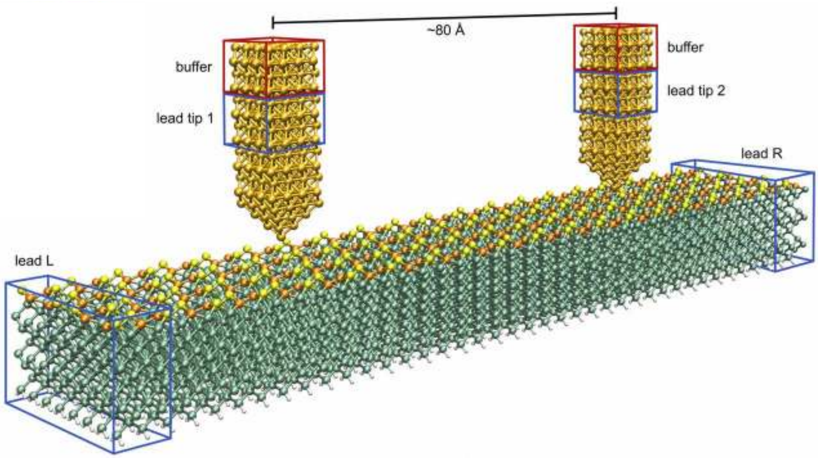
Electron quantum optics with graphene-based nanostructures

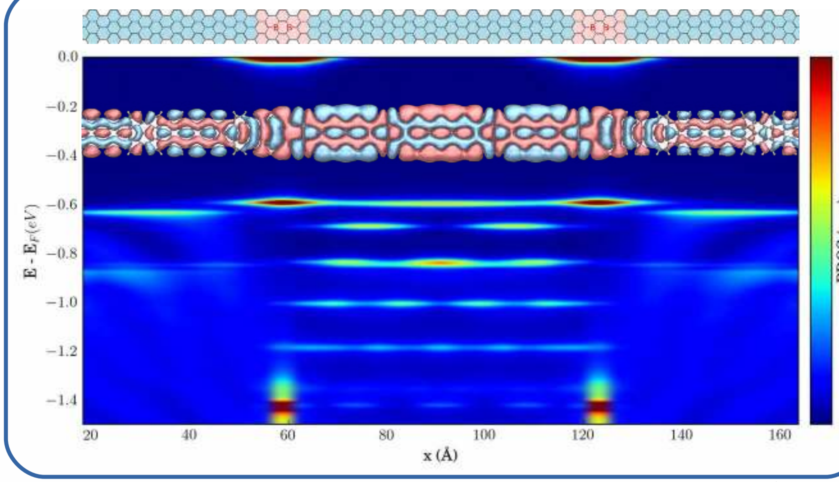
Pedro Brandimarte

Donostia International Physics Center
San Sebastián, Spain

May 2018



M. Kolmer, P. Brandimarte *et al*. ***In preparation!***



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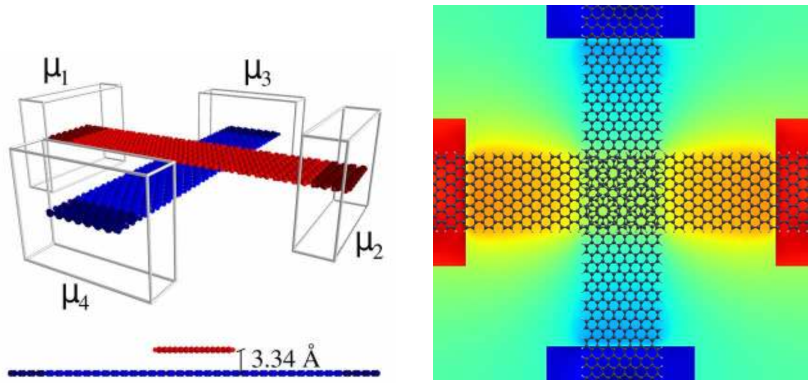

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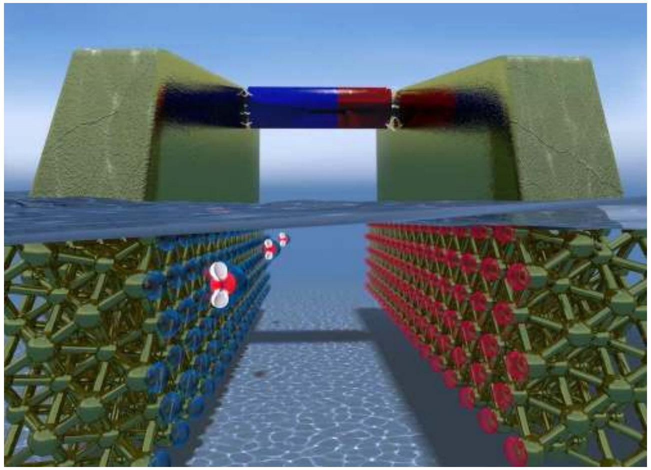

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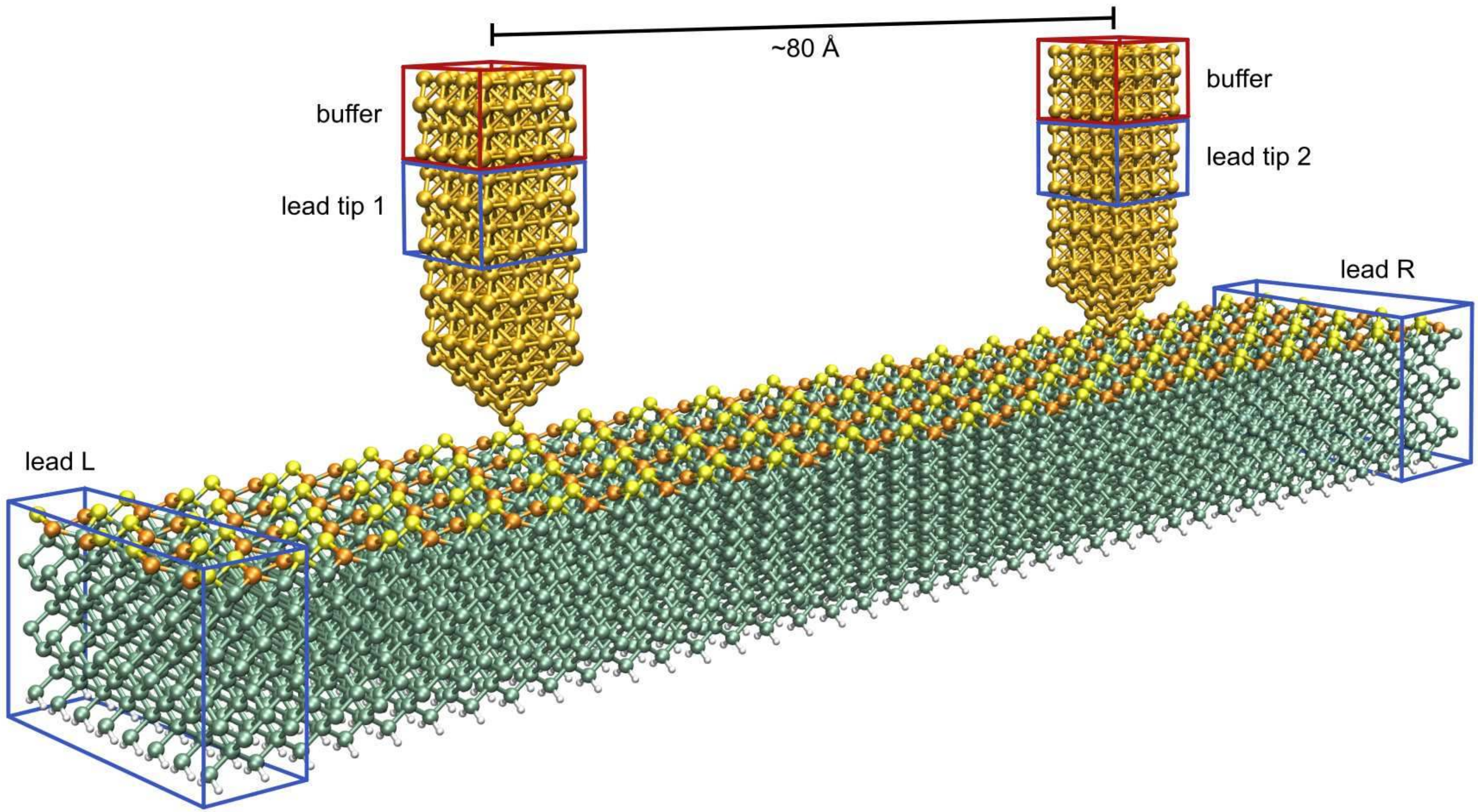

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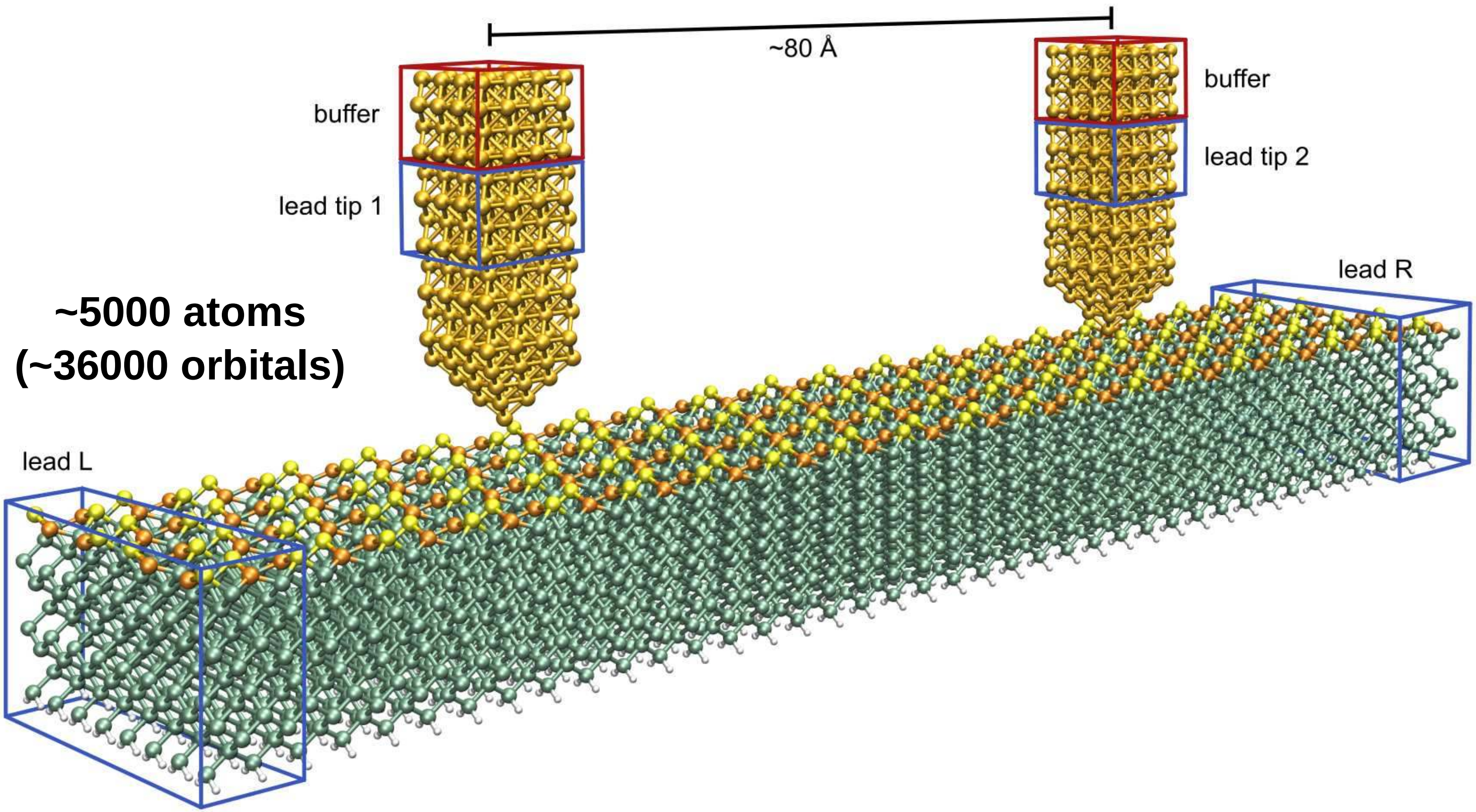

~5000 atoms
(~36000 orbitals)

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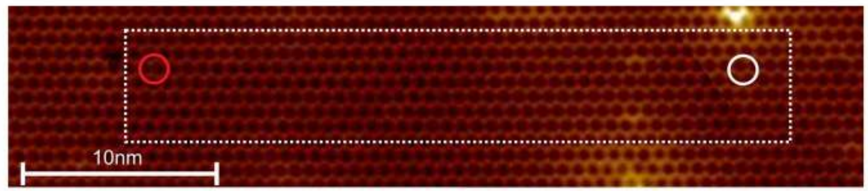

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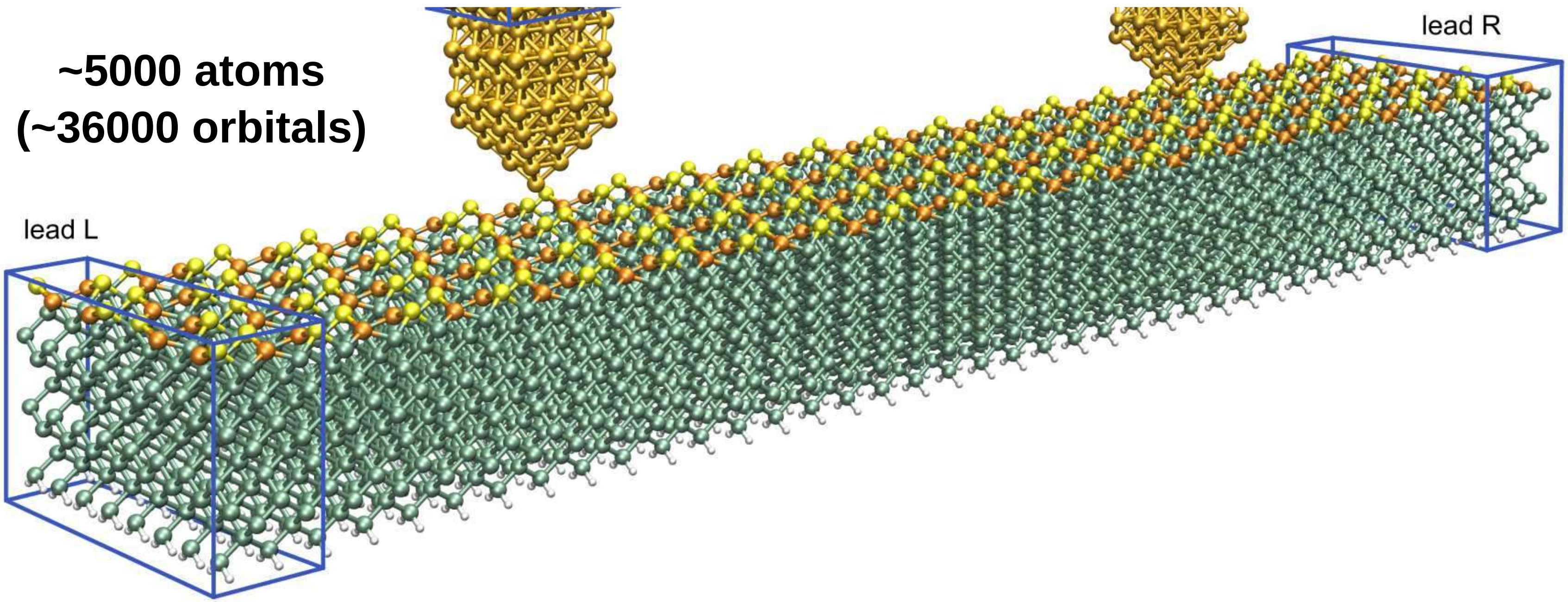

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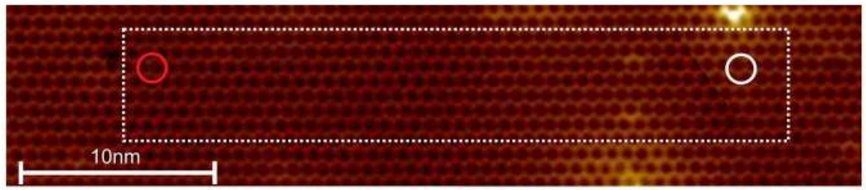

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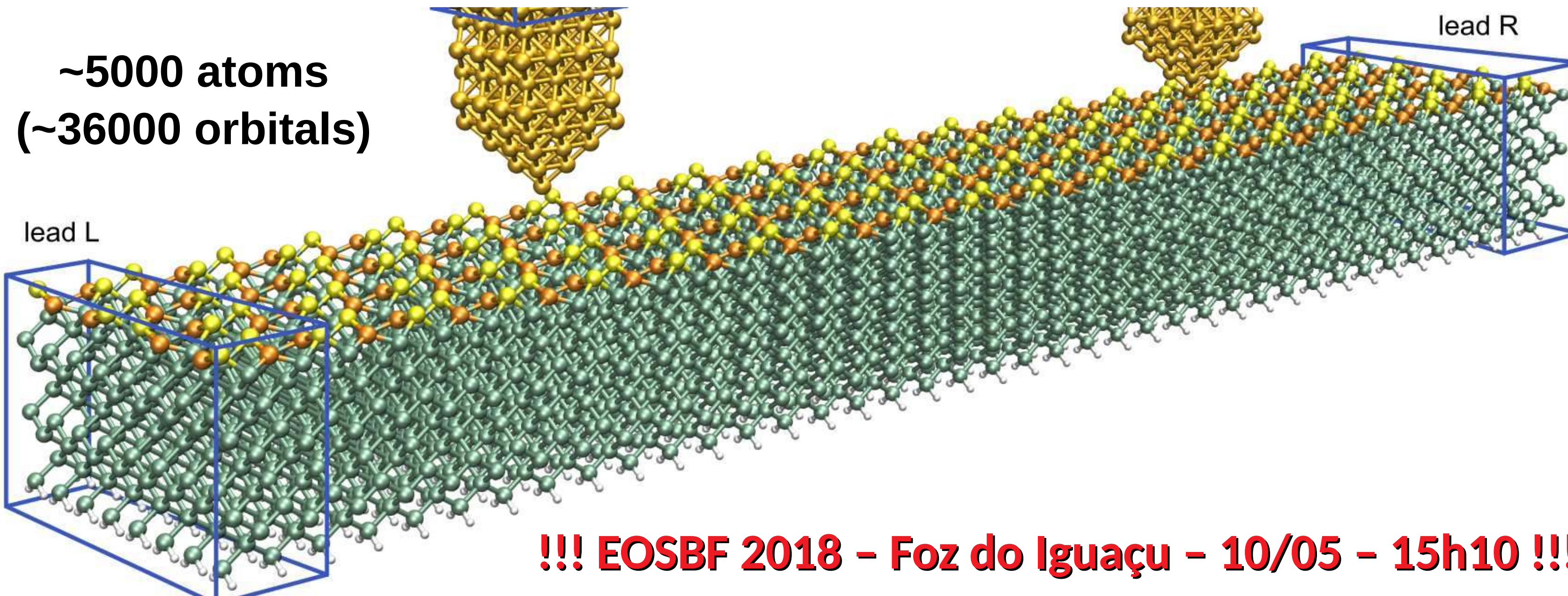

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NANOMATERIALS: GROWTH AND CHARACTERIZATION

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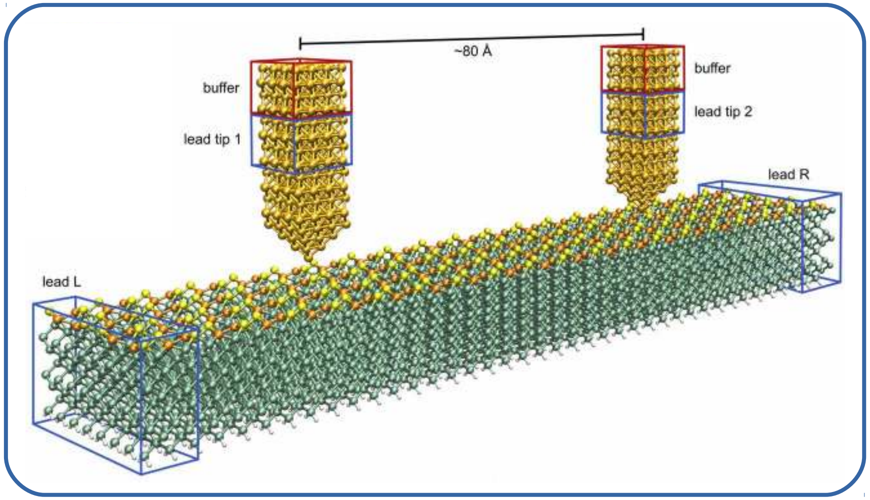

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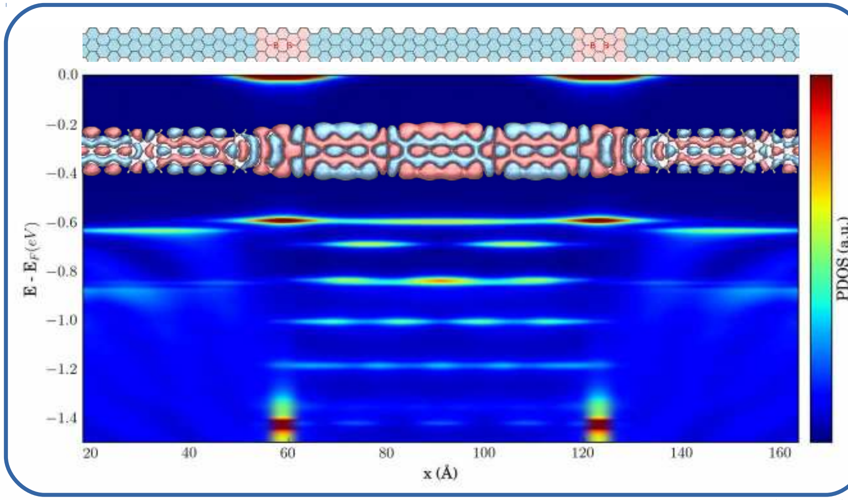

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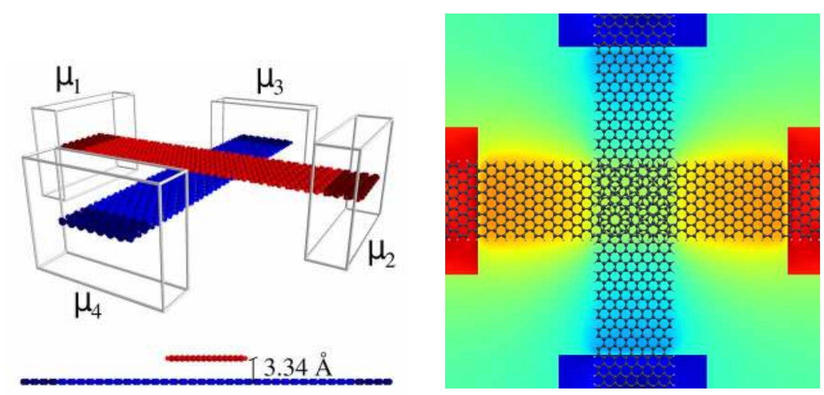

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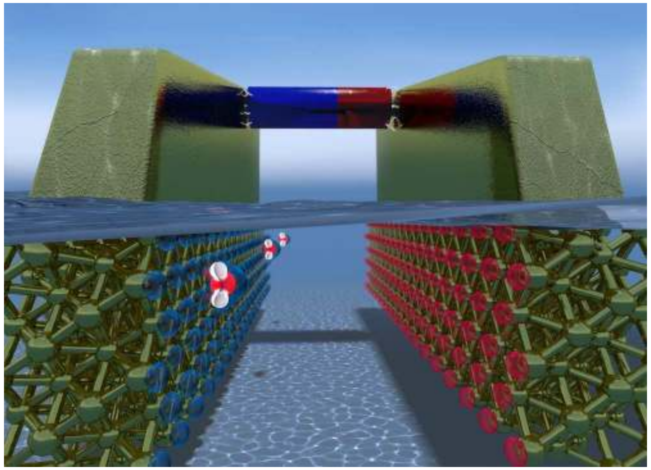

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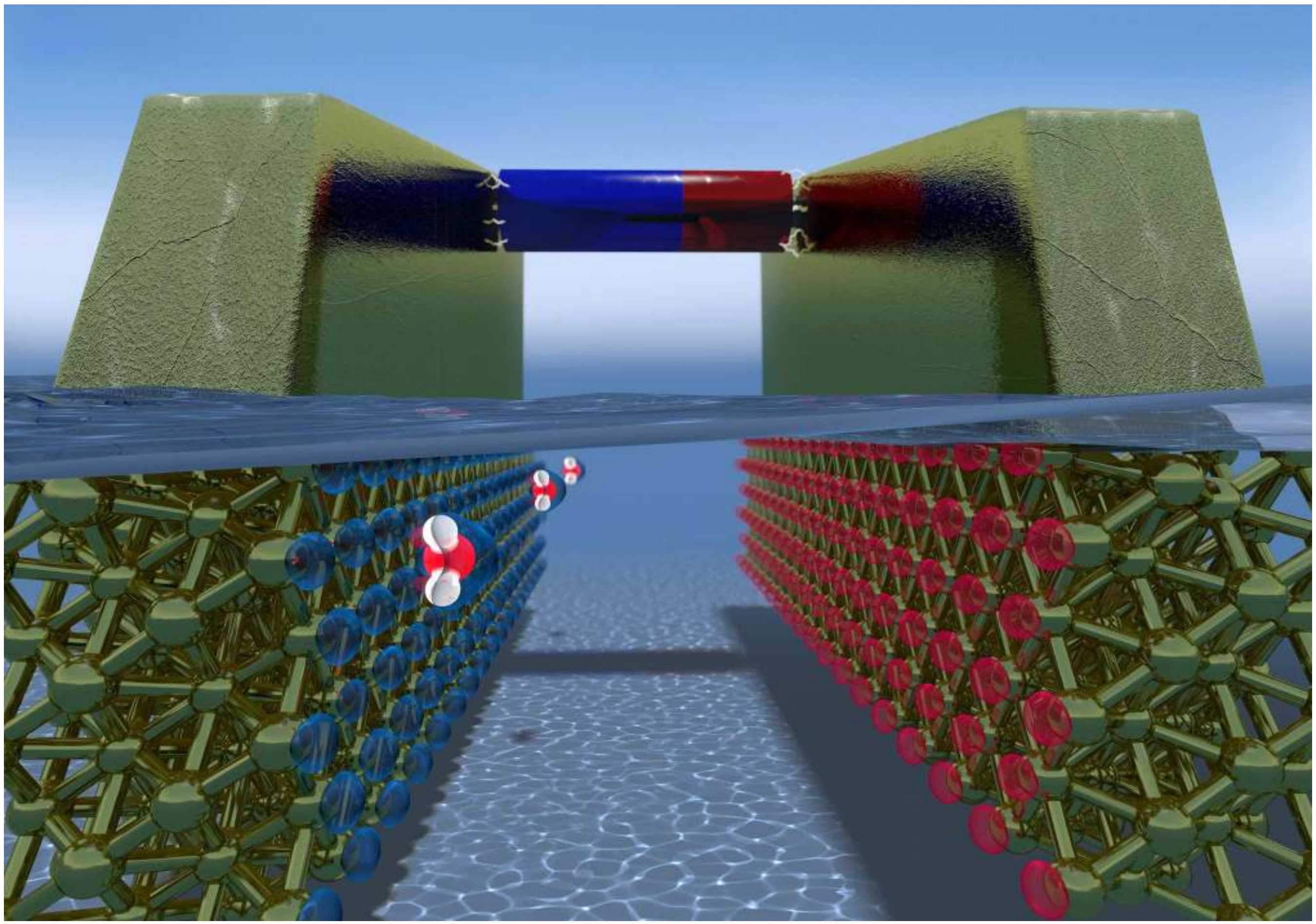

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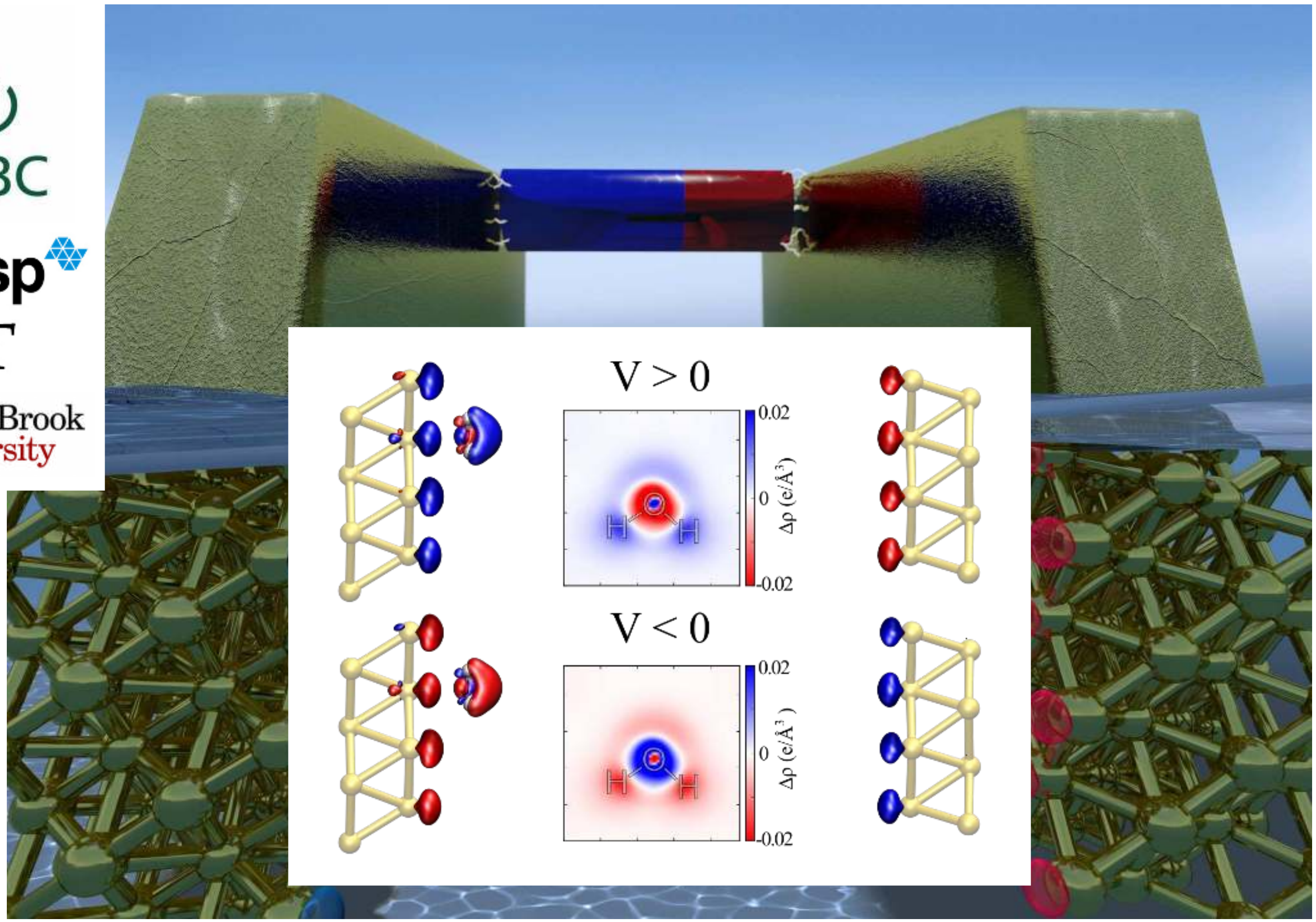

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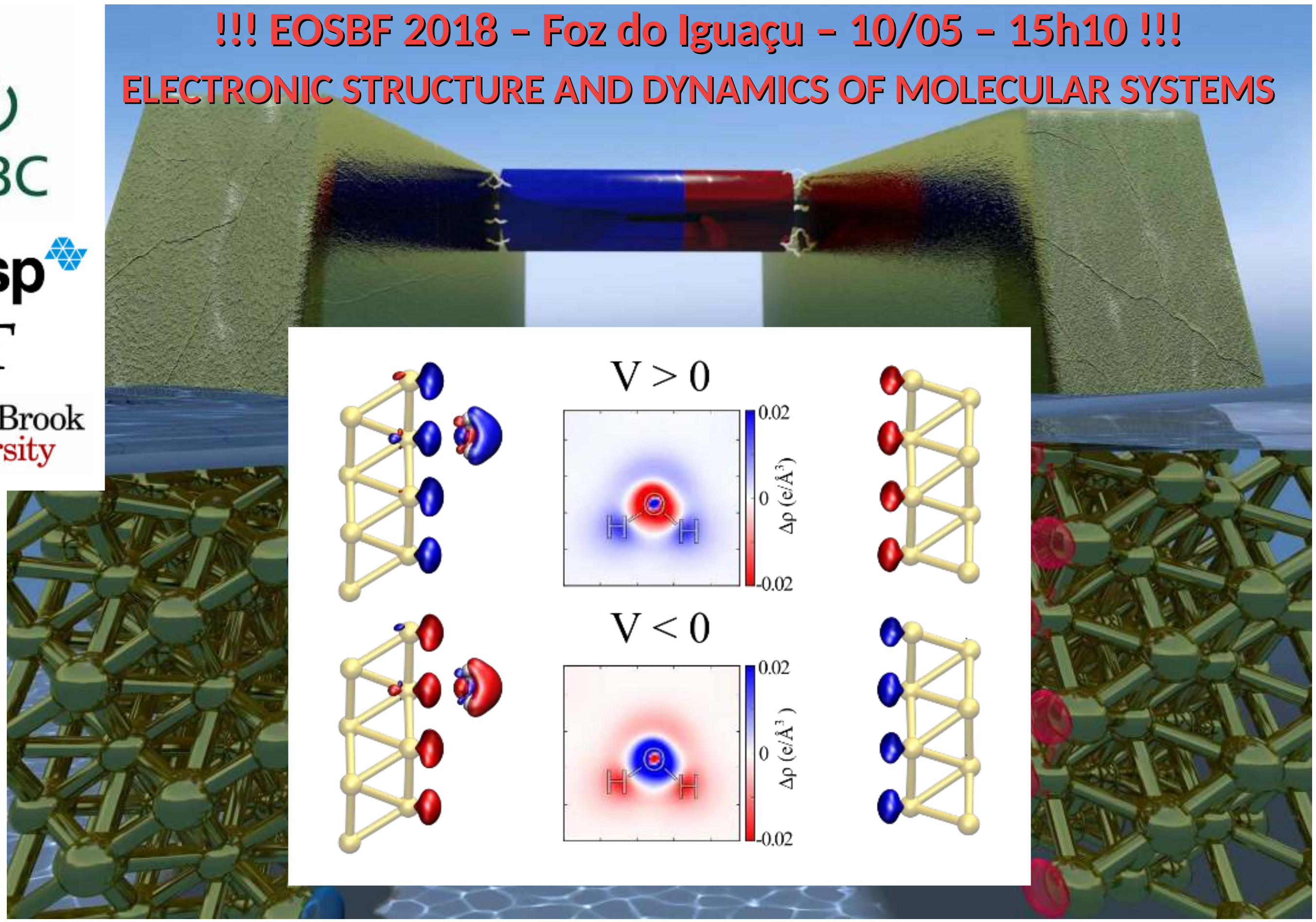

