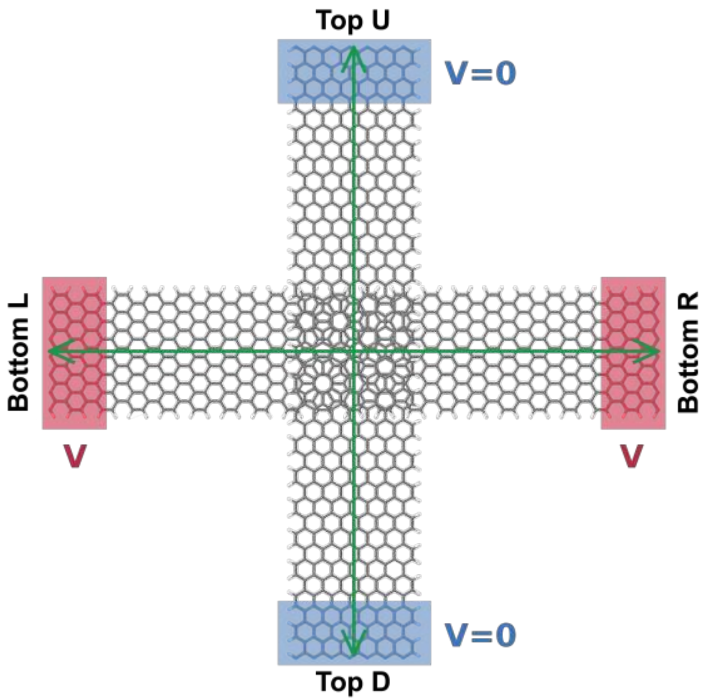
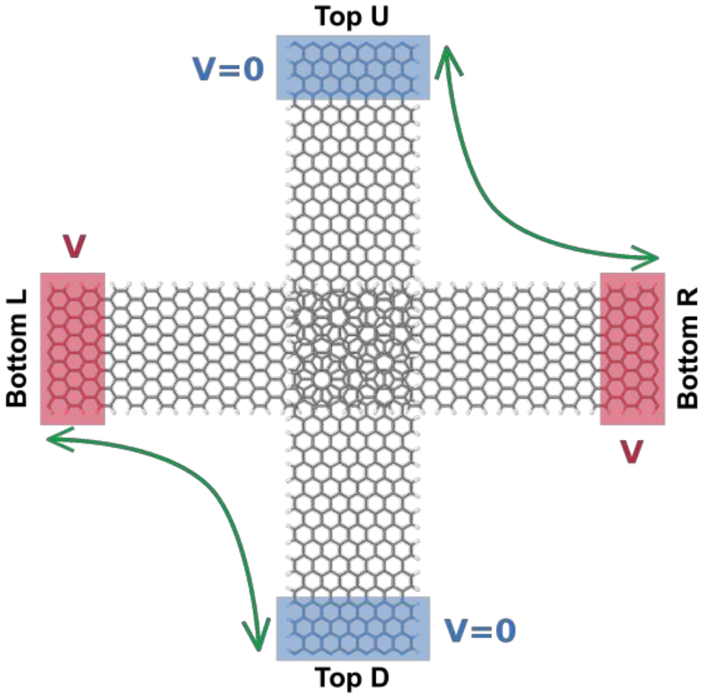
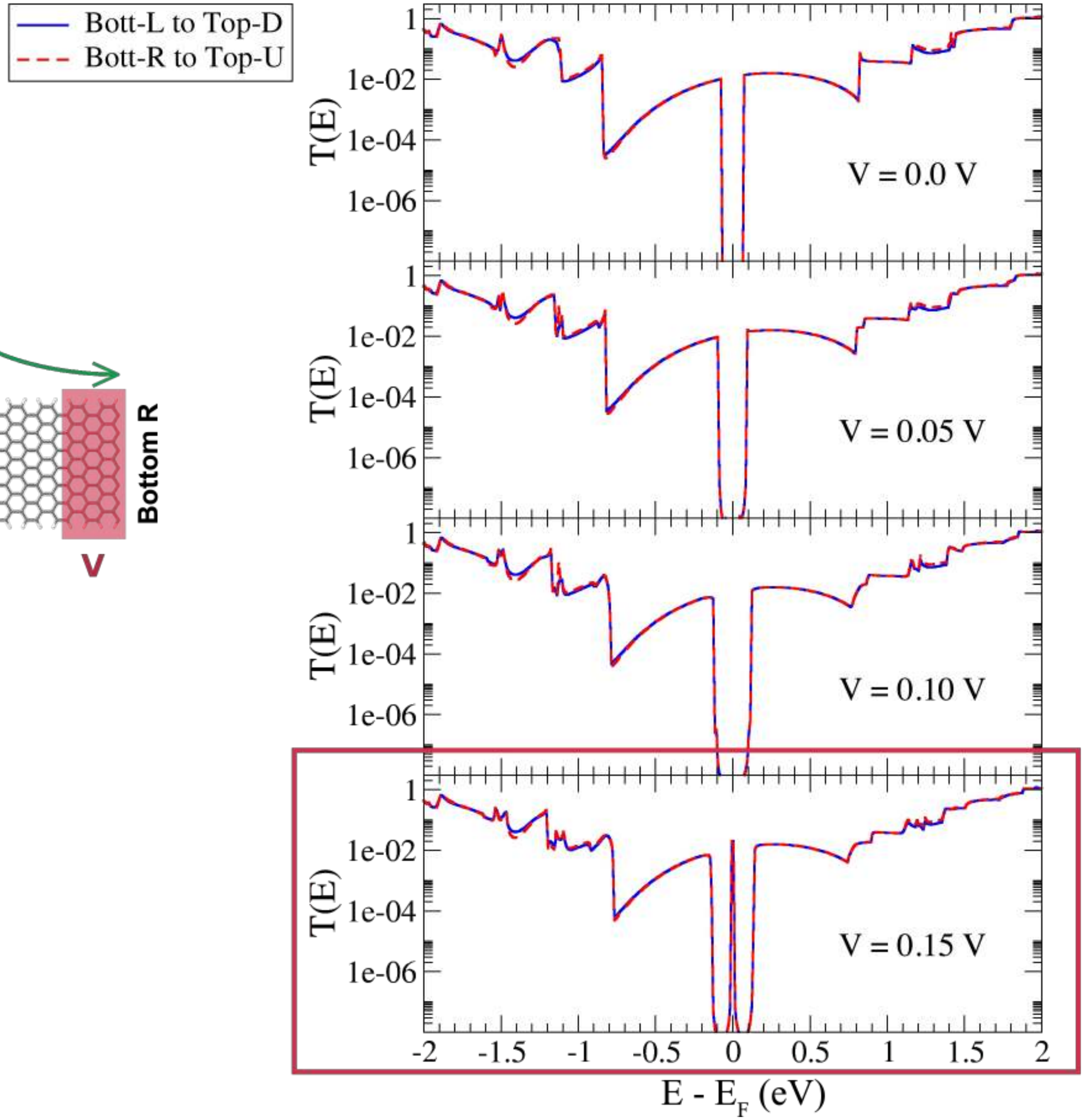


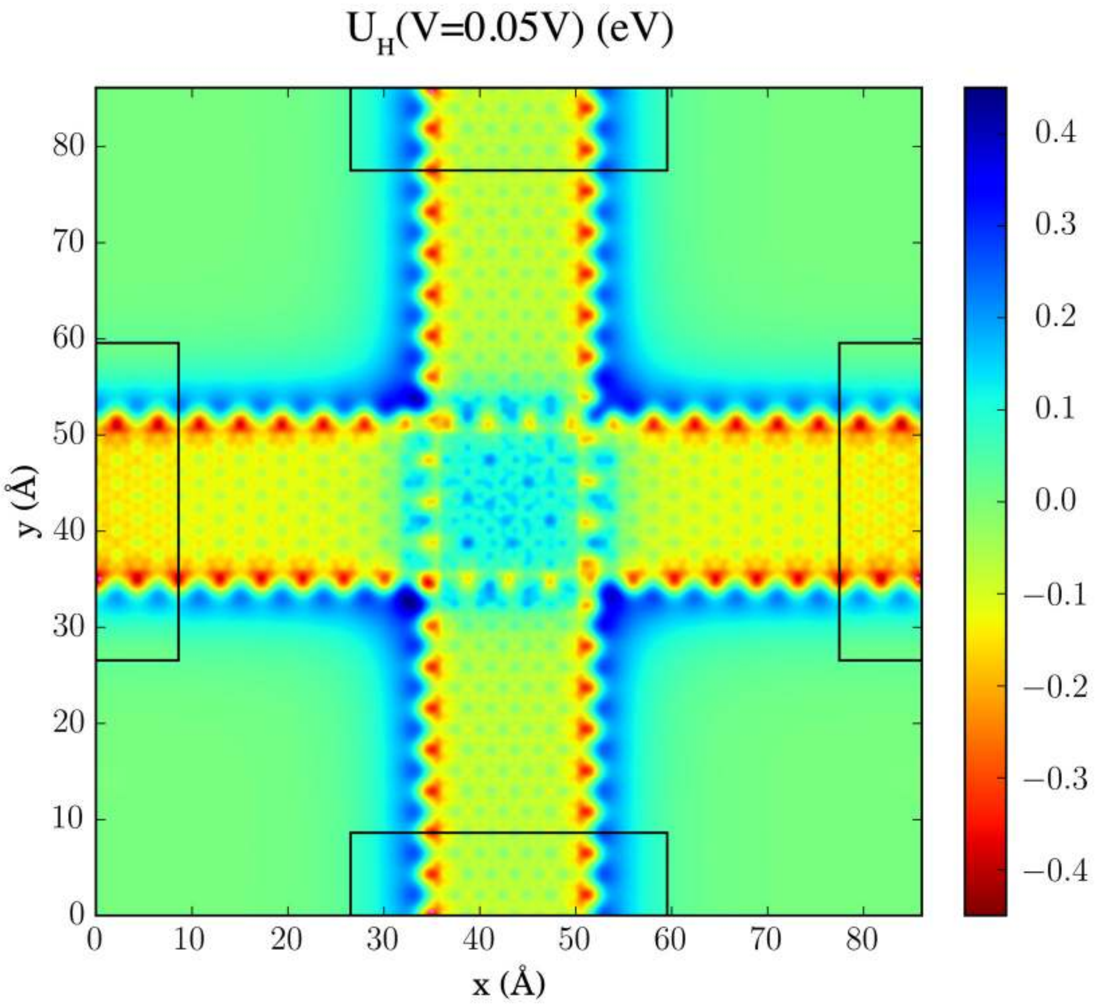


Inter-ribbon transmission





Electrostatic potential at 0.05 V



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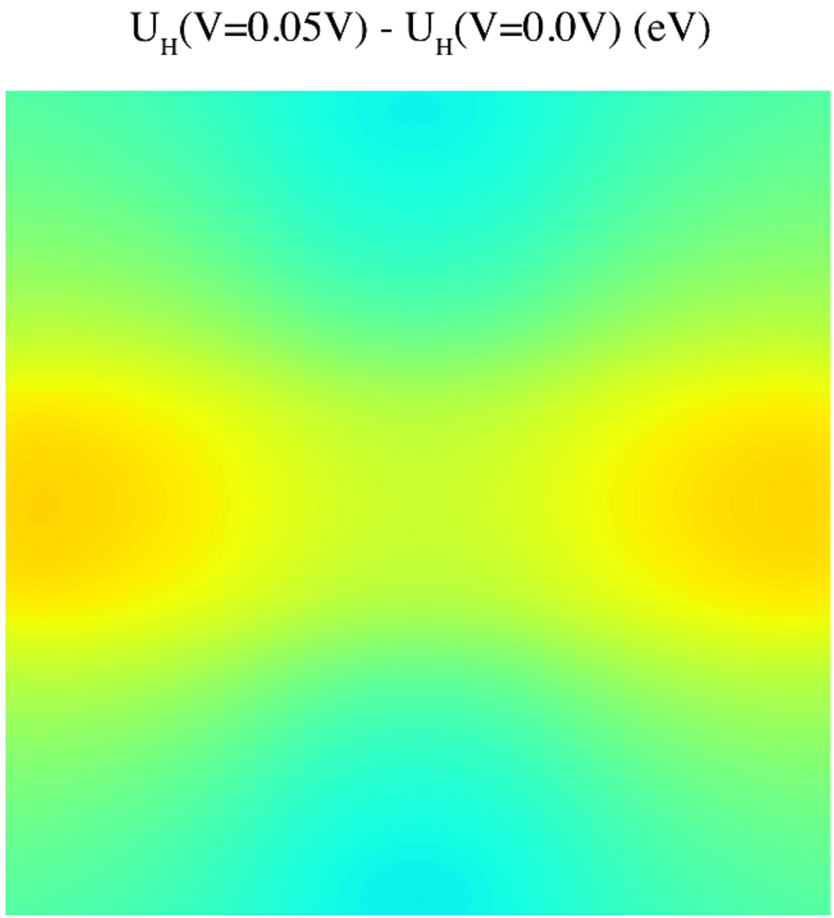
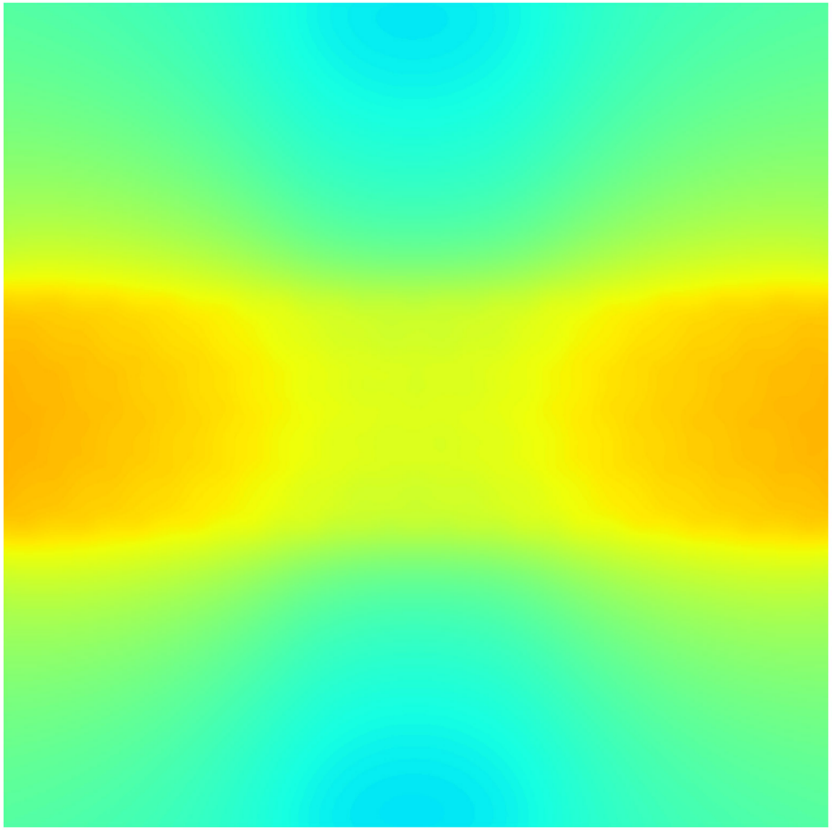


Electrostatic potential at 0.05 V

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



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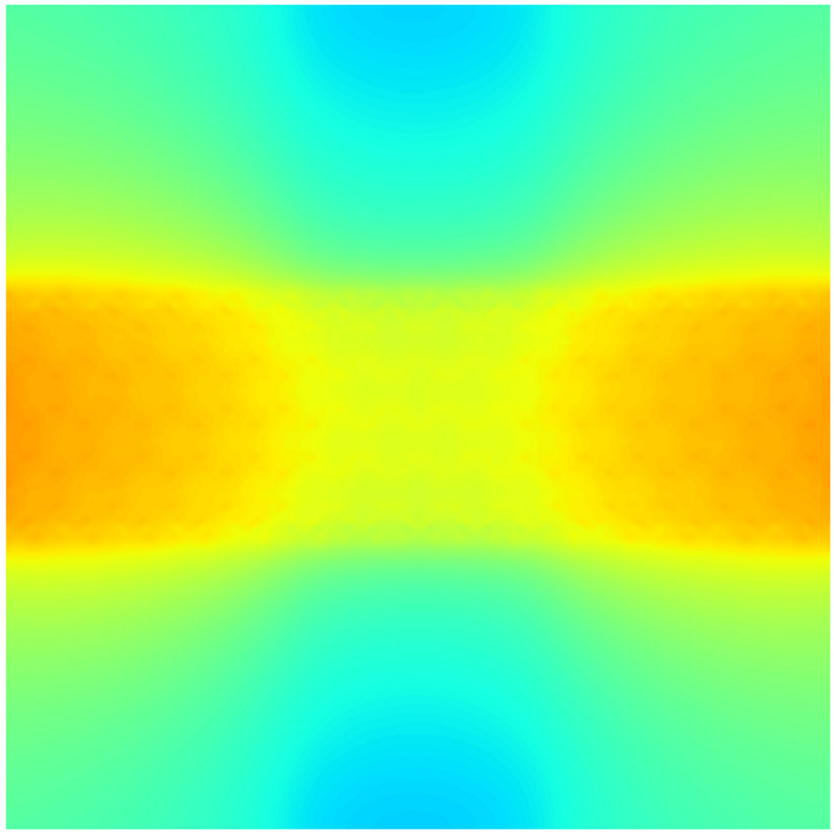