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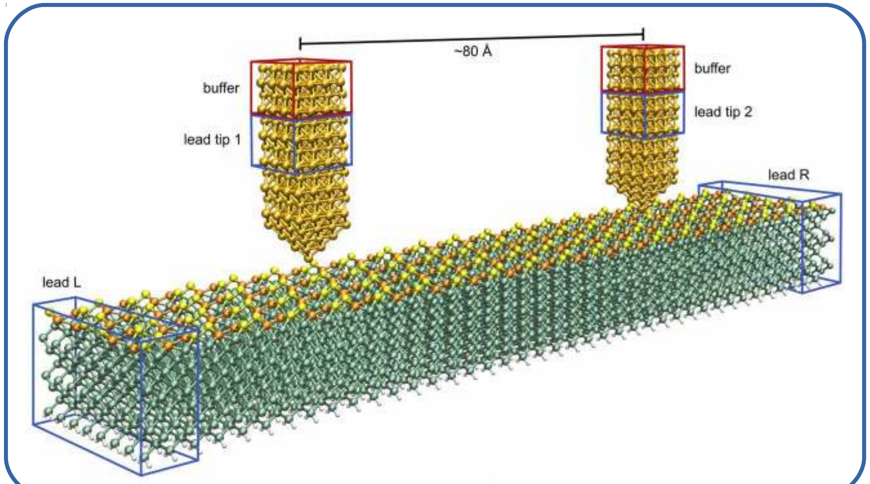

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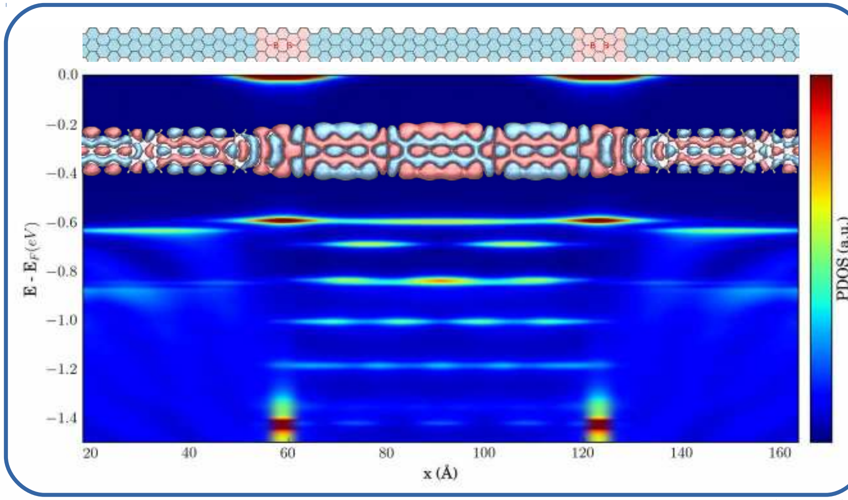

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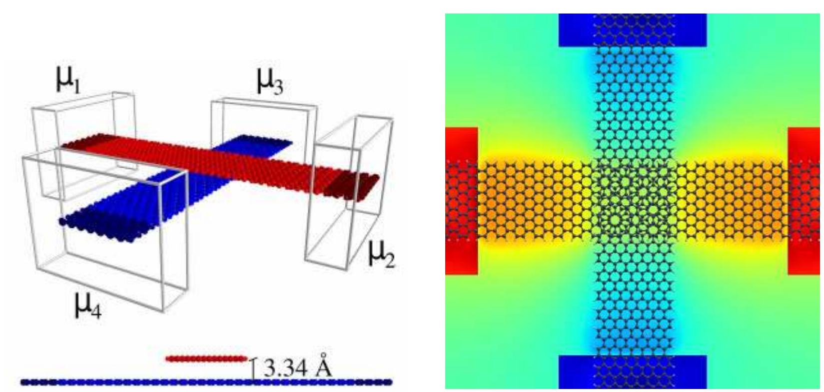

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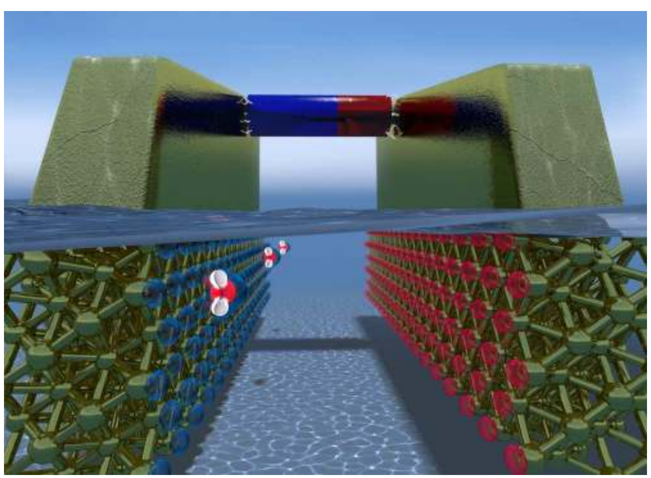

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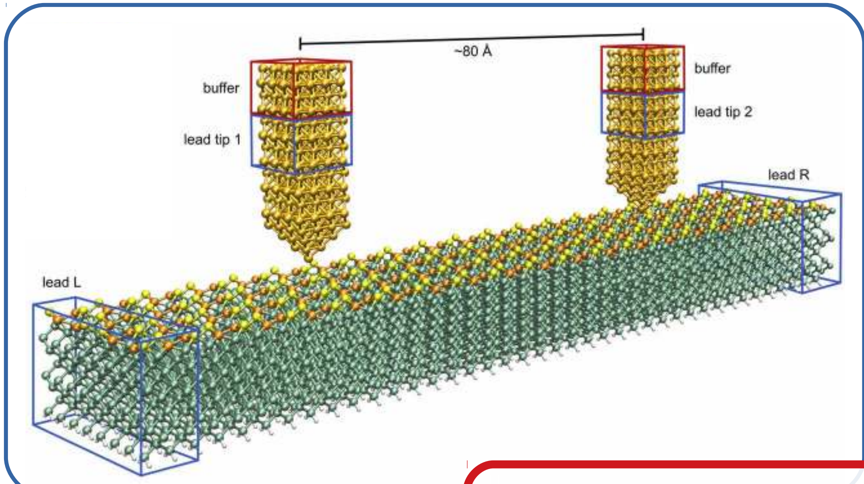
OPEN QUANTUM SYSTEMS



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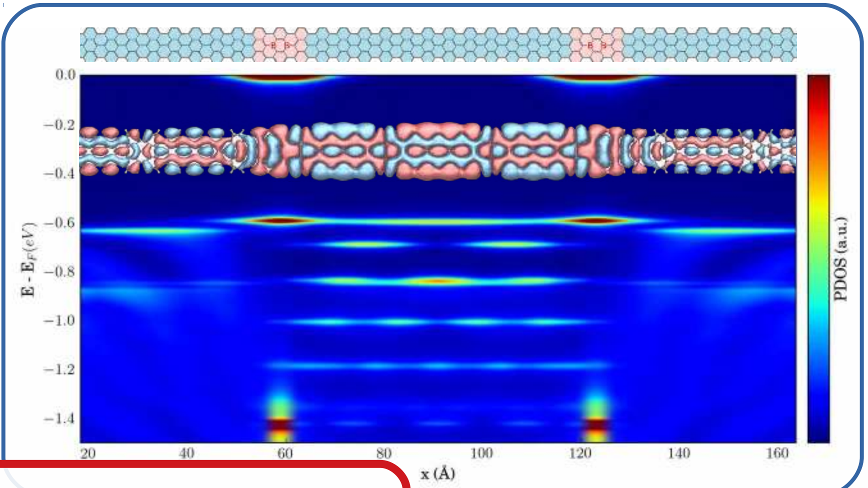

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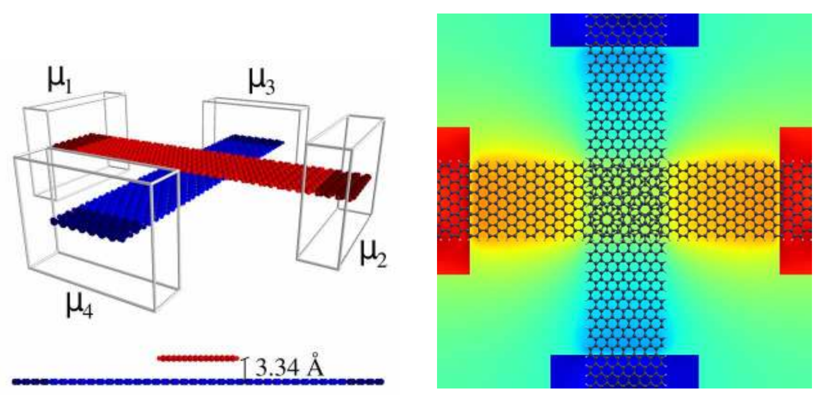

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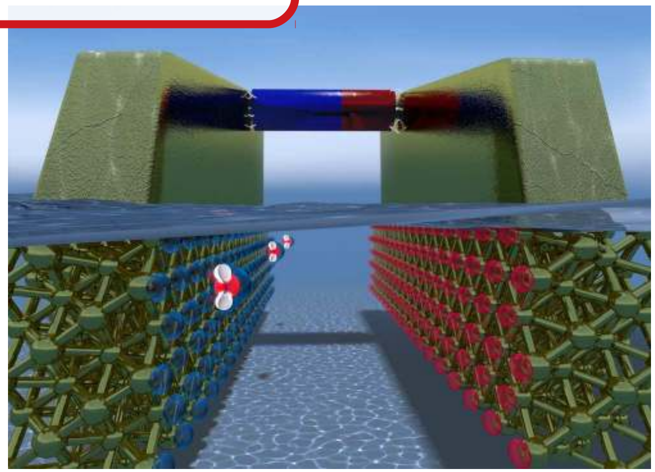

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Donostia - San Sebastián

Good for tourism… and for SCIENCE!!!

Acknowledgments

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Daniel Sánchez-Portal

Thomas Frederiksen

Aran Garcia-Lekue

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Geza Giedke

DTU (Denmark)

Nick Papior

CIC nanoGune/CFM

Jose Ignacio Pascual

Eduard Carbonel-Sanromà

Martina Corso

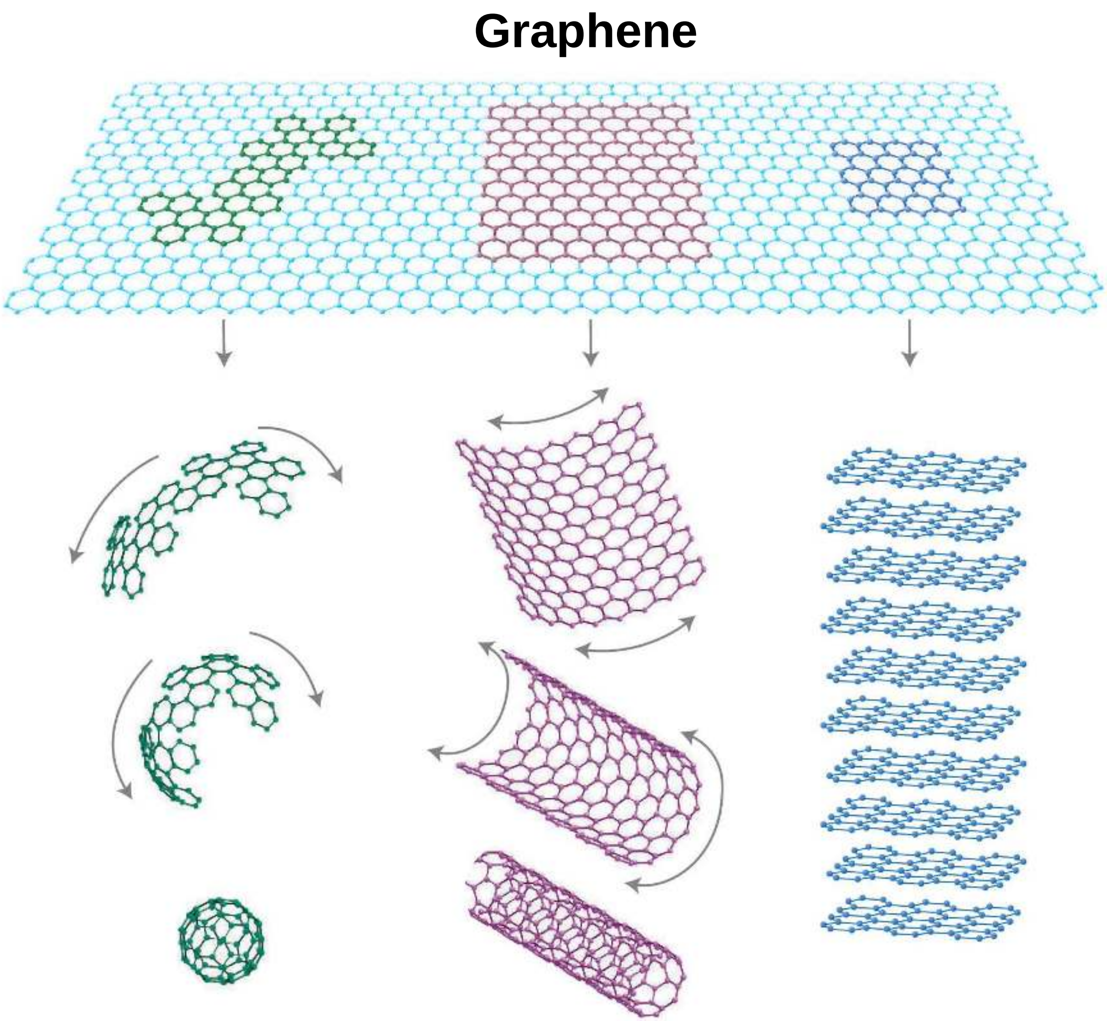
Outline

- Motivation
- 1-Dimension quantum well states on doped GNRs
- Tunable electronic beam splitter with crossed GNRs
- Summary

What is GNR?

What is GNR?

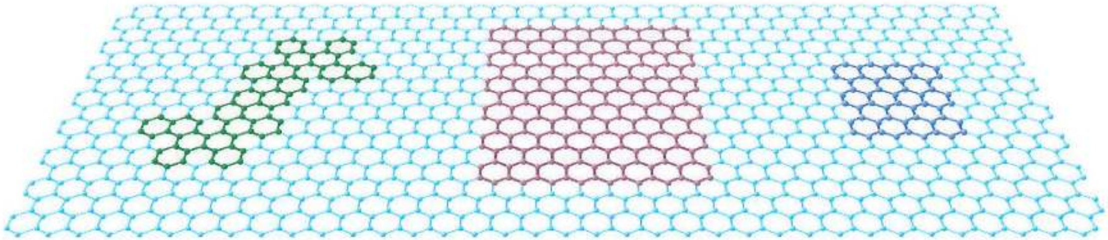
What is GNR?

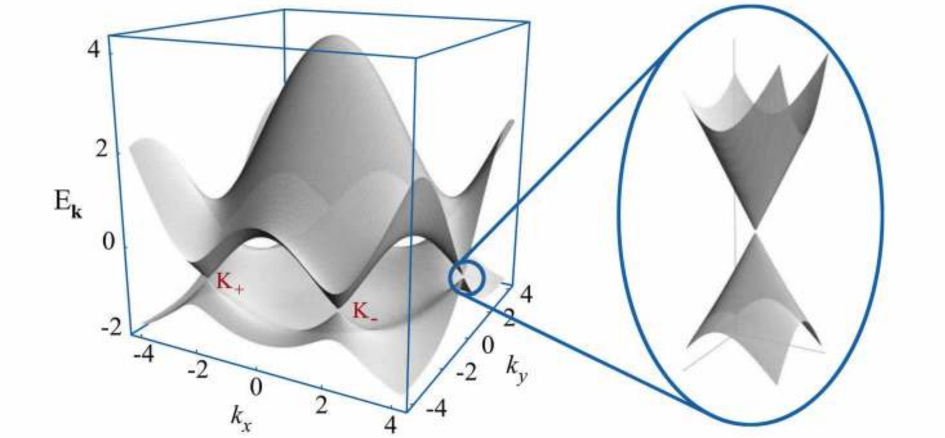


A. Geim and K. Novoselov. *Nature Mat.* **6**(3), 183 (2007).

What is GNR?

Graphene





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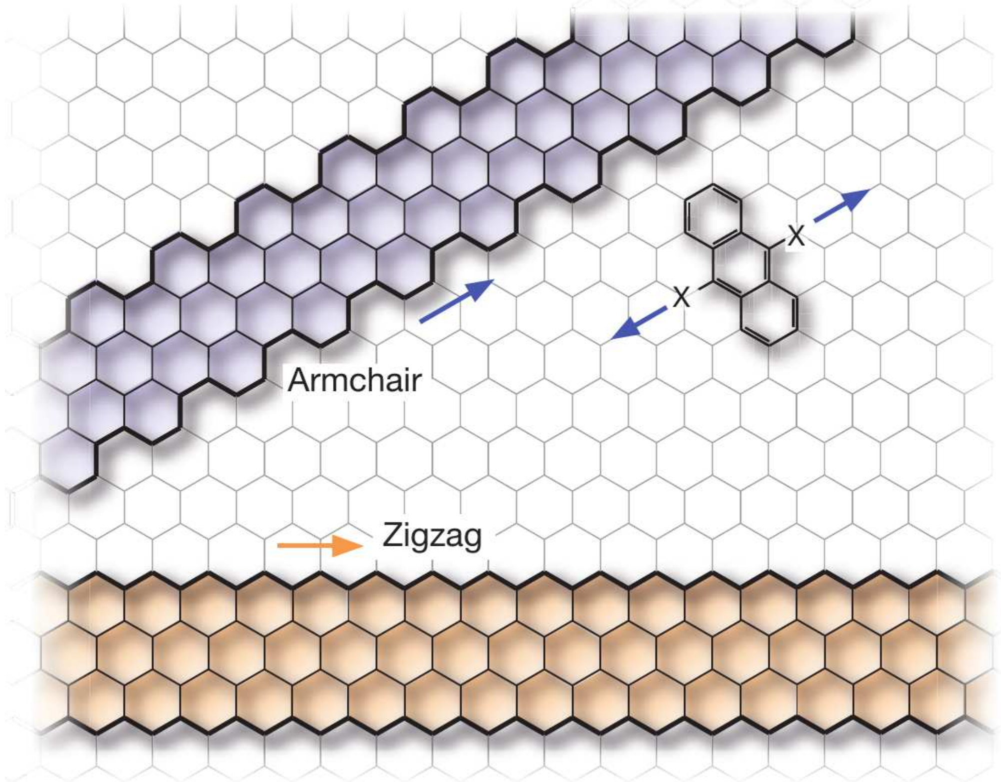
A. Castro Neto *et al*. *Rev. Mod. Phys.* **81**, 109 (2009).

What is GNR?

Graphene NanoRibbon (GNR)



P. Ruffieux *et al*. *Nature* **531**, 489 (2016).

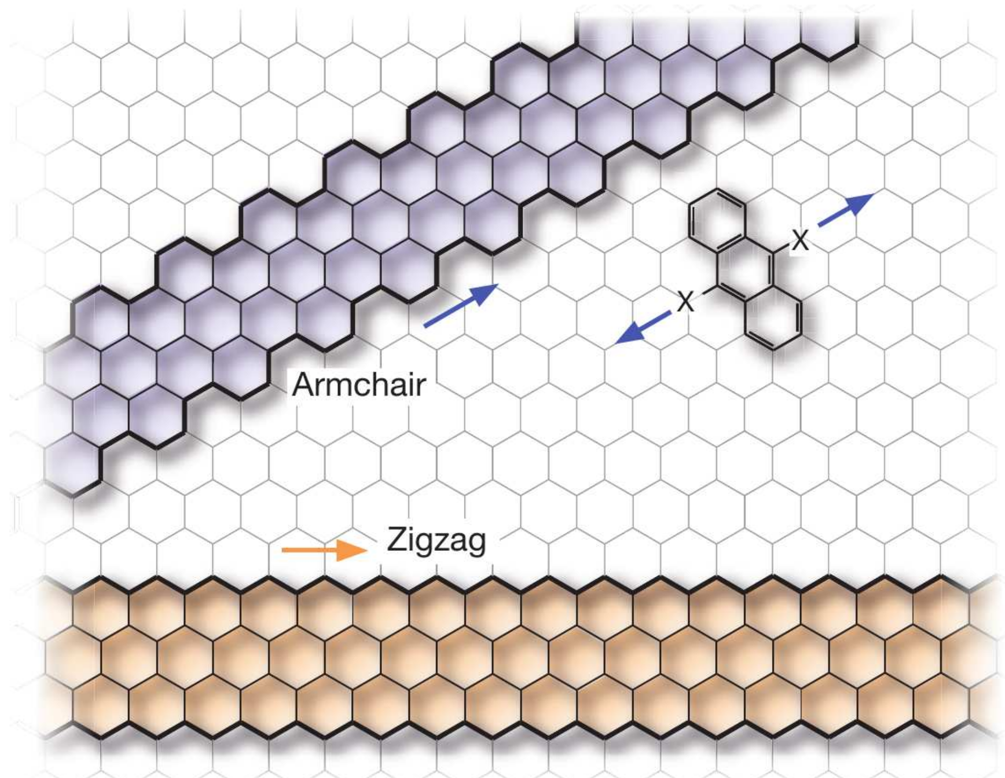
What is GNR?

Armchair **G**raphene **N**ano**R**ibbon

AGNR

+

Graphene NanoRibbon (GNR)



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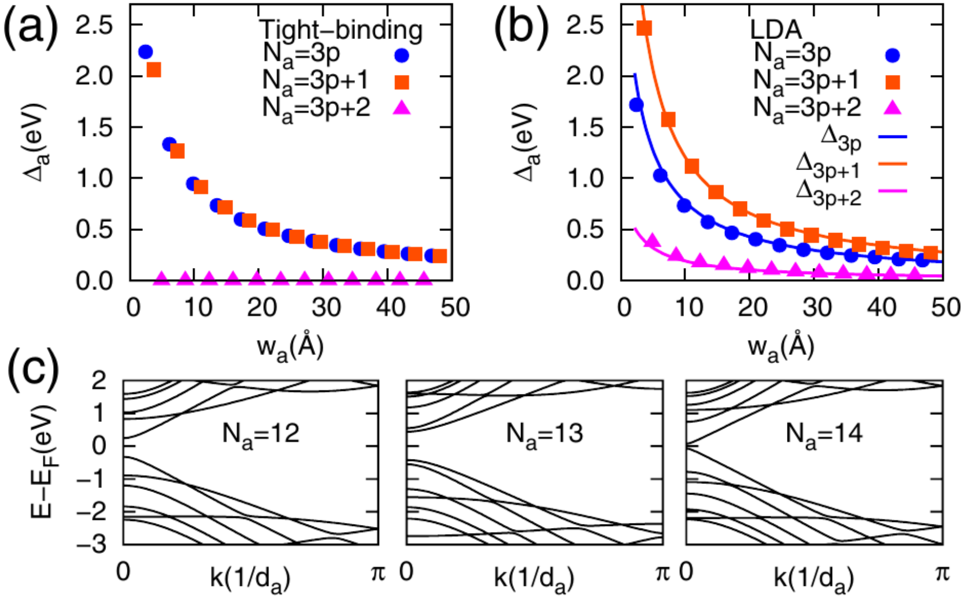
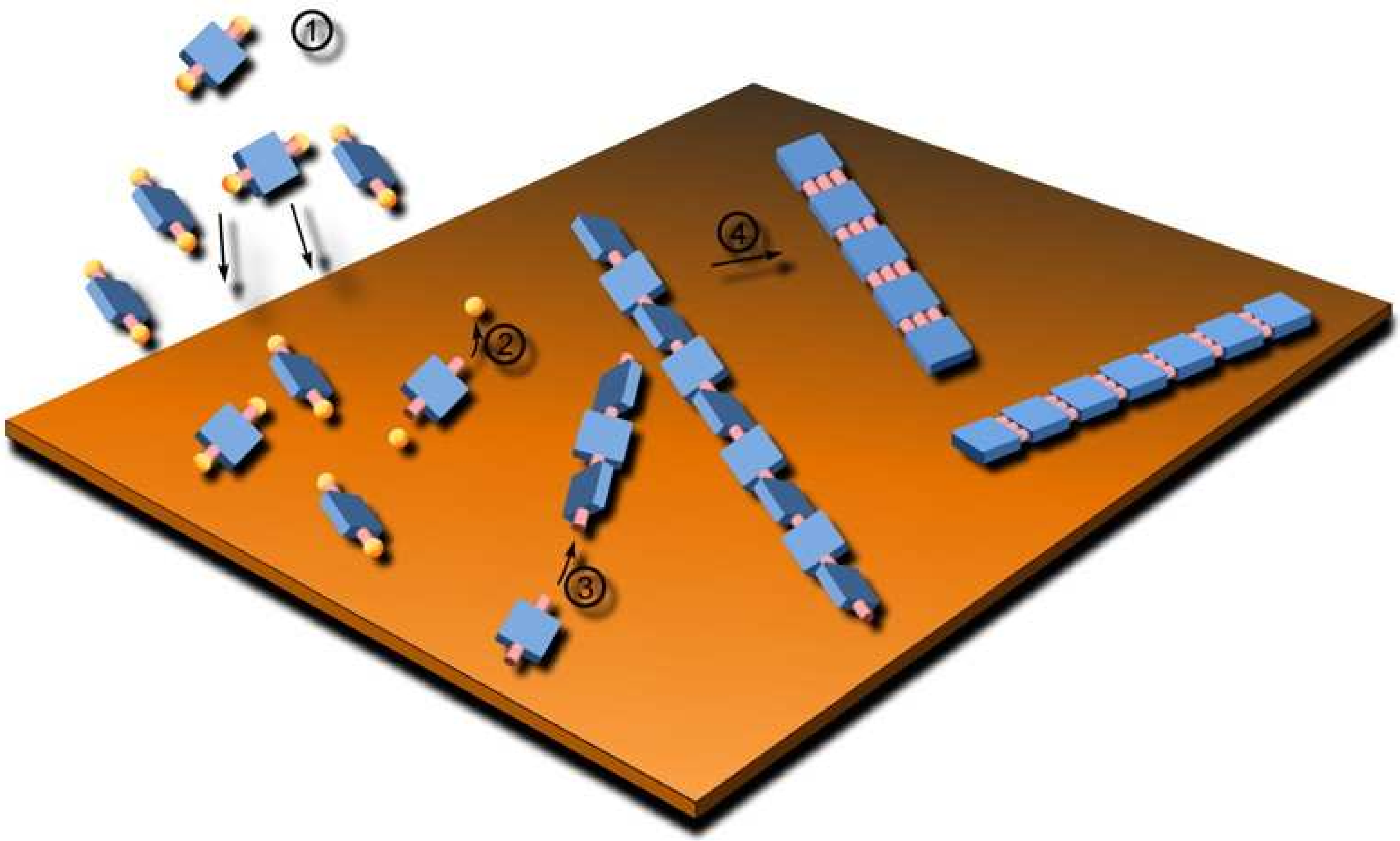


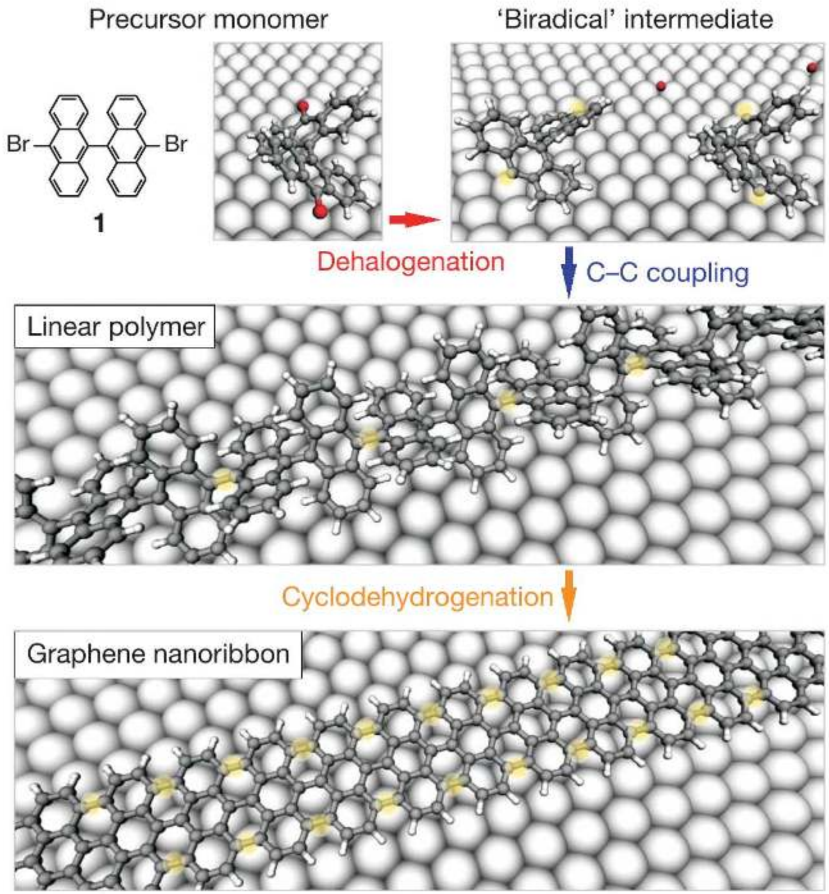
Y.-W. Son et al. *Phys. Rev. Lett.* **97**, 216803 (2006).

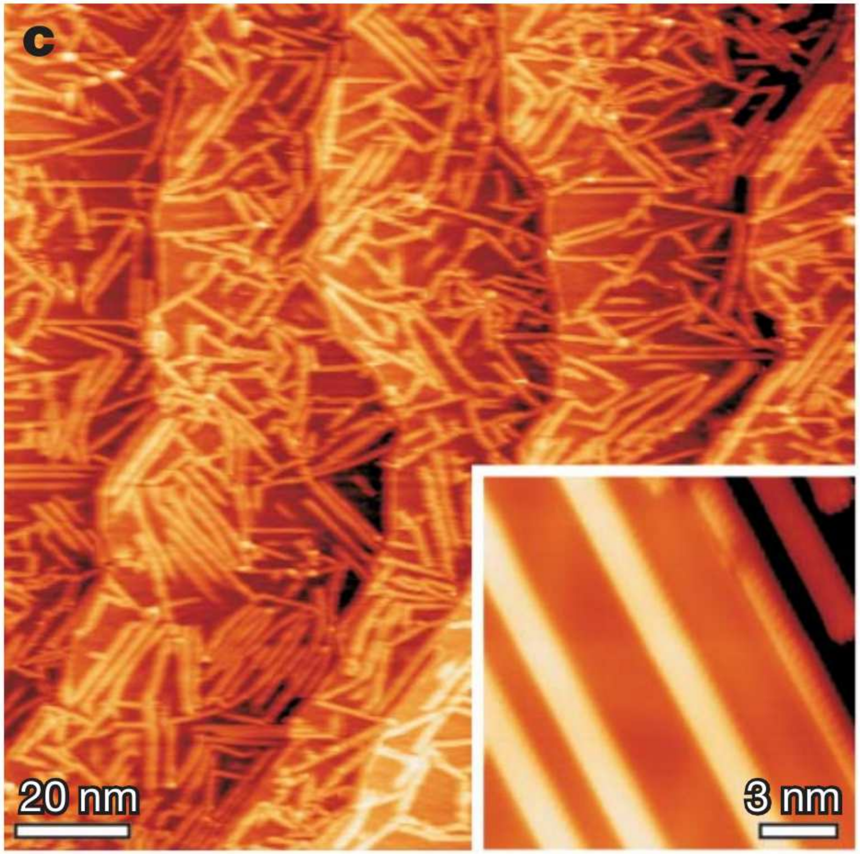
GNR on-surface synthesis



P. Ruffieux. *Swiss Phys. Soc. - Progress in Physics* (2013).

GNR on-surface synthesis





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

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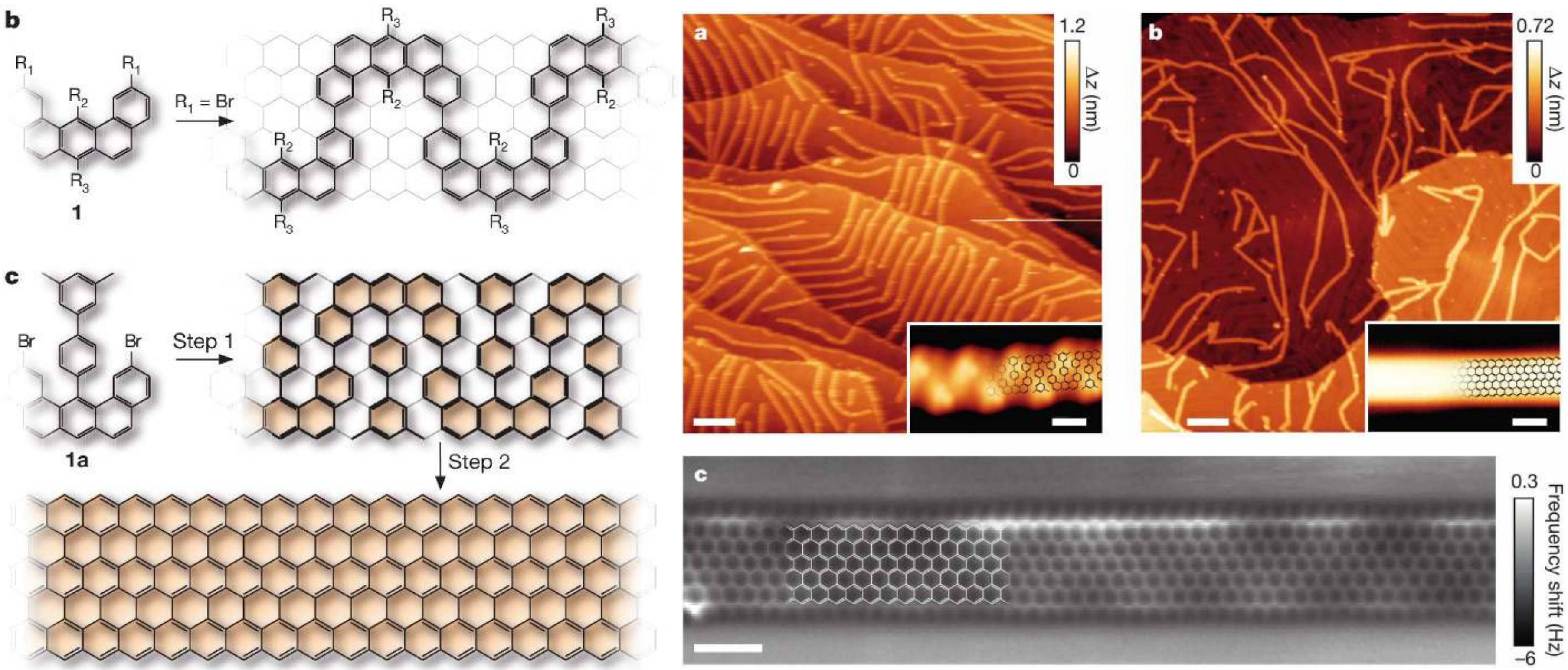