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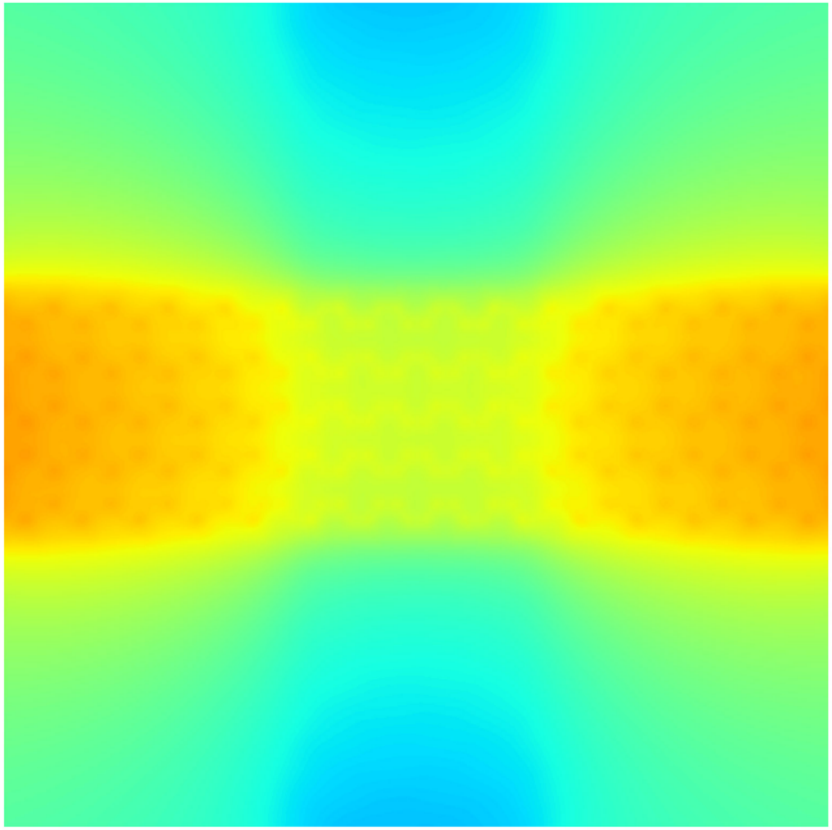
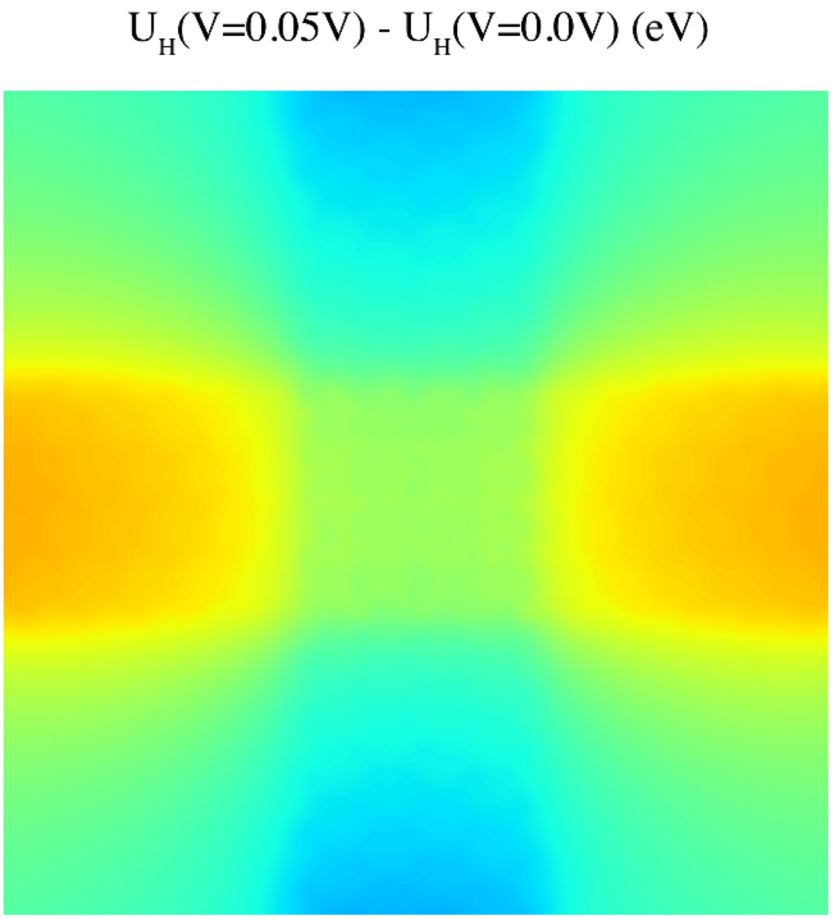


Electrostatic potential at 0.05 V



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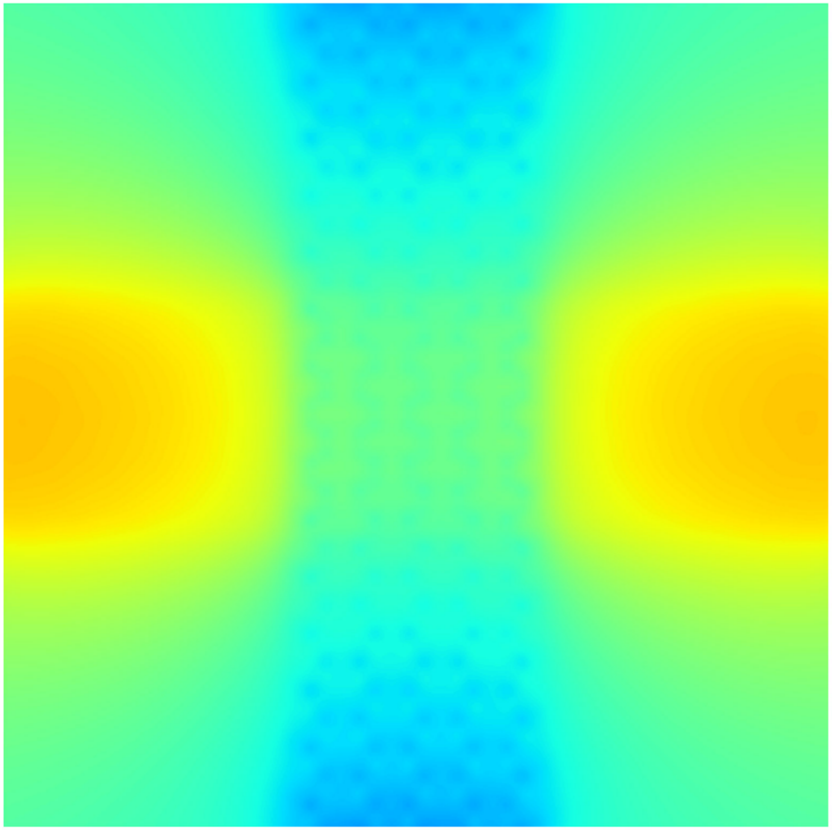

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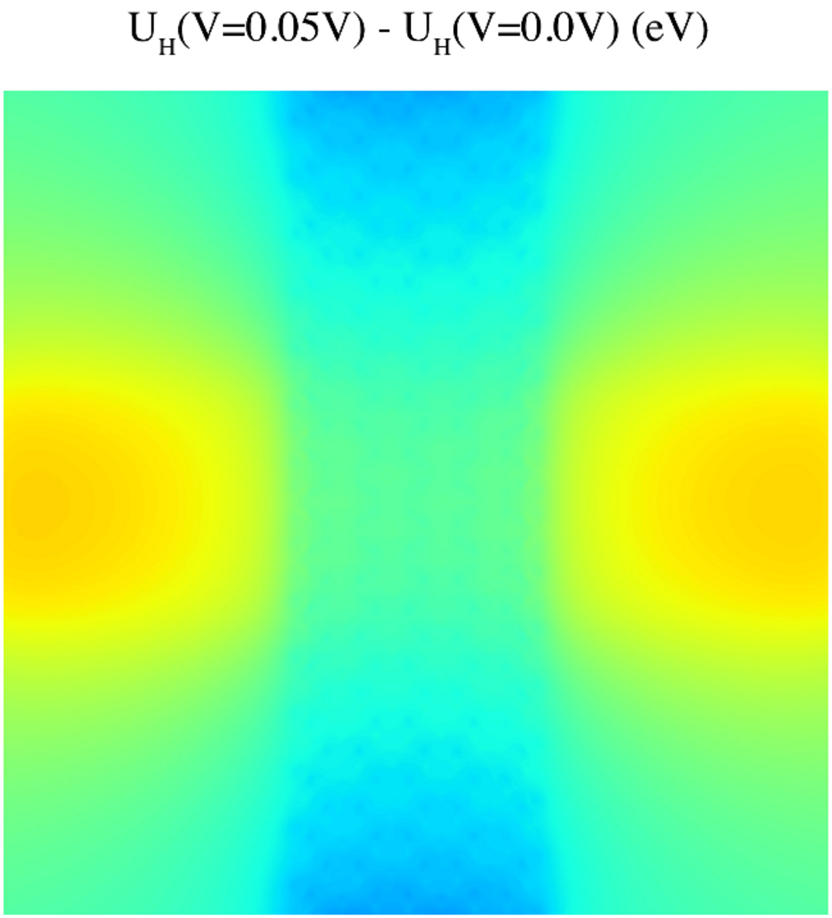

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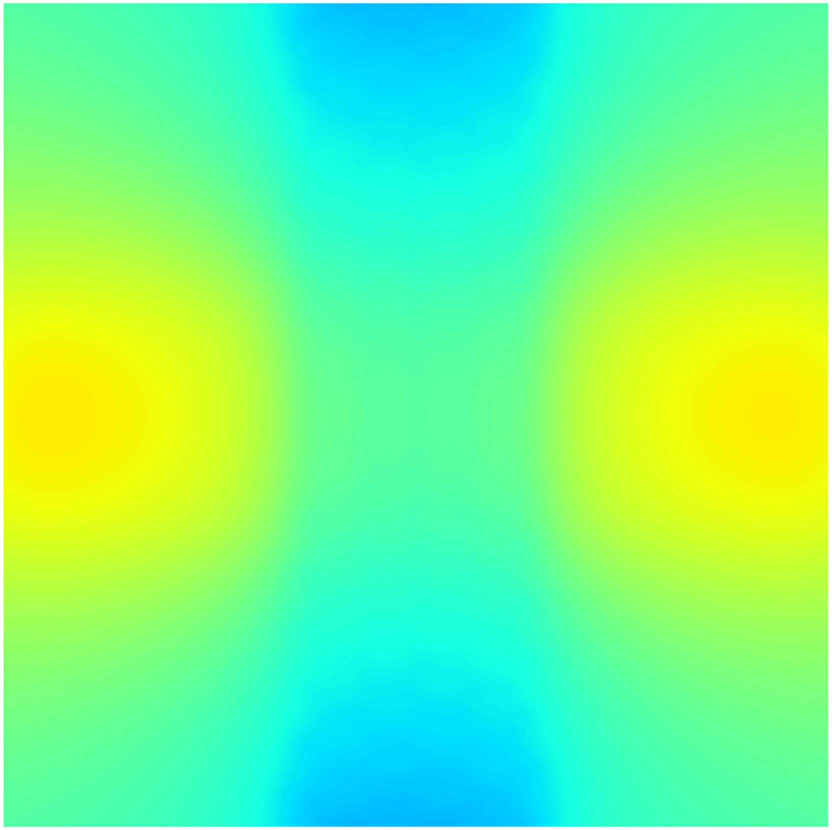
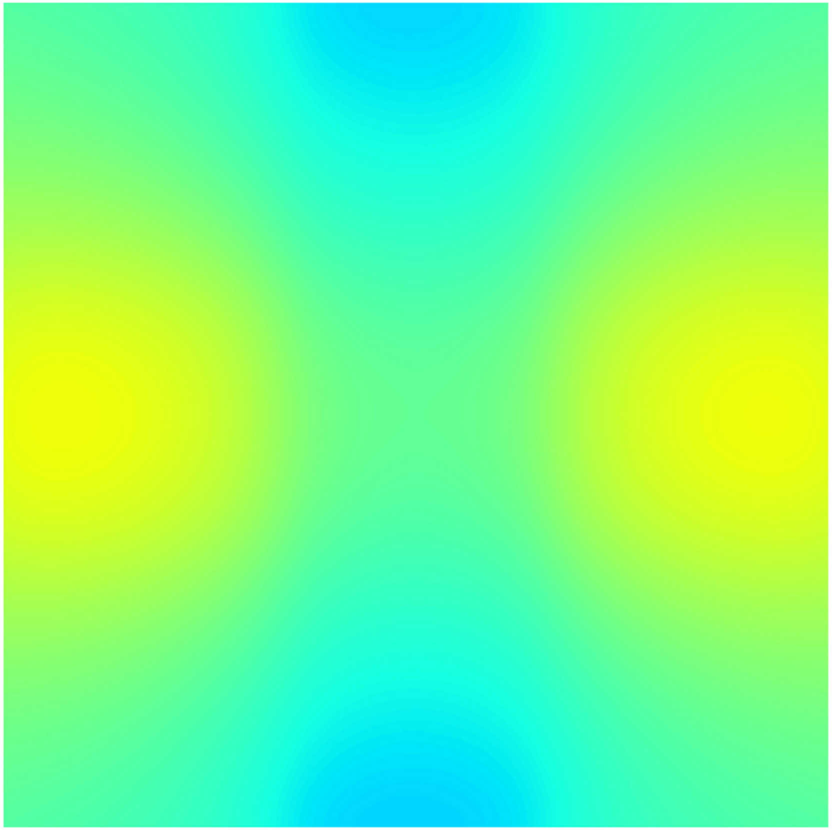
$U_H(V=0.05V) - U_H(V=0.0V)$ (eV)

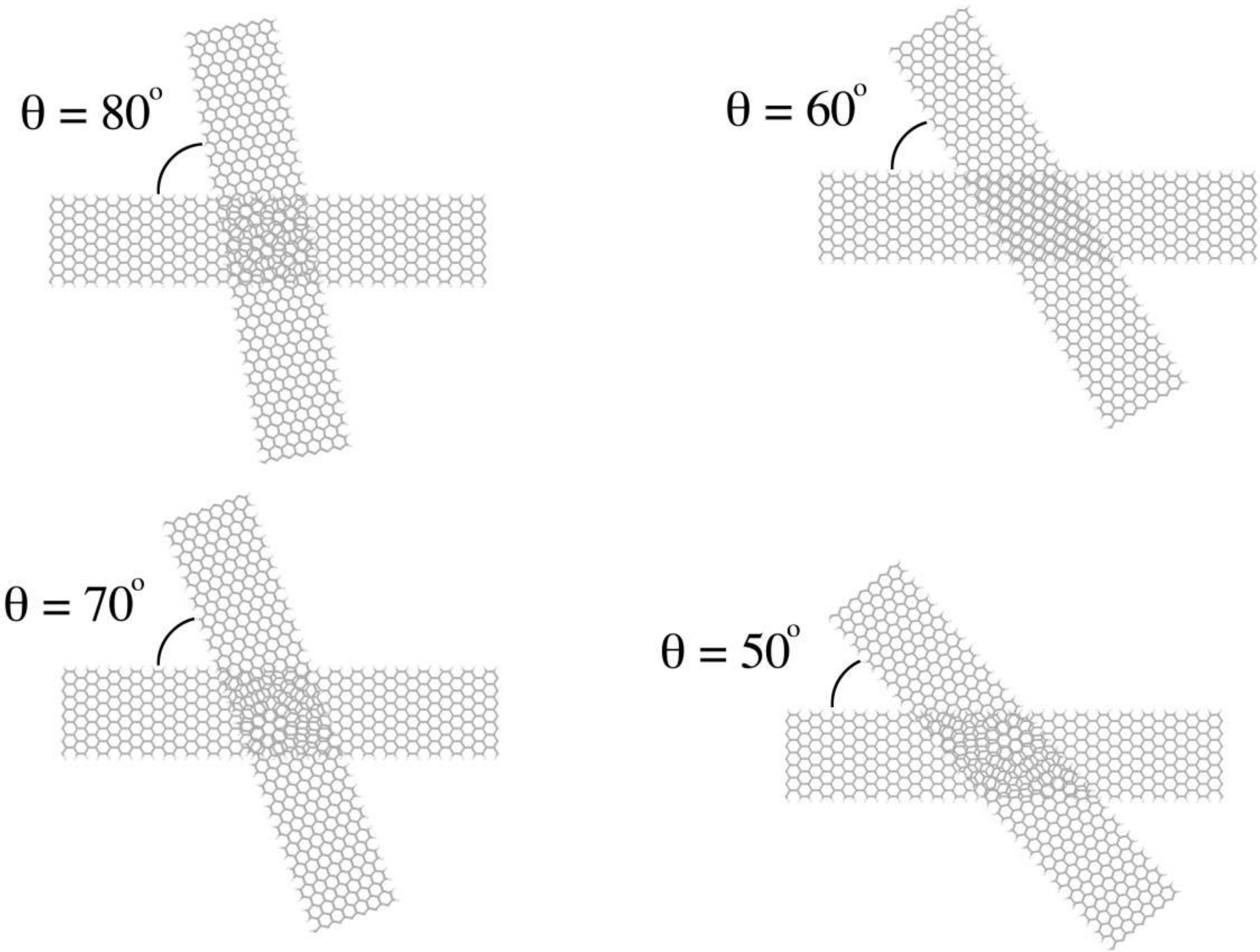


Electrostatic potential at 0.05 V

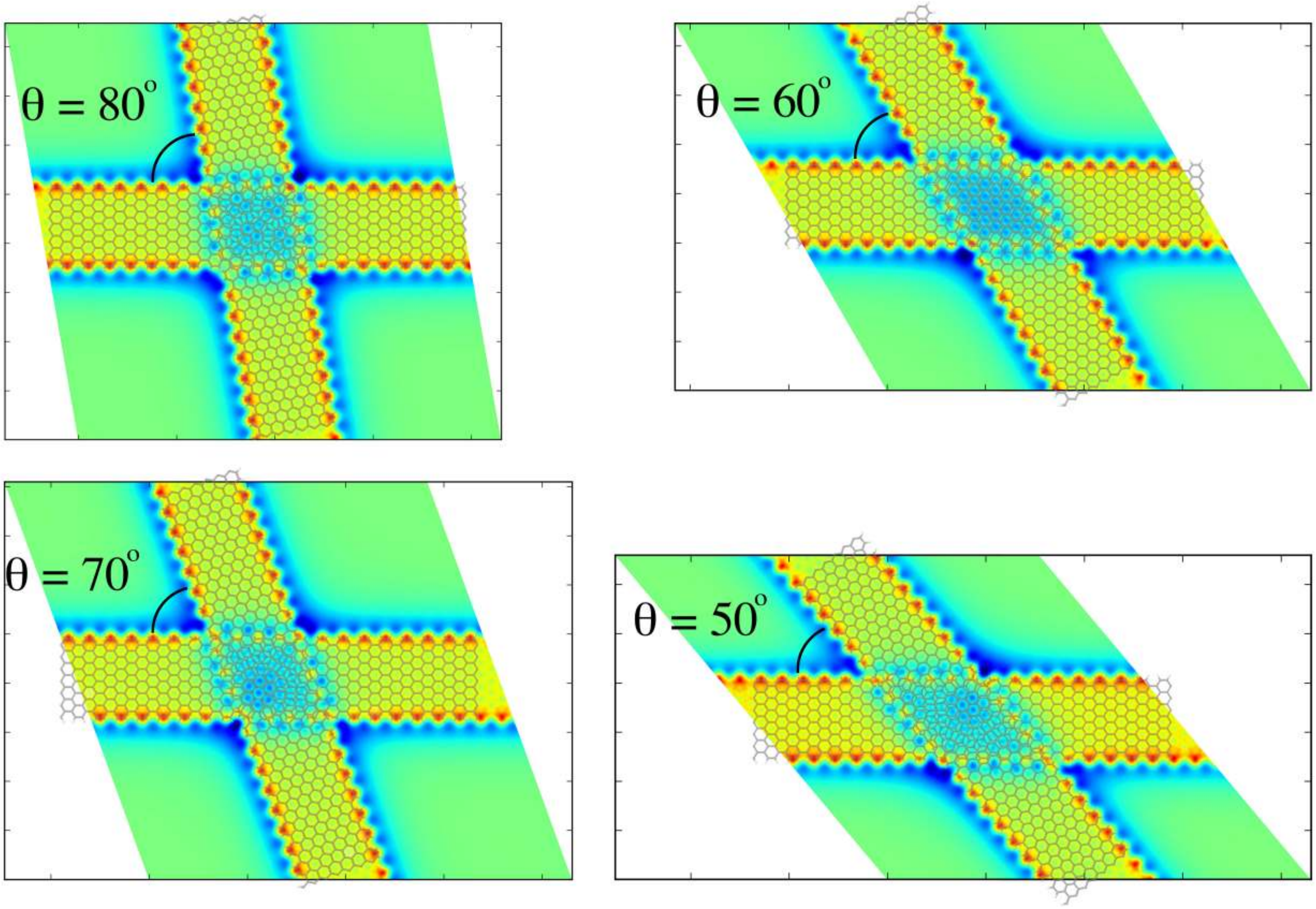
$U_H(V{=}0.05V) - U_H(V{=}0.0V)$ (eV)



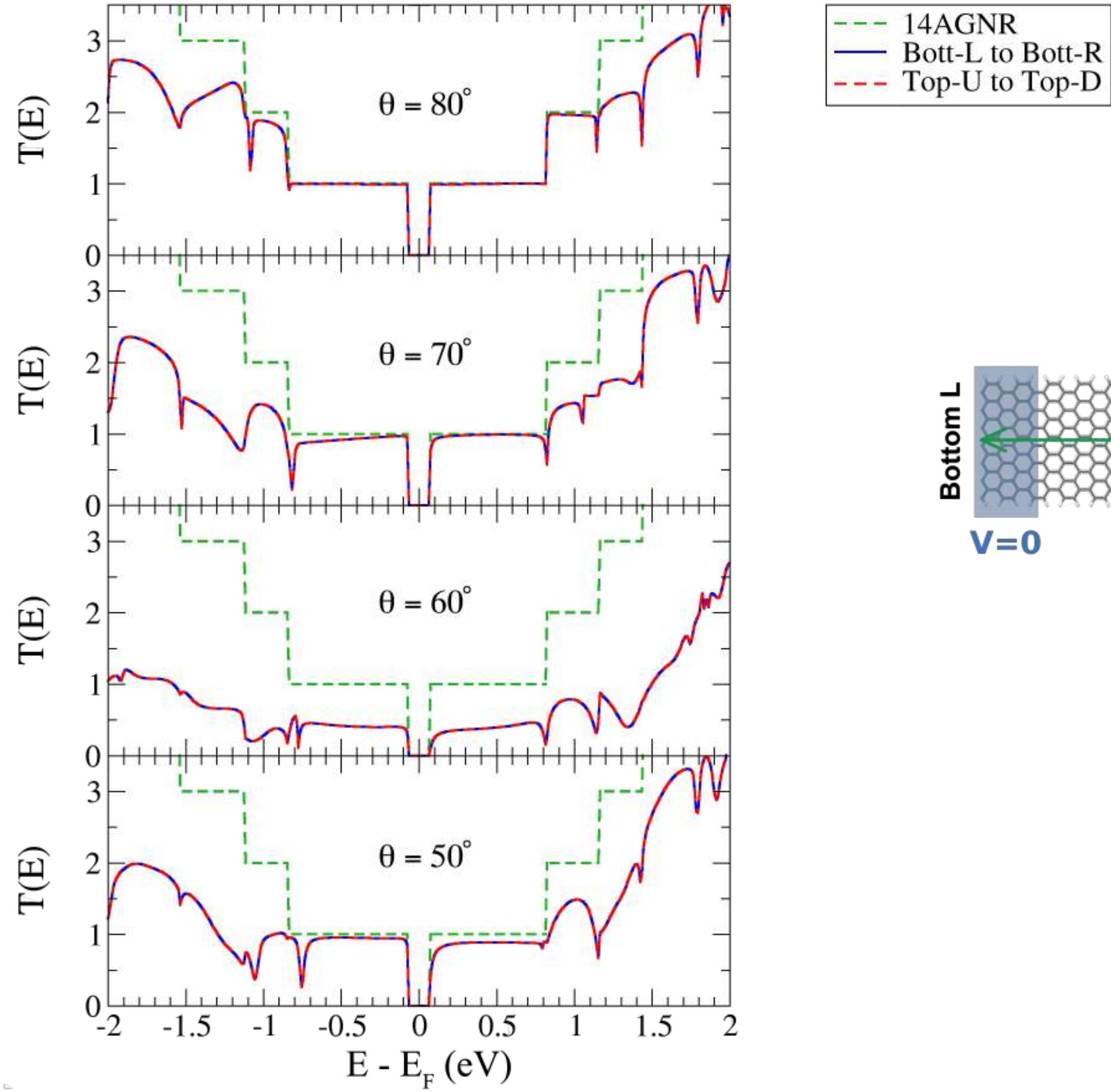
Rotated crossbar

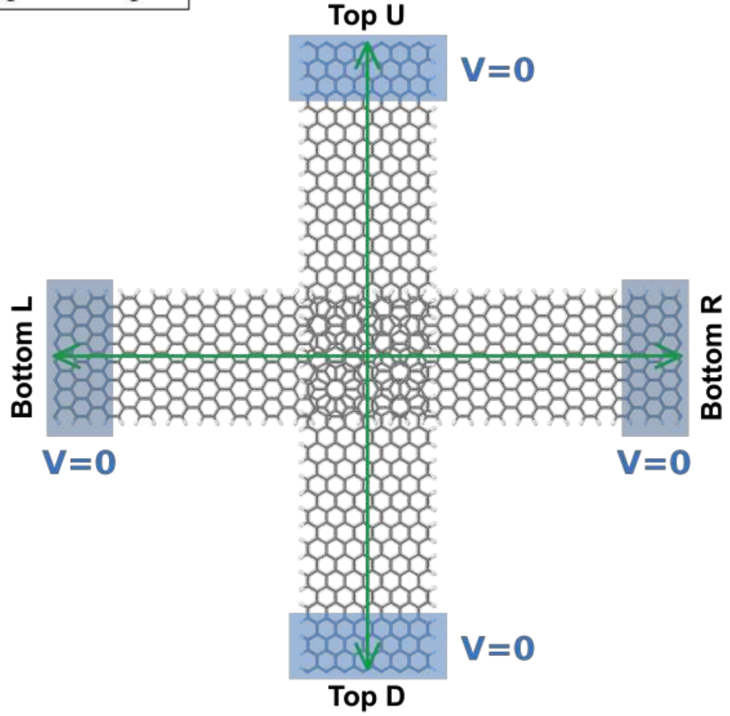


Electrostatic potential at V = 0

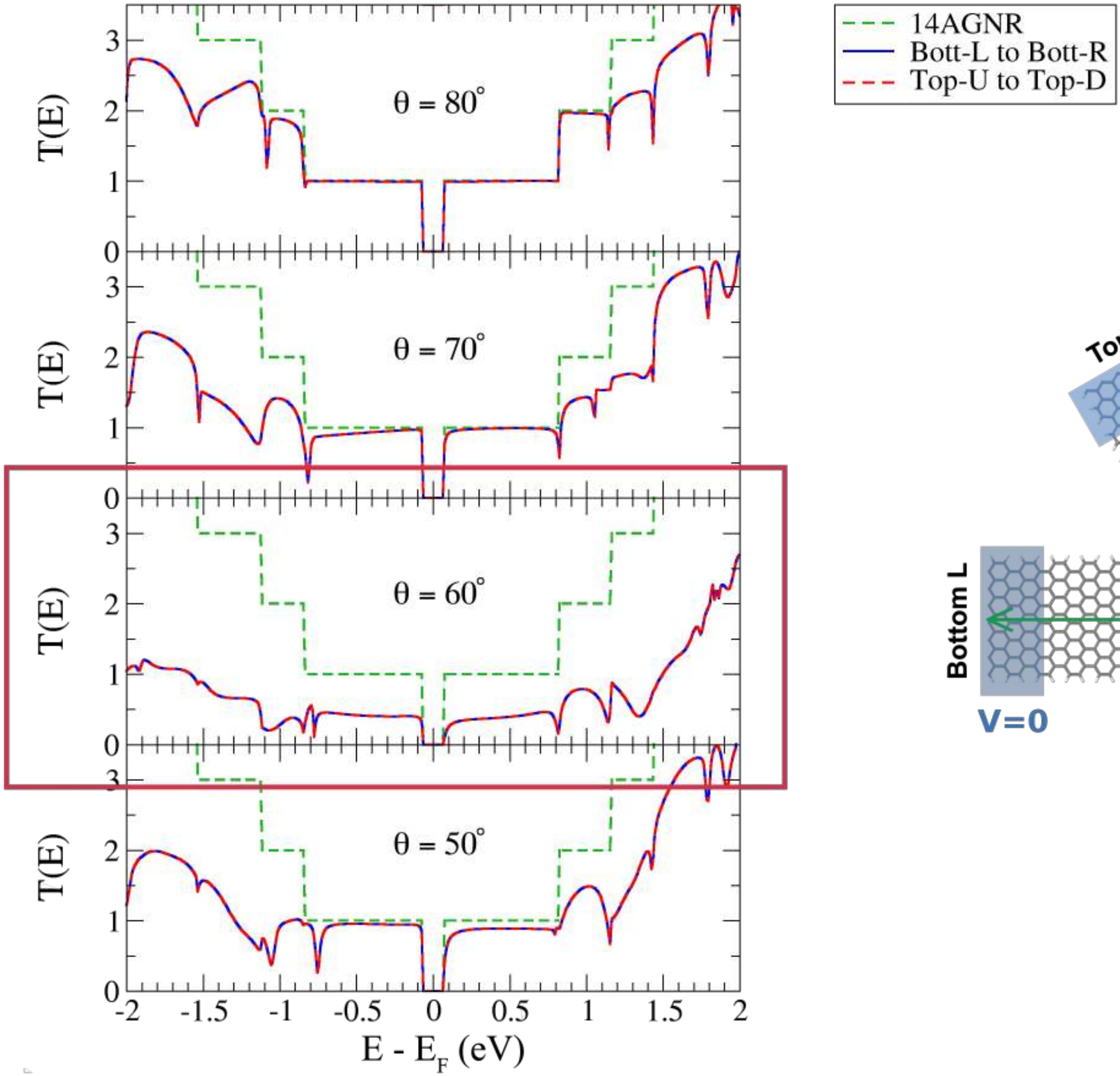


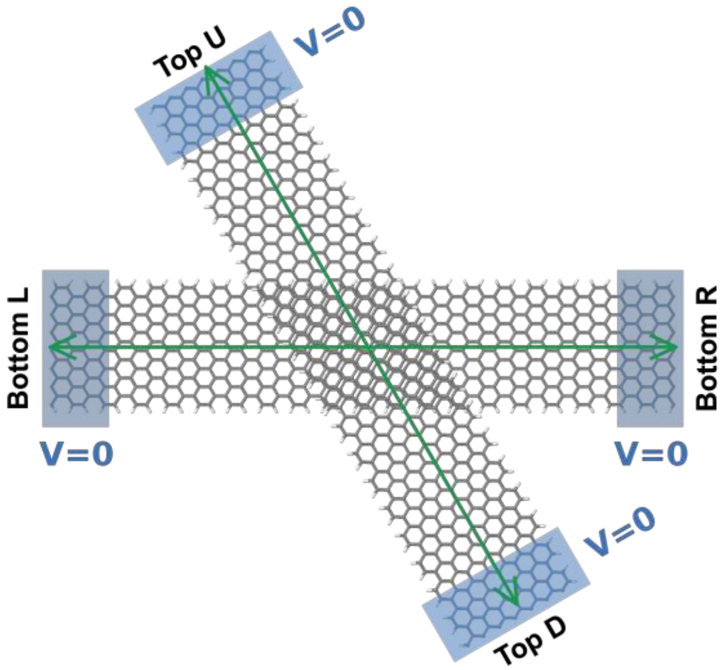
Direct transmission at V = 0



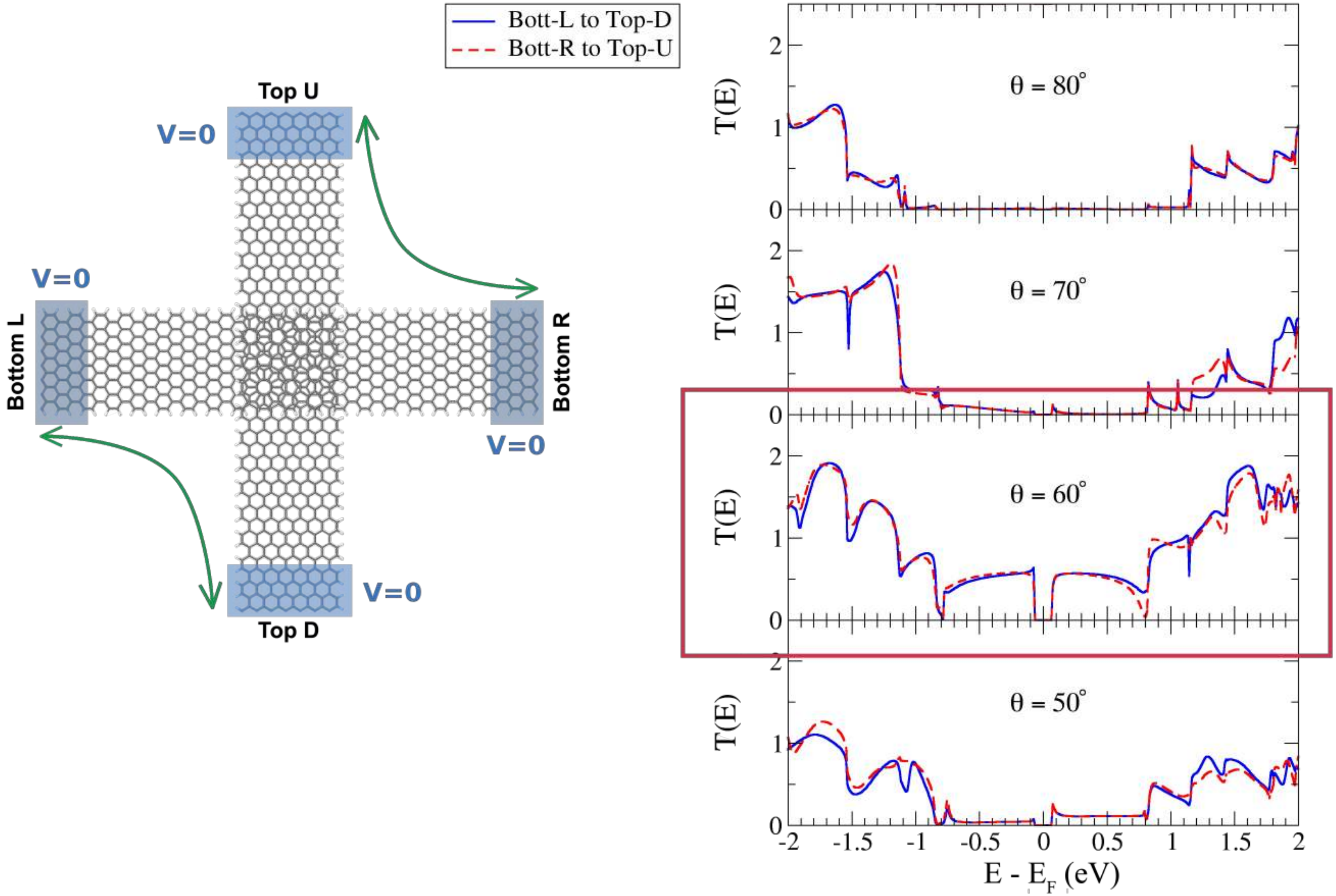


Direct transmission at V = 0

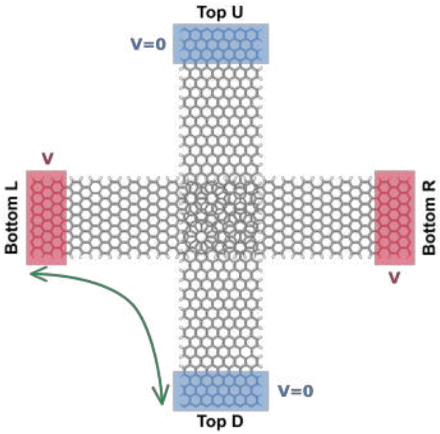


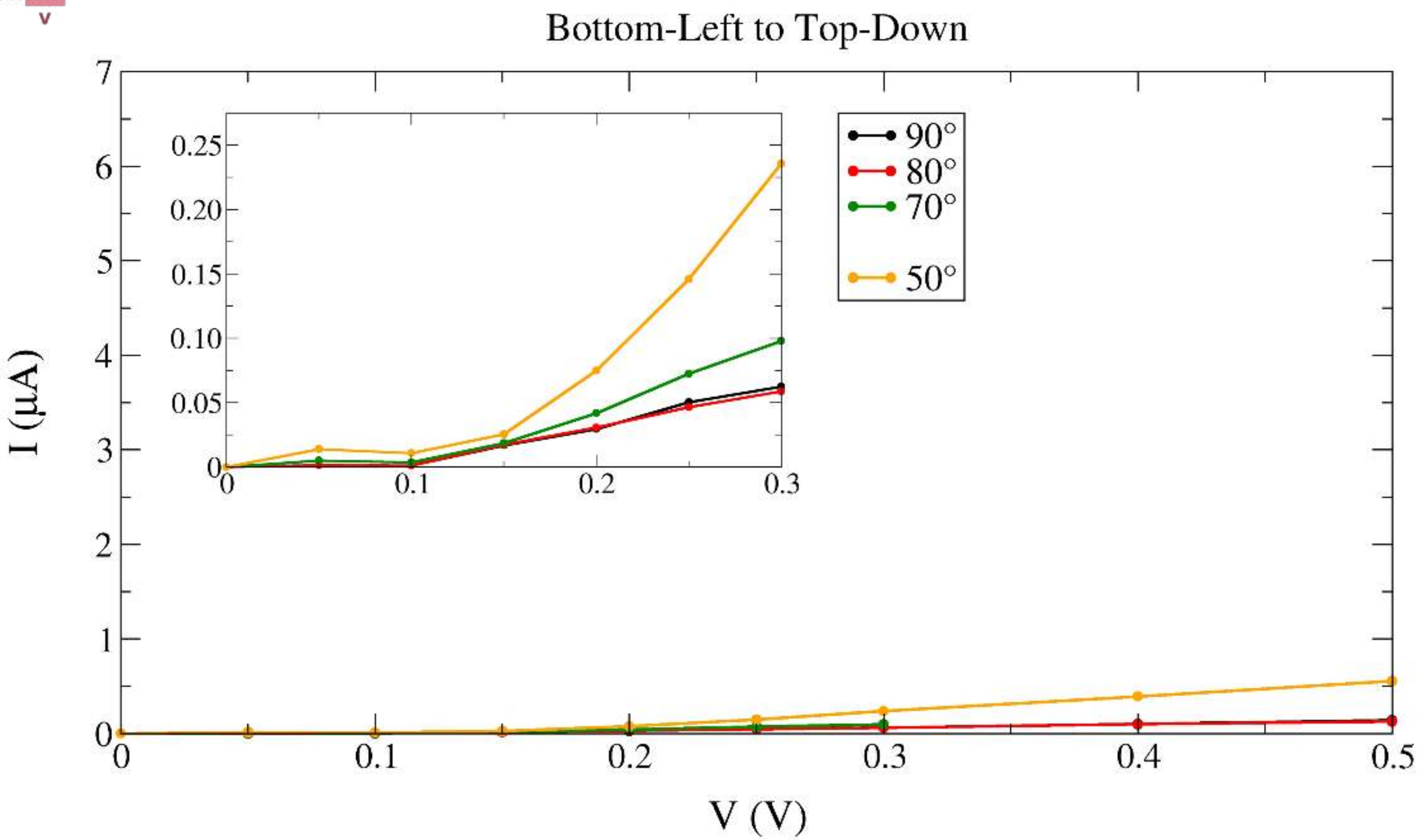


Inter-ribbon transmission at V = 0

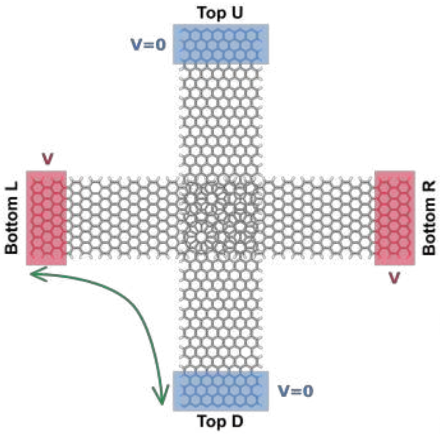


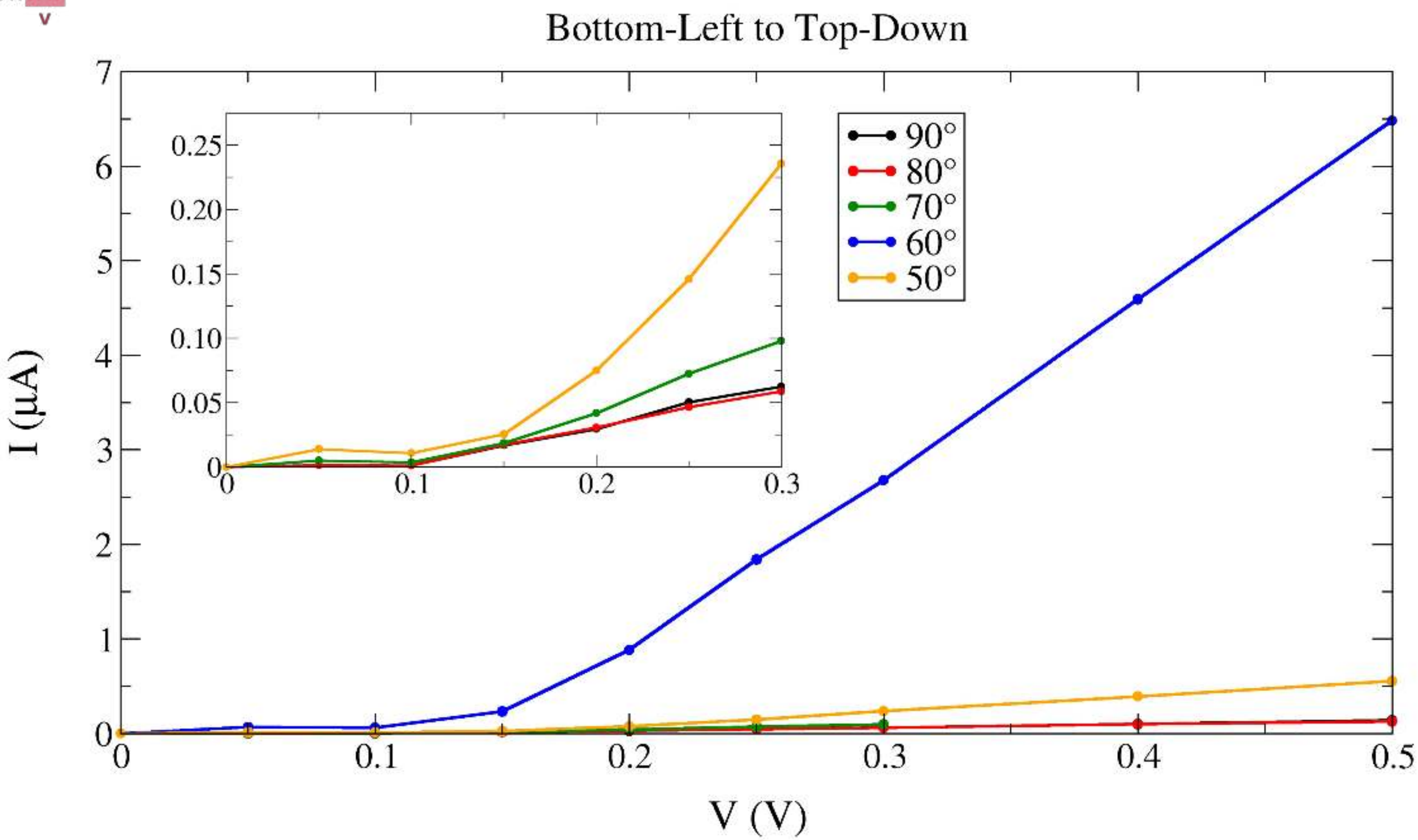
Inter-ribbon current



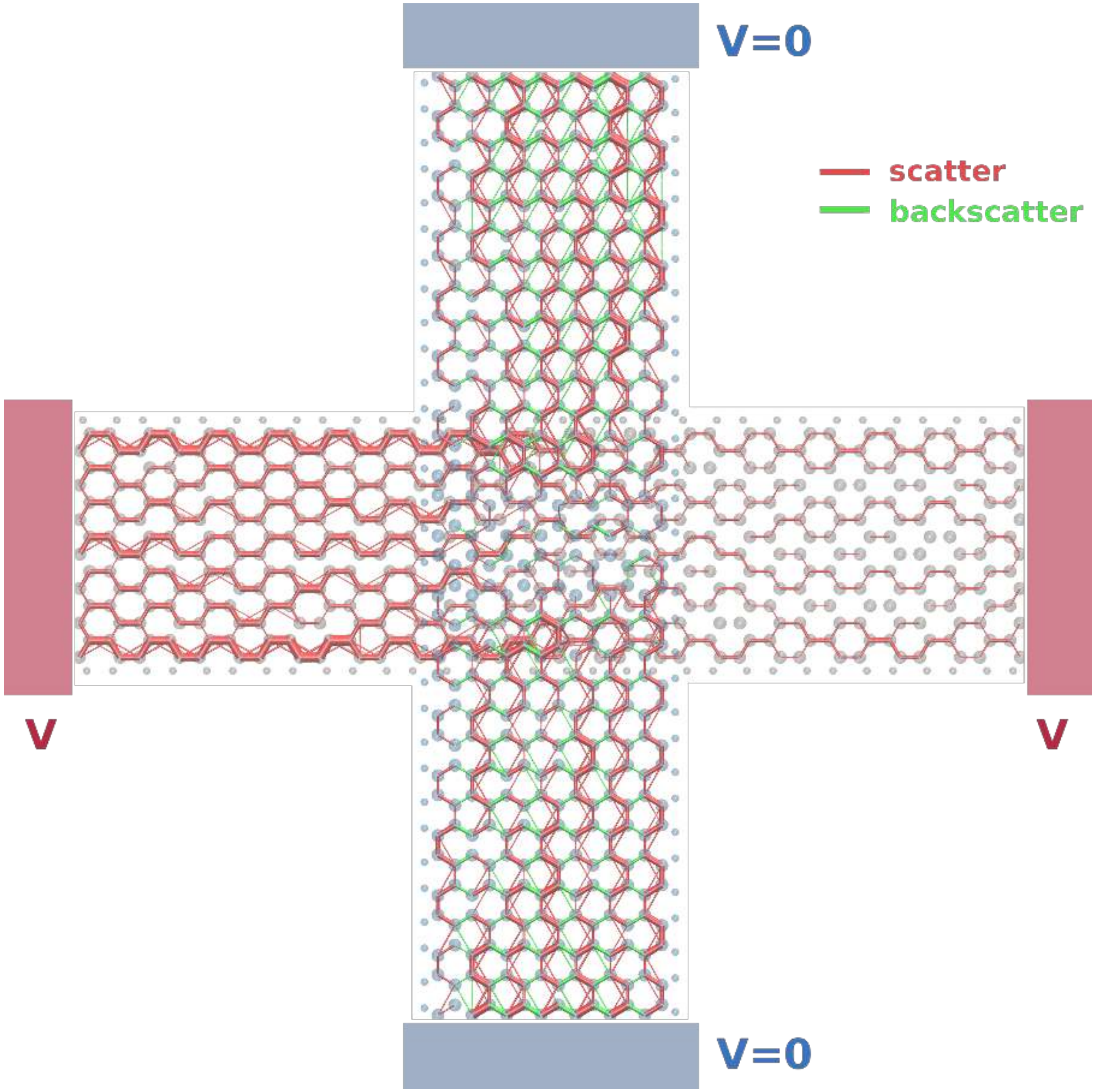


Inter-ribbon current