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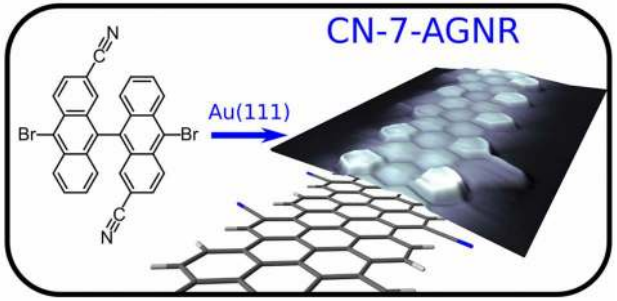
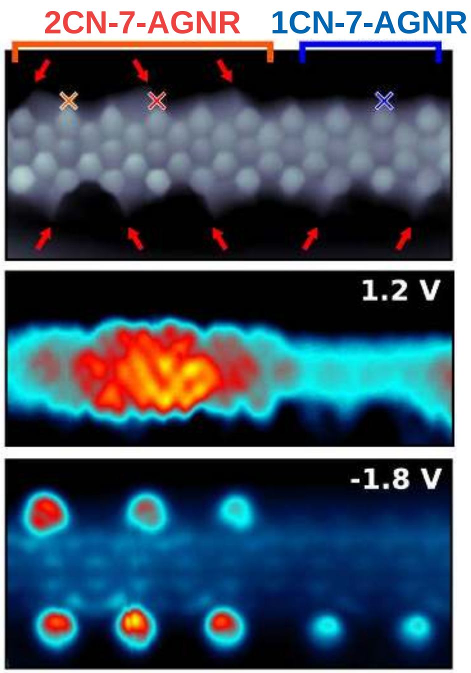
Chemical functionalization of GNR





E. Carbonell-Sanromà, ..., P. Brandimarte *et al*. *ACS Nano* **11**(7), 7355 (2017).

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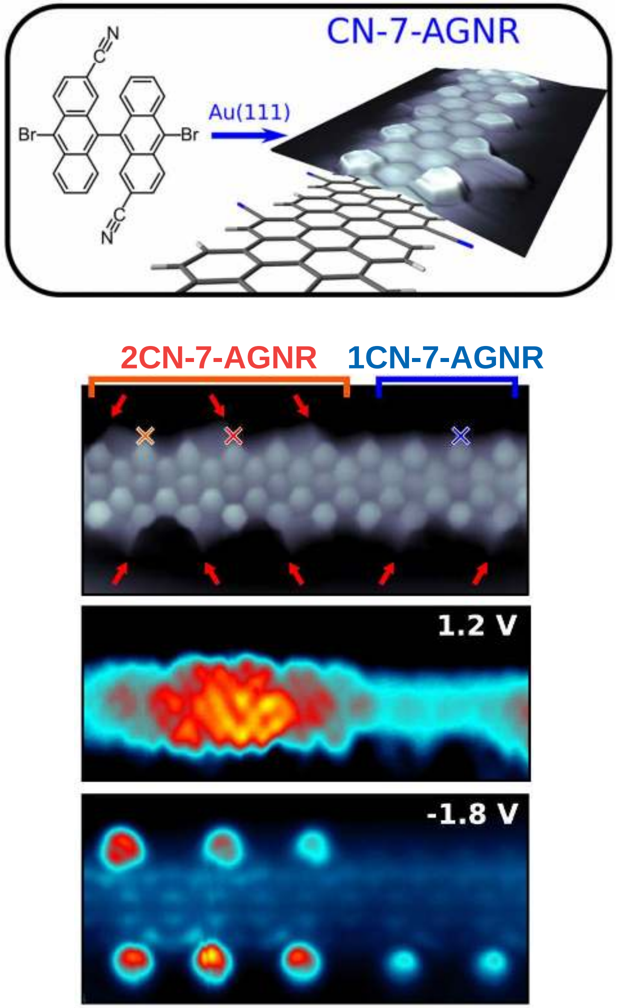

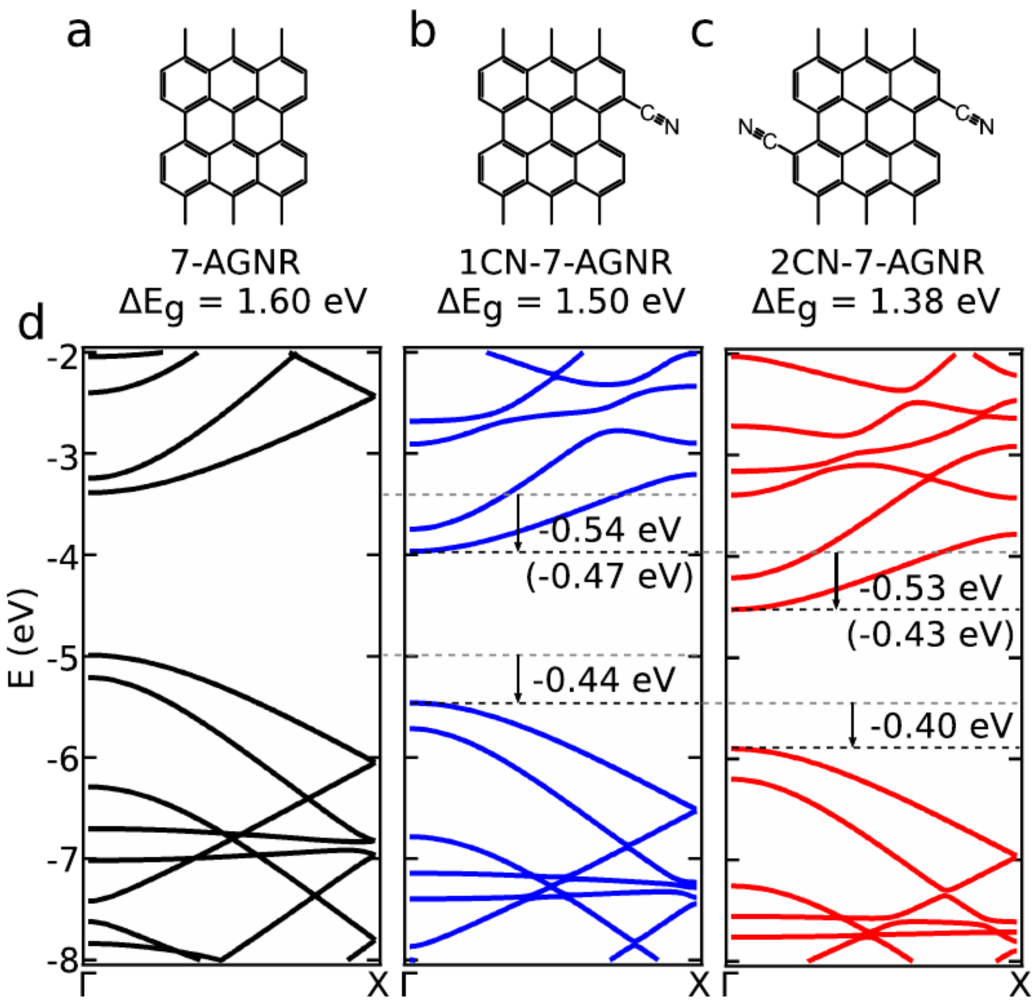

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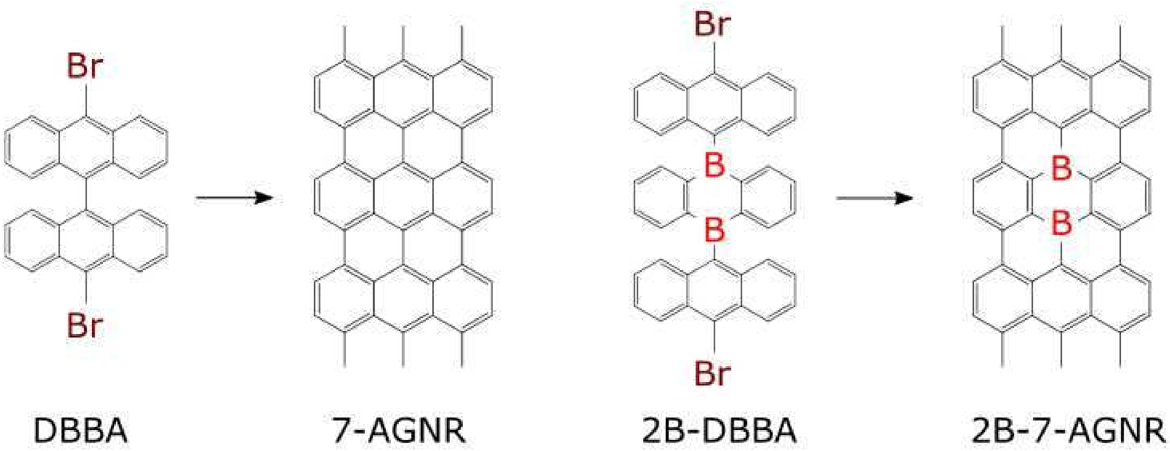
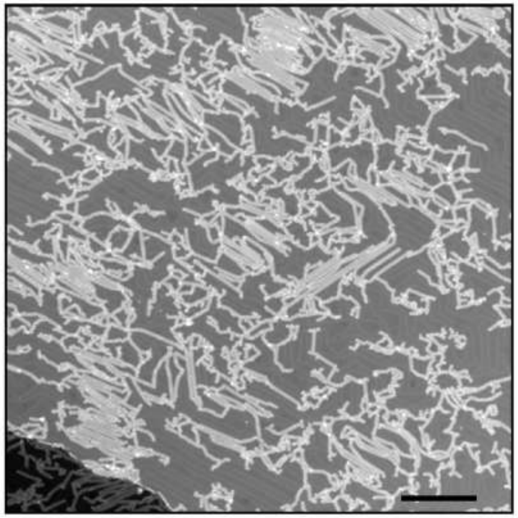
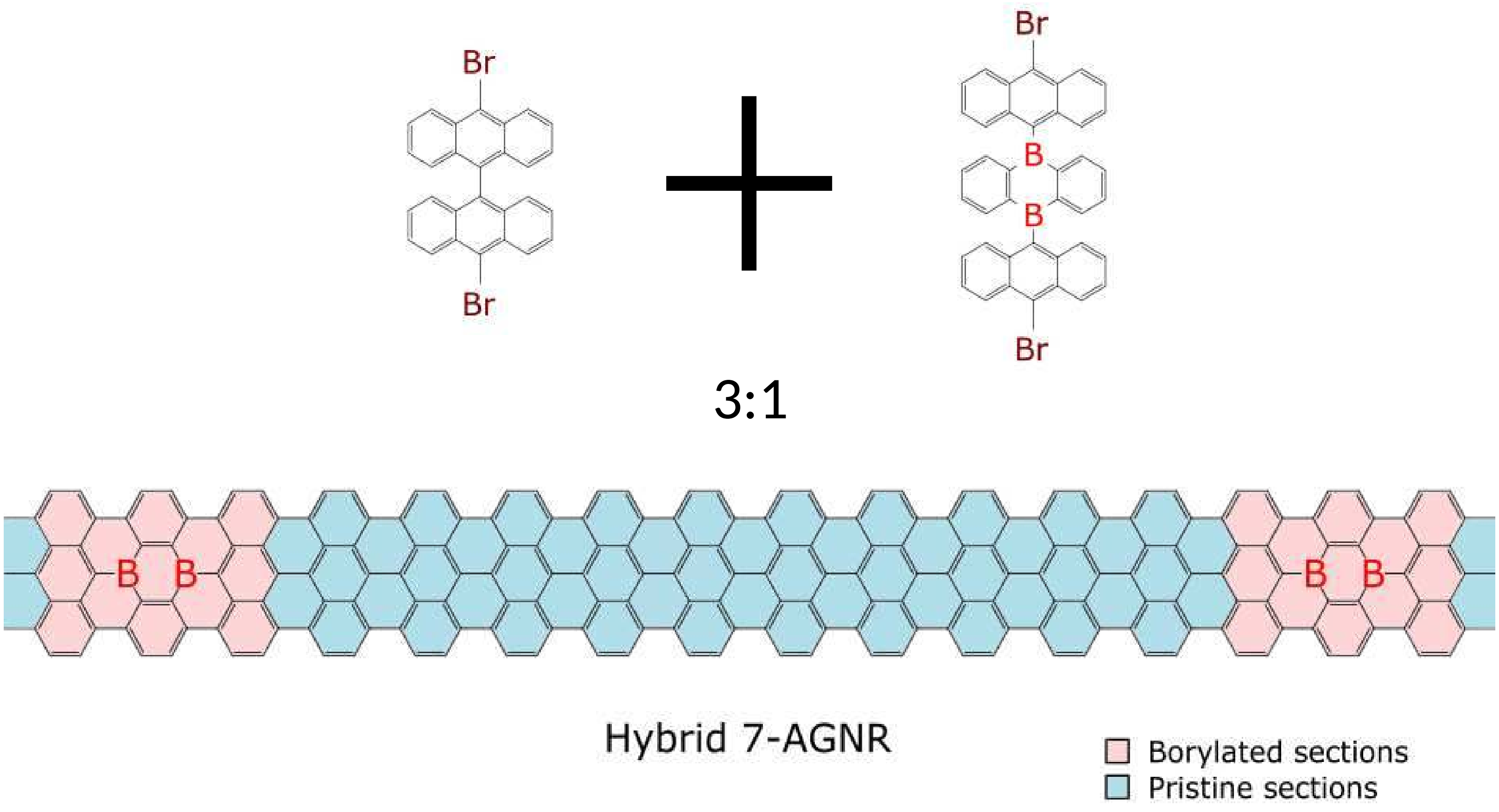




S. Kawai *et al*. *Nature Comm*. **6**, 8098 (2015).
R. R. Cloke et al. *J. A. Chem. Soc.* 137, 8872 (2015).

Hybrid 7-AGNR



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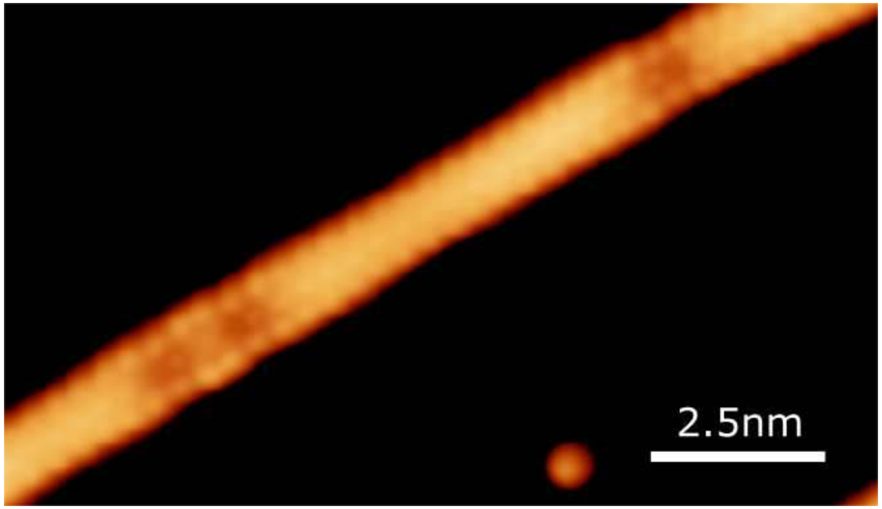

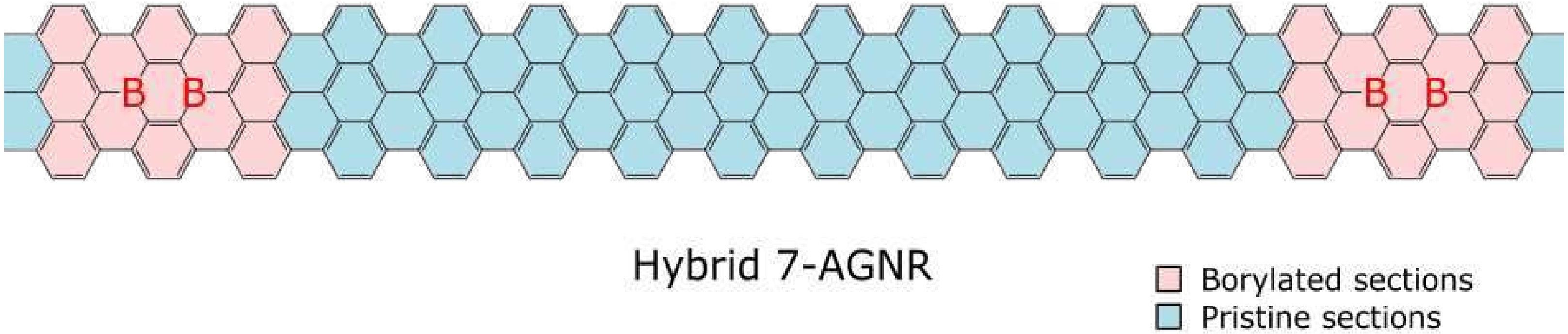

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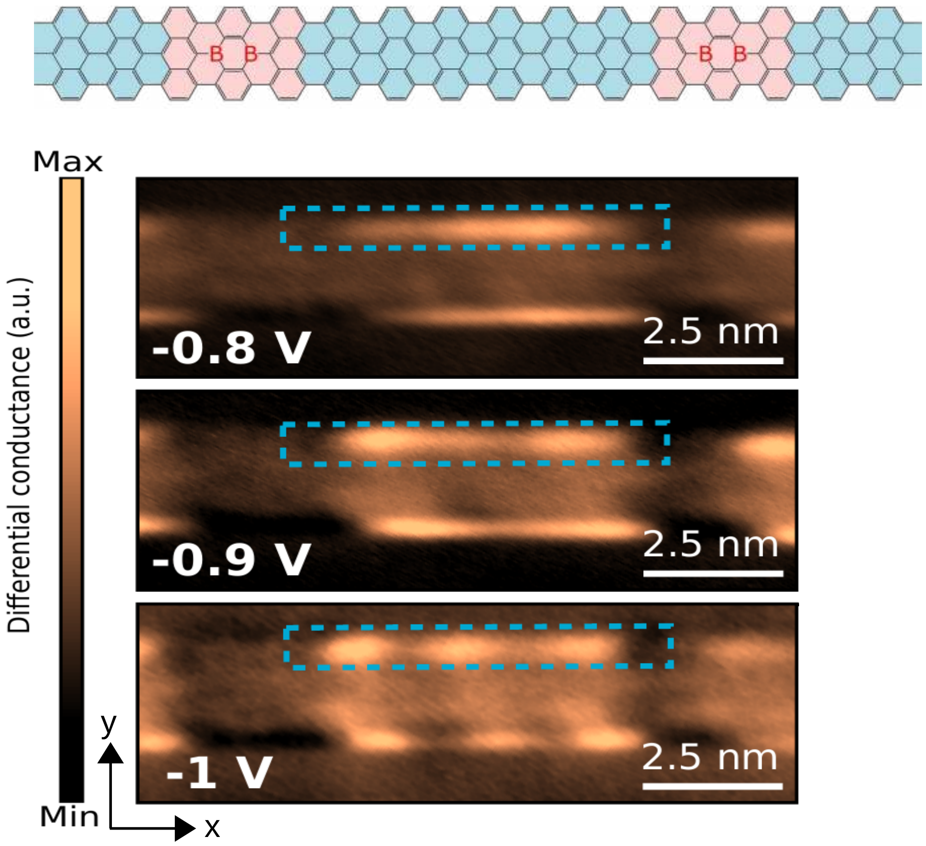

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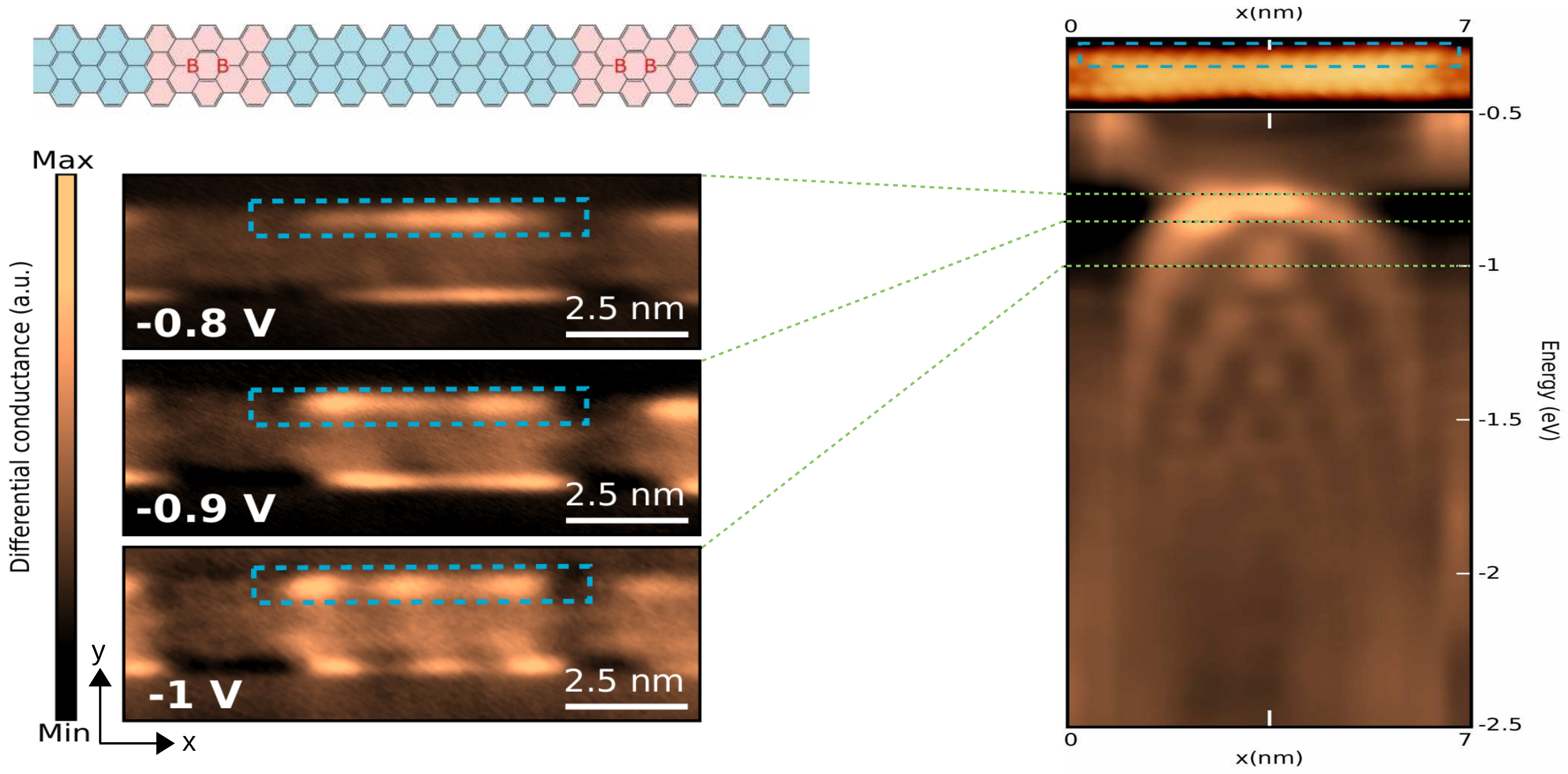

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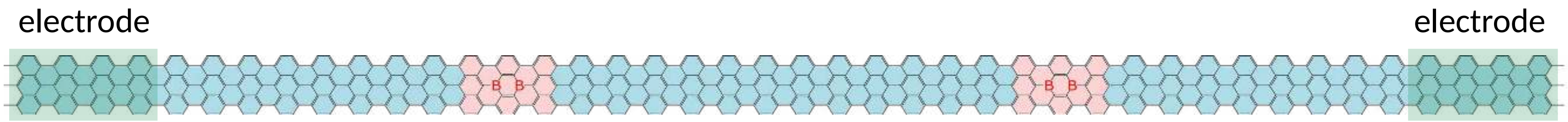
Pedro Brandimarte (brandimarte@pm.me)

Transport simulation setup



Density-Functional Theory (DFT)

+

Non-Equilibrium Green's Function (NEGF)

TranSIESTA

J. M. Soler *et al*. *J. Phys. Condens. Matter.* **14**, 2745 (2002).
M. Brandbyge *et al*. *Phys. Rev. B* **65**, 165401 (2002).
N. Papior *et al*. *Comp. Phys. Commun.* **212**, 8 (2017).

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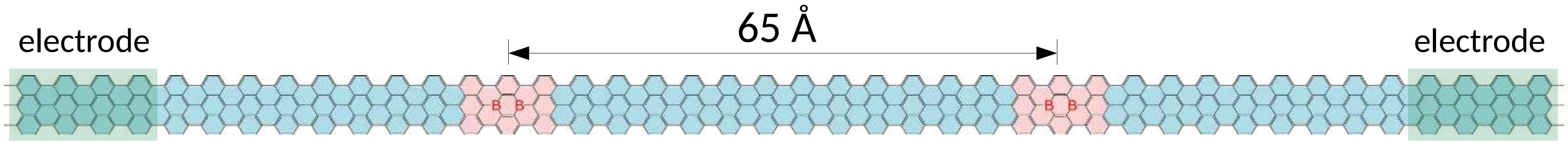

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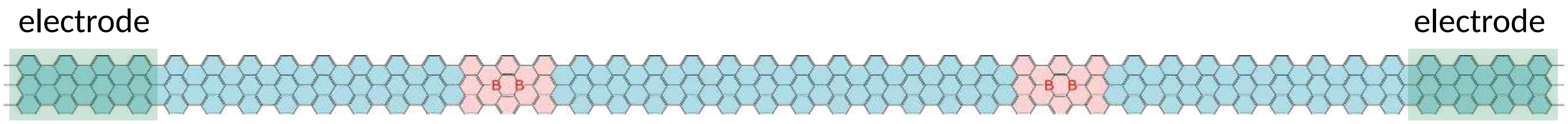
N. Papior *et al*. *Comp. Phys. Commun.* **212**, 8 (2017).

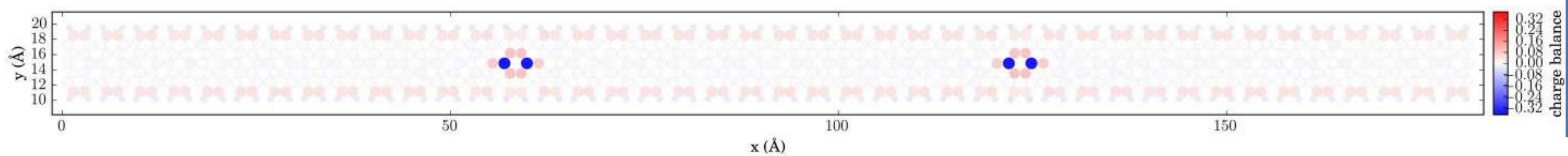
Simulation characteristics:

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

E. Carbonell-Sanromà, P. Brandimarte *et al*. *Nano Letters* **17**, 50 (2017).

Mulliken population





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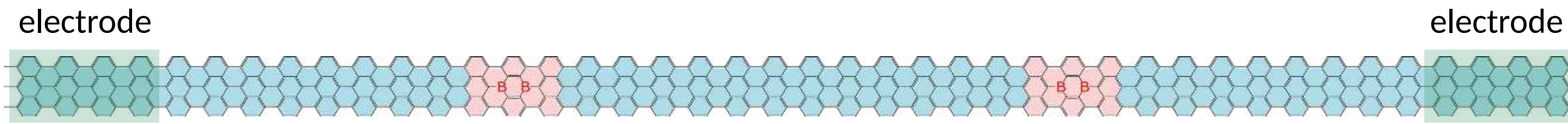

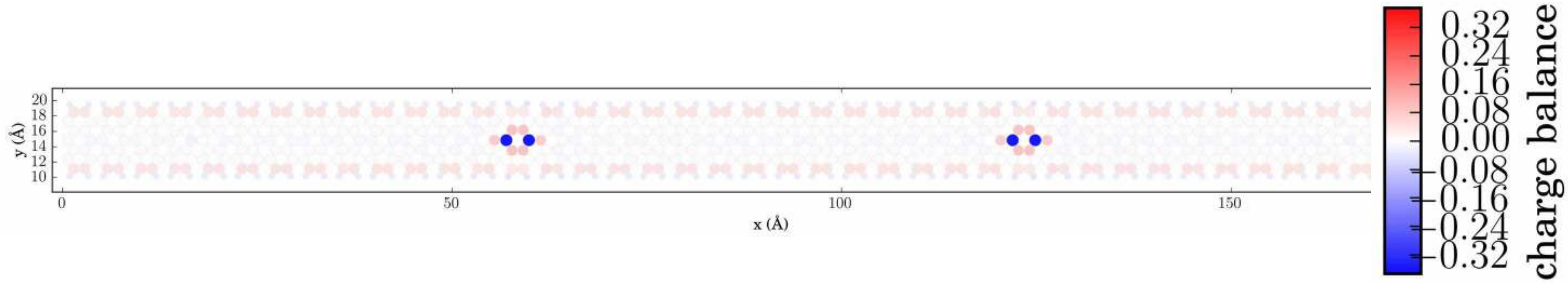

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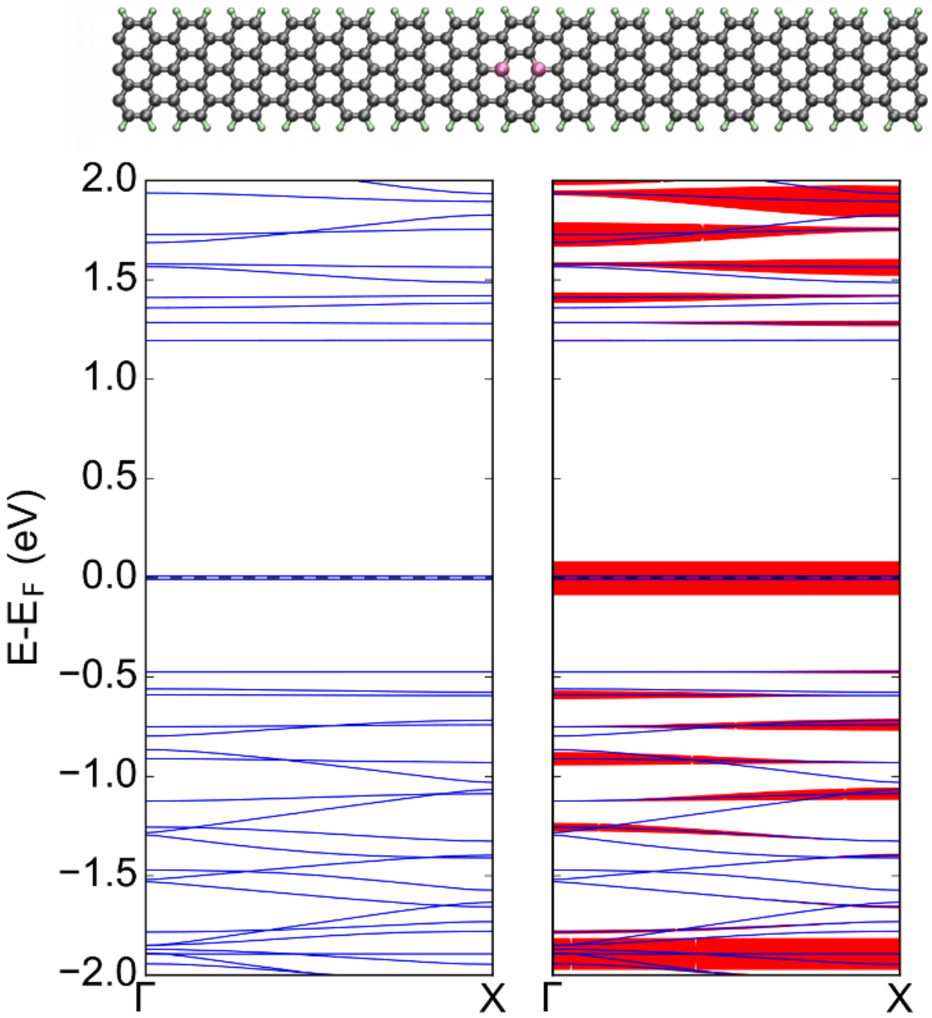
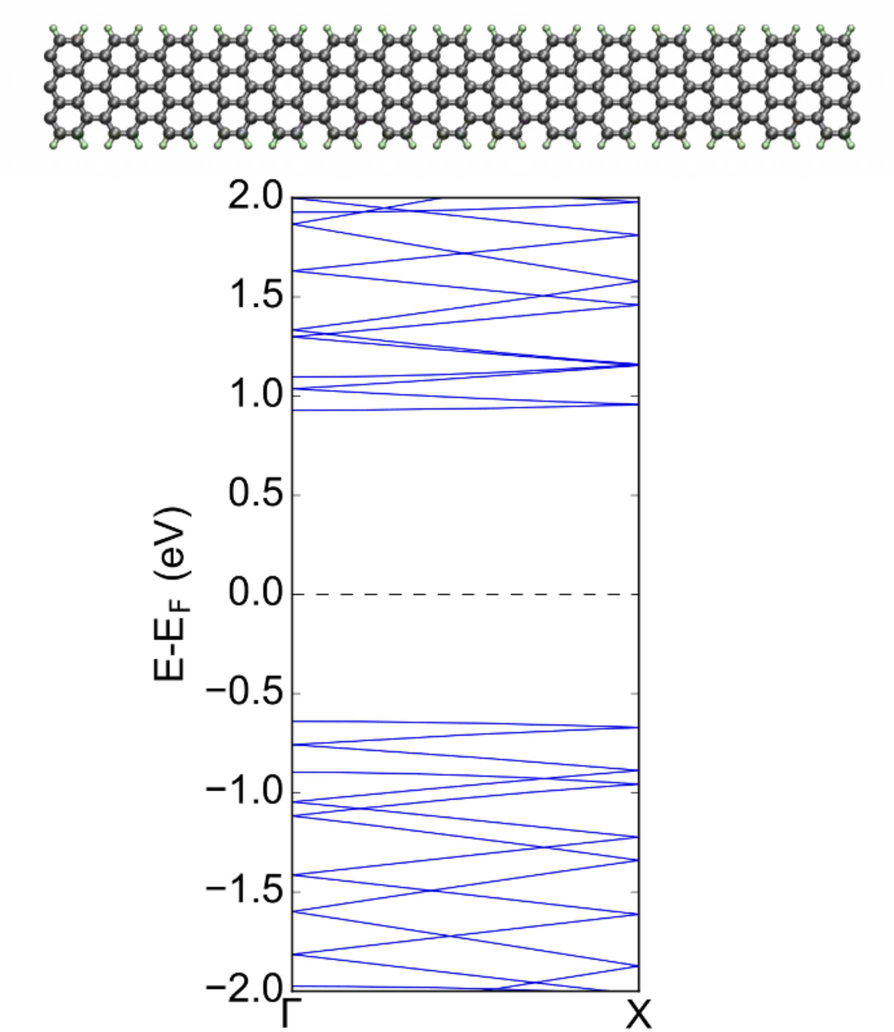
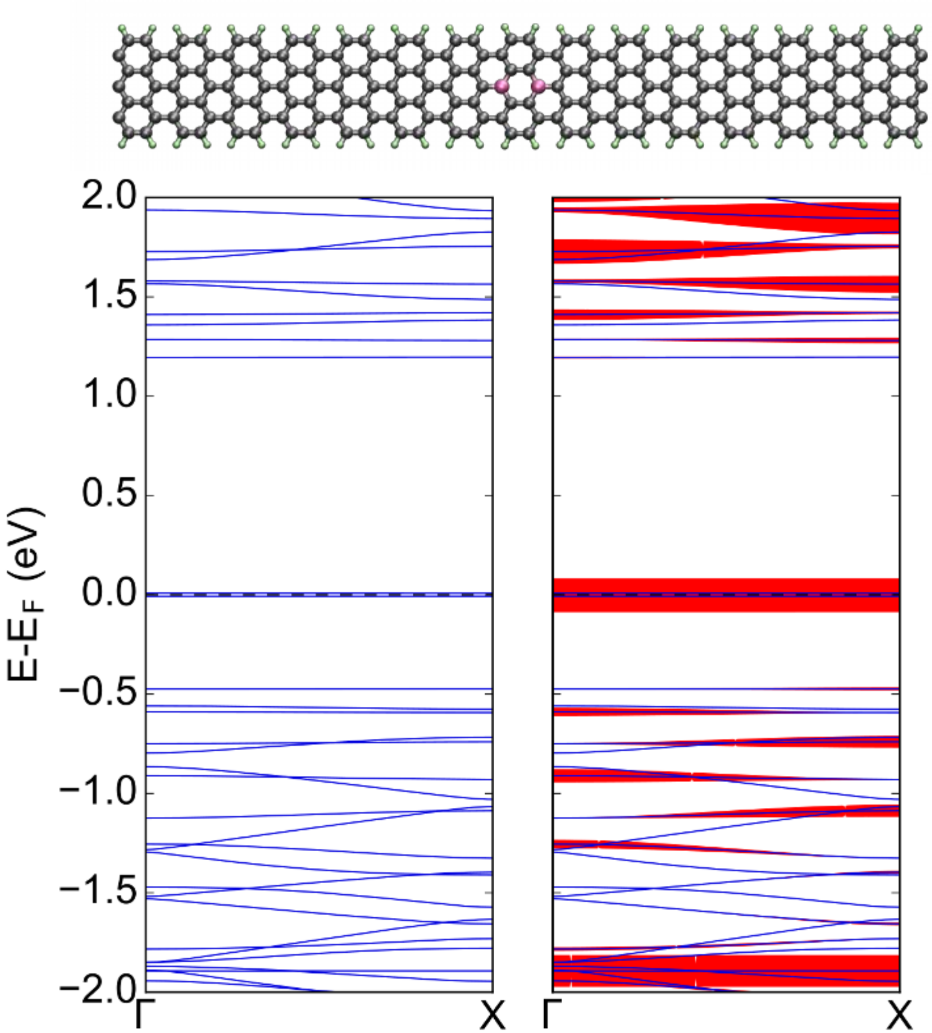
Periodic calculation