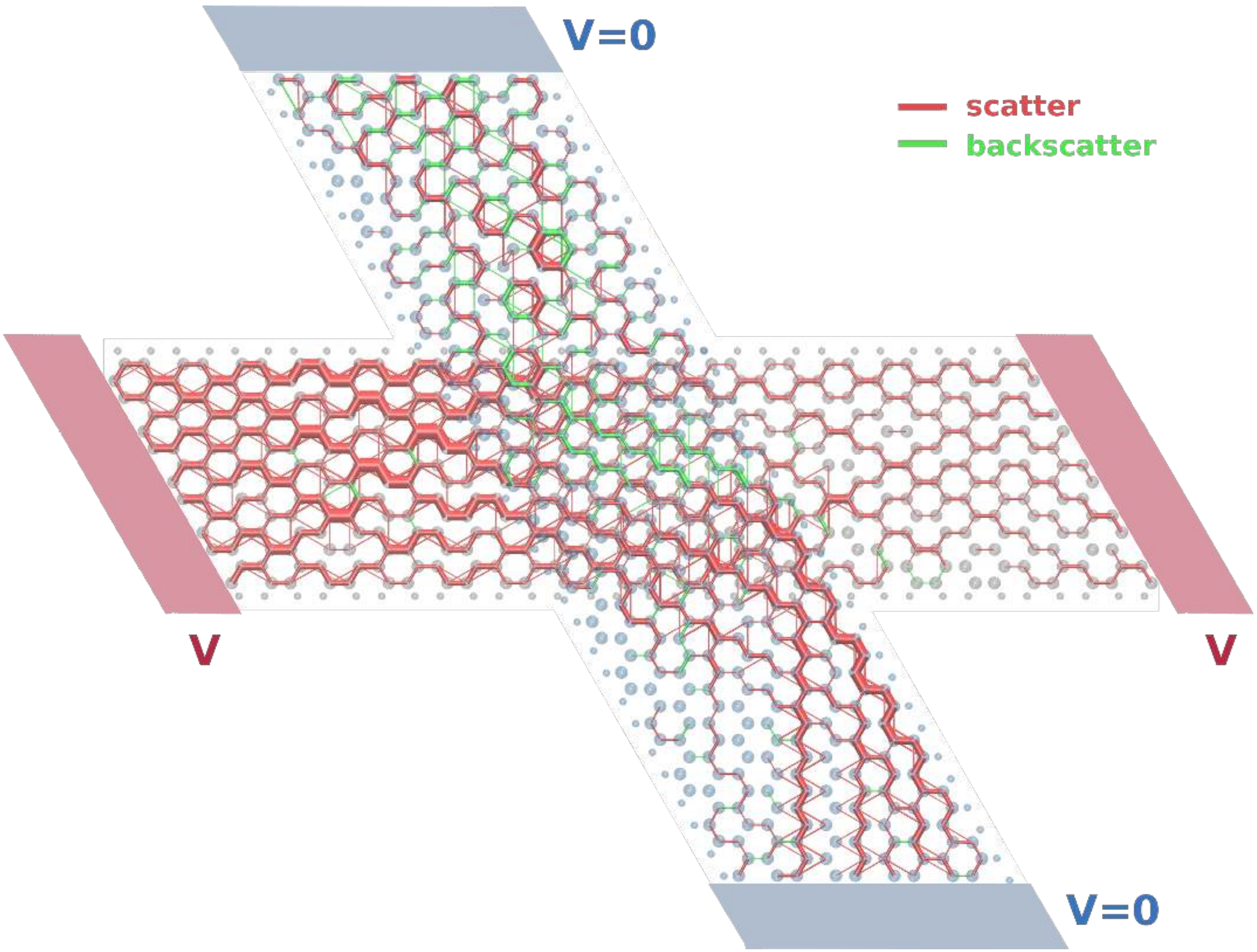




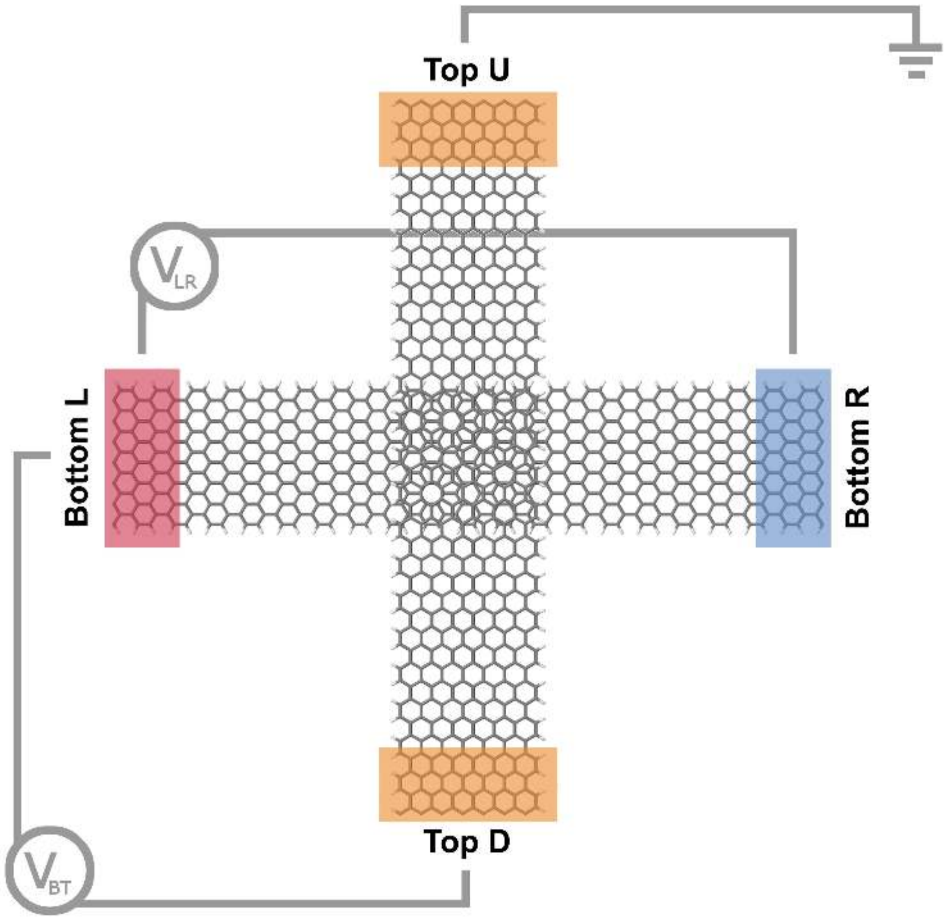
Bond currents for 90° at 0.5 V



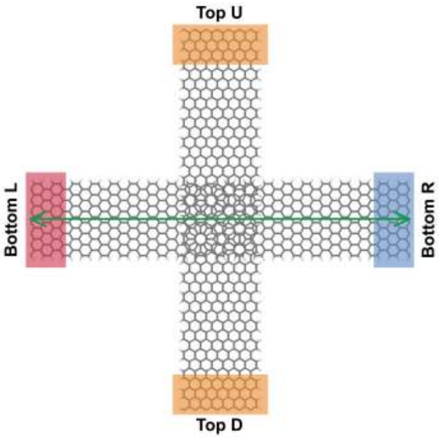
Bond currents for 60° at 0.5 V

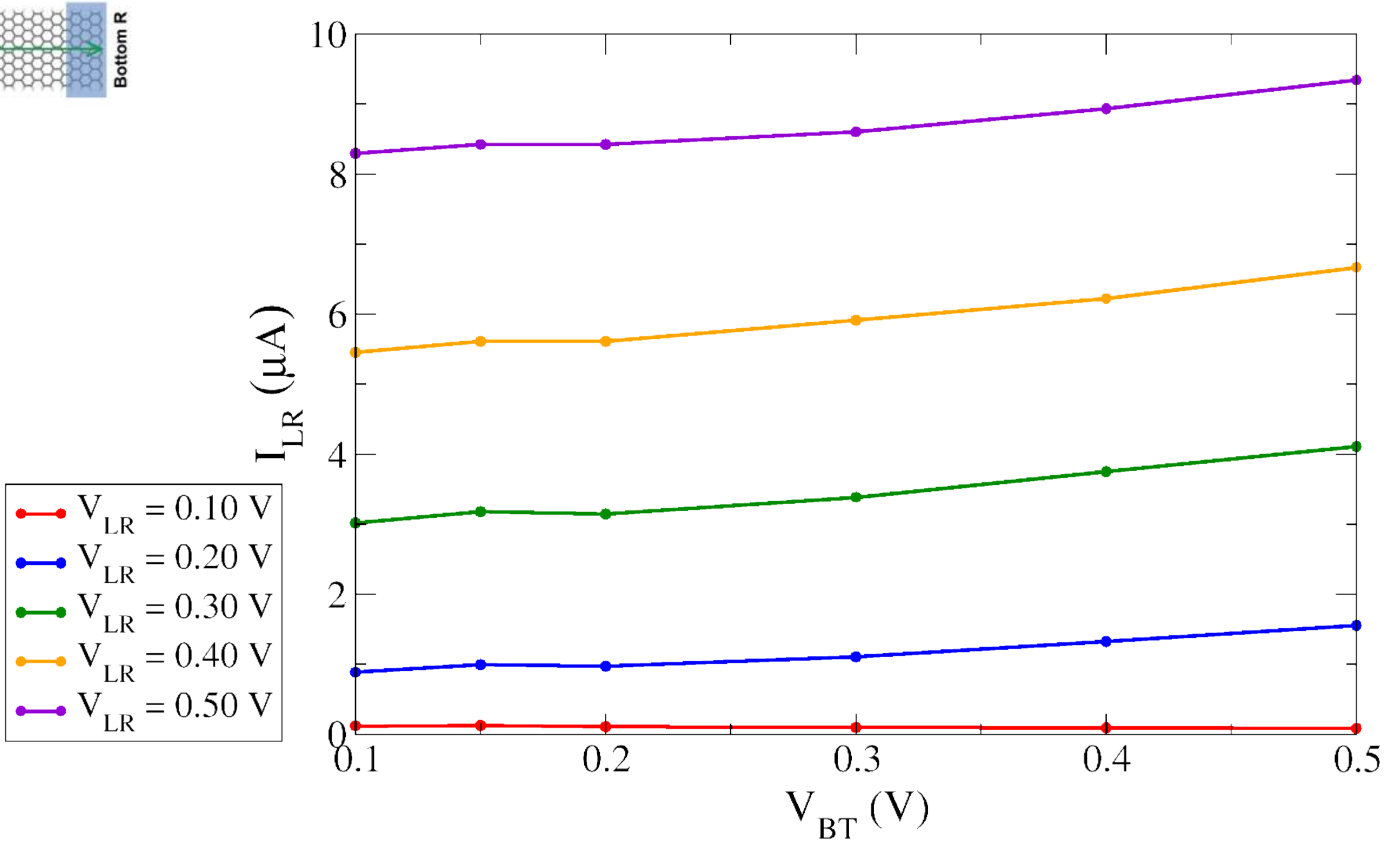


Intralayer bias

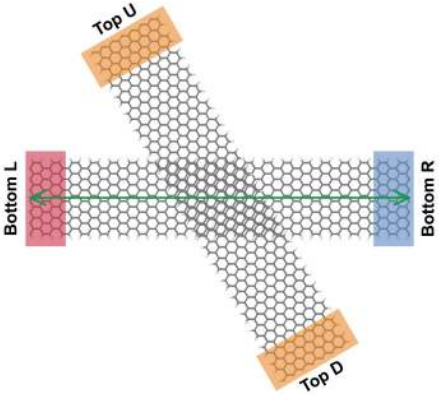


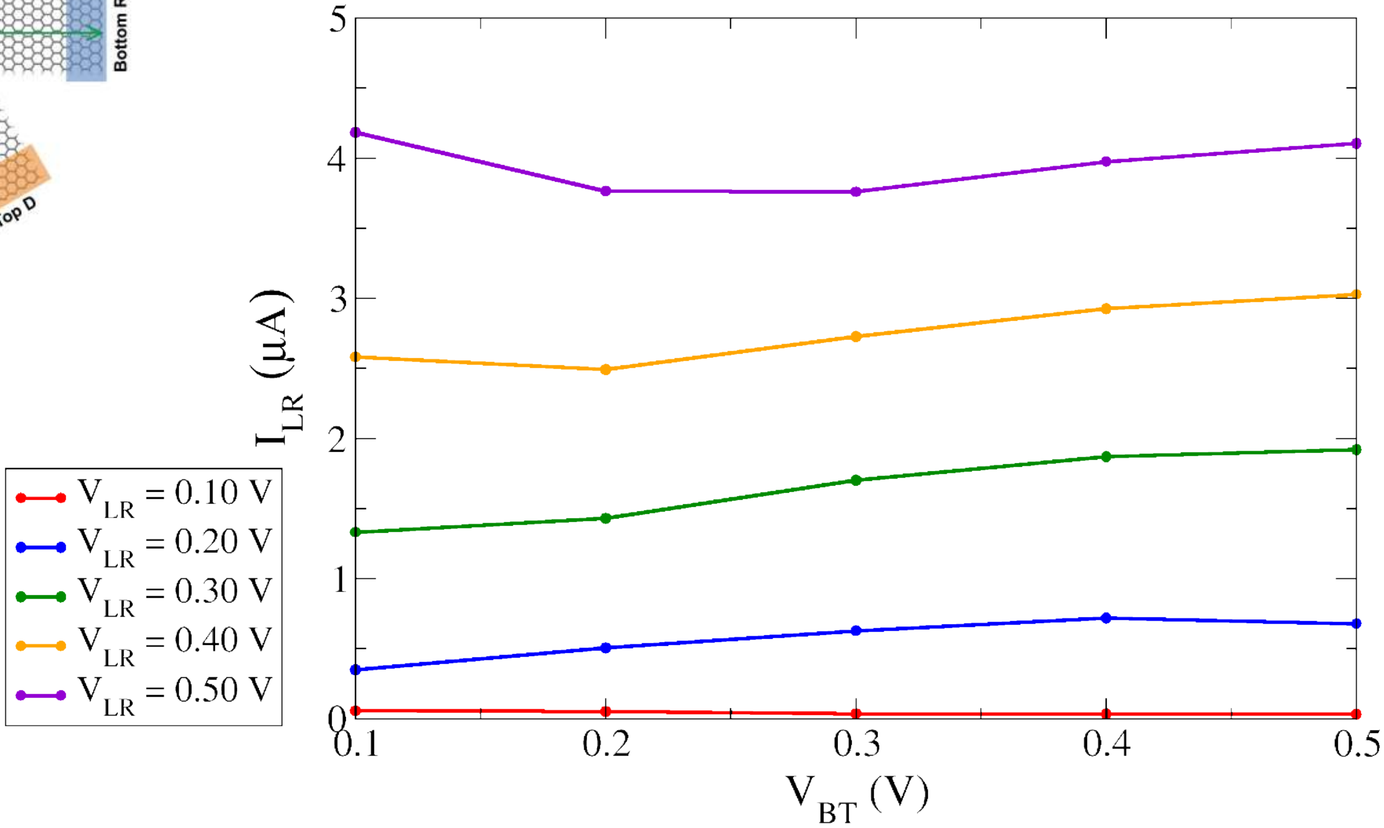
Intralayer bias





Intralayer bias





Conclusions

- Application of TranSIESTA for **N=4 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.

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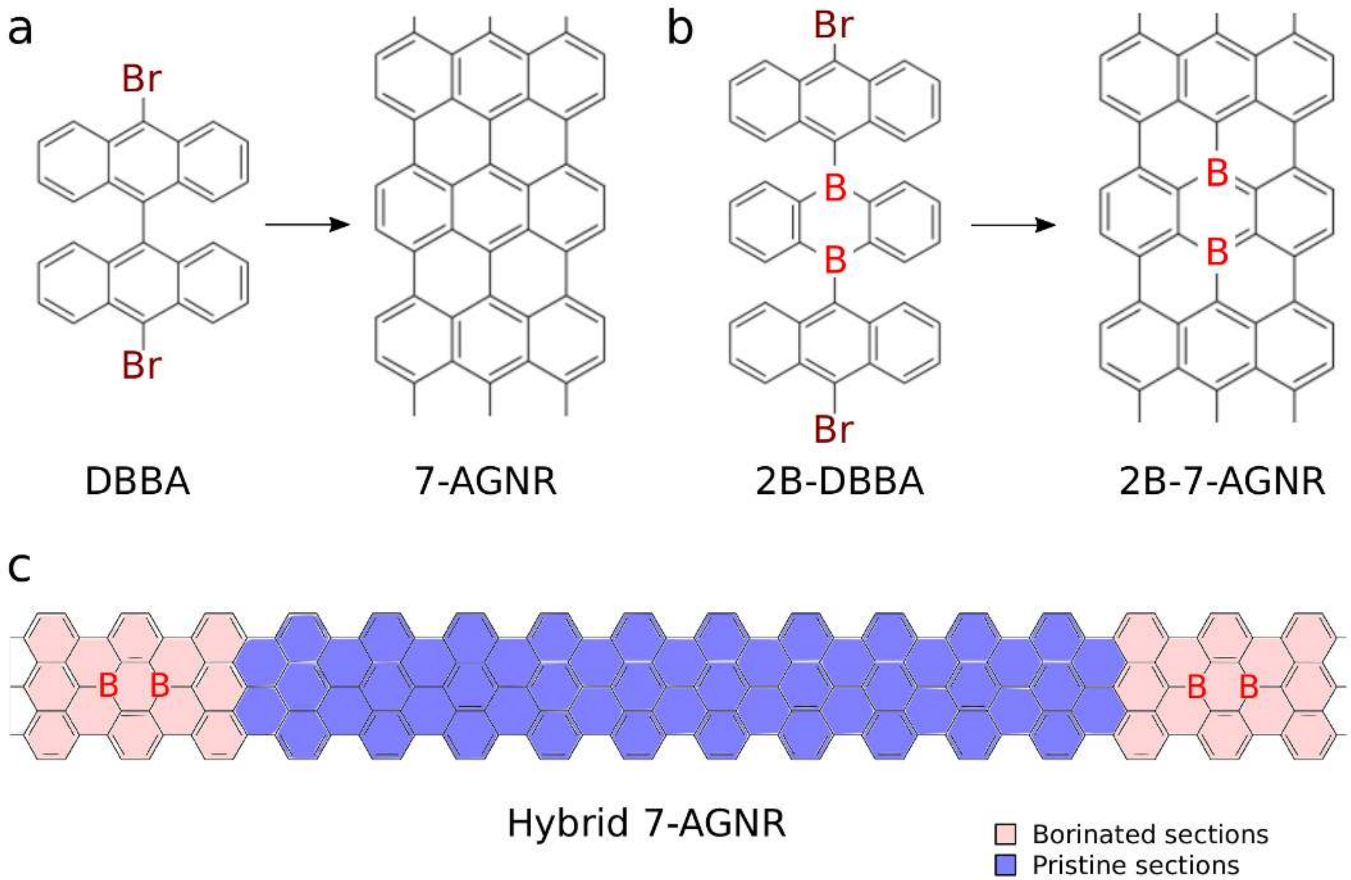