E. Carbonell-Sanromà, P. Brandimarte *et al*. *Nano Letters* **17**, 50 (2017).

Periodic calculation





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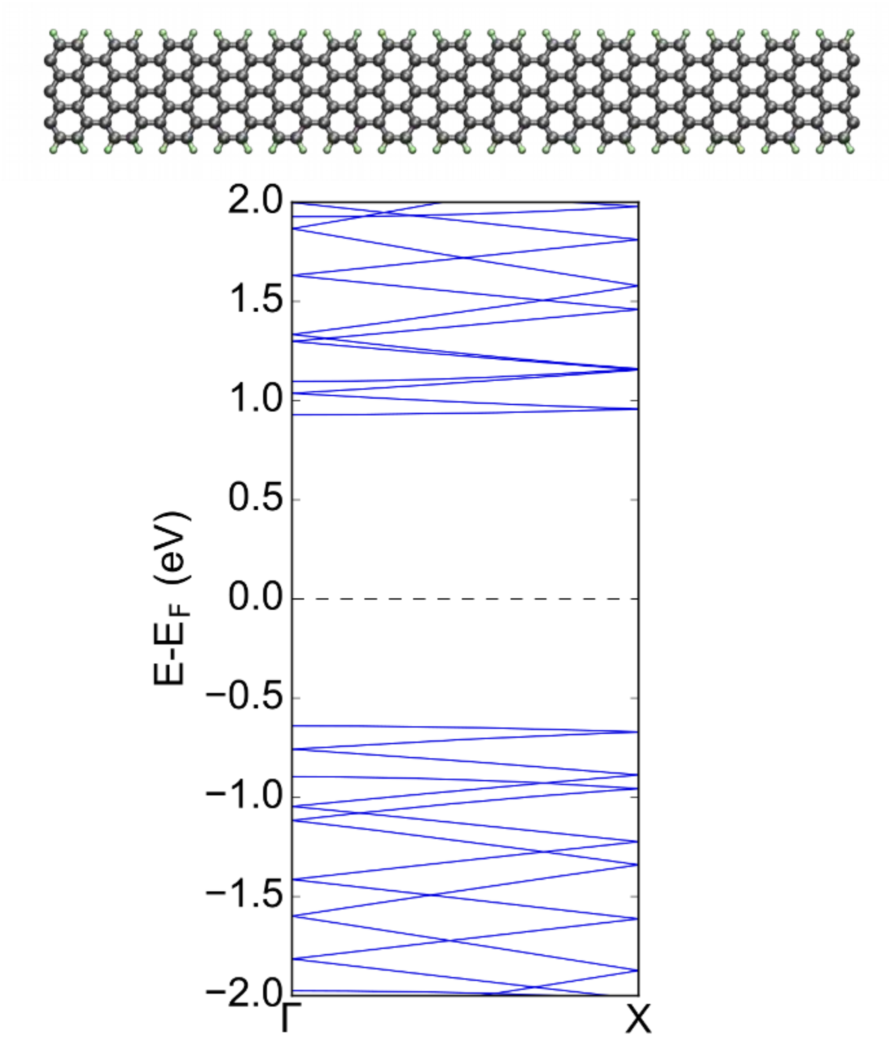

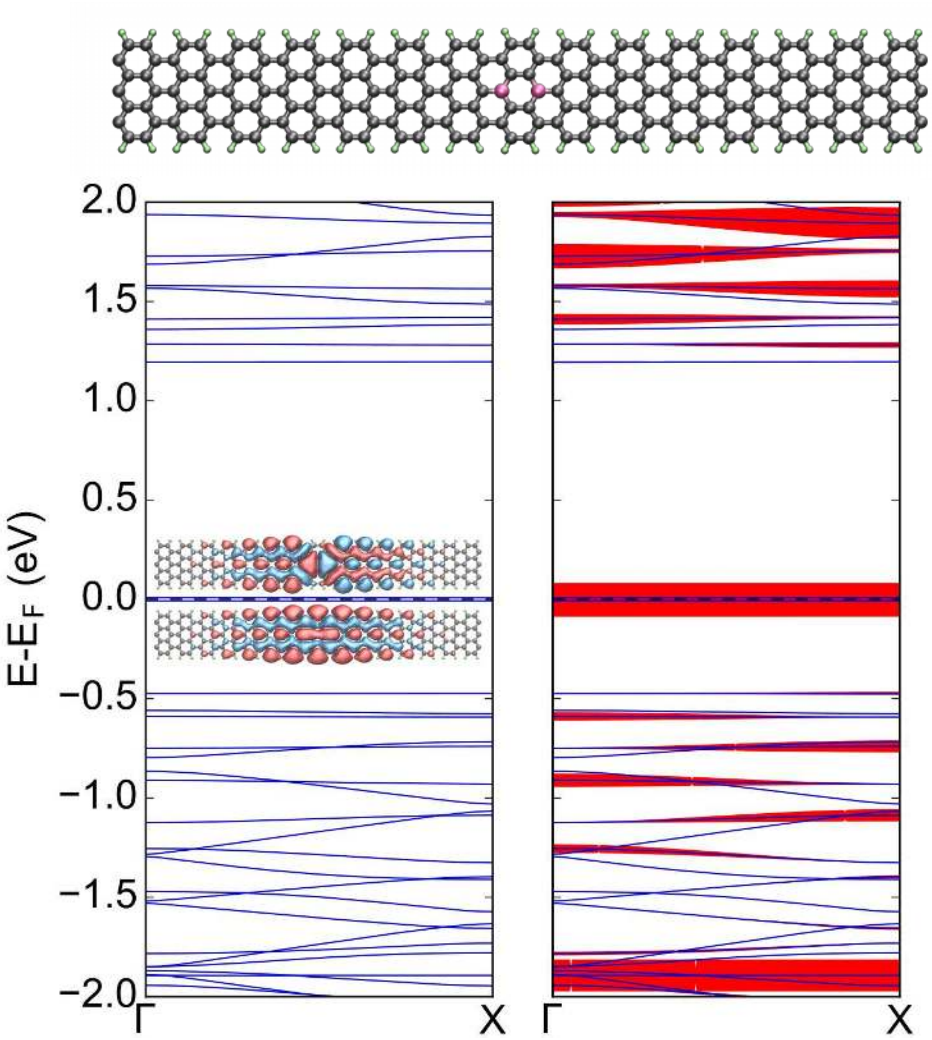

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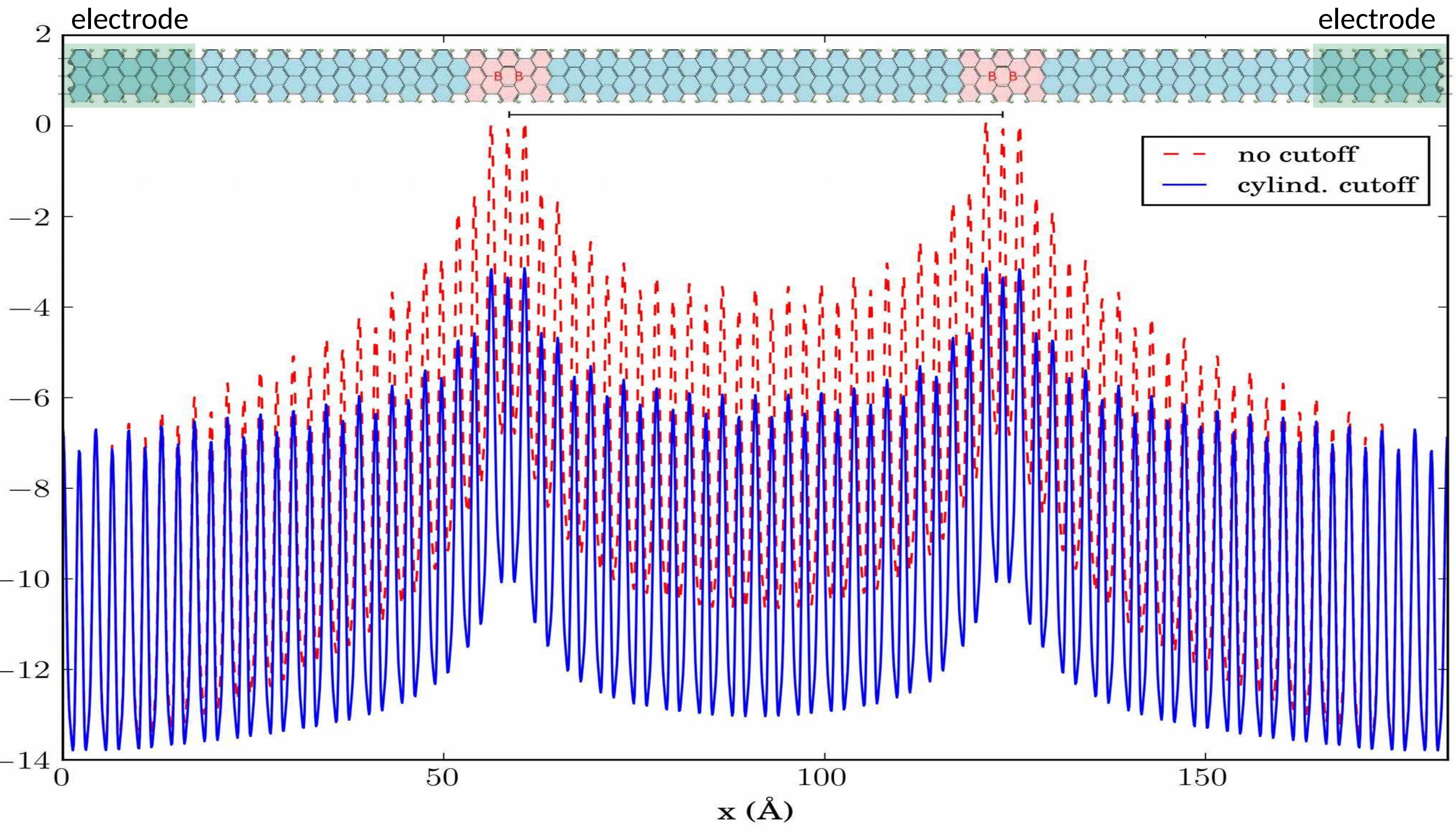
Electrostatic potential



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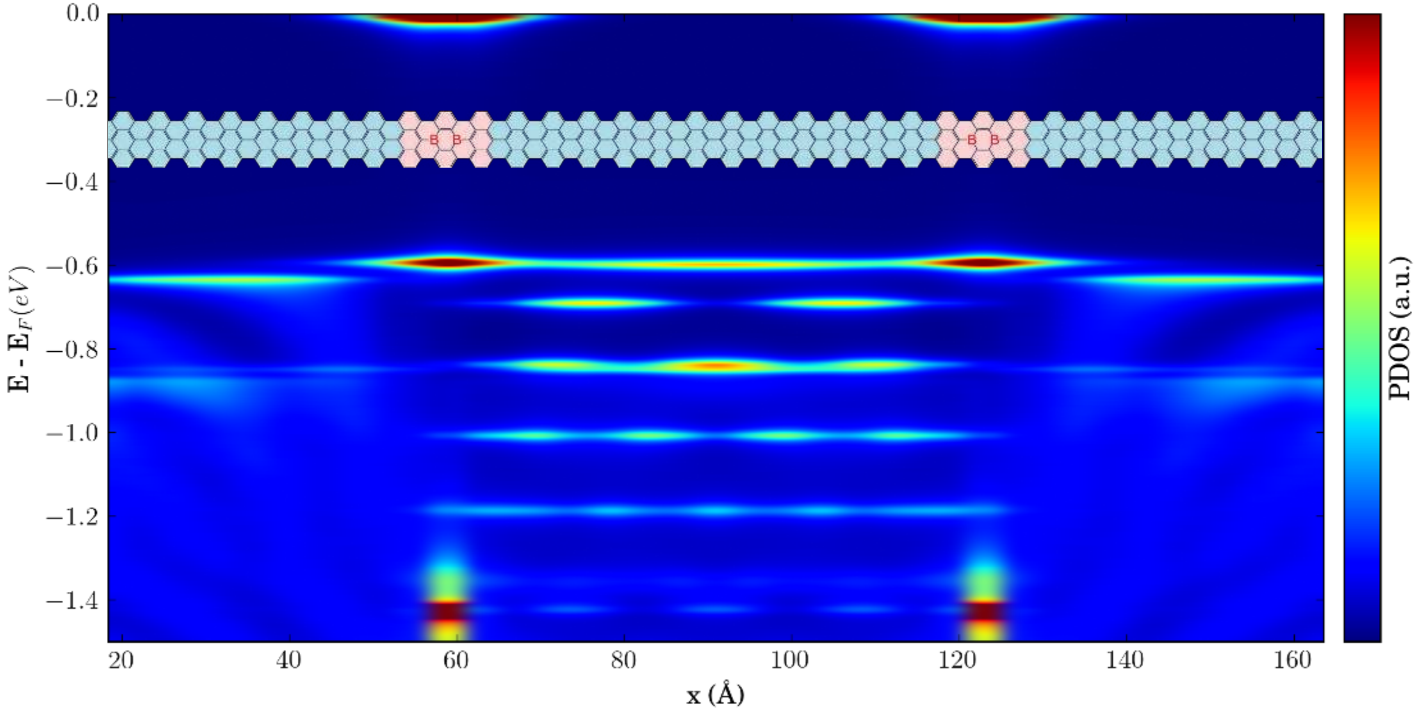
DOS projected on each GNR "row"



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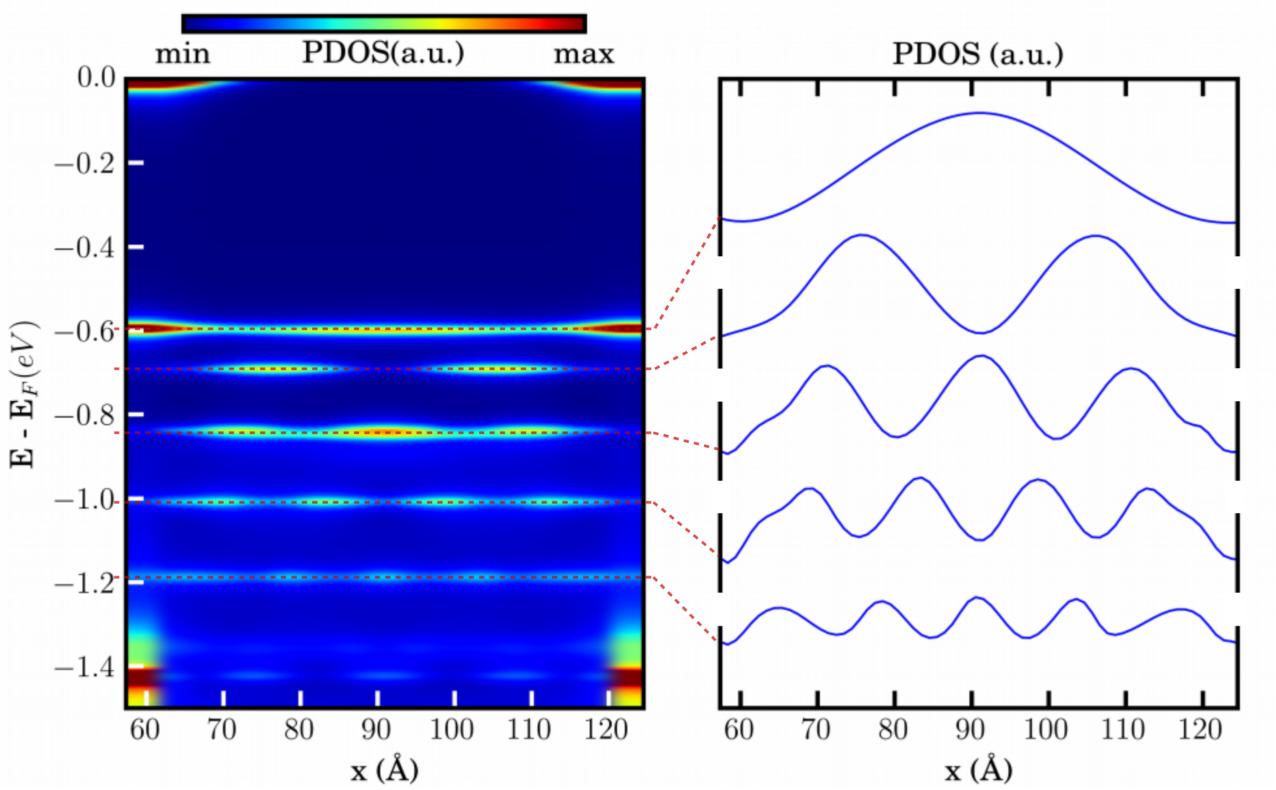

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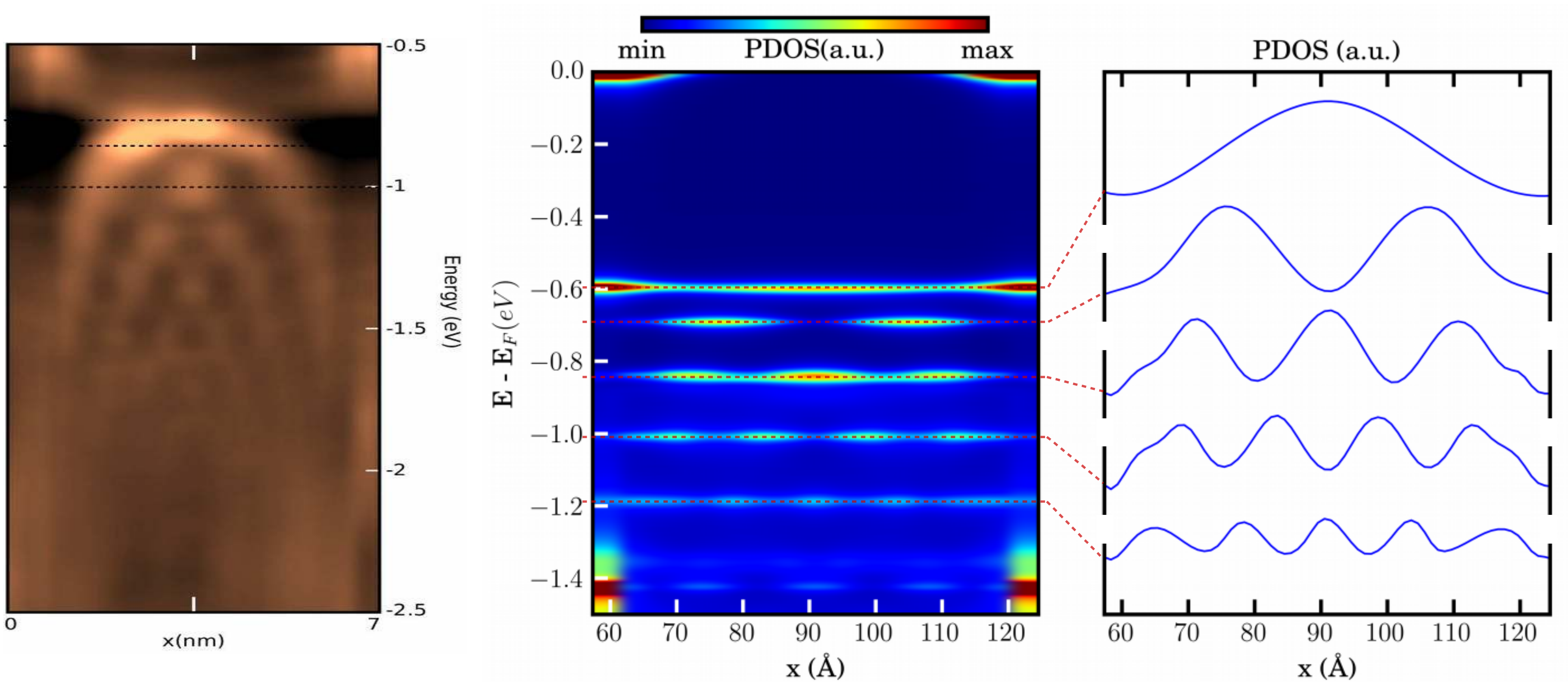

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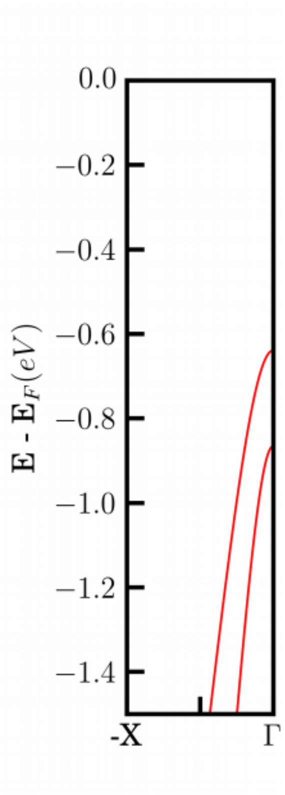
Zero bias transmission



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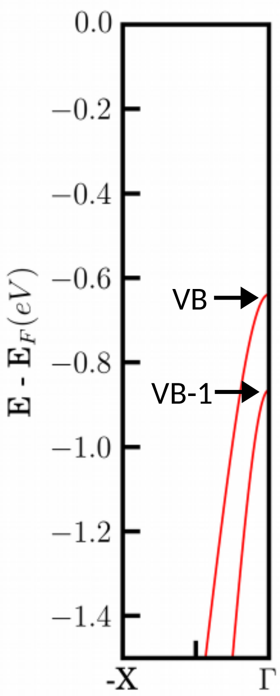

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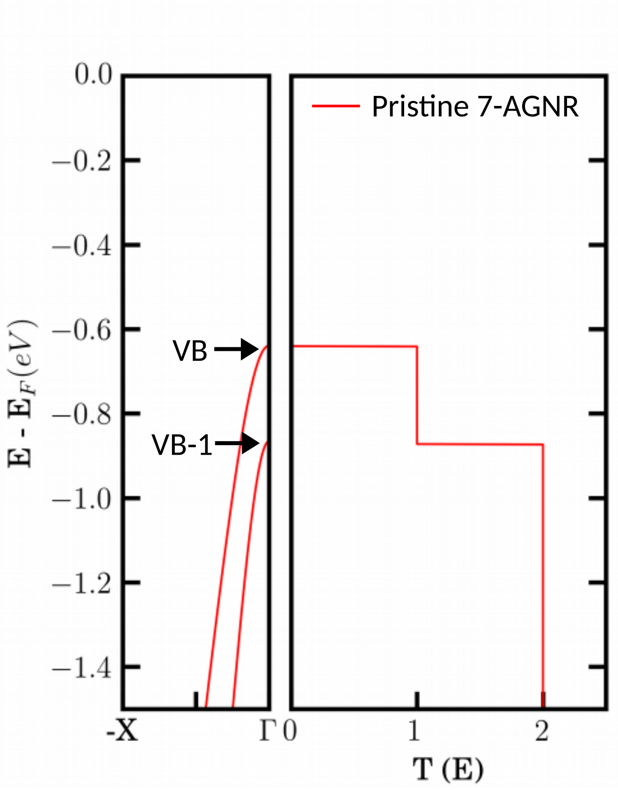

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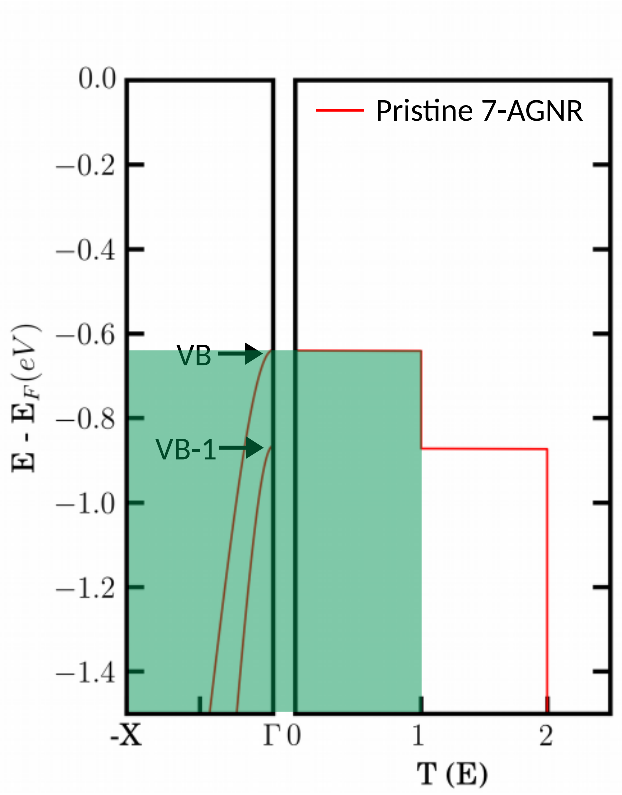

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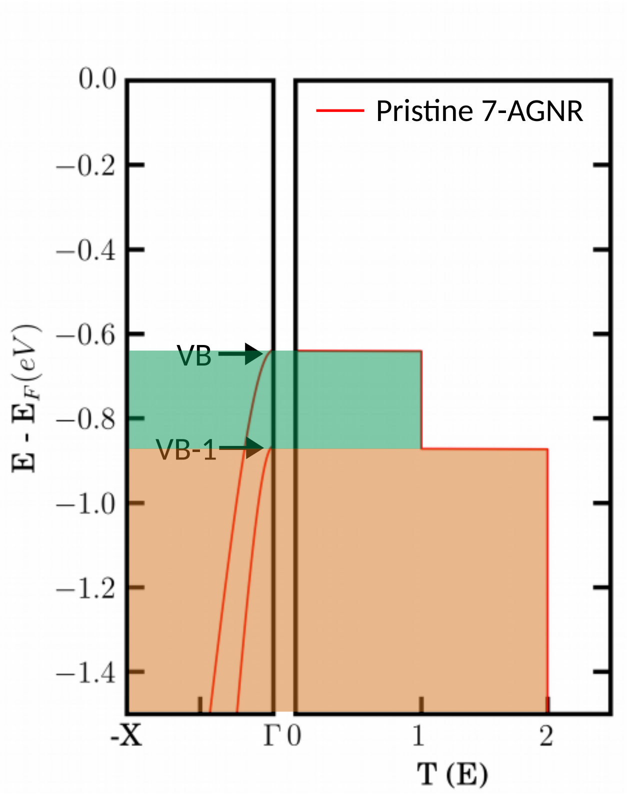

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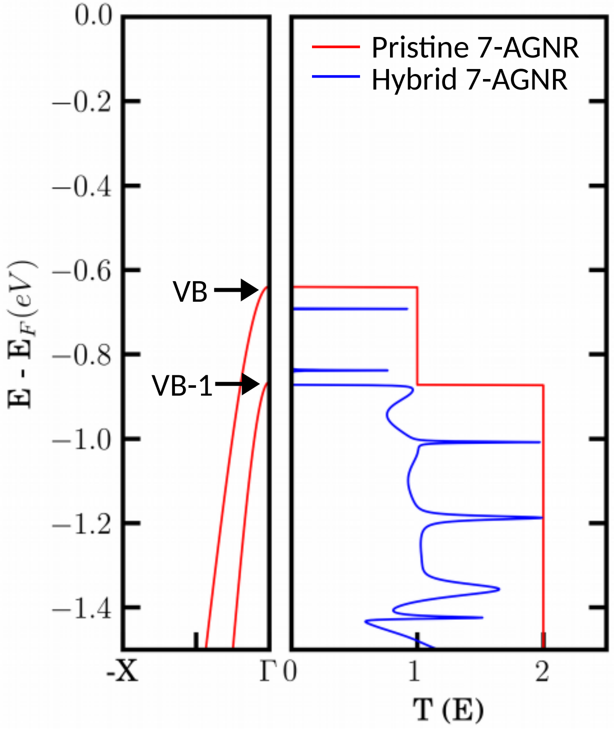

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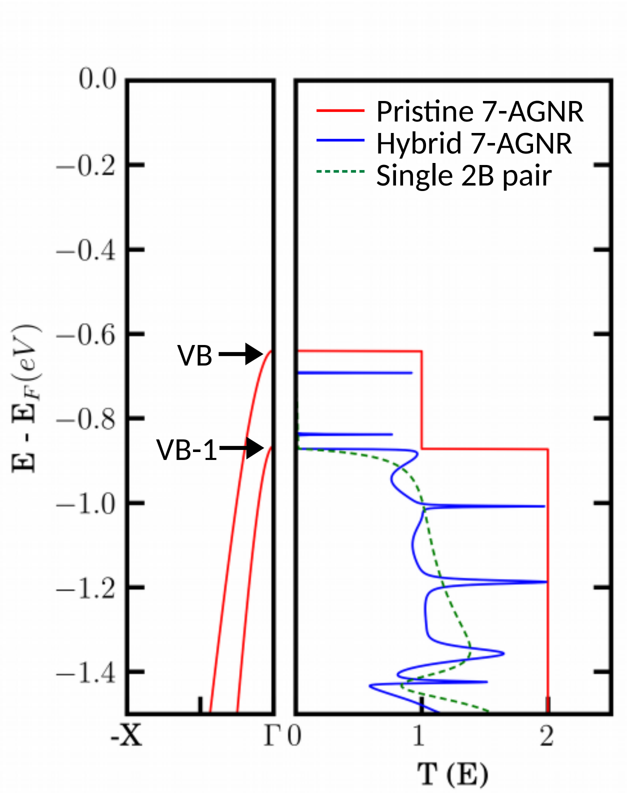

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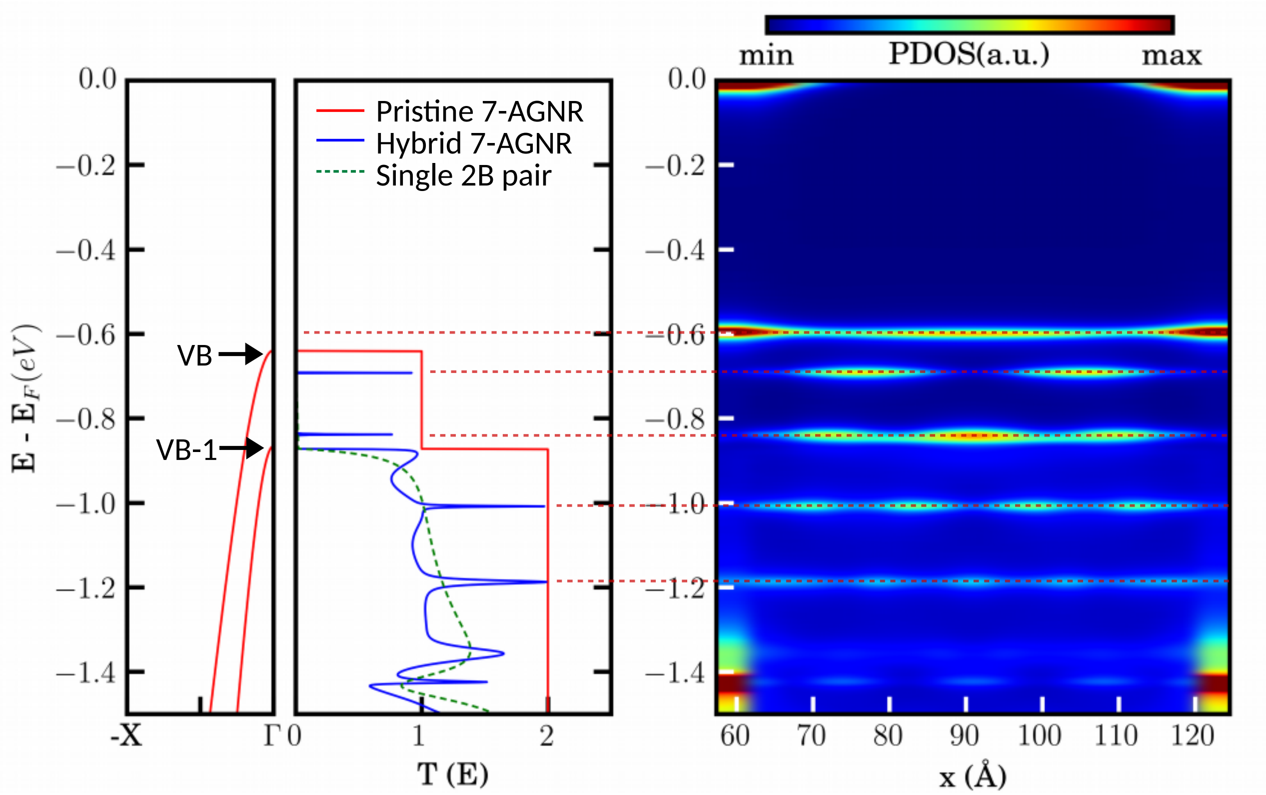

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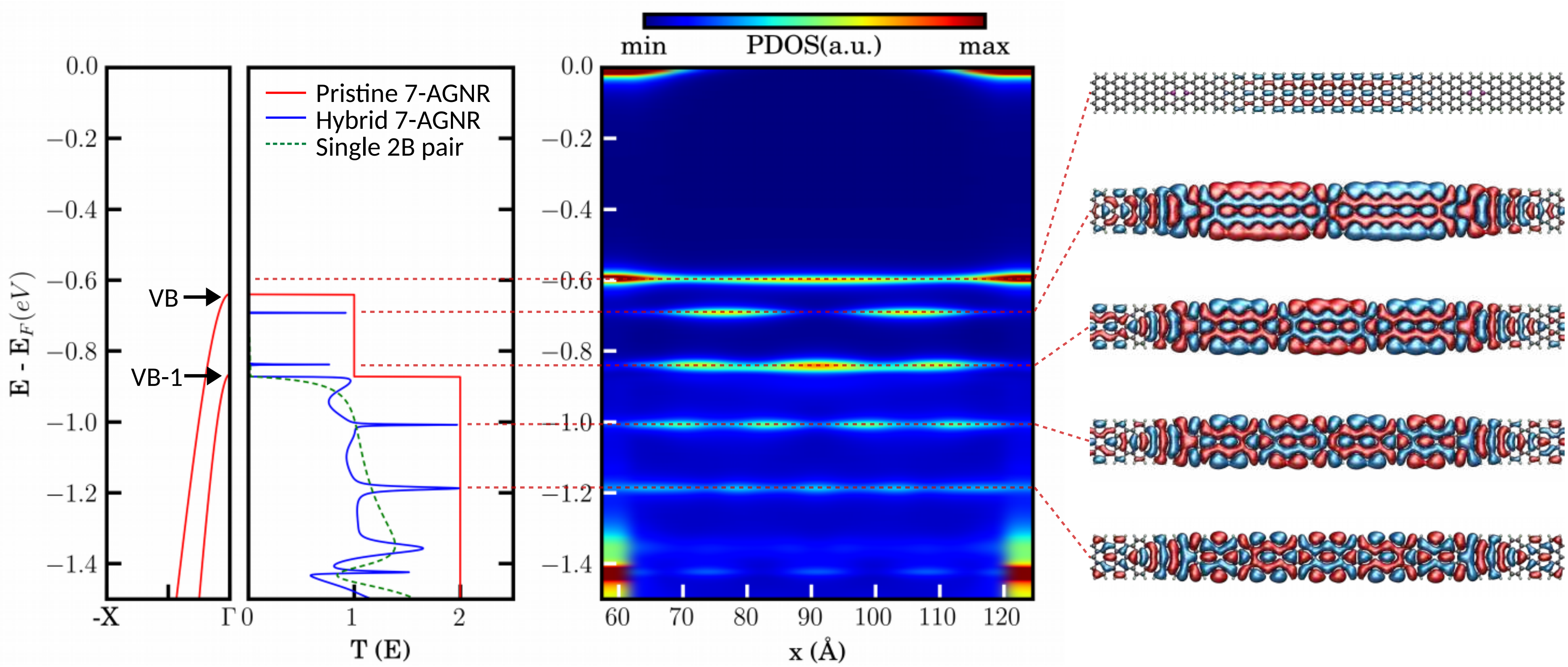
Scattering states



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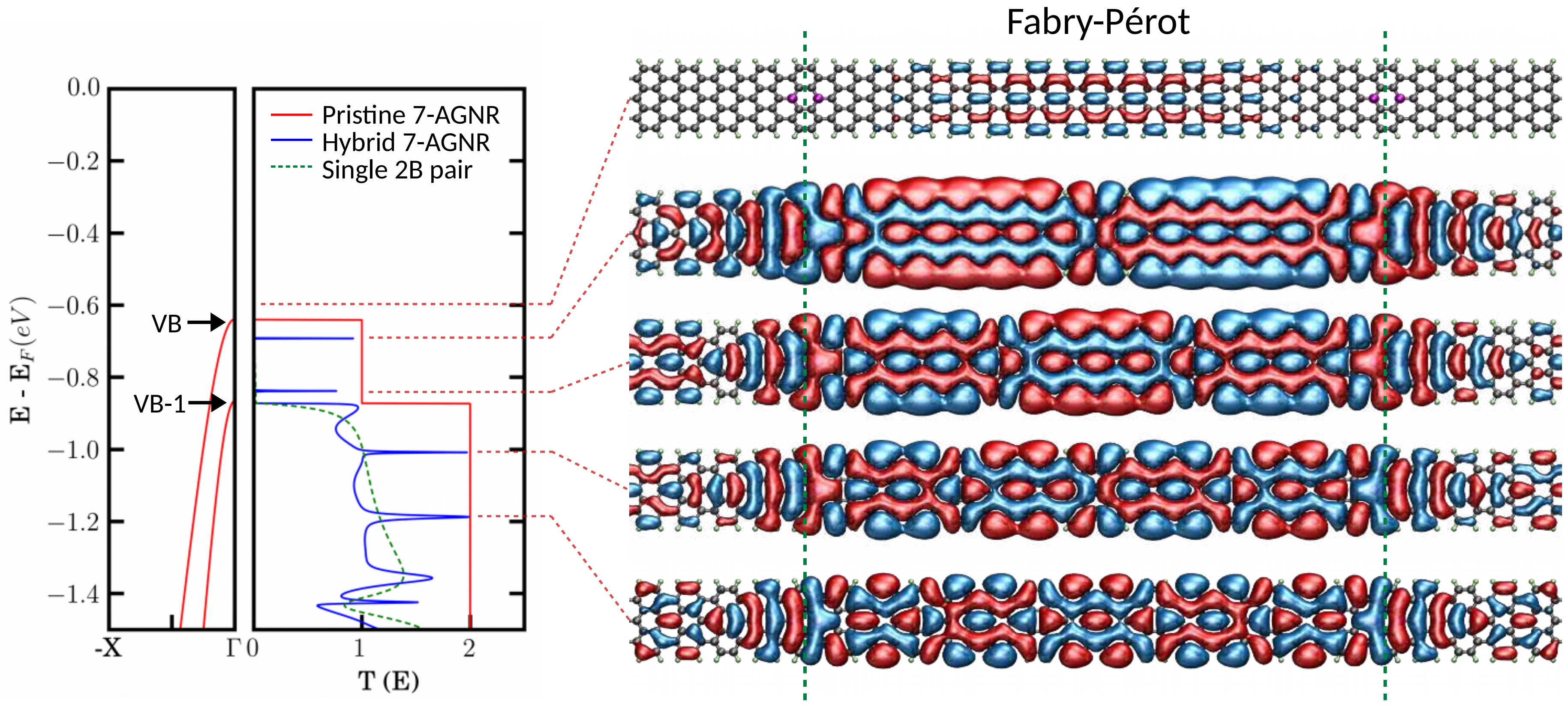

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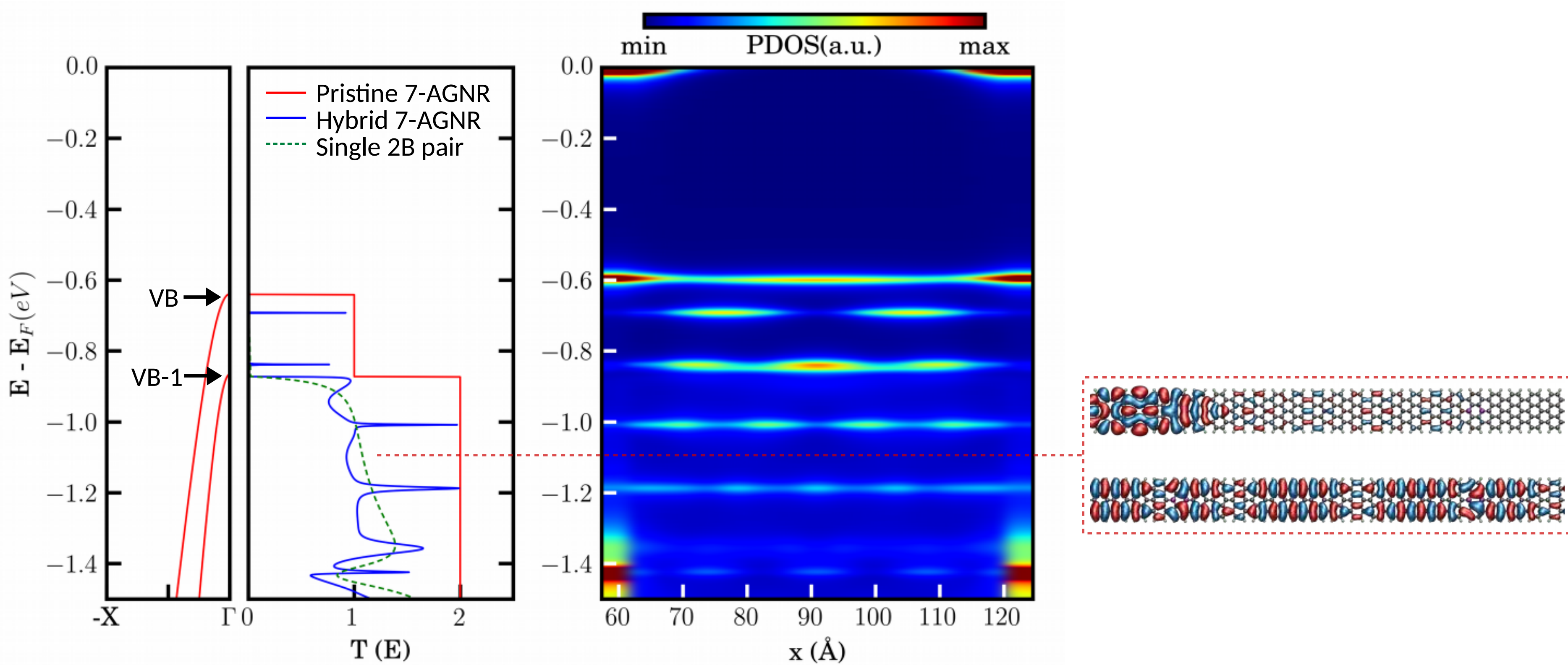

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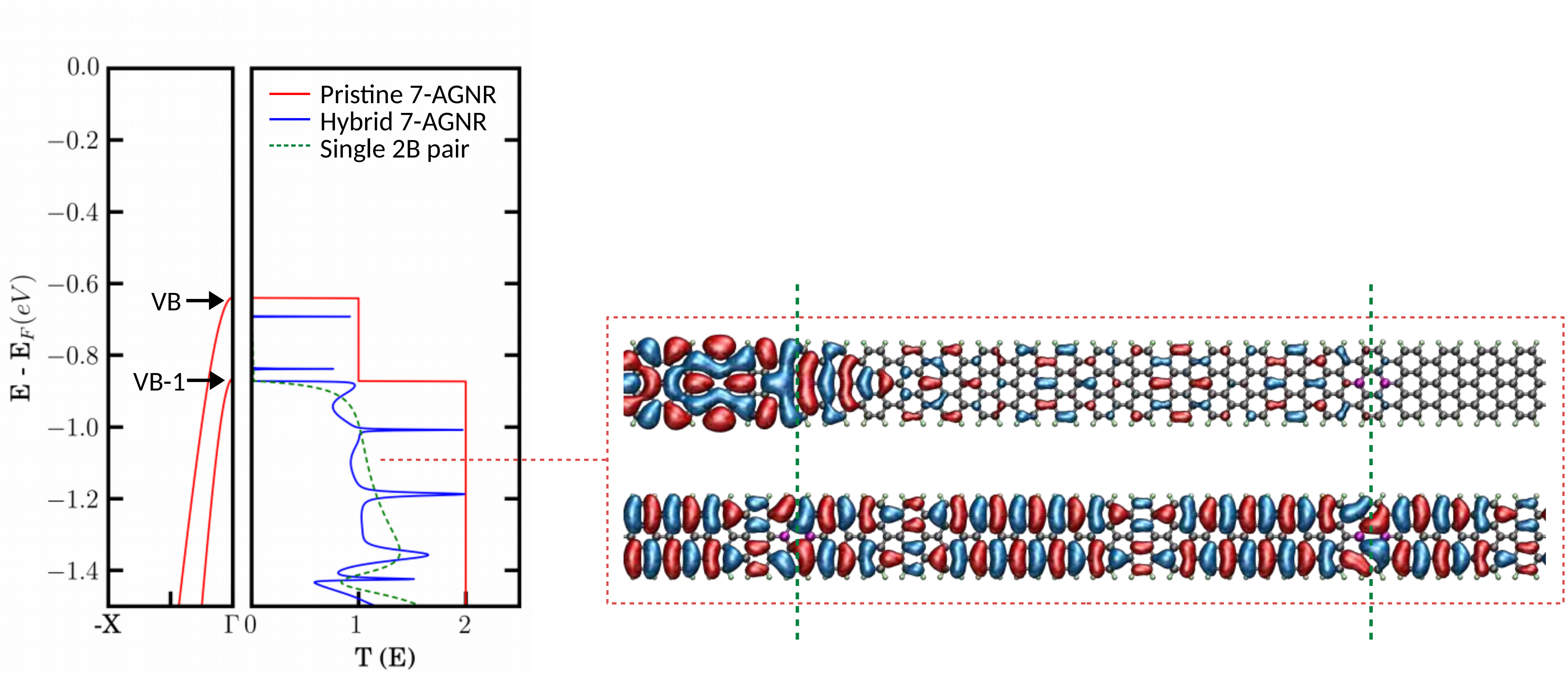
Band selectivity



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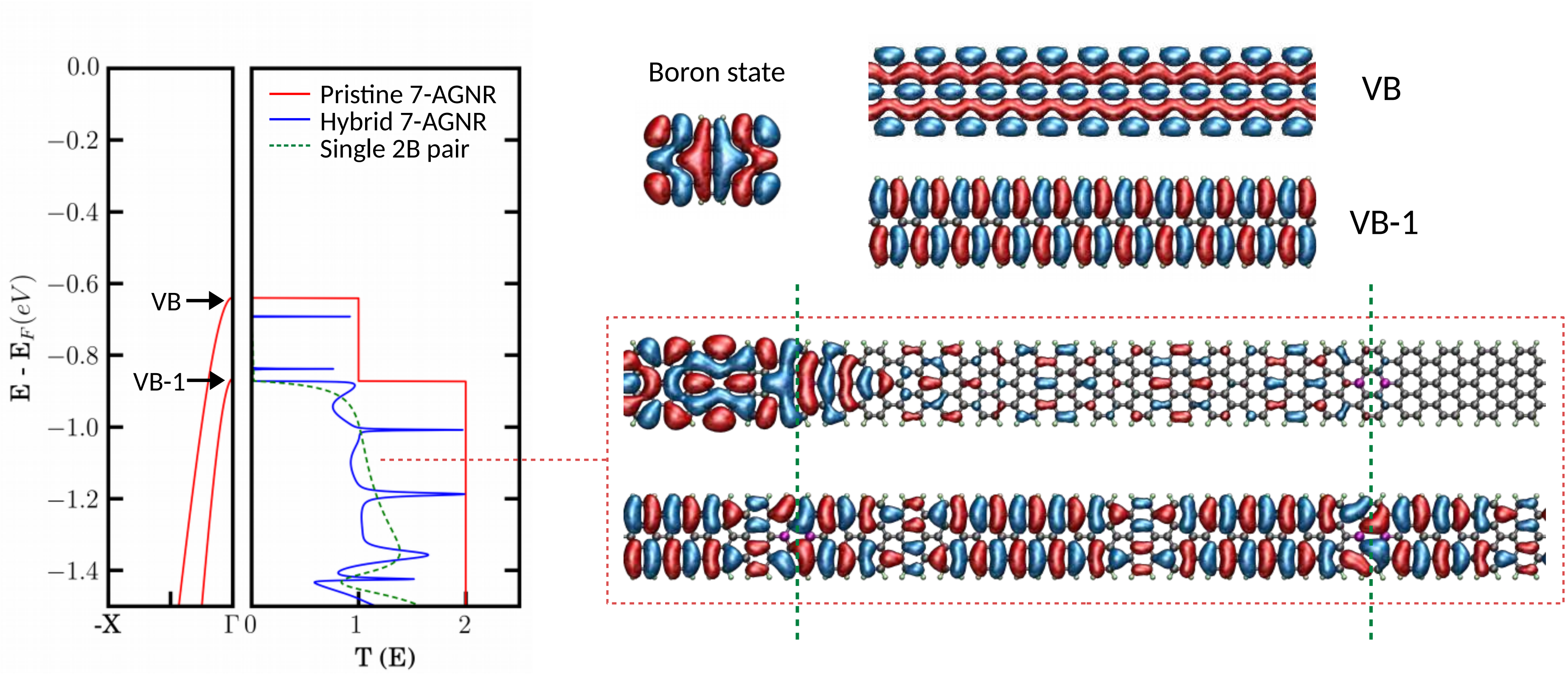

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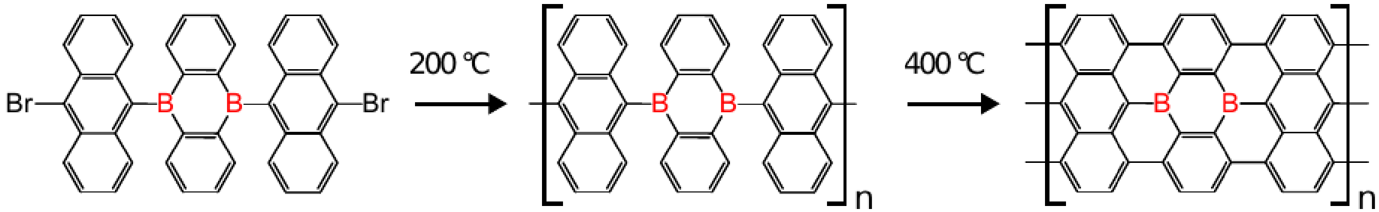
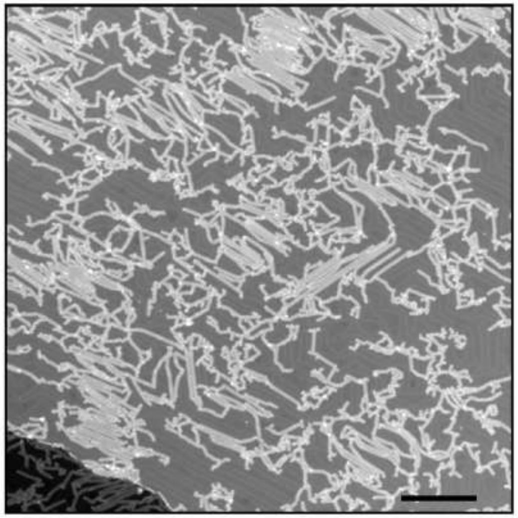
Fully borylated GNR





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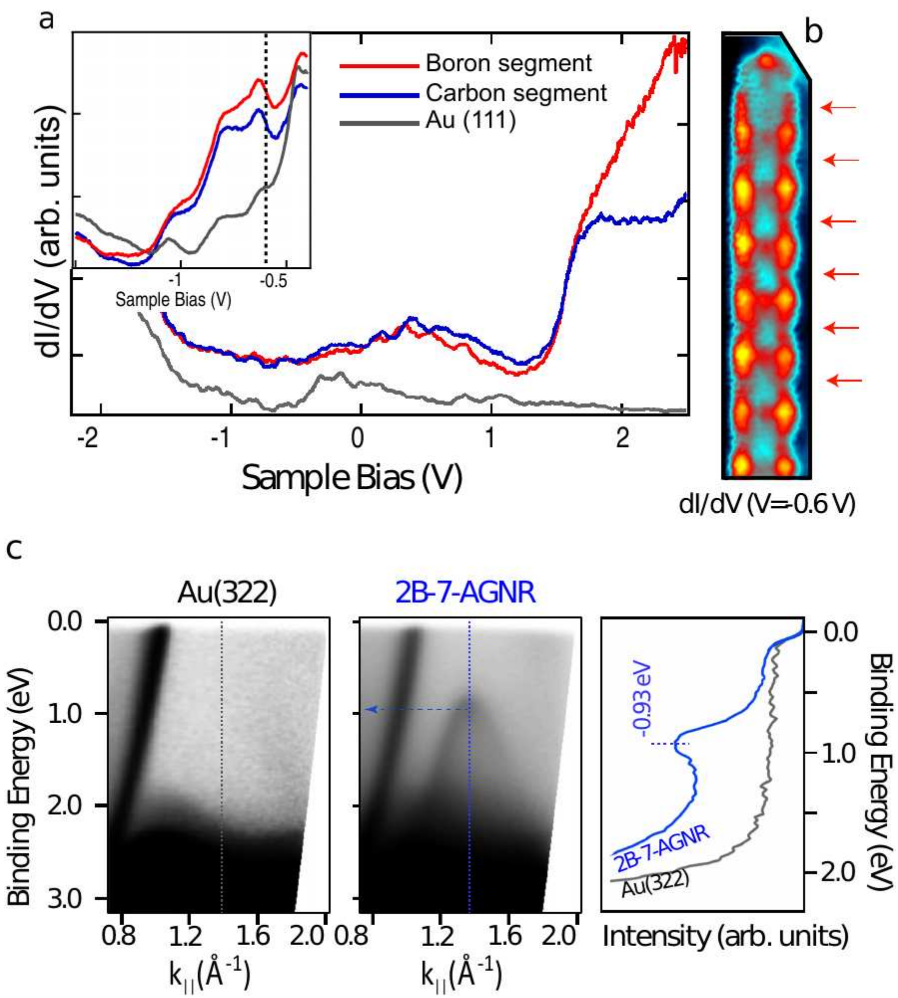

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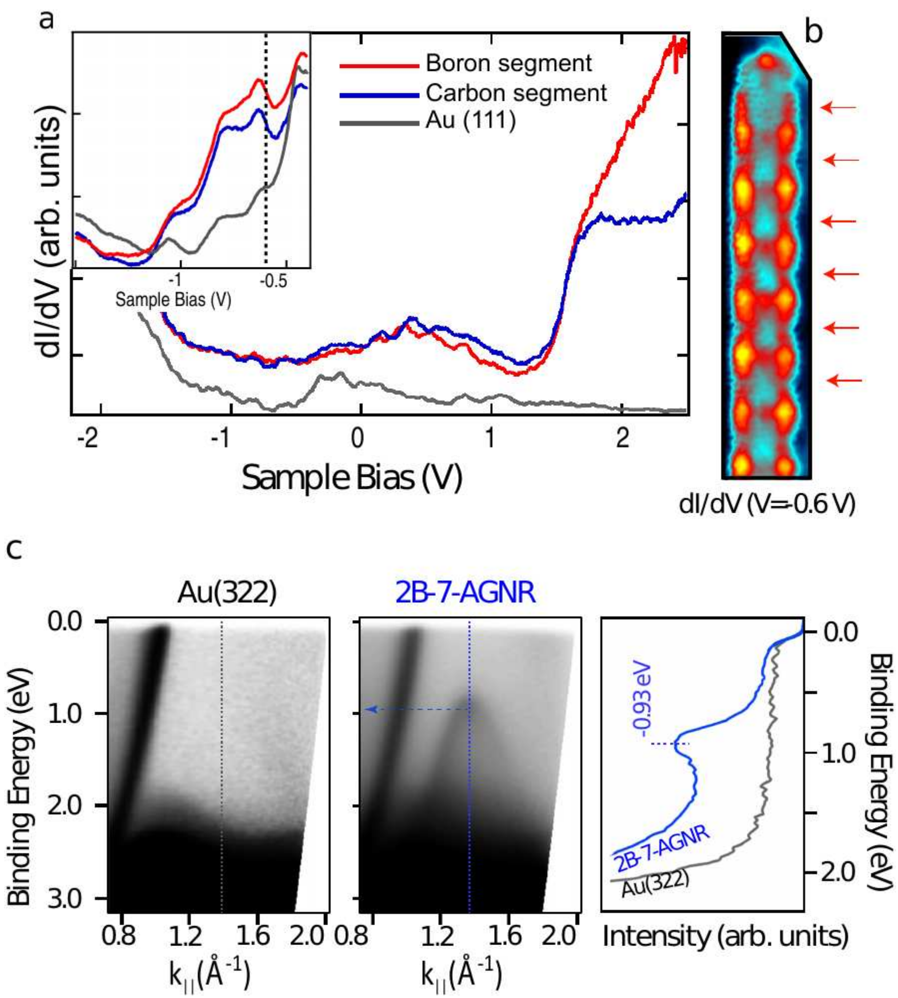

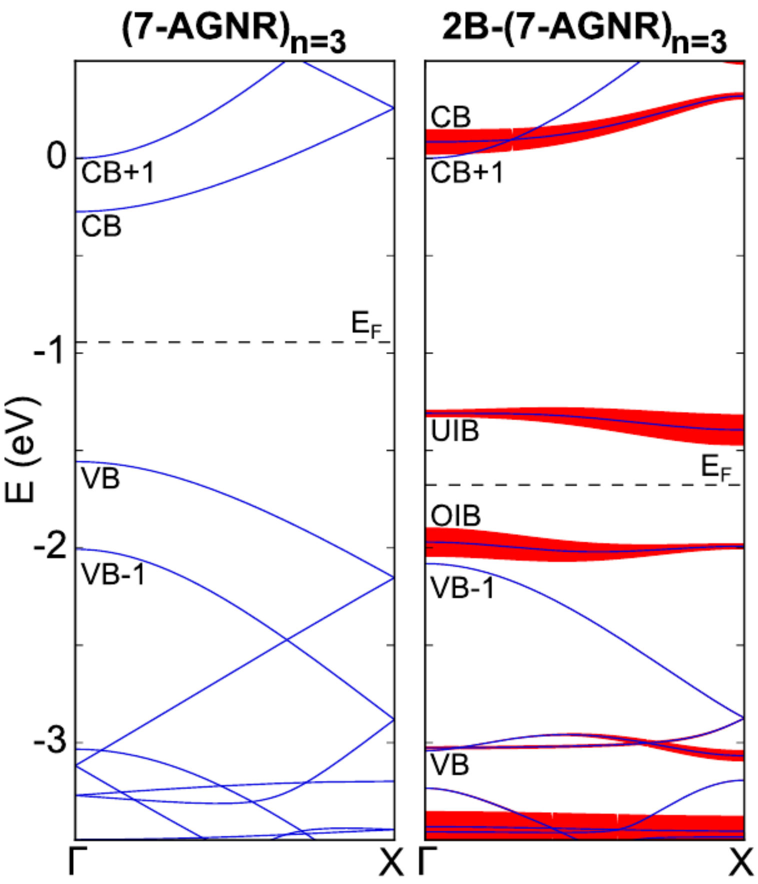

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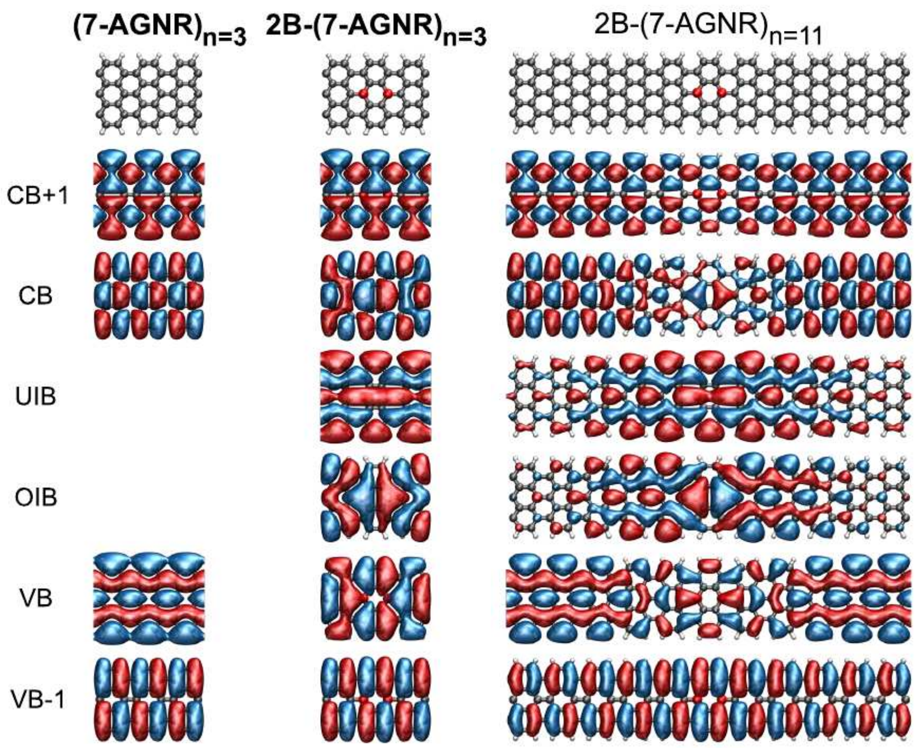

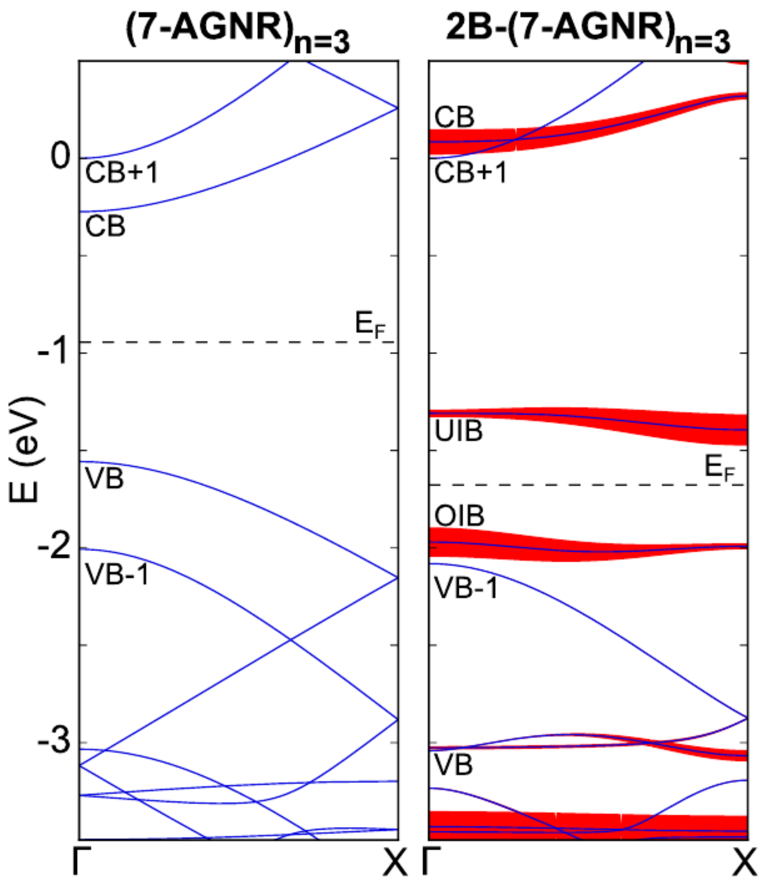

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Conclusions

- Transport simulations can **reproduce** observed quantum well states
- The theoretical analysis **reveals a band selectivity** mechanism
- **Fabry-Pérot** analogue for **electrons**

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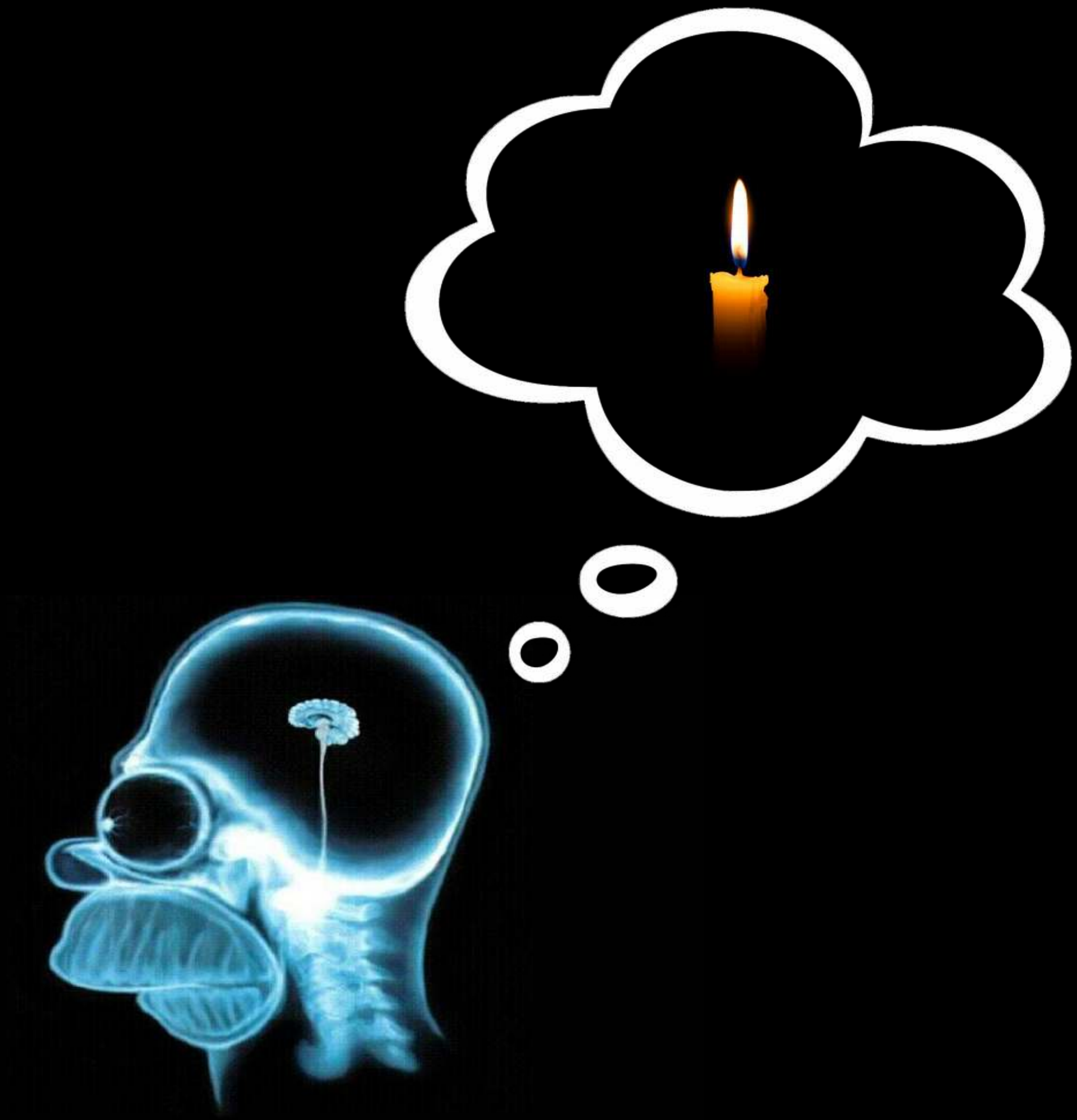