1-D Quantum Well States on Doped Graphene Nanoribbons Revealed by Transport Simulations

Pedro Brandimarte, Aran Garcia-Lekue, Eduard Carbonell-Sanromà, Martina Corso, Richard Balog, Shigeki Kawaii, Shohei Saito, Shinichiro Osumi, Shigehiro Yamaguchi, Jose I. Pascual, and Daniel Sánchez-Portal

June 13, 2016



S. Kawai *et al*. *Nature Communications* **6**, 8098 (2015).
R. R. Cloke *et al*. *J. A. Chem. Soc.* **137**, 8872 (2015).

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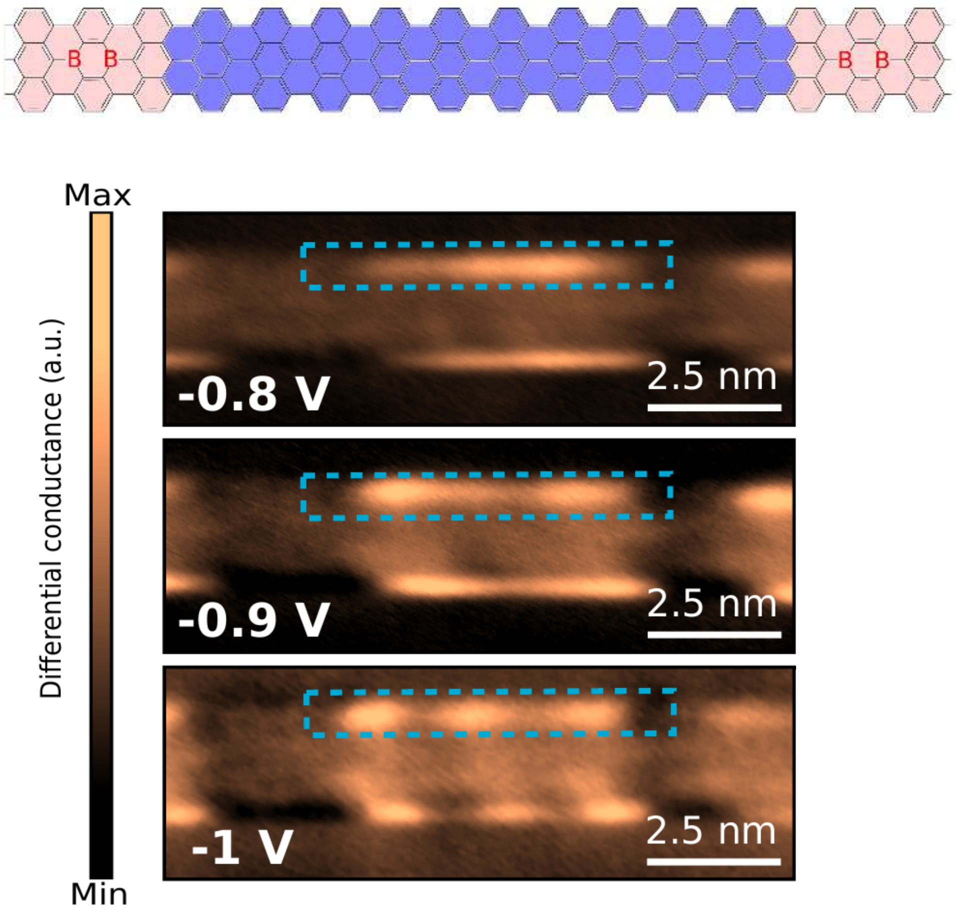
Pedro Brandimarte



1-D Quantum Well States on Doped Graphene Nanoribbons Revealed by Transport Simulations