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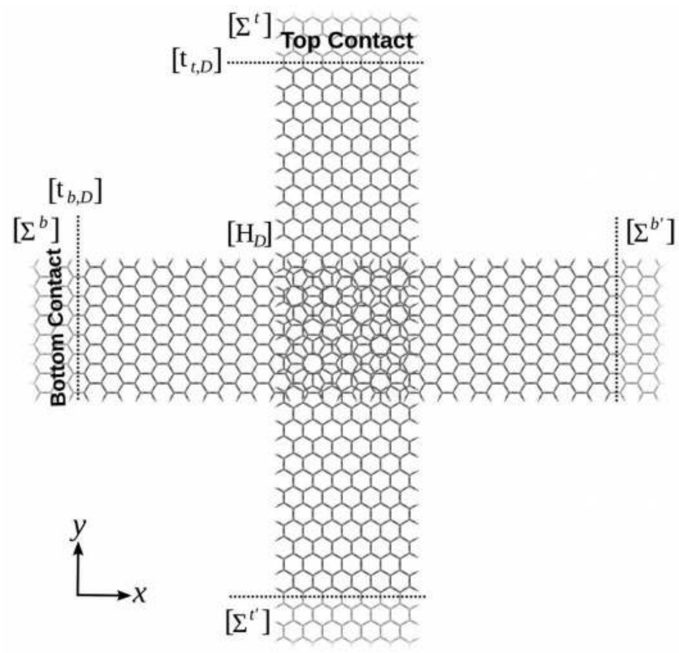
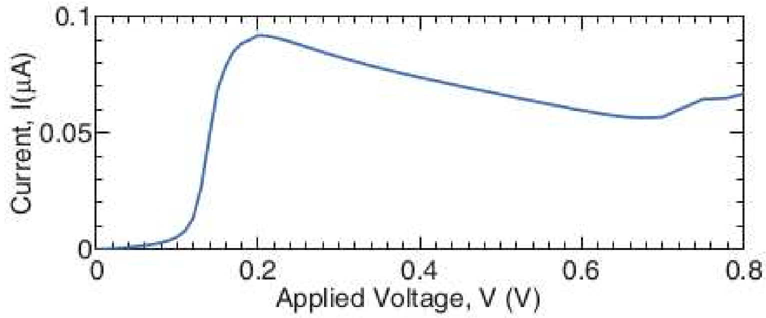
Crossed 14-AGNR device





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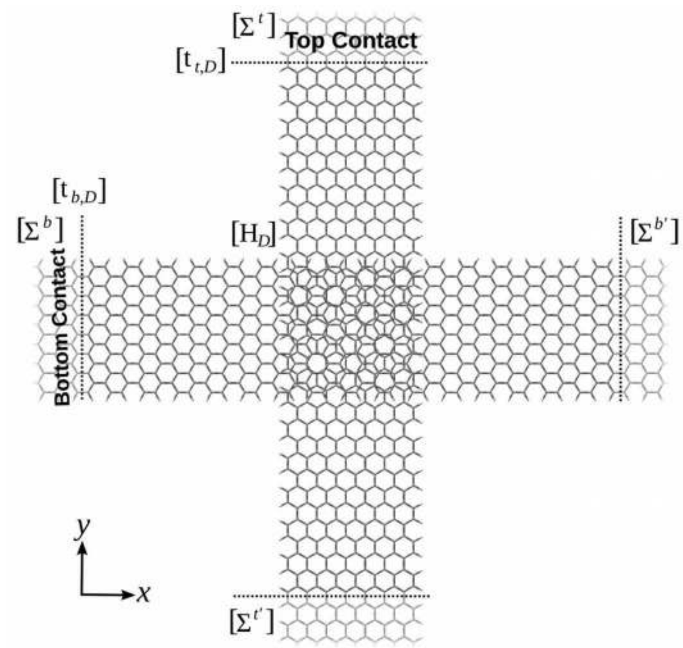

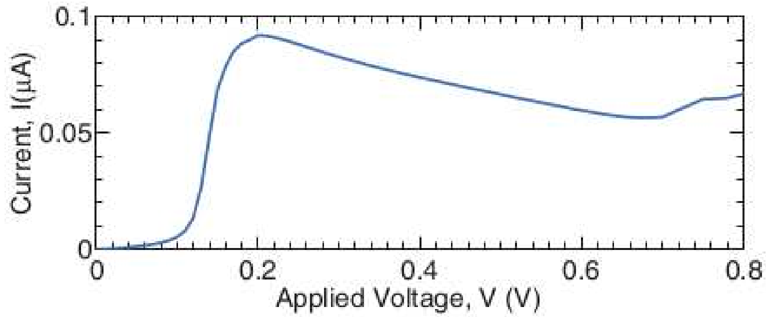

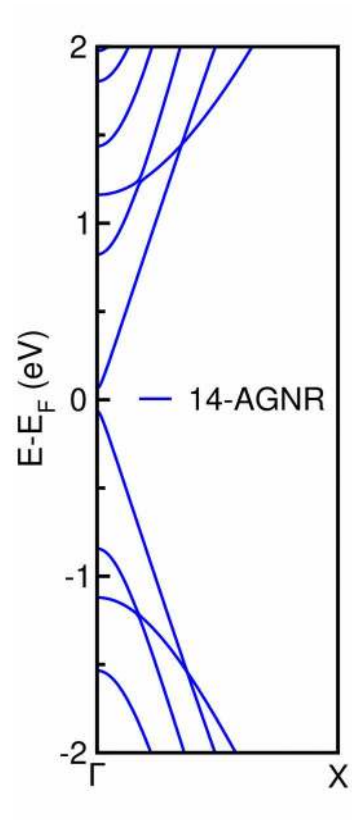

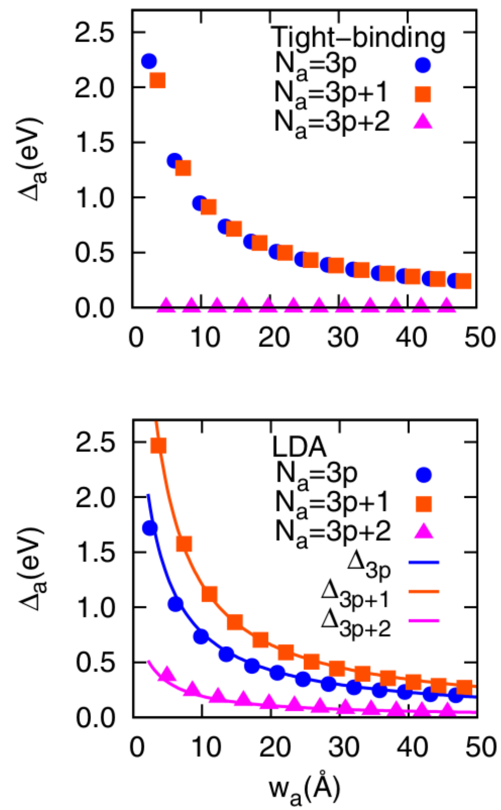

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Y.-W. Son et al. *Phys. Rev. Lett.* **97**, 216803 (2006).

Transport simulation setup

Density-Functional Theory (DFT)

+

Non-Equilibrium Green's Function (NEGF)

TranSIESTA

J. M. Soler *et al*. *J. Phys. Condens. Matter.* **14**, 2745 (2002).
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N. Papior *et al*. *Comp. Phys. Commun.* **212**, 8 (2017).

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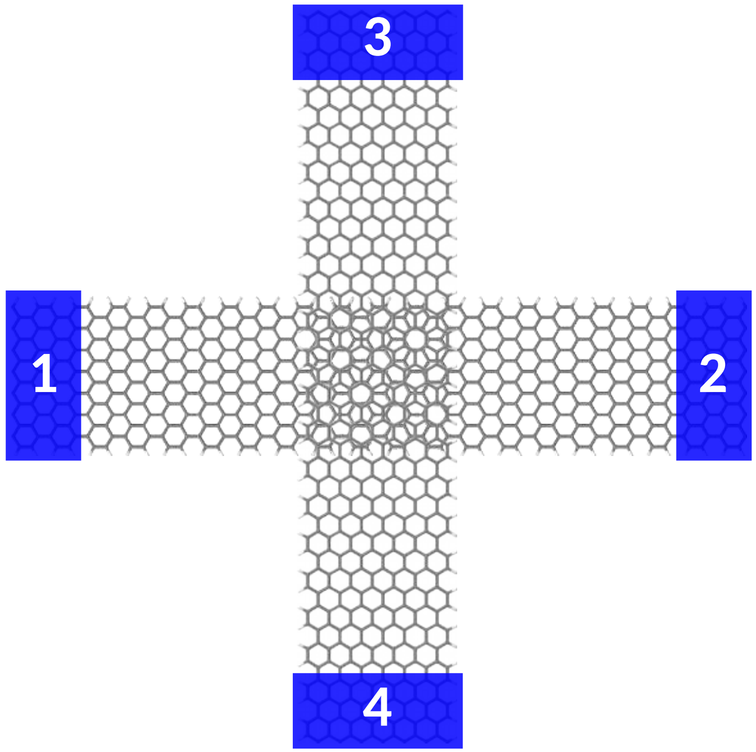
!!! multi-terminal !!!



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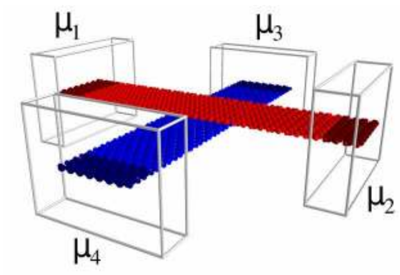

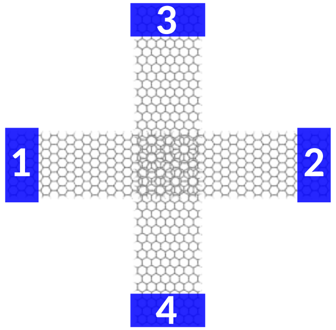

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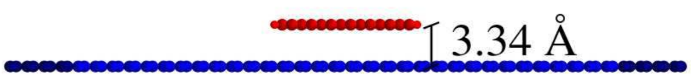
!!! multi-terminal !!!

Simulation characteristics:

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



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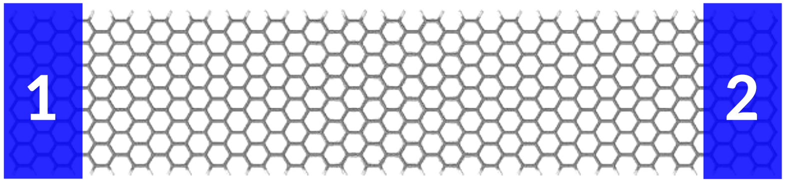
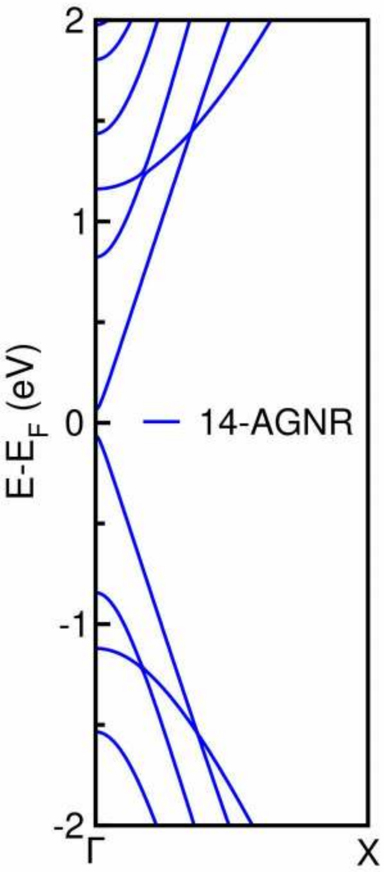
Pristine 14-AGNR





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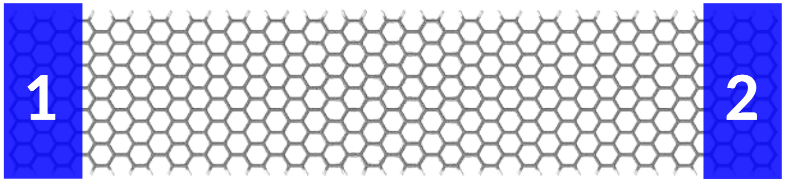

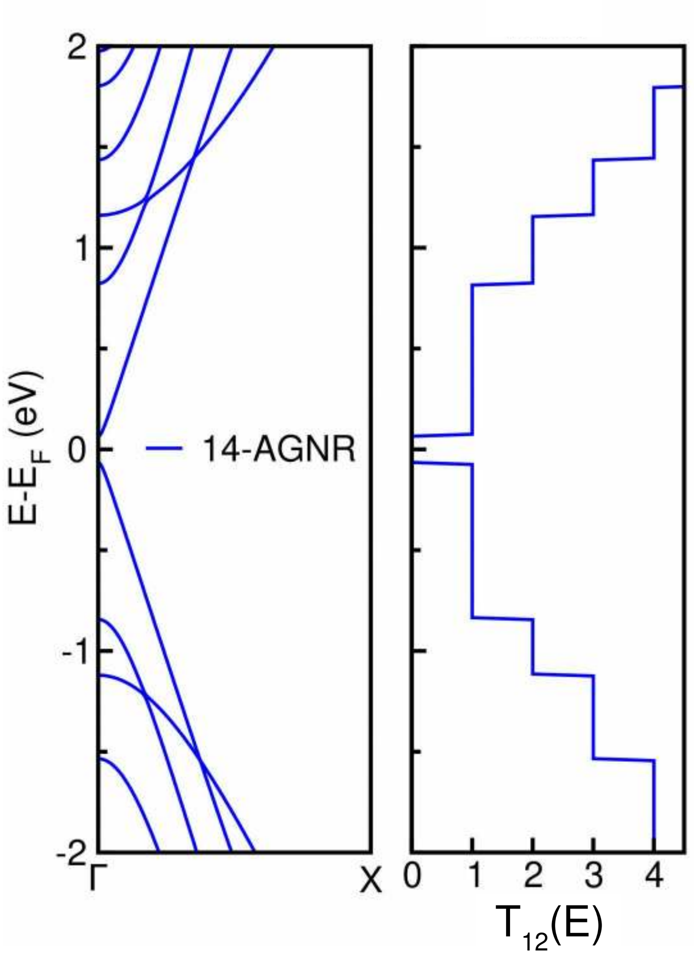

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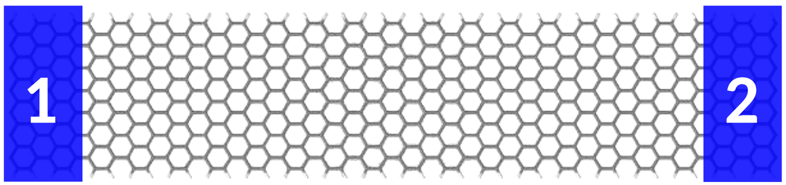

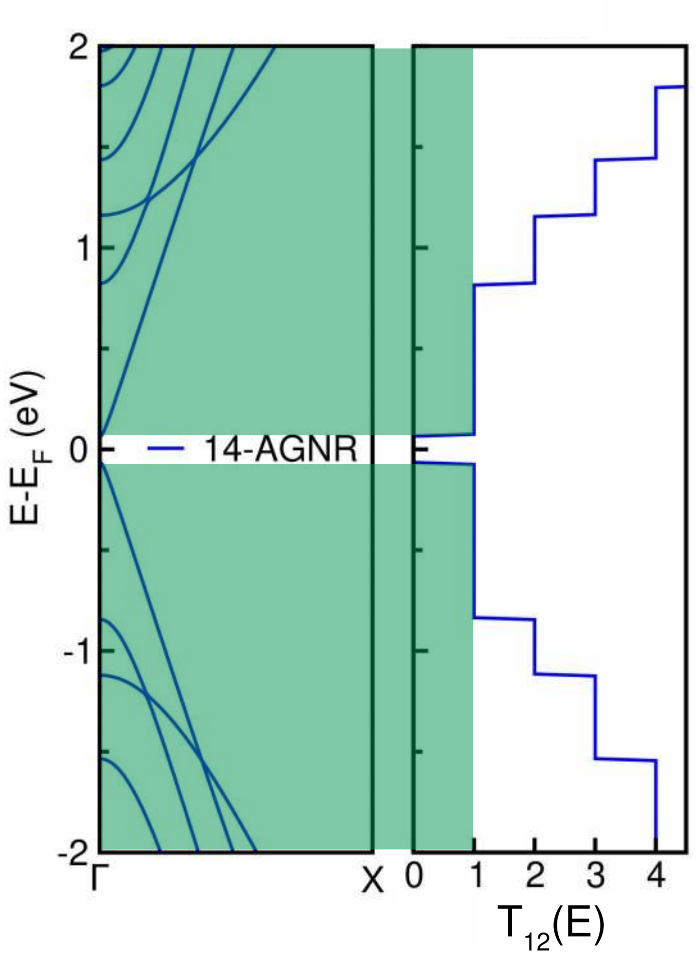

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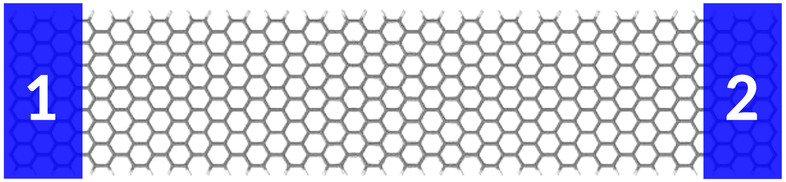

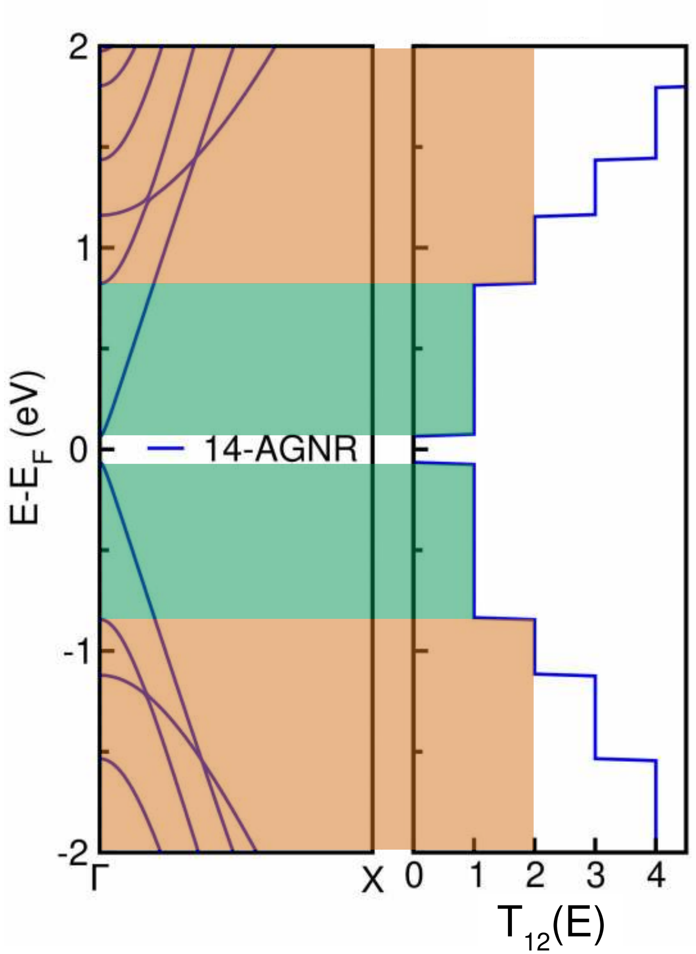

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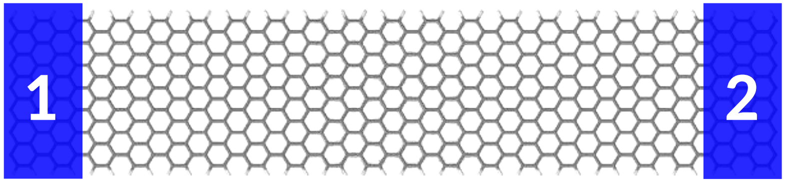

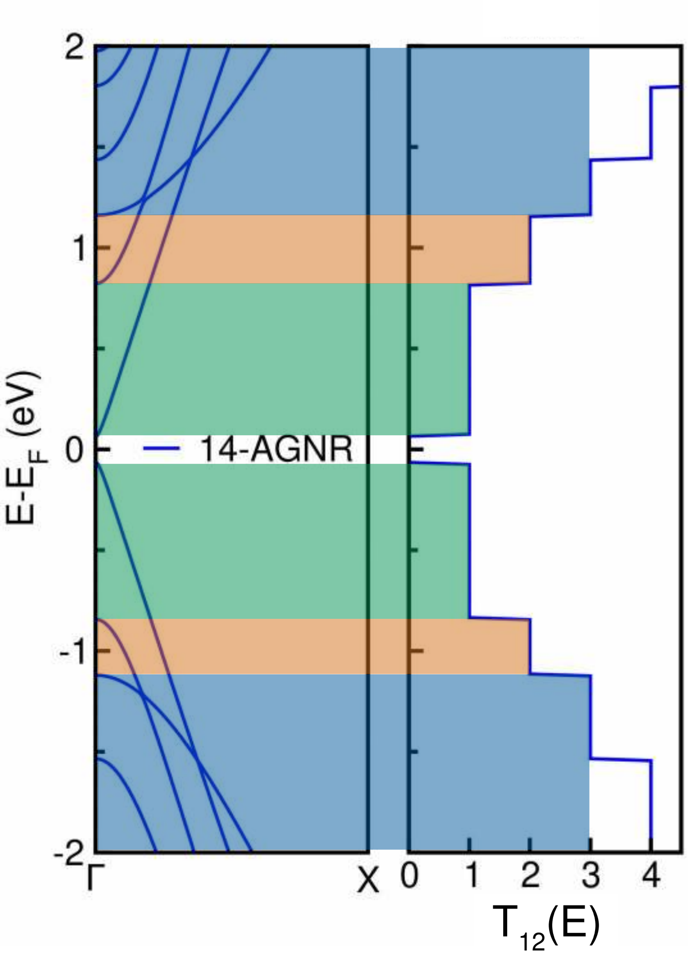

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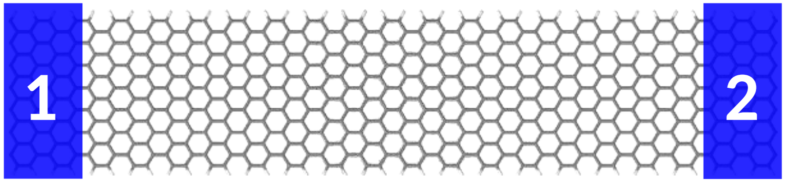

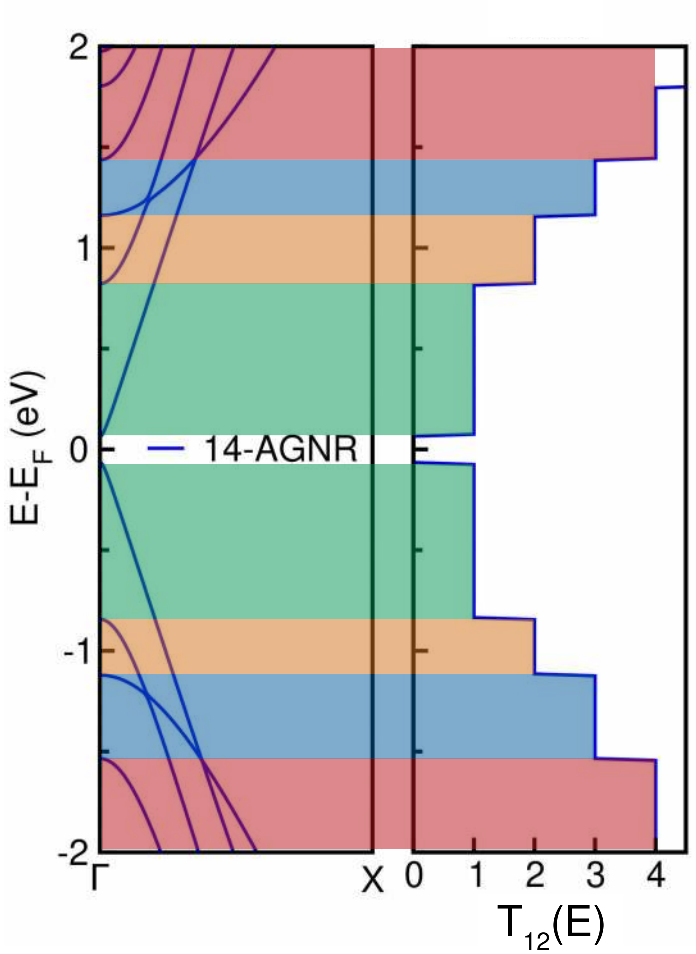

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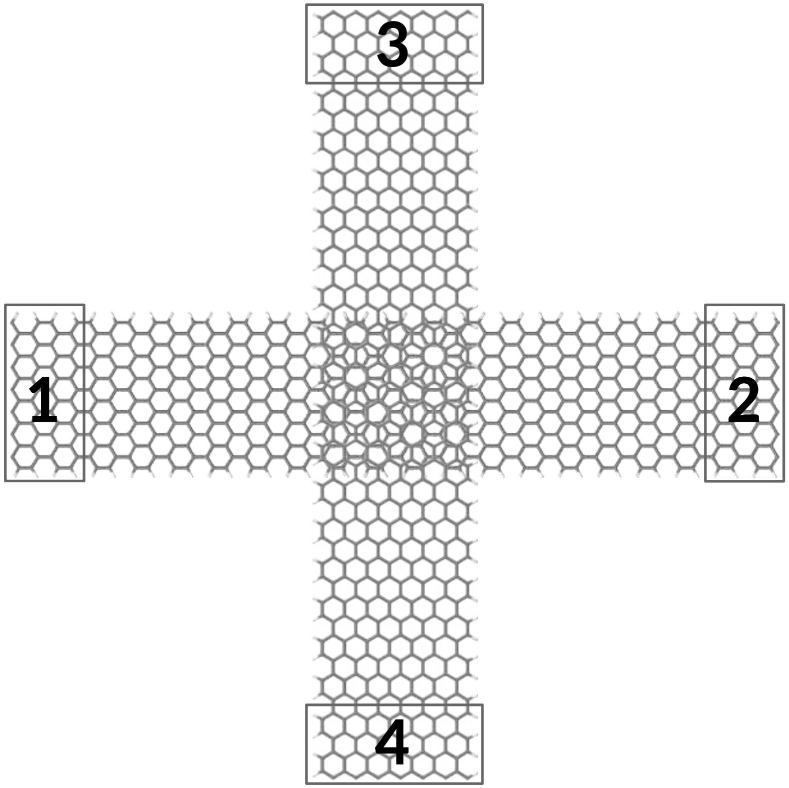
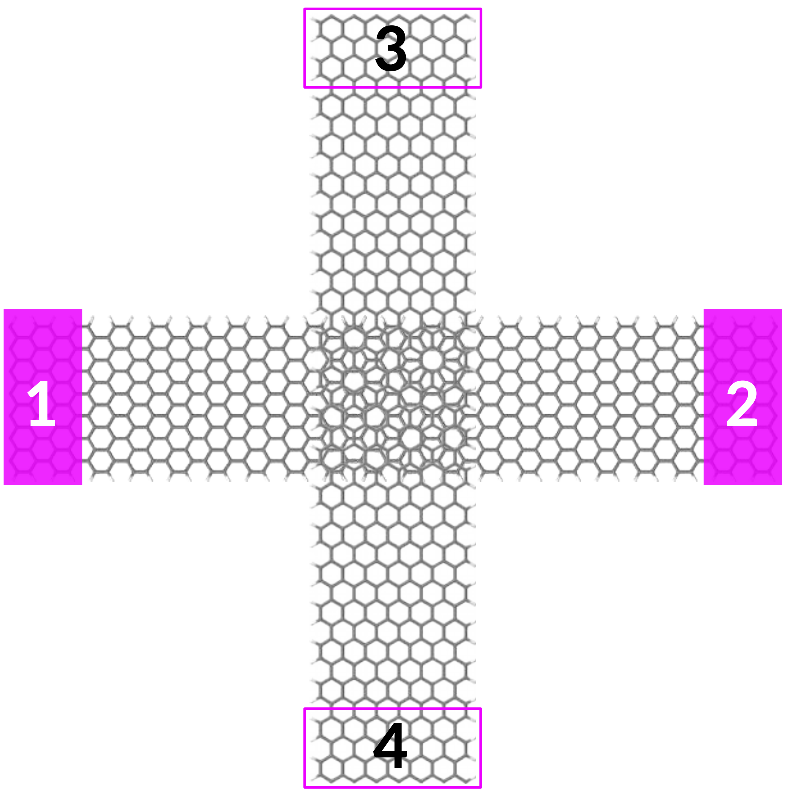


interlayer separation of 3.34 Å

P. Brandimarte *et al*. *J. Chem. Phys.* **146**, 092318 (2017).

Intra-GNR transmission at V=0



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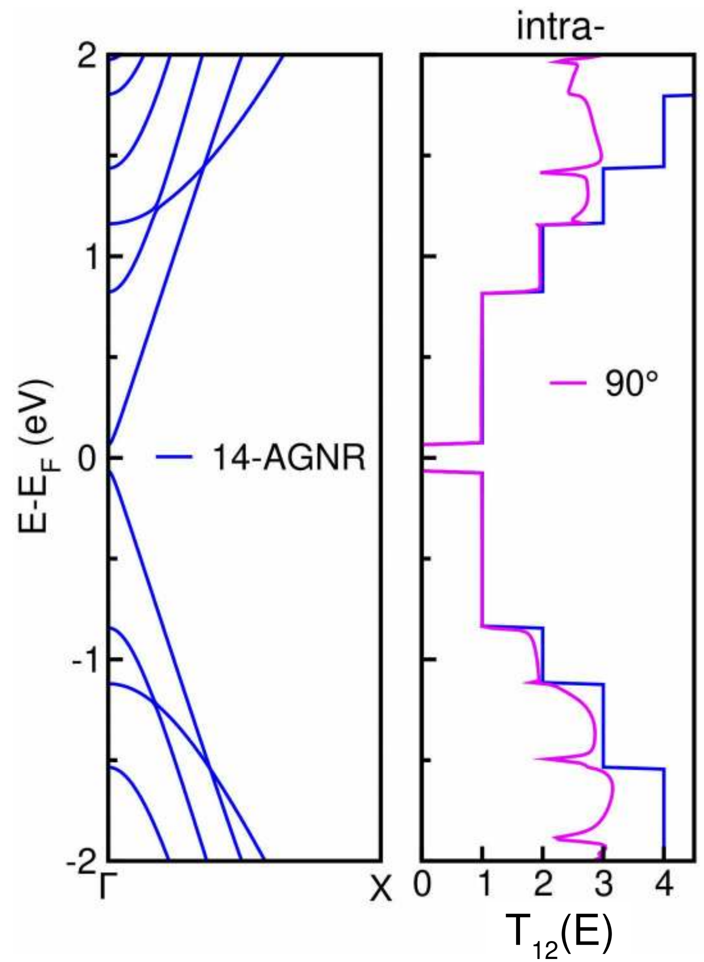

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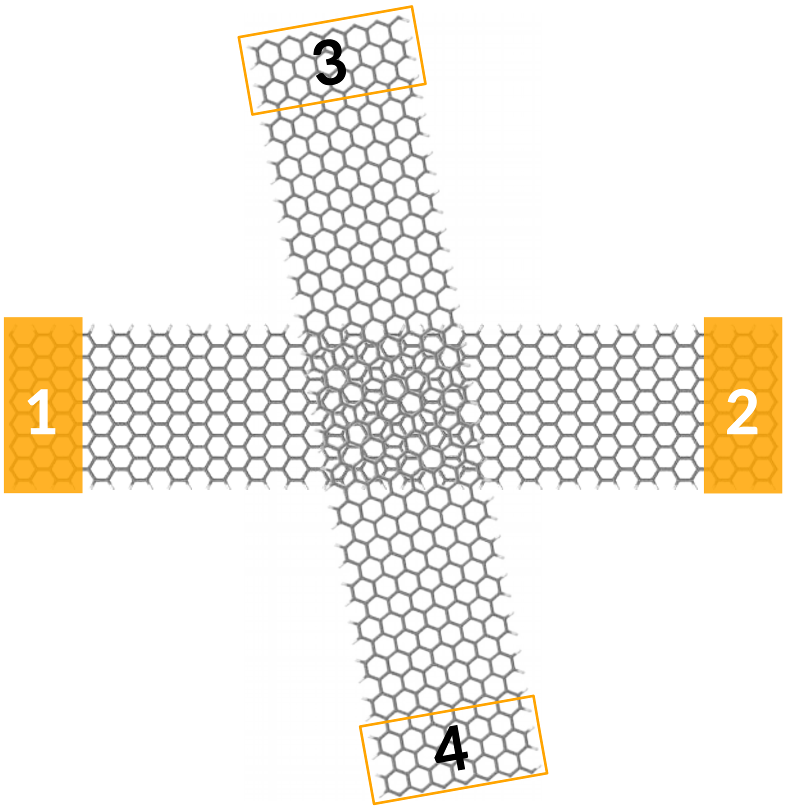

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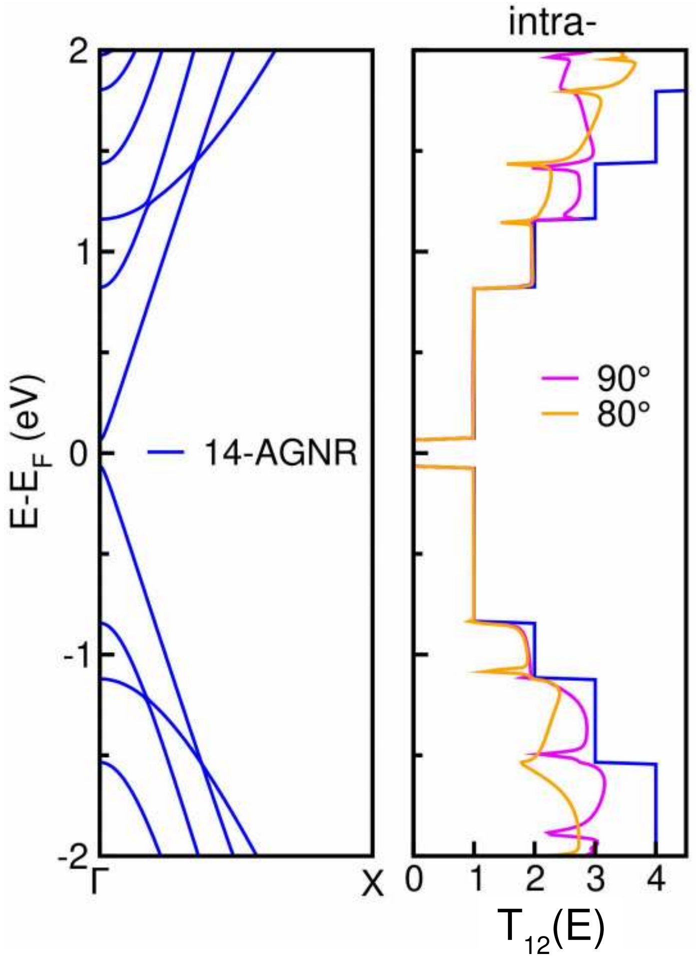

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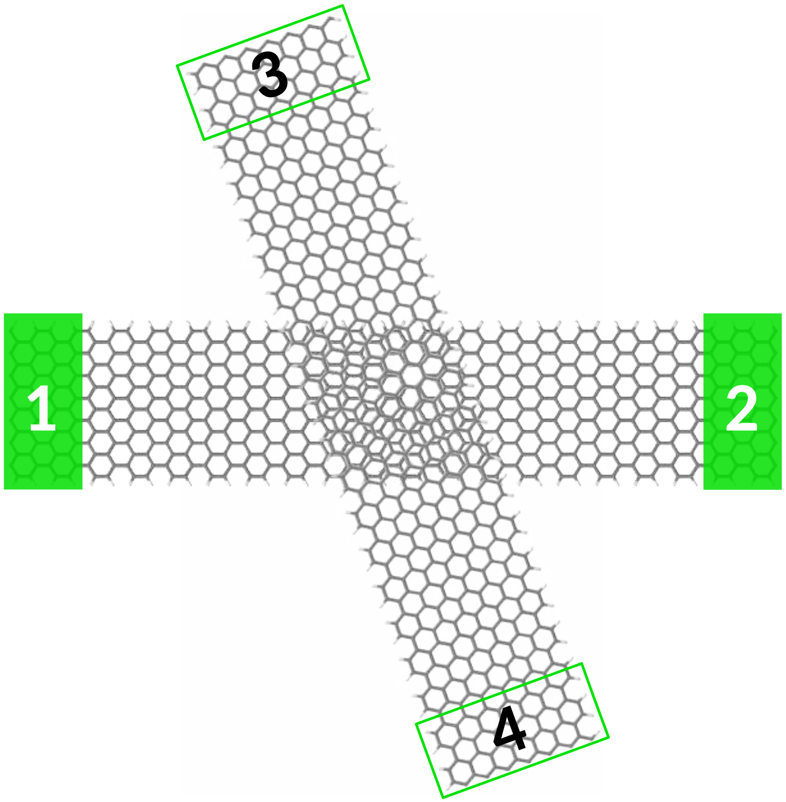
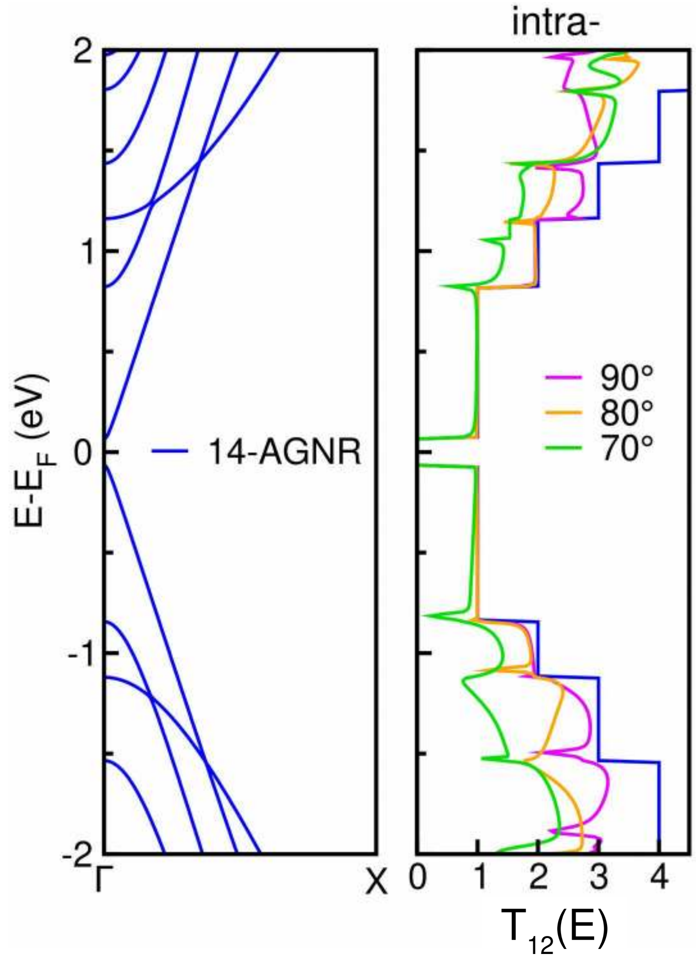


interlayer separation of 3.34 Å



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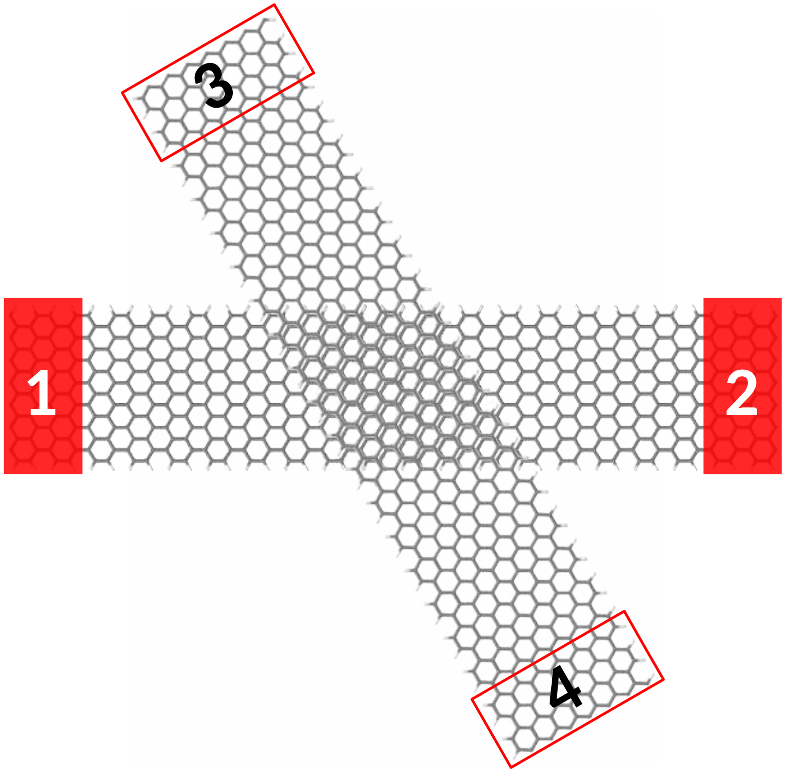
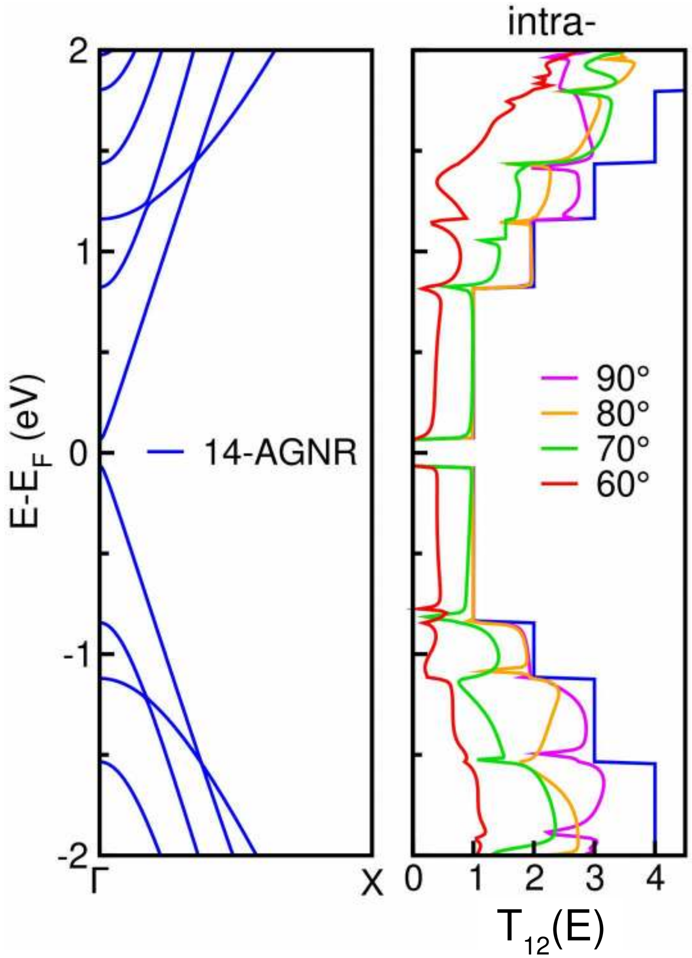
Intra-GNR transmission at V=0



interlayer separation of 3.34 Å



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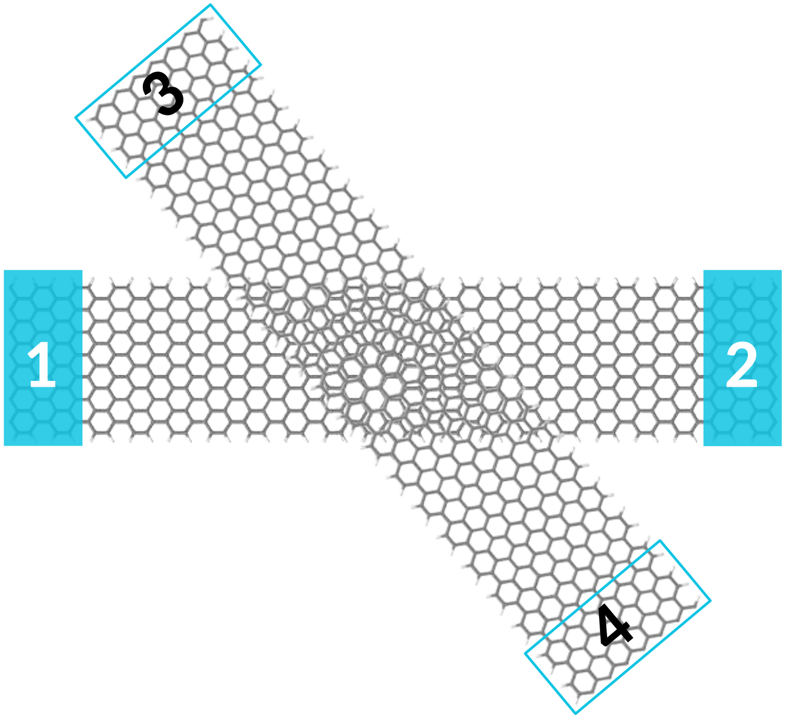
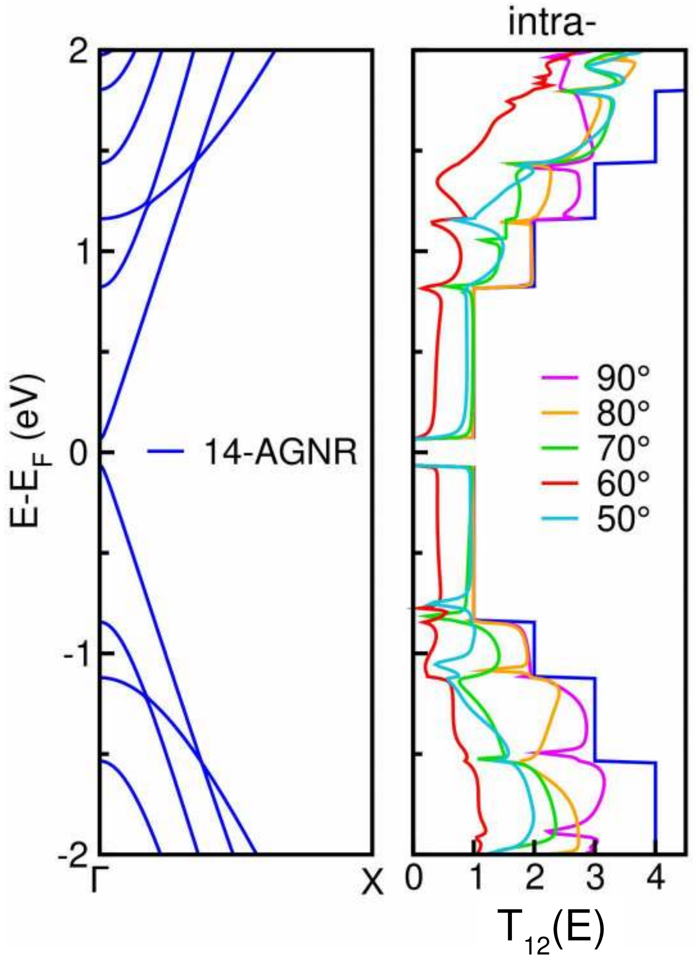
Intra-GNR transmission at V=0



interlayer separation of 3.34 Å



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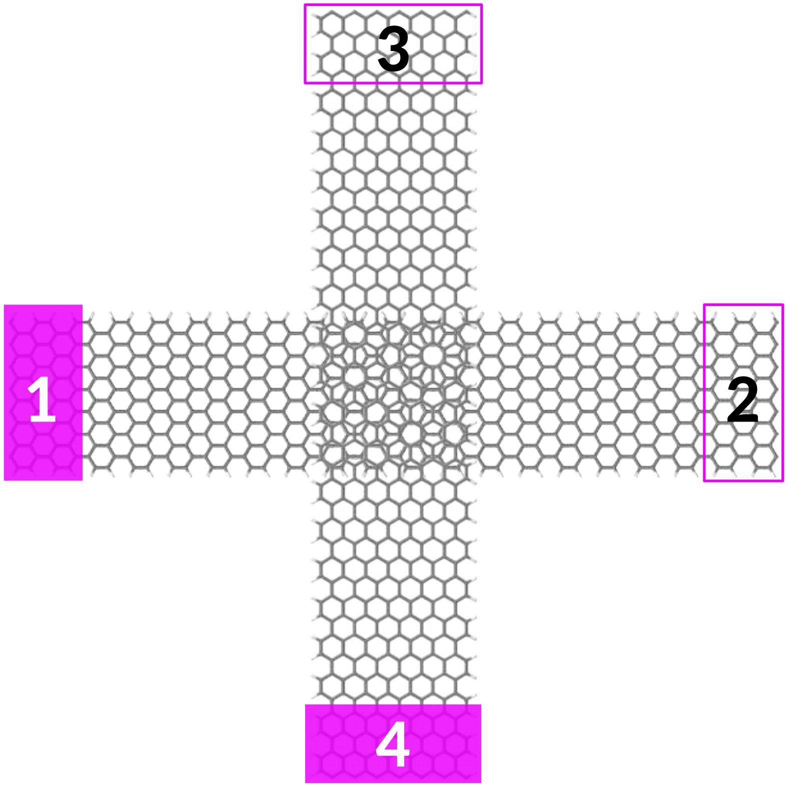
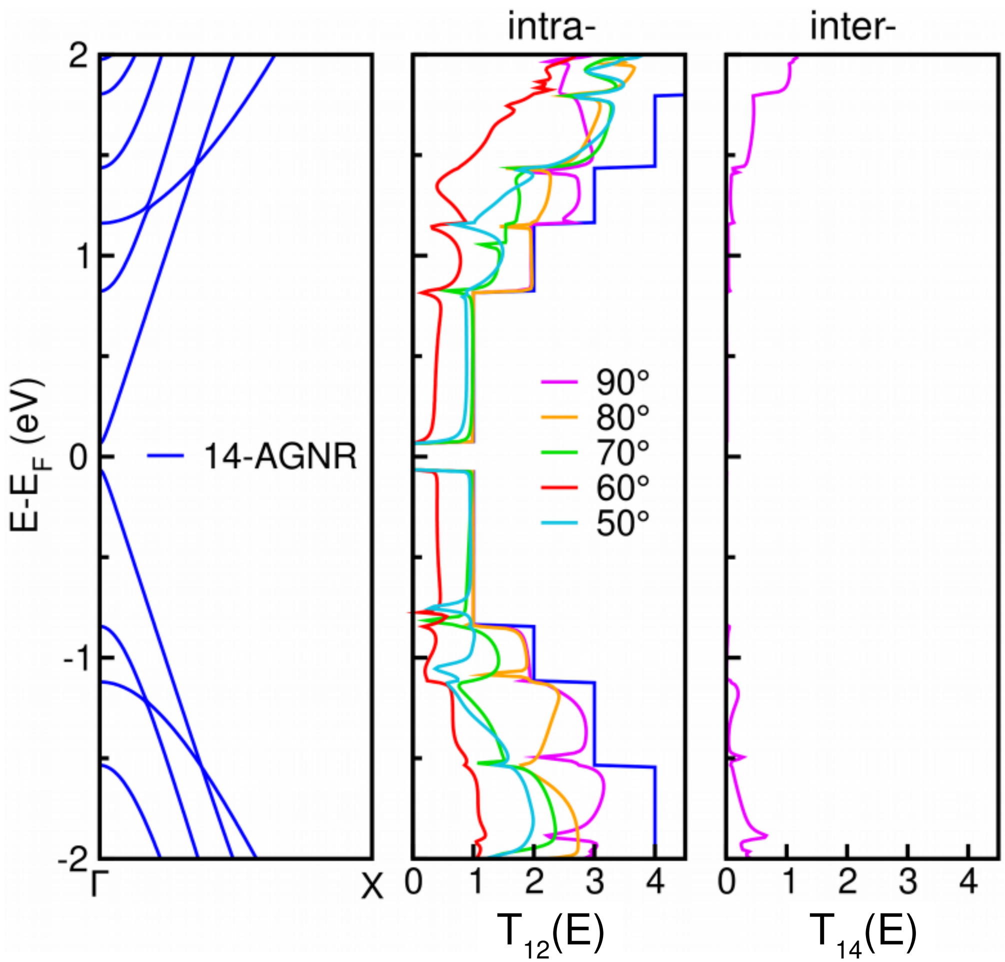
Inter-GNR transmission at V=0



interlayer separation of 3.34 Å



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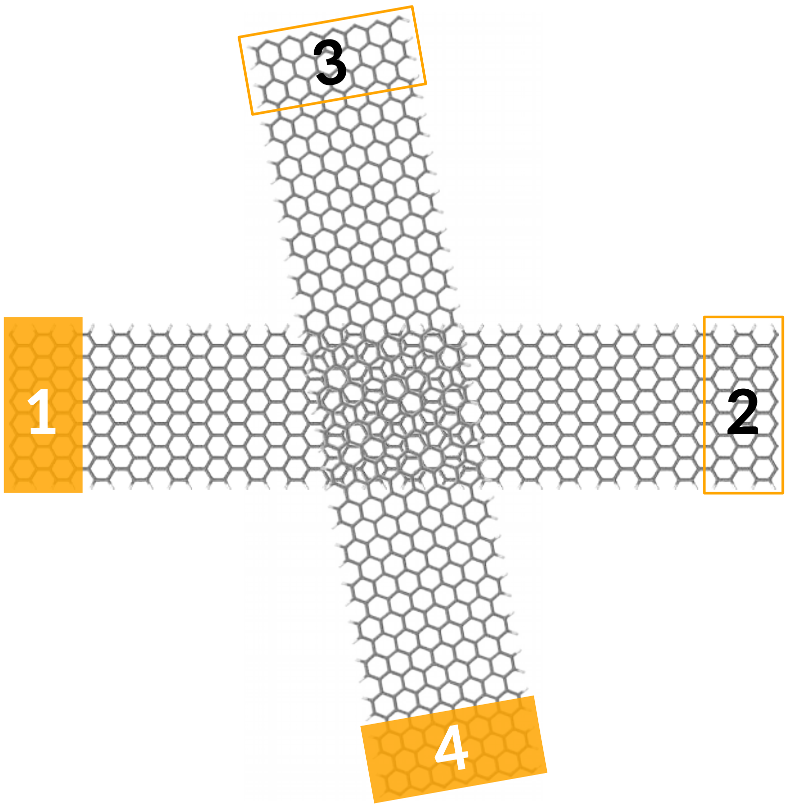
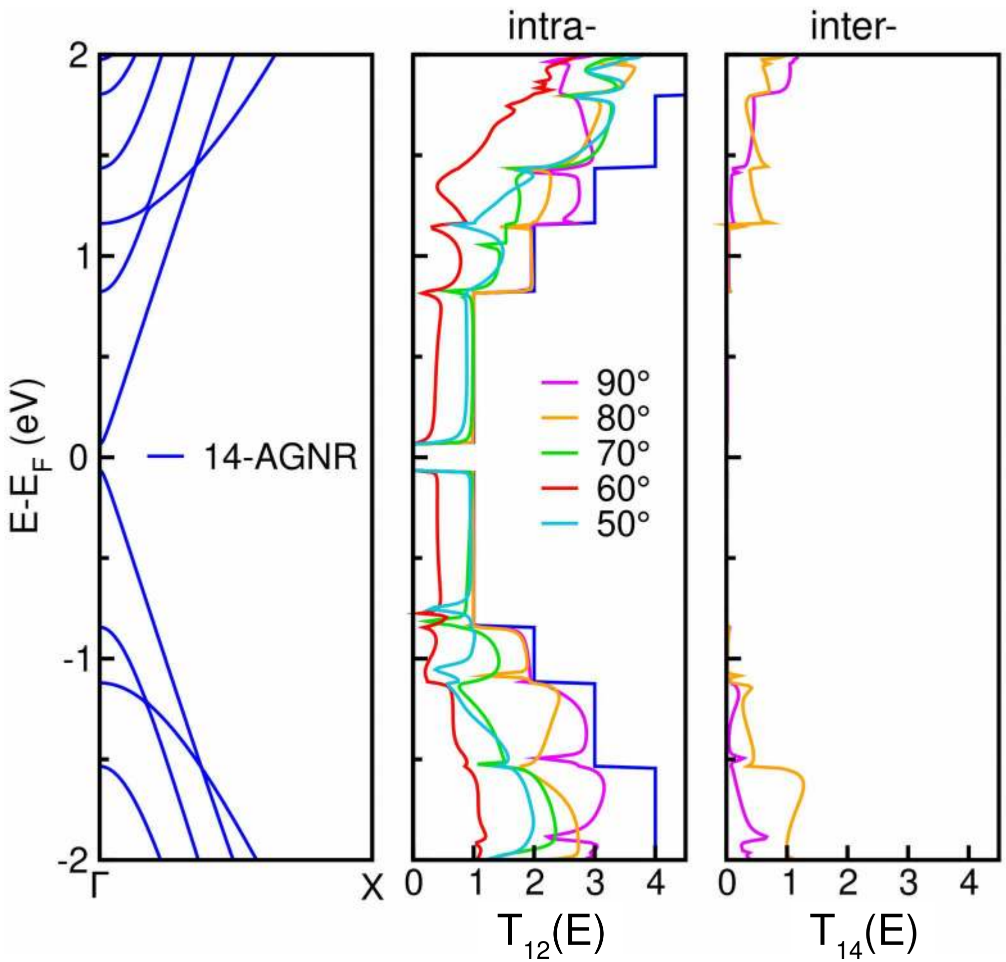
Inter-GNR transmission at V=0



interlayer separation of 3.34 Å



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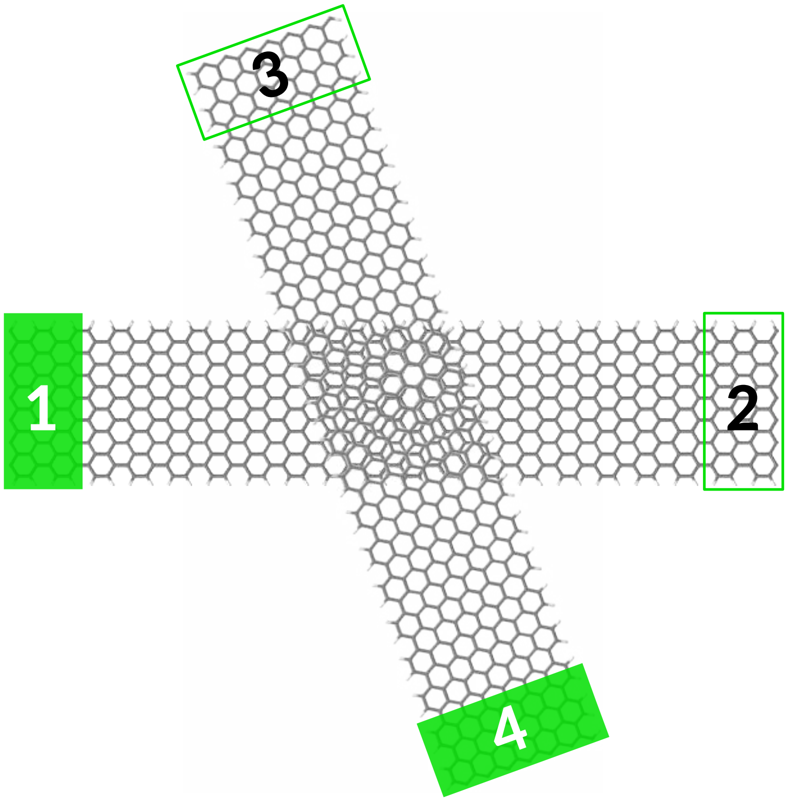
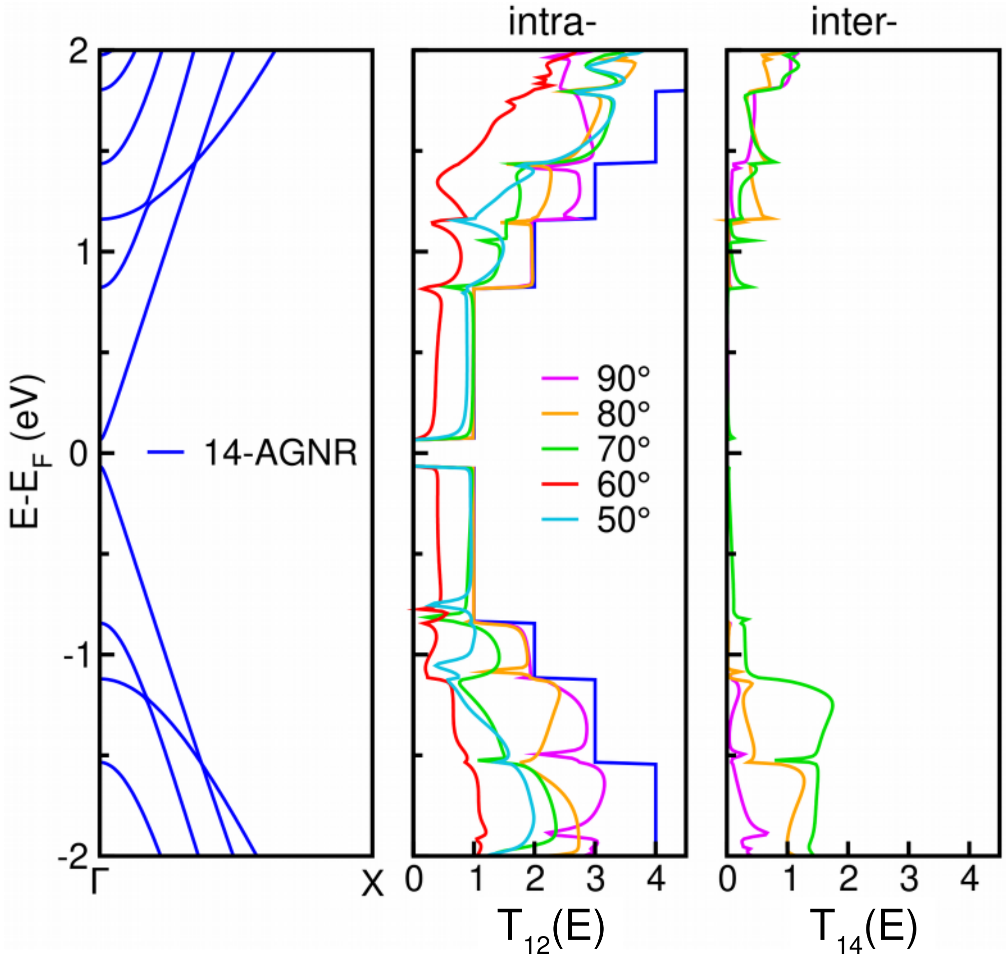
Inter-GNR transmission at V=0



interlayer separation of 3.34 Å



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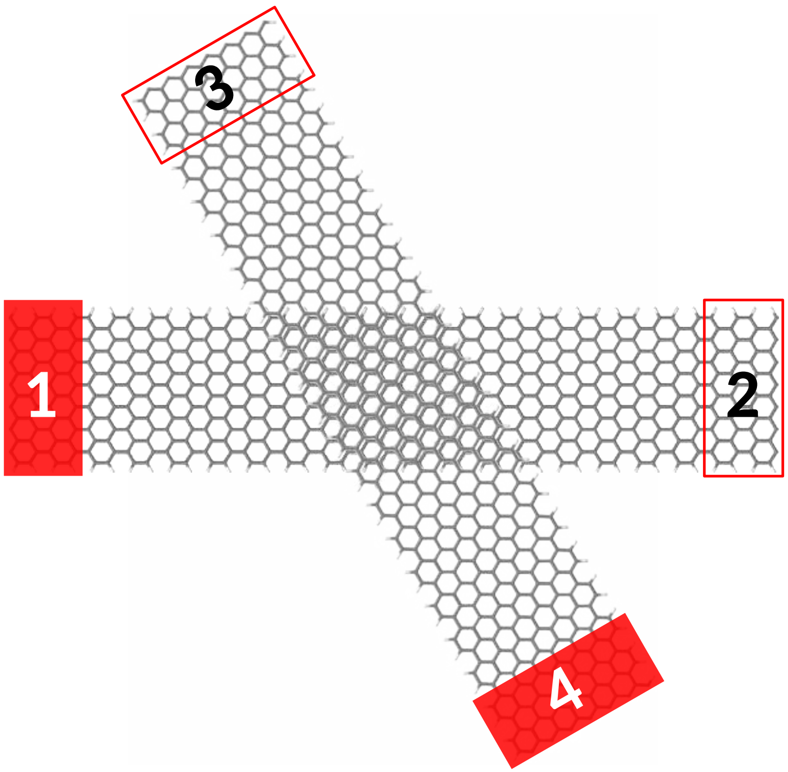
Inter-GNR transmission at V=0



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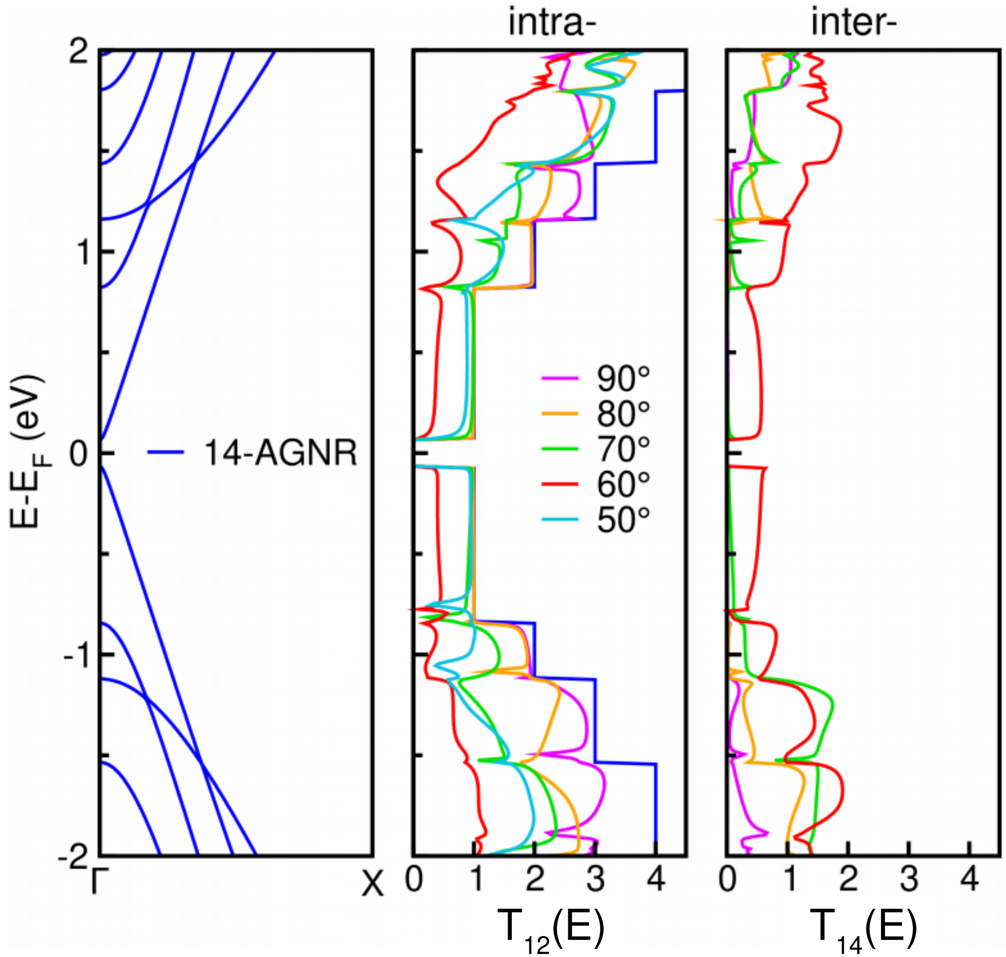

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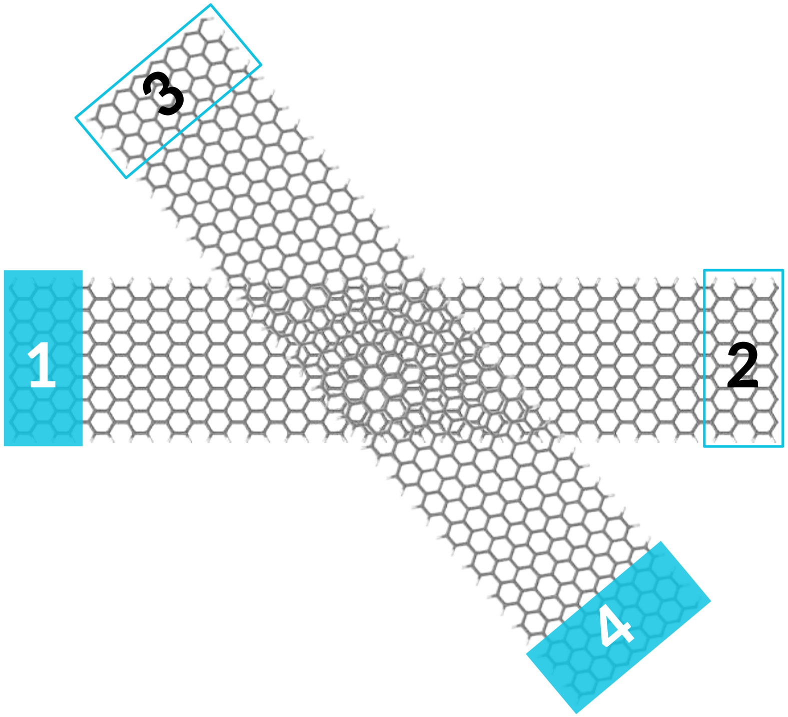
Inter-GNR transmission at V=0



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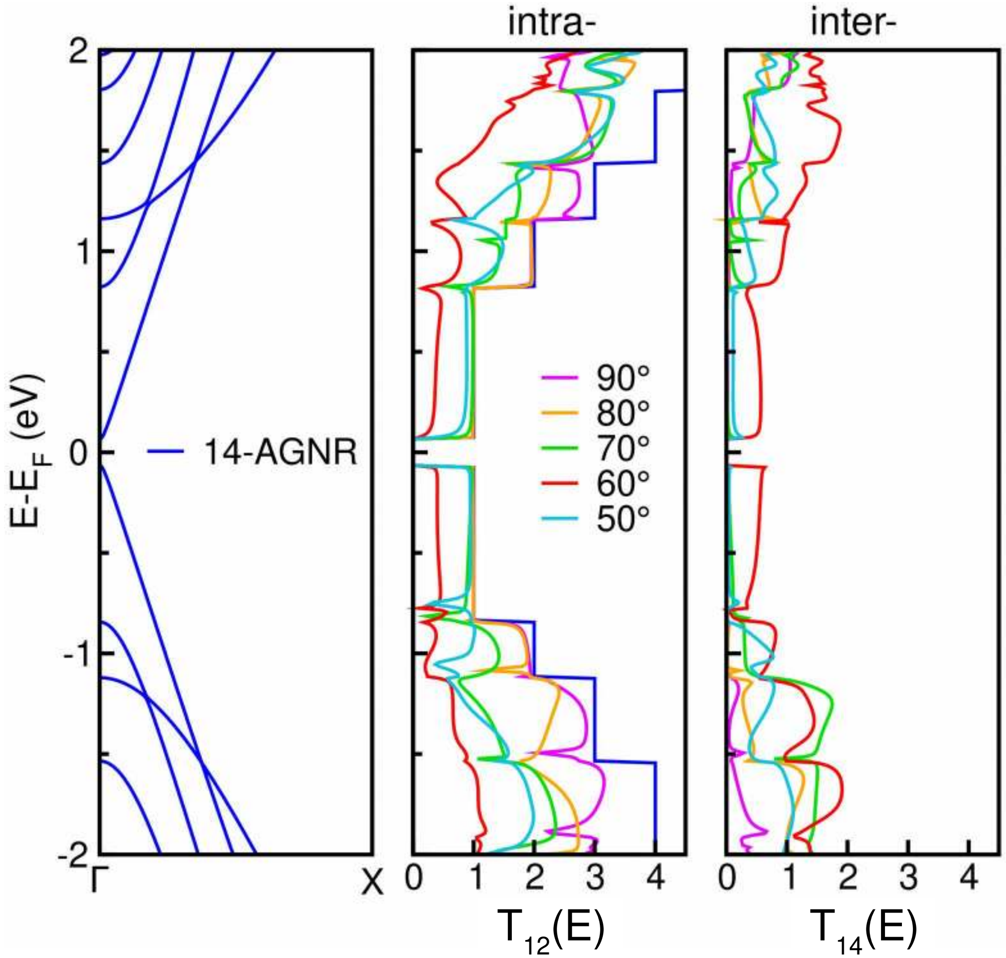

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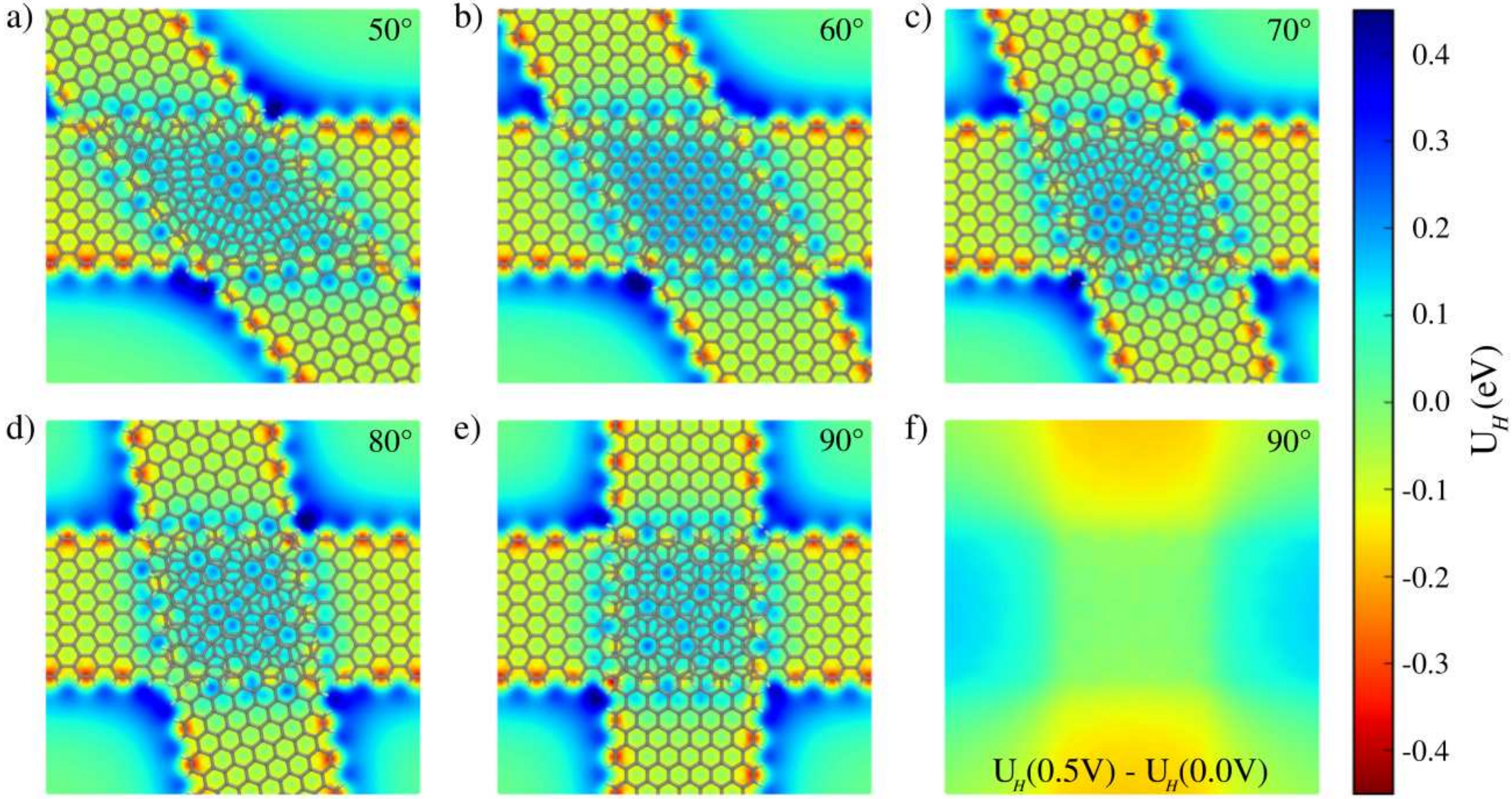
Electrostatic potential at V=0.5V



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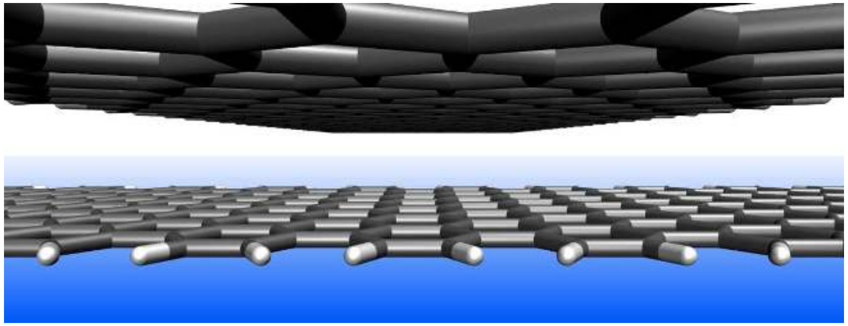
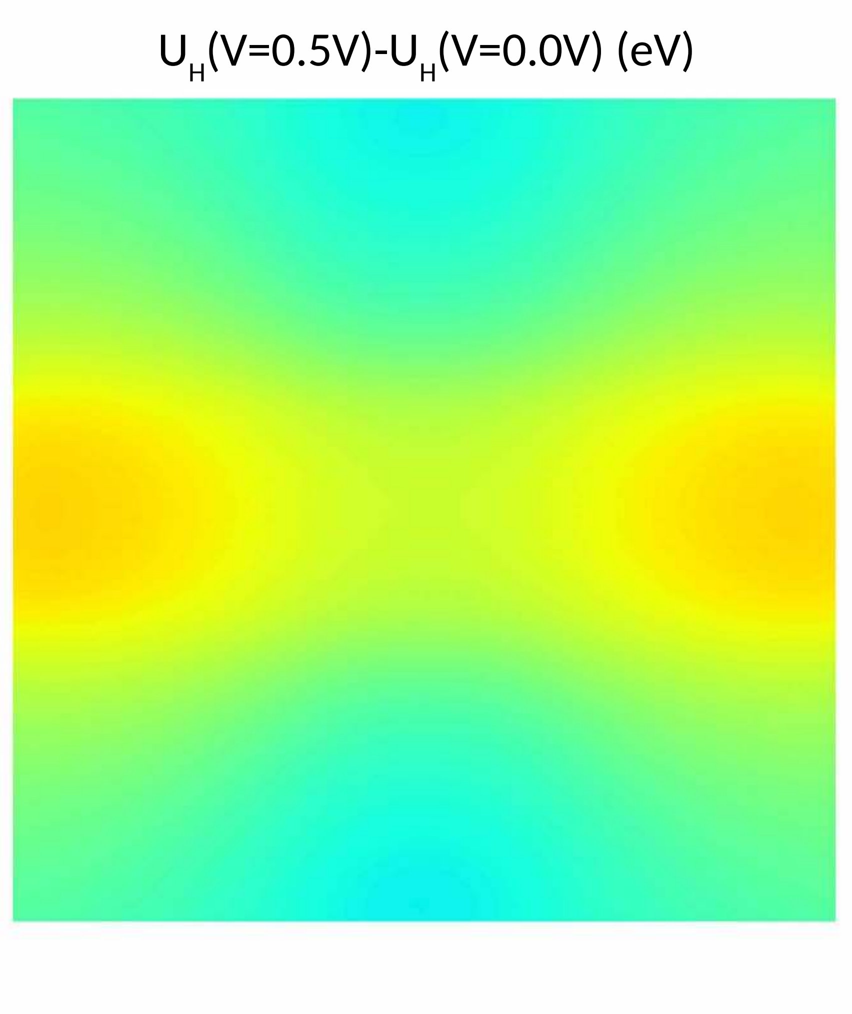
Pedro Brandimarte (brandimarte@pm.me)

Electrostatic potential profile at V=0.5V





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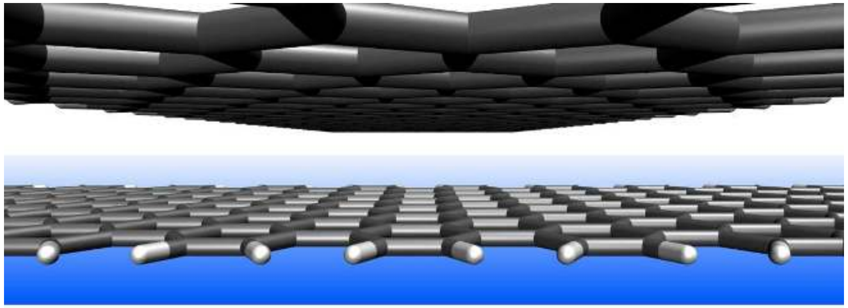
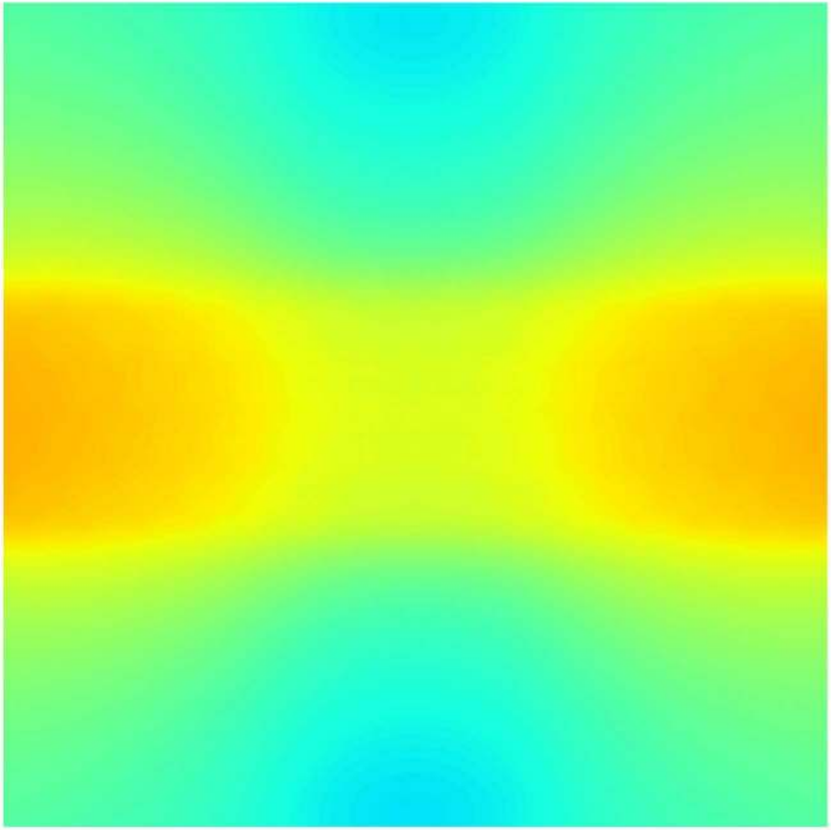
Electrostatic potential profile at V=0.5V



$U_H(V=0.5V)-U_H(V=0.0V)$ (eV)



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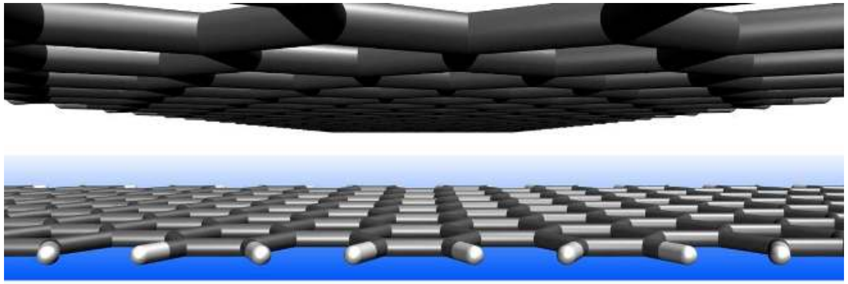

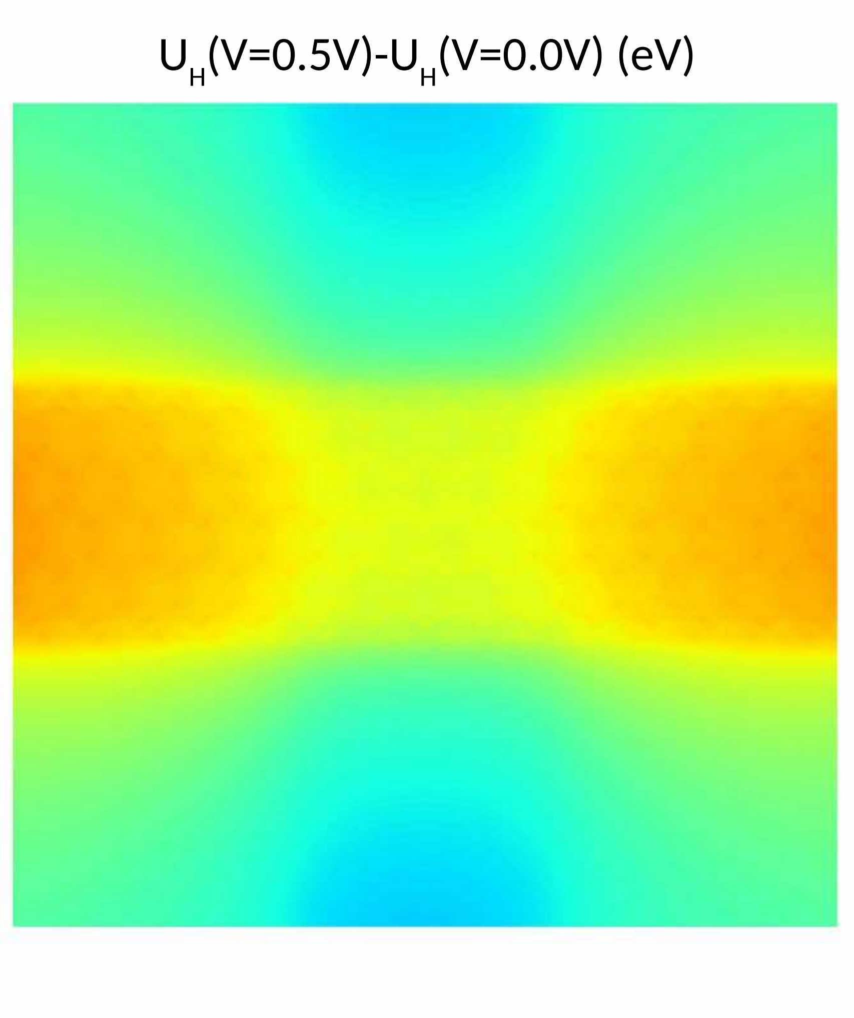

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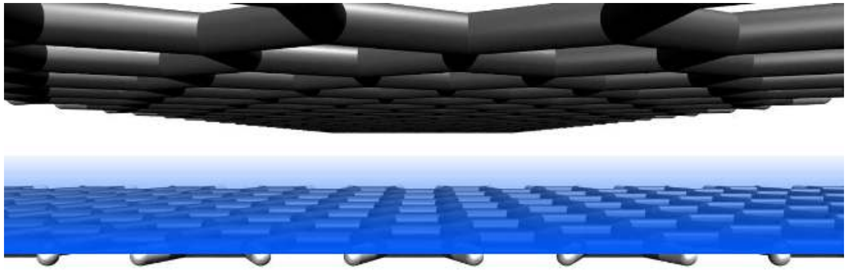

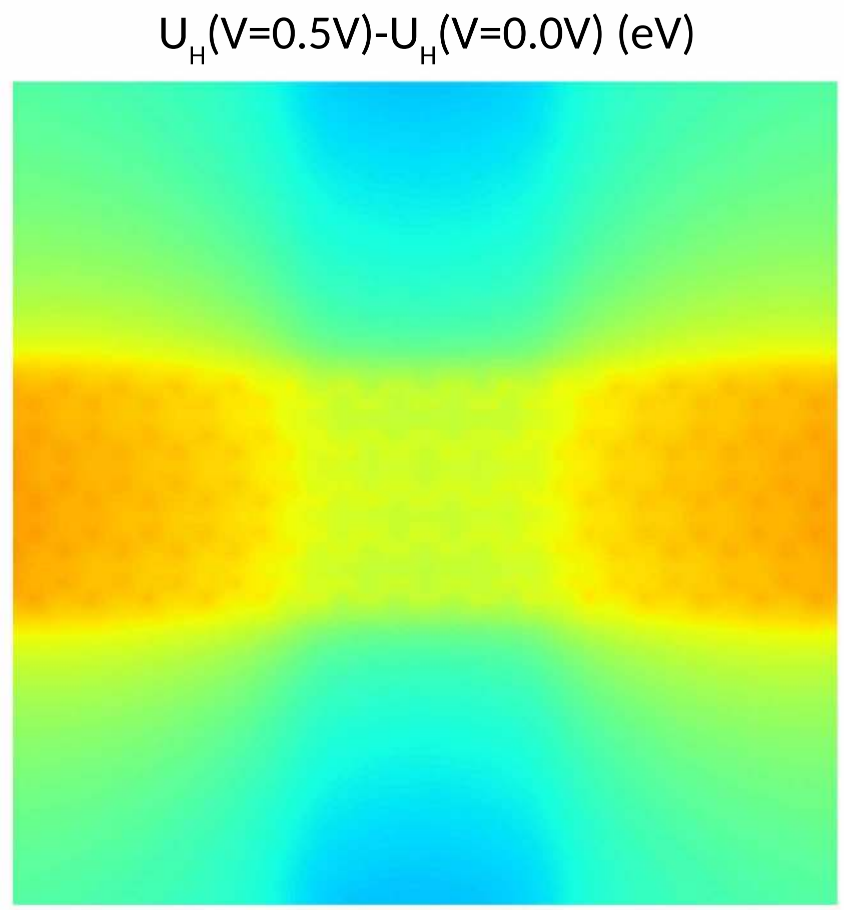

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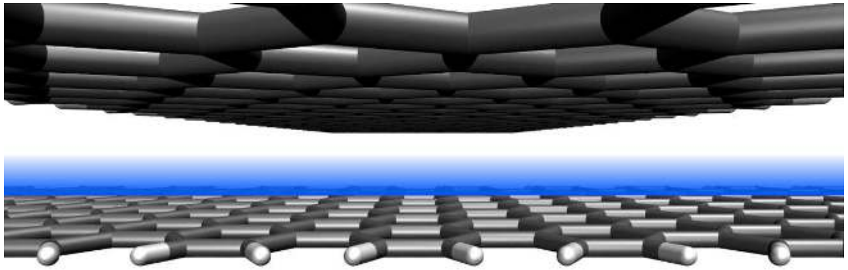

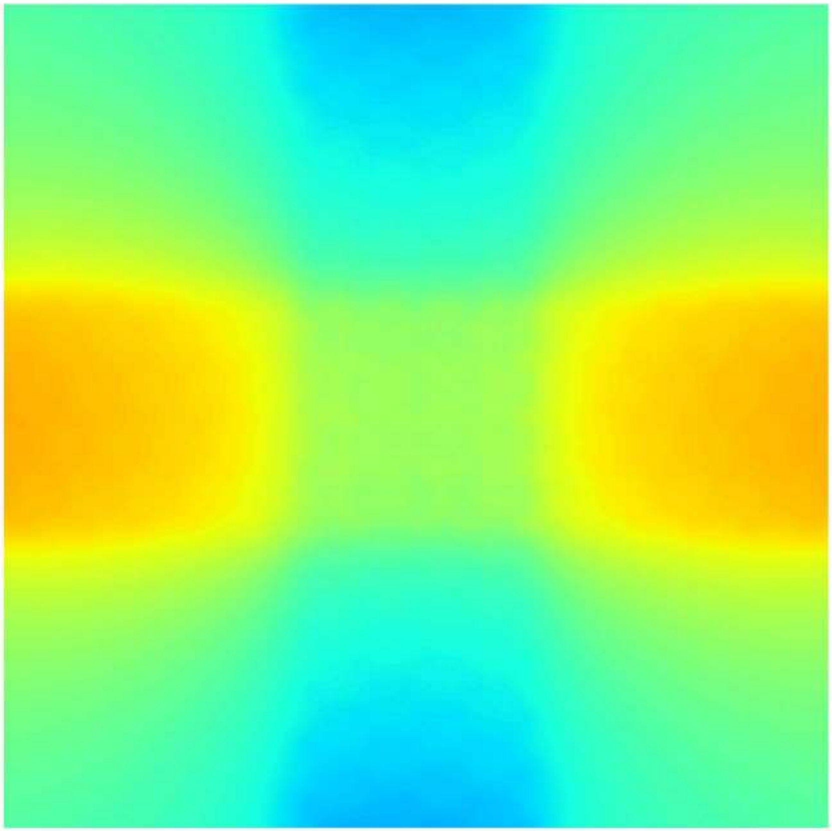

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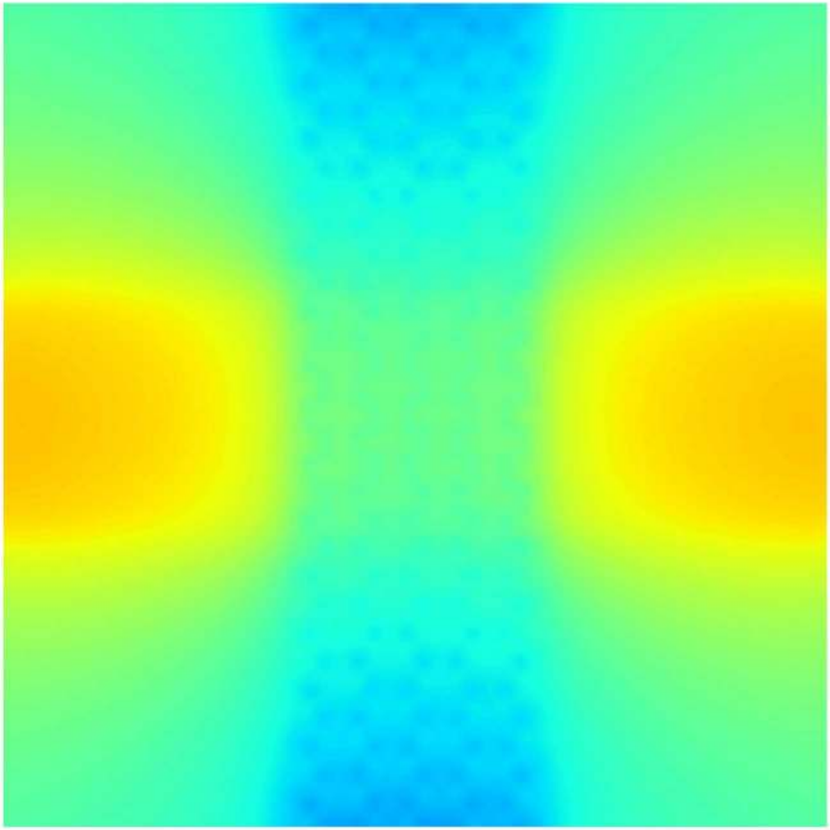
Electrostatic potential profile at V=0.5V

$U_H(V=0.5V)-U_H(V=0.0V)$ (eV)



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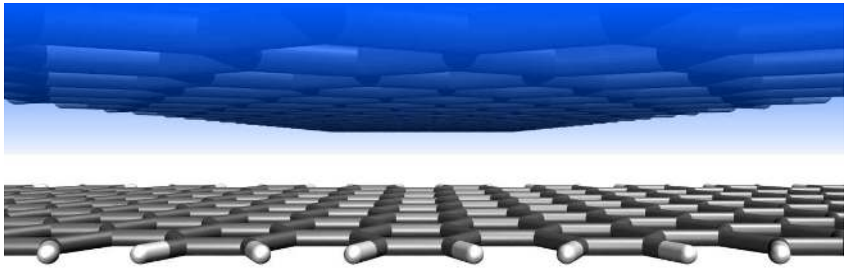
Electrostatic potential profile at V=0.5V



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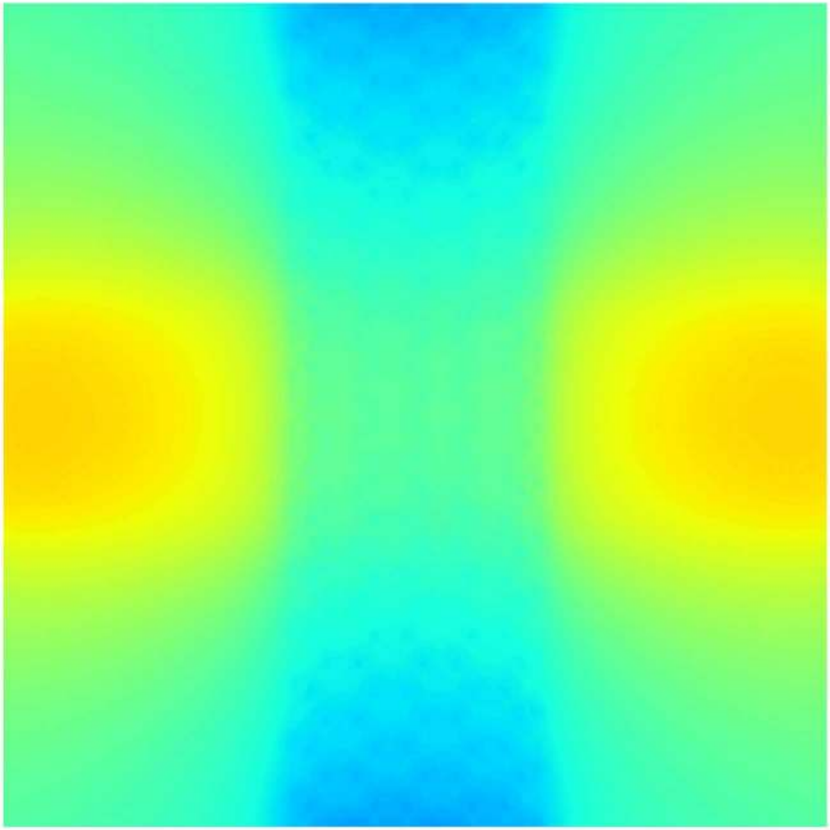

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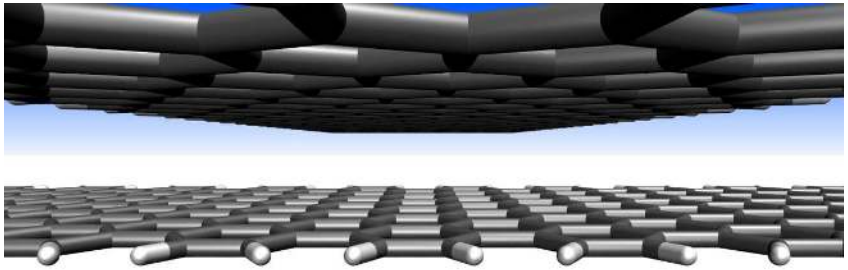
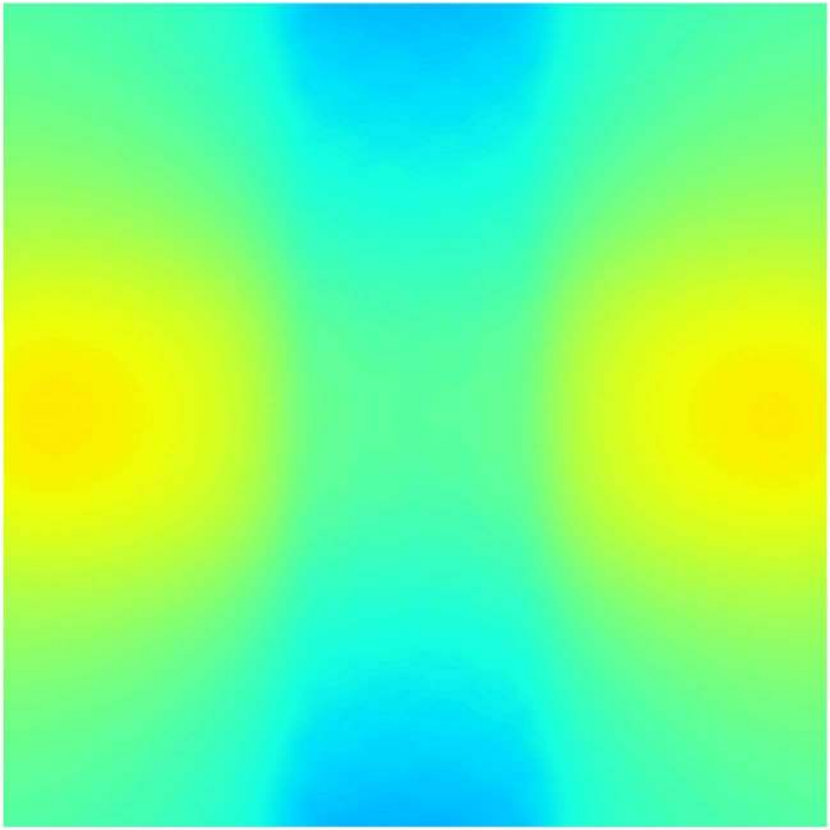
Electrostatic potential profile at V=0.5V



$U_H(V=0.5V)-U_H(V=0.0V)$ (eV)



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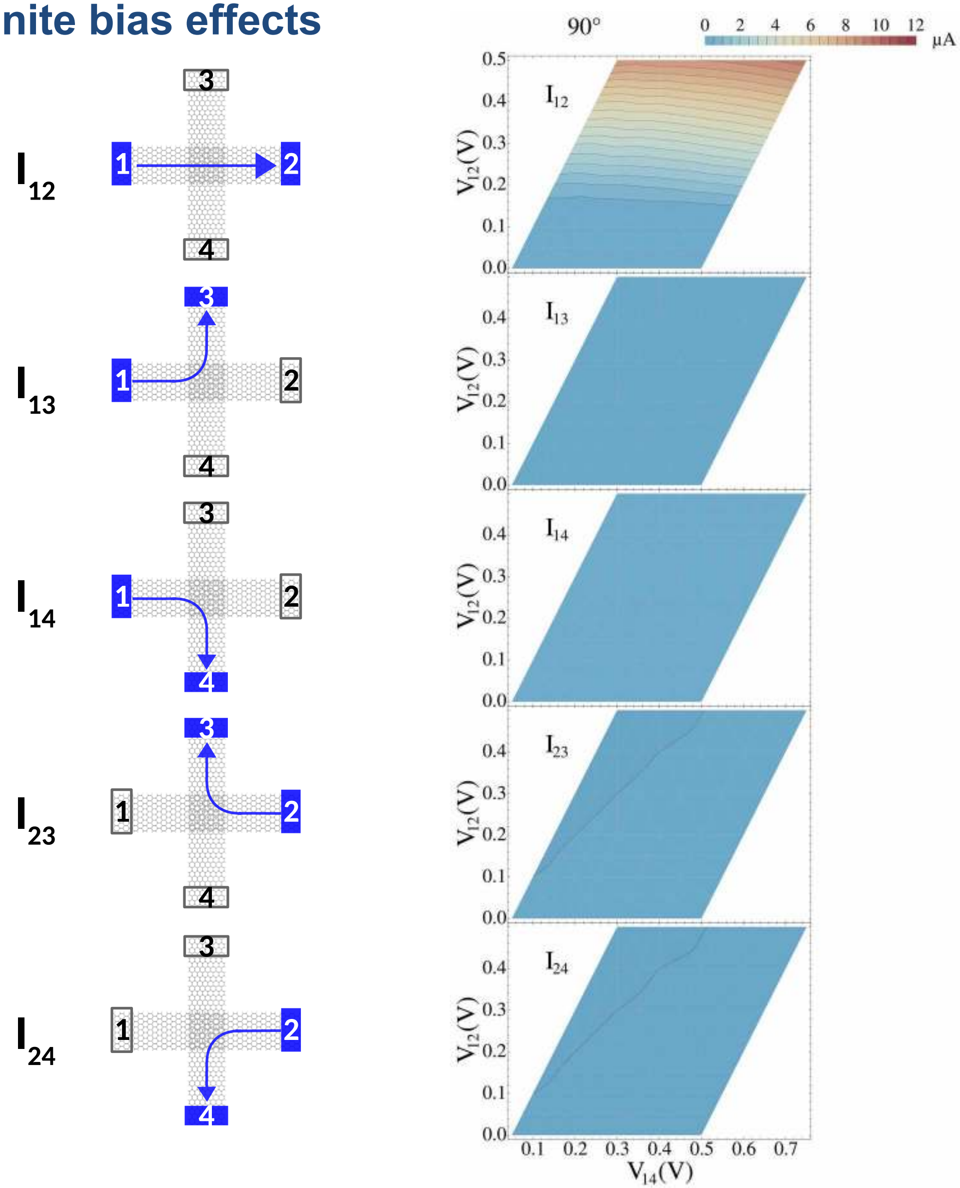
Finite bias effects



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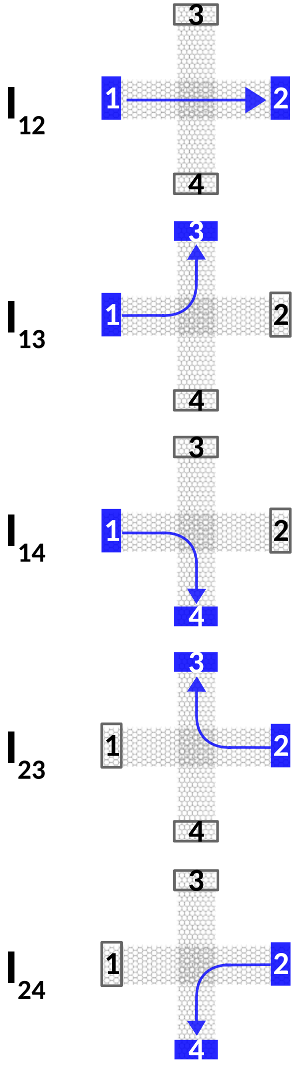