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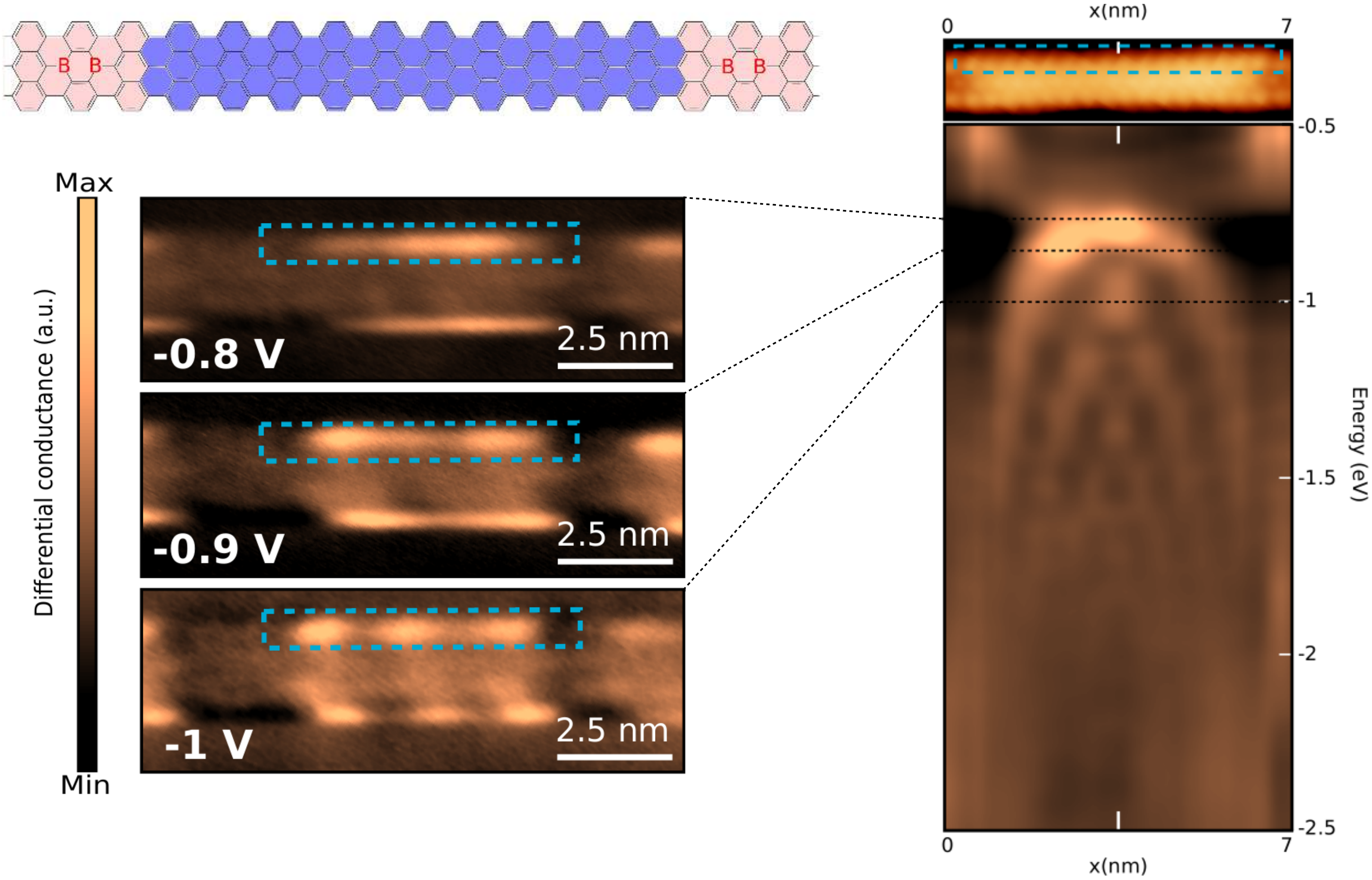
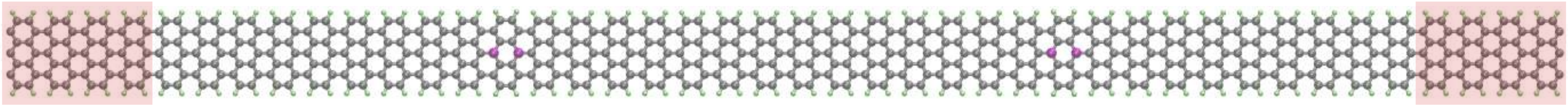
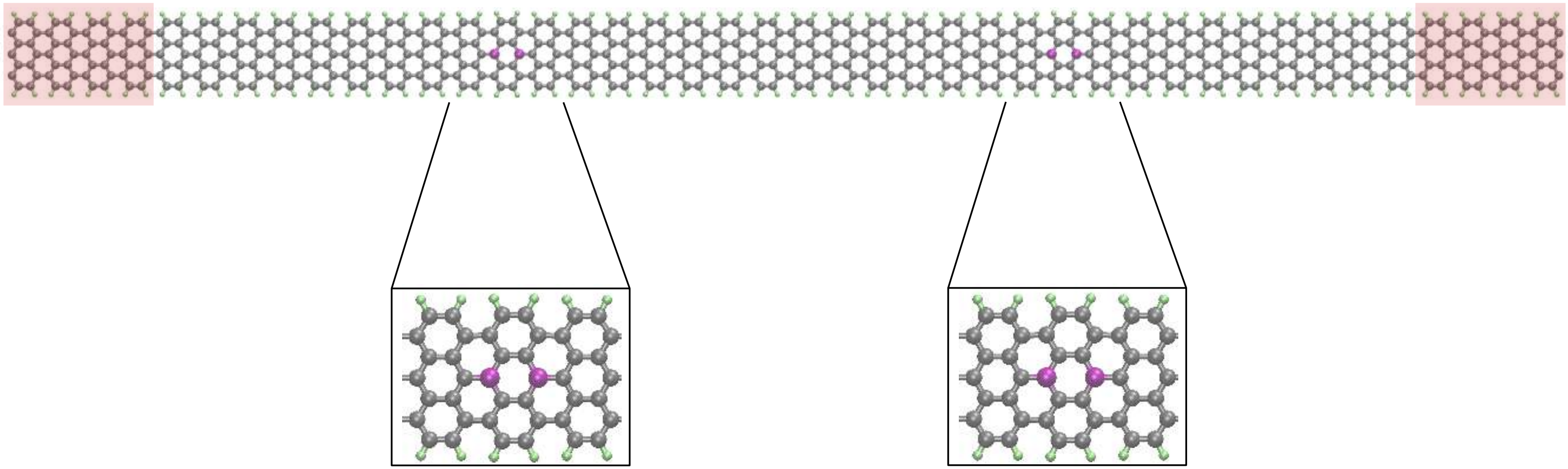


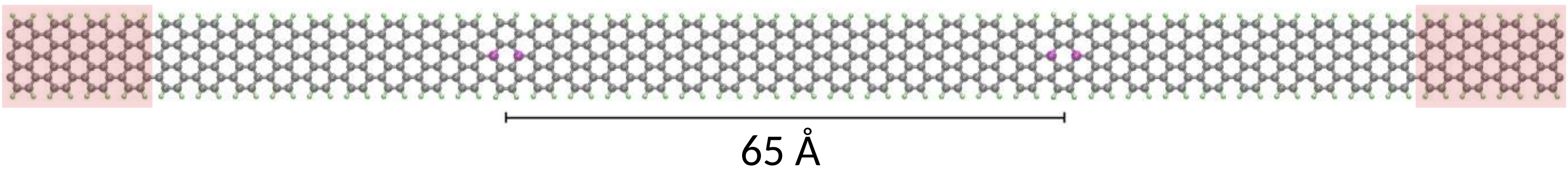
TranSIESTA



TranSIESTA



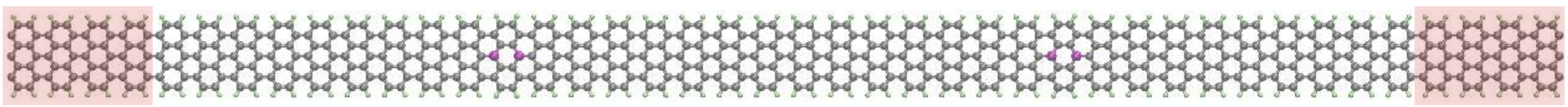
TranSIESTA

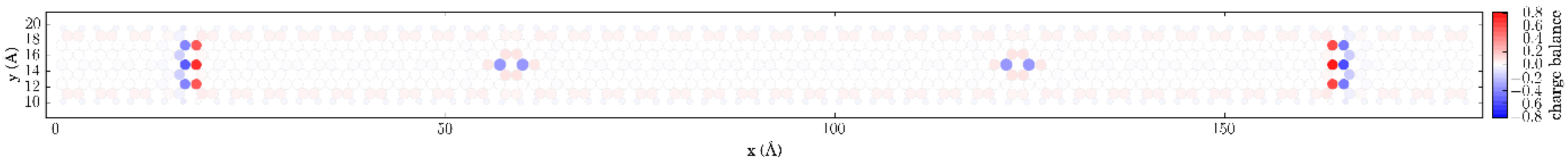


Simulation characteristics:

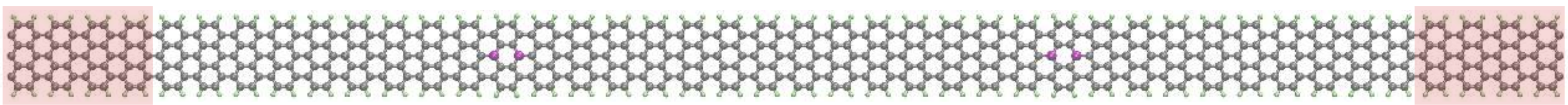
- 756 atoms;
- double-ζ (5040 orbitals);
- vdW (optB88);
- real space grid cutoff: 250 Ry;
- forces < 10 meV/Å.

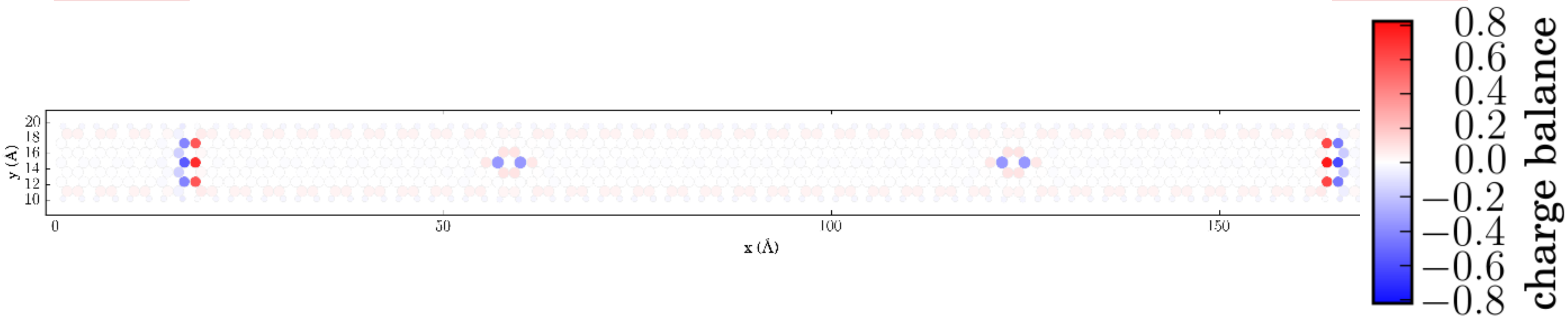
Mulliken population



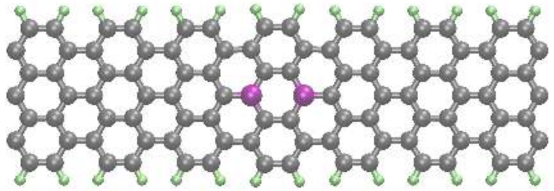


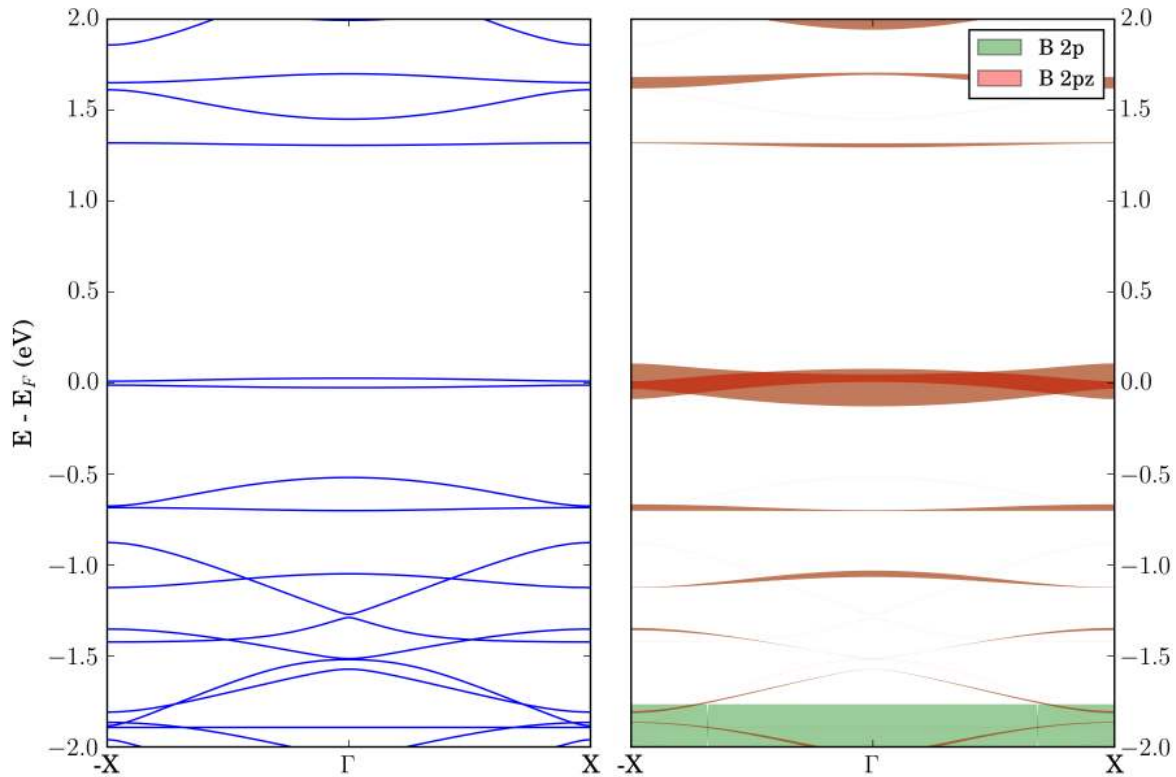
Mulliken population





Periodic calculation





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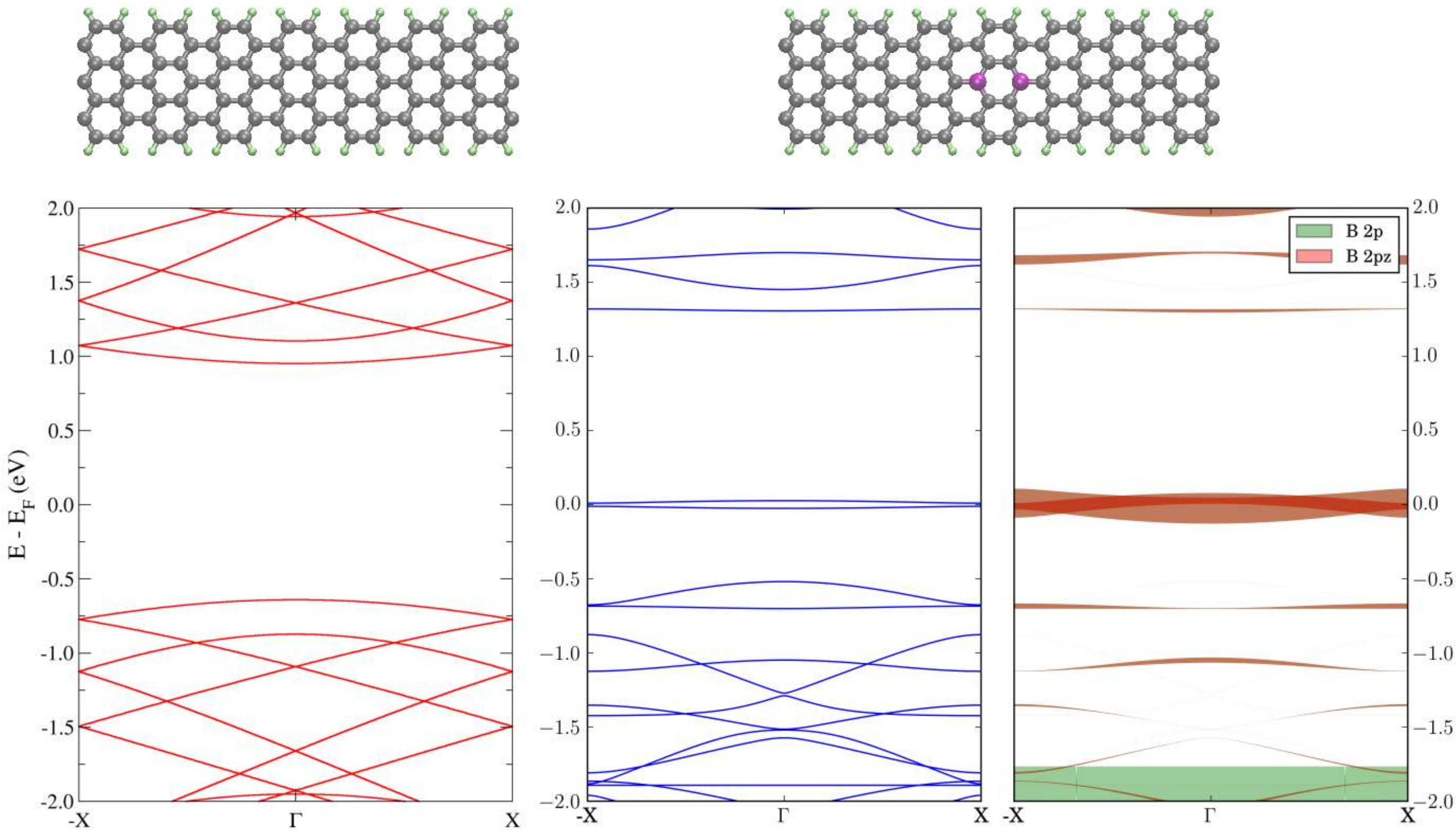

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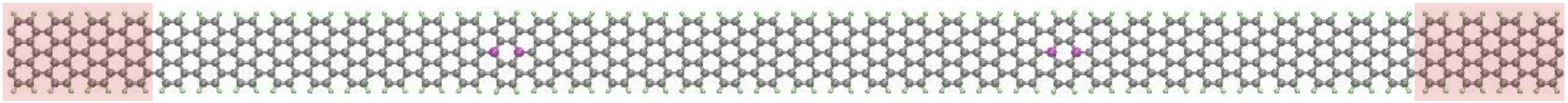
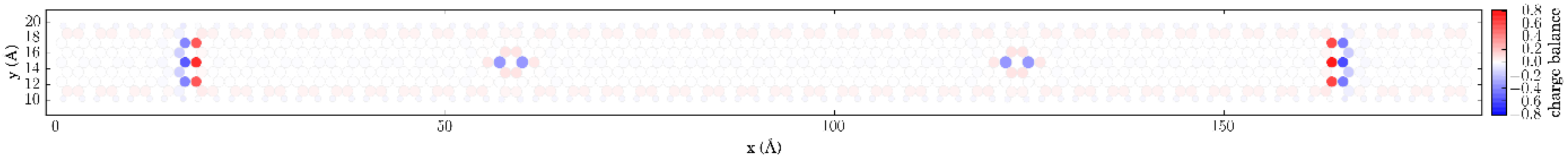
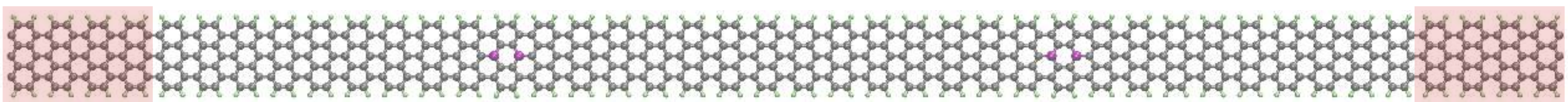
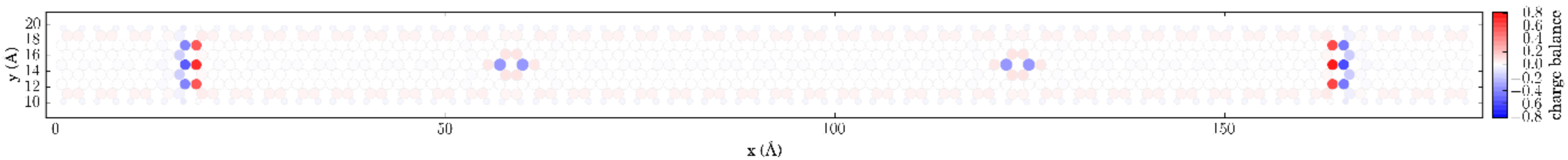
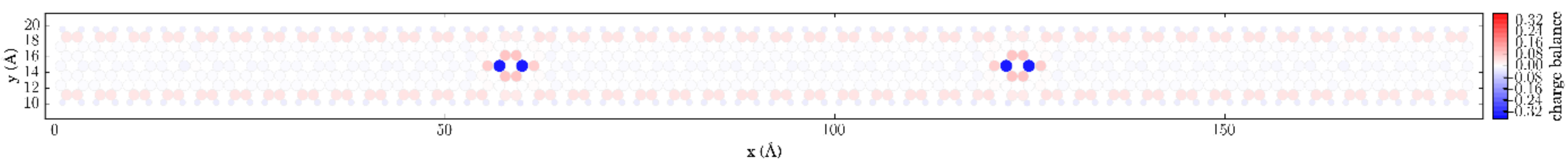




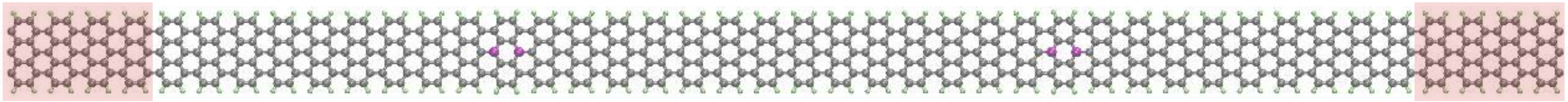
Mulliken population

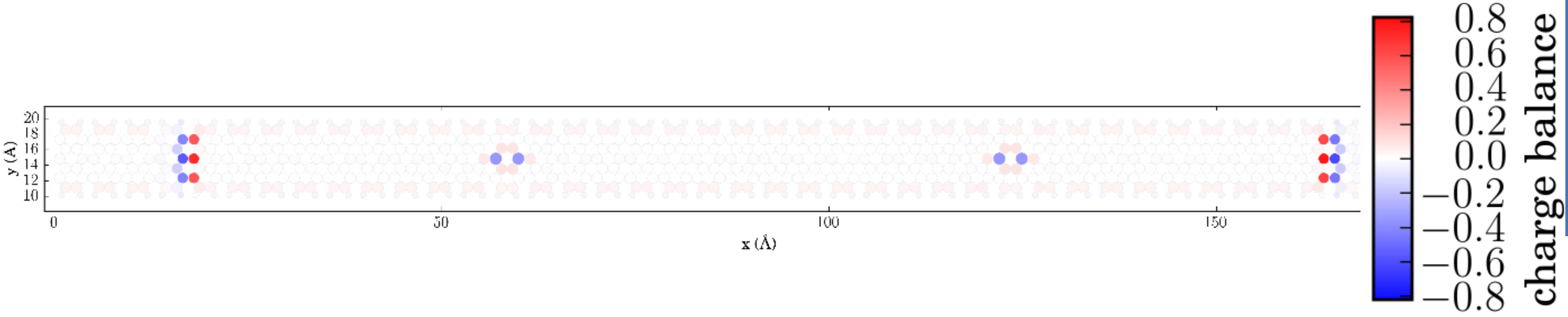


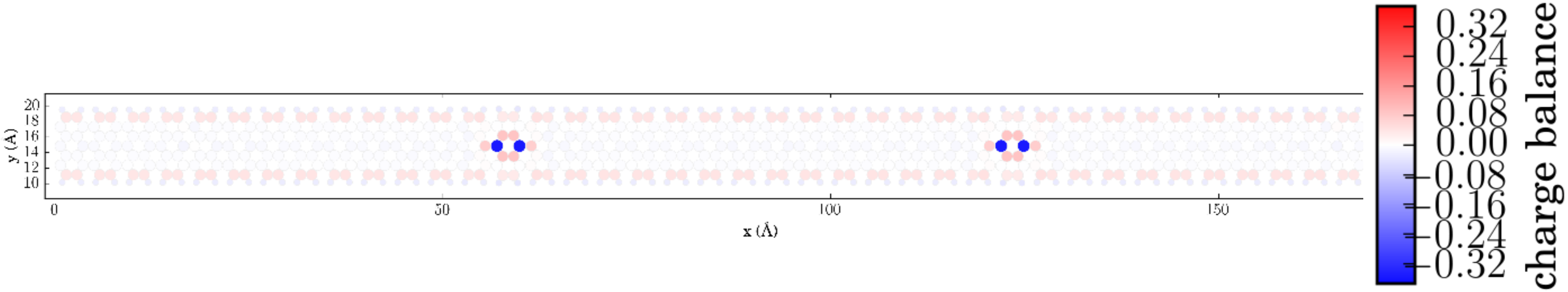




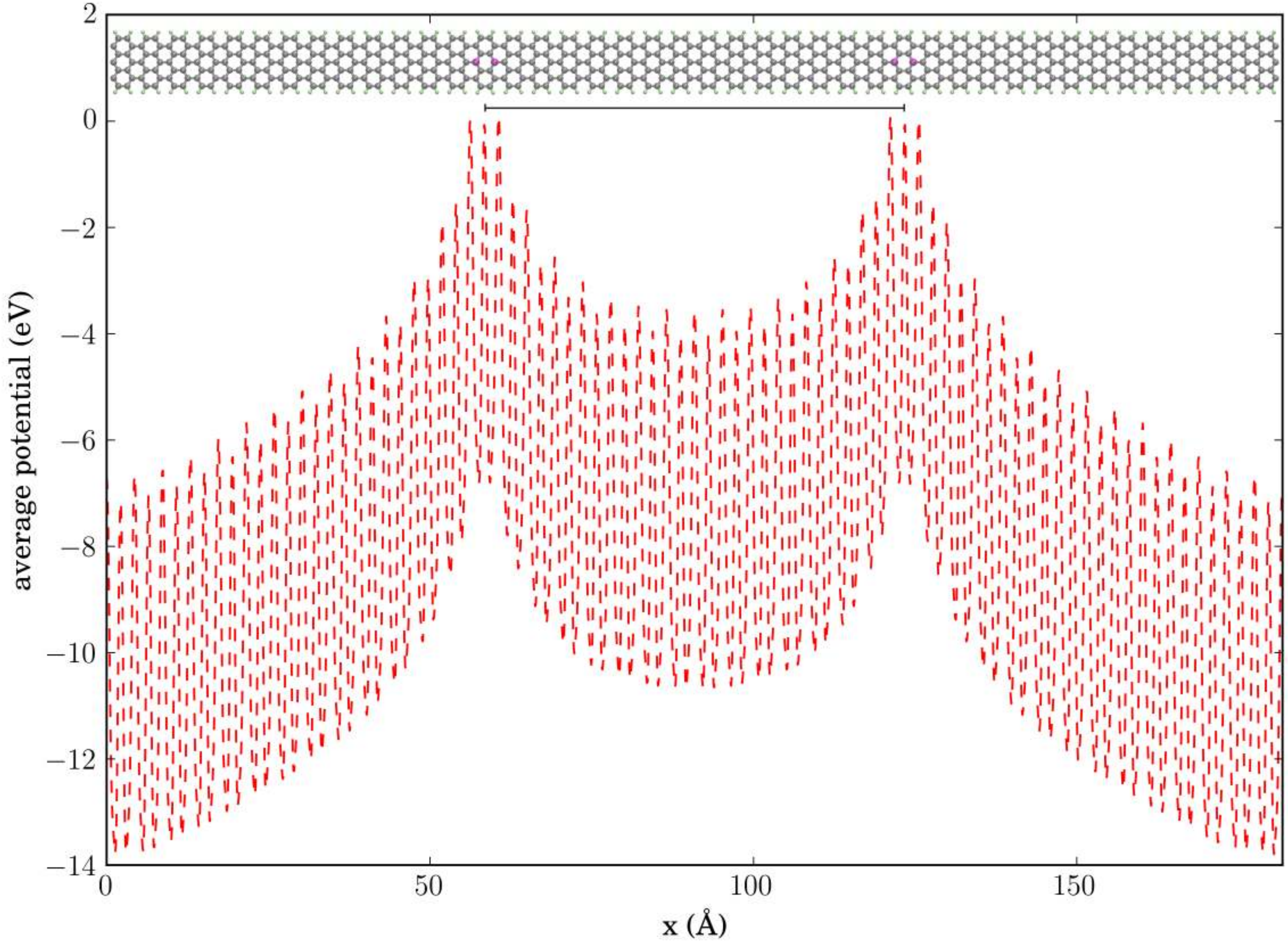
Mulliken population







Electrostatic potential



Coulomb cutoff

$$\tilde{v}(\mathbf{G}) = \int\int\int_{space} \tilde{v}(r) e^{-i\mathbf{G}\cdot\mathbf{r}} d^3\mathbf{r} = \int\int\int_{\mathcal{D}} v(r) e^{-i\mathbf{G}\cdot\mathbf{r}} d^3\mathbf{r}$$

C. A. Rossi *et al*. *Phys. Rev. B* **73**, 205119 (2006).

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- 1-D: $\tilde{v}^{1\mathrm{D}}(G_x, G_\perp) = \frac{4\pi}{G^2}[1 + G_\perp R J_1(G_\perp R) K_0(G_x R) - G_x R J_0(G_\perp R) K_1(G_x R)]$

C. A. Rossi *et al*. *Phys. Rev. B* **73**, 205119 (2006).

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$$\approx -4\pi \int_0^R r J_0(G_\perp r) \ln(r) dr + 4\pi R \ln(2h) \frac{J_1(G_\perp R)}{G_\perp}$$

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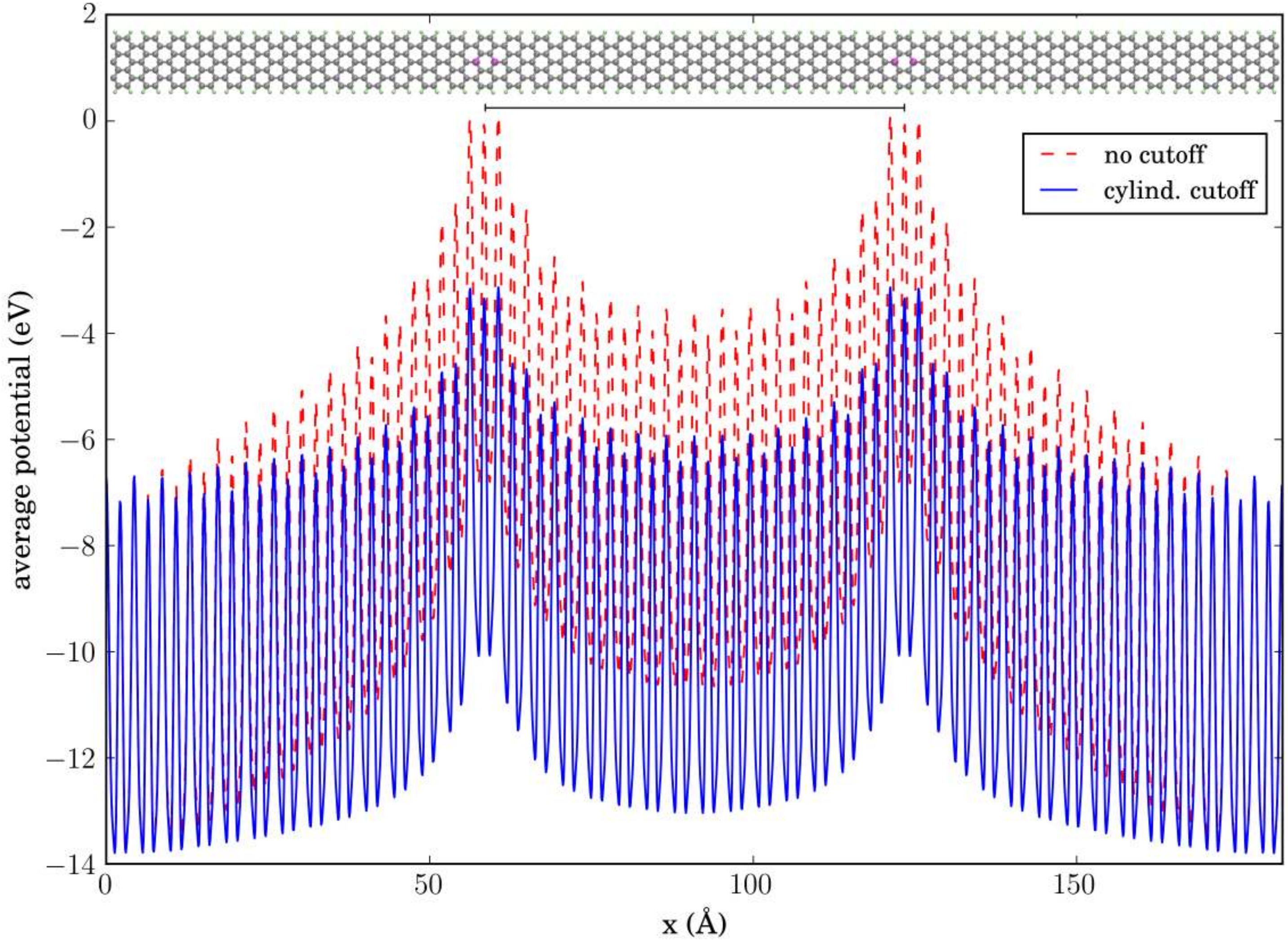
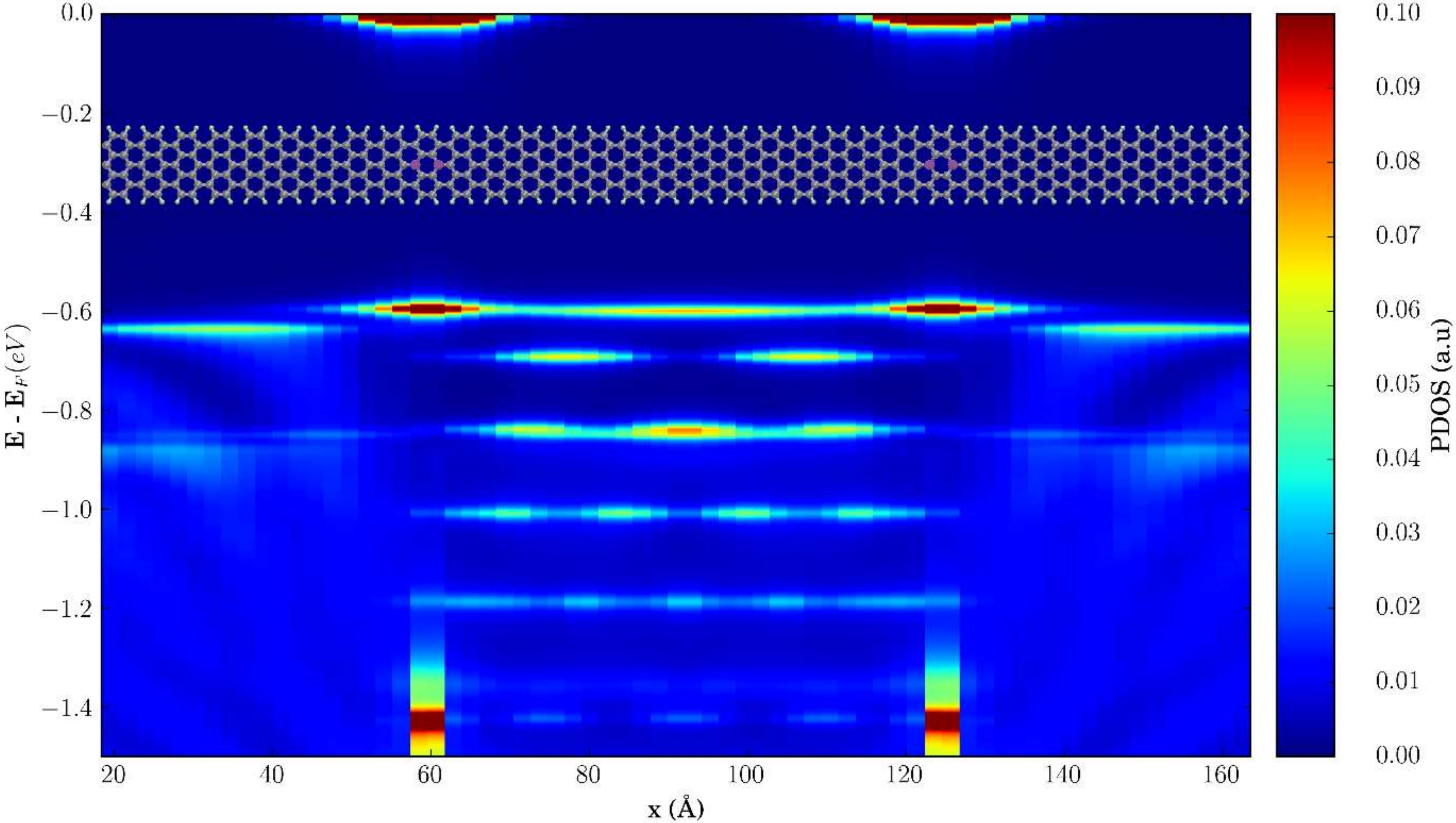
$= 0$

C. A. Rossi *et al*. *Phys. Rev. B* **73**, 205119 (2006).

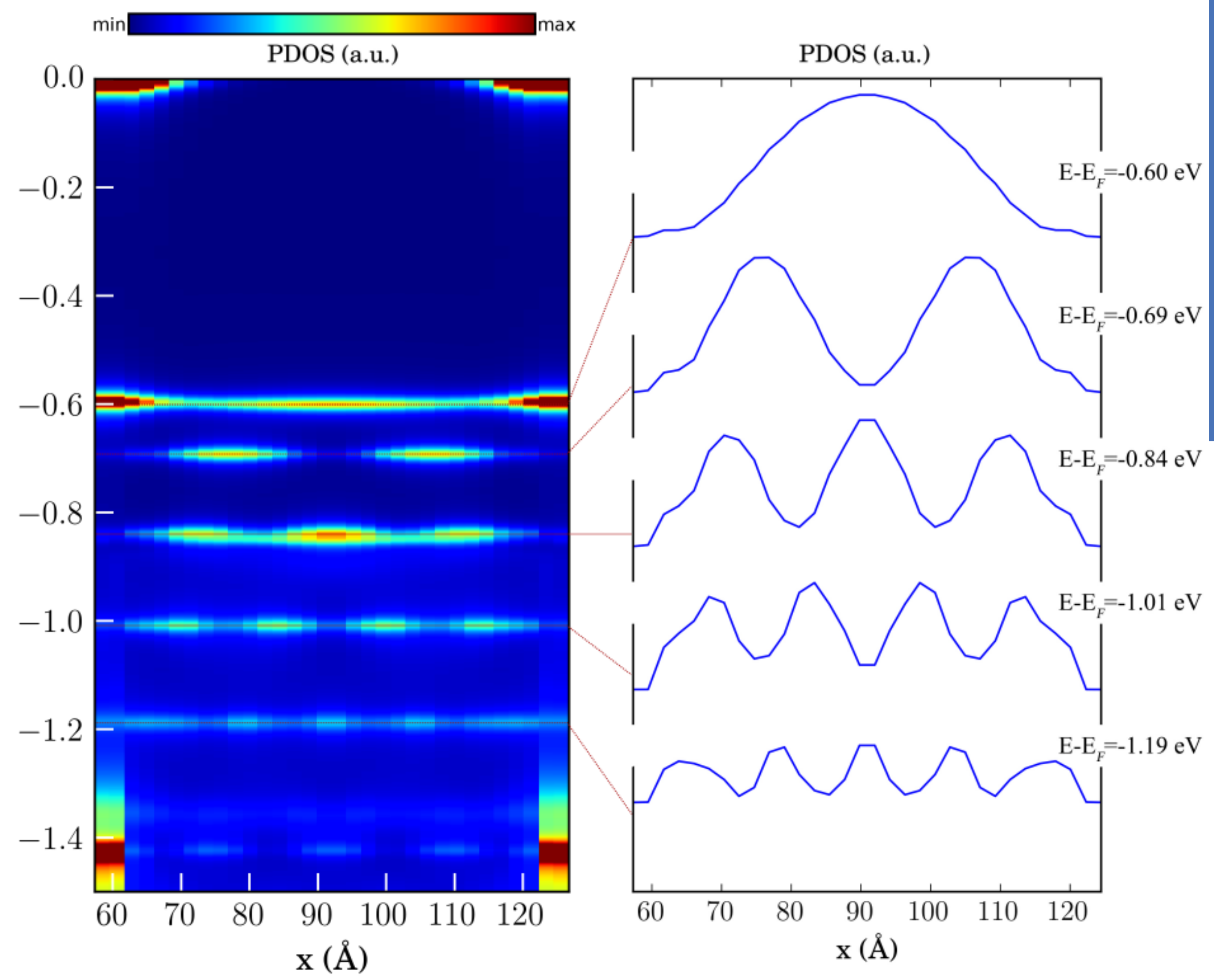
Electrostatic potential



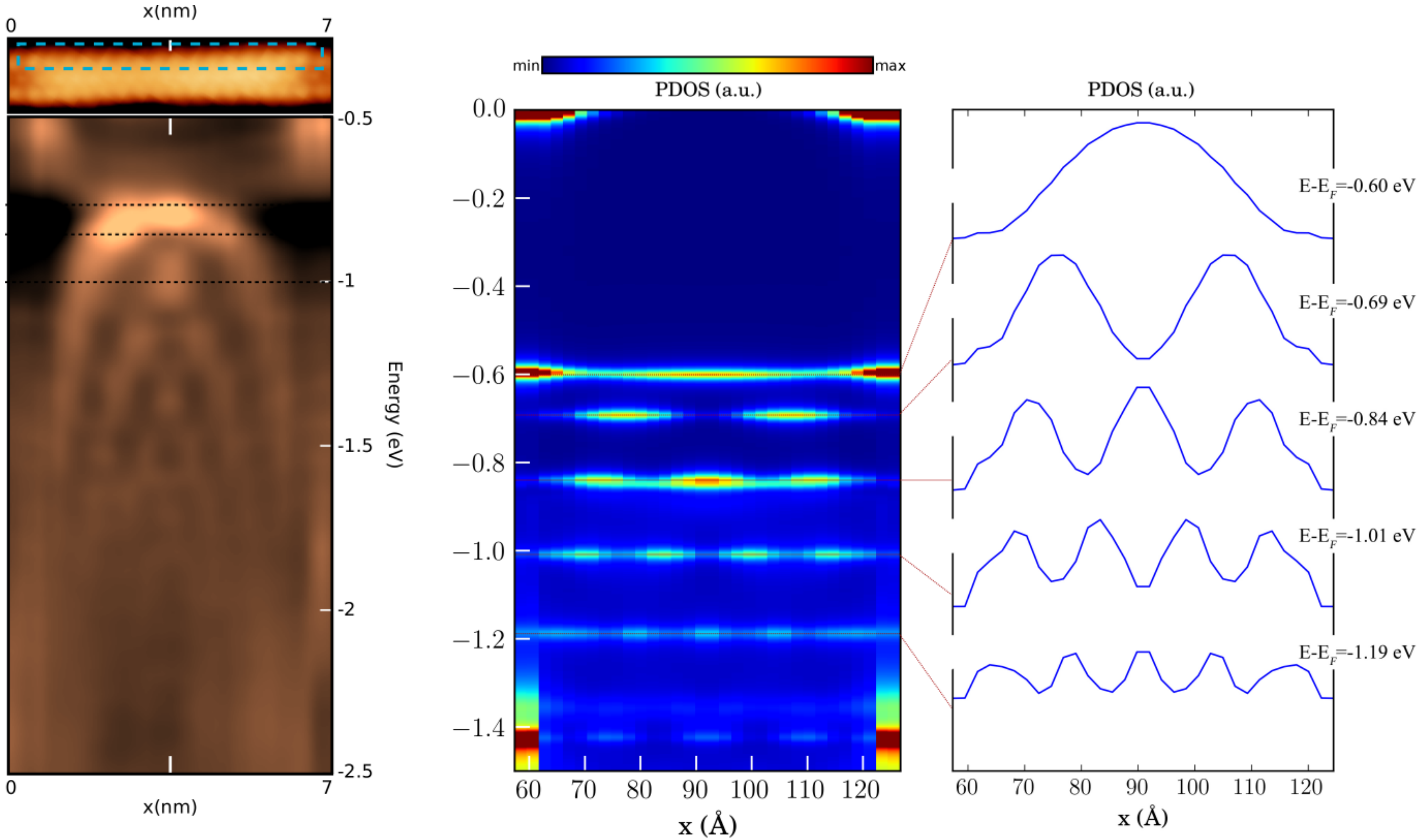
DOS projected on each ribbon “row”



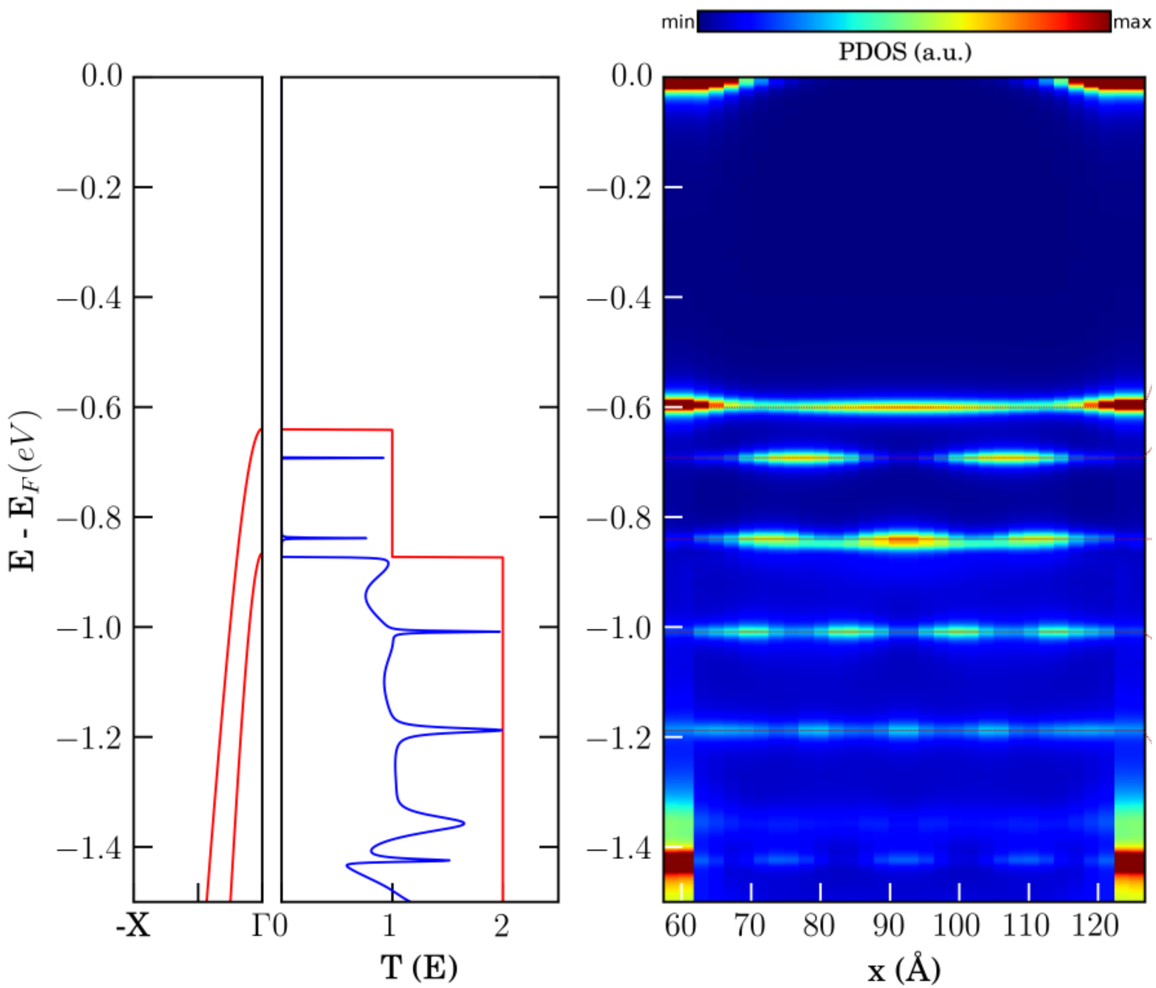
DOS projected on each ribbon "row"



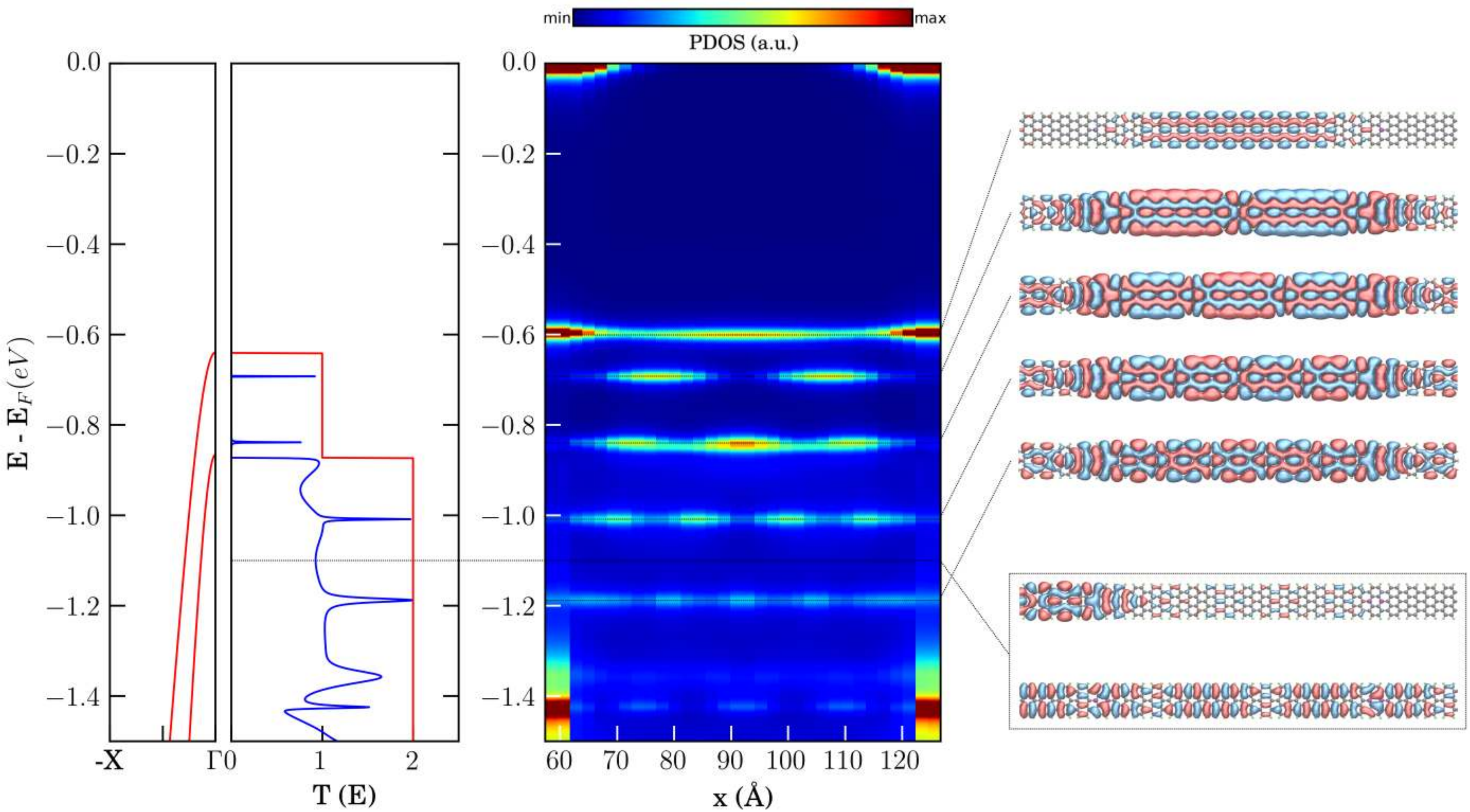
DOS projected on each ribbon "row"



Zero bias transmission

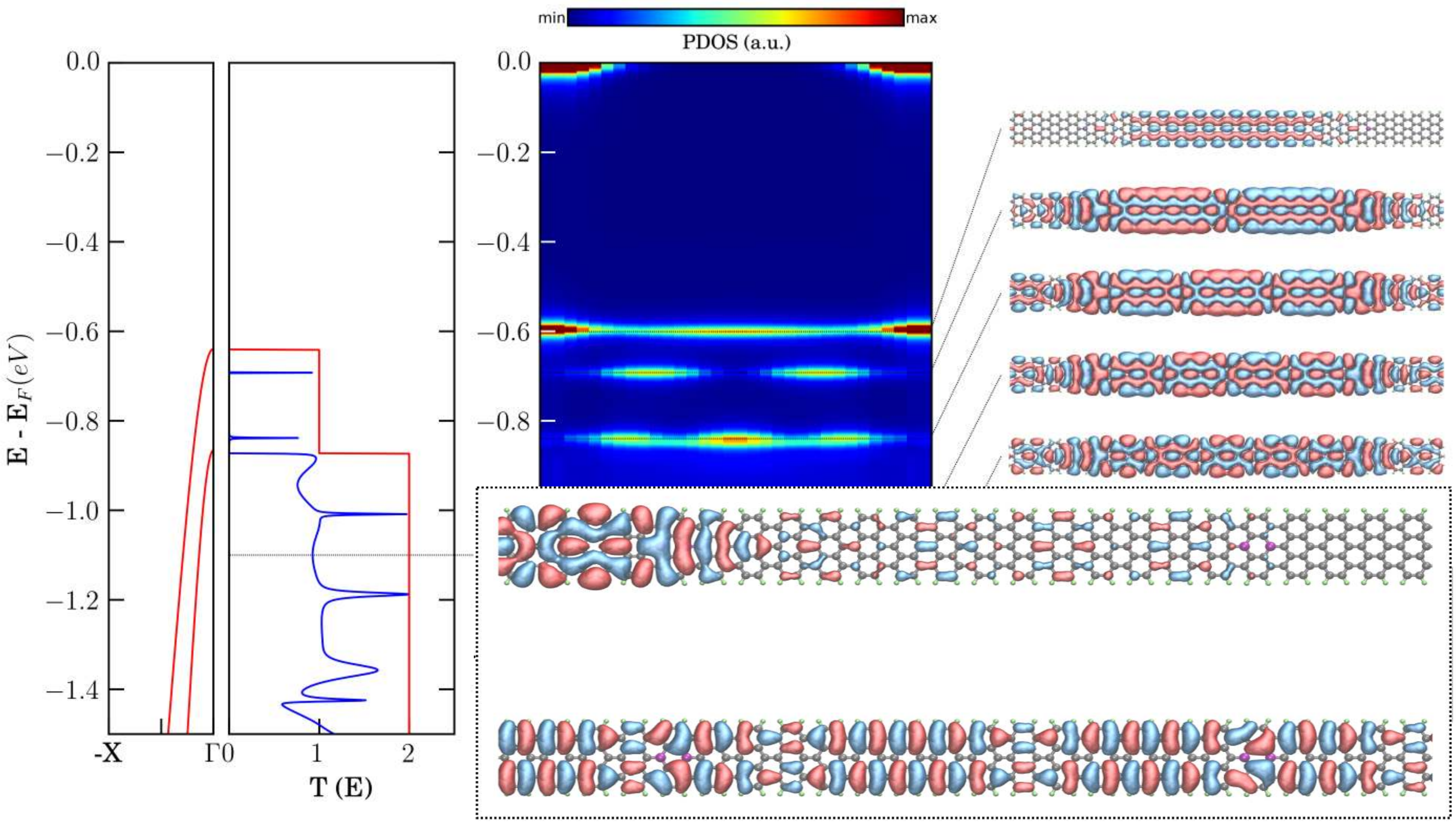


Eigenchannels



M. Paulsson and M. Brandbyge. *Phys. Rev. B* **76**, 115117 (2007).

Eigenchannels



M. Paulsson and M. Brandbyge. *Phys. Rev. B* **76**, 115117 (2007).

Conclusions

- Semiconductor electrodes: **use with caution!**
- **Coulomb cutoff in TranSIESTA** for low dimensionality systems;
- Transport simulations can **reproduce** observed quantum well states and **explain** their mechanism.

Thank you!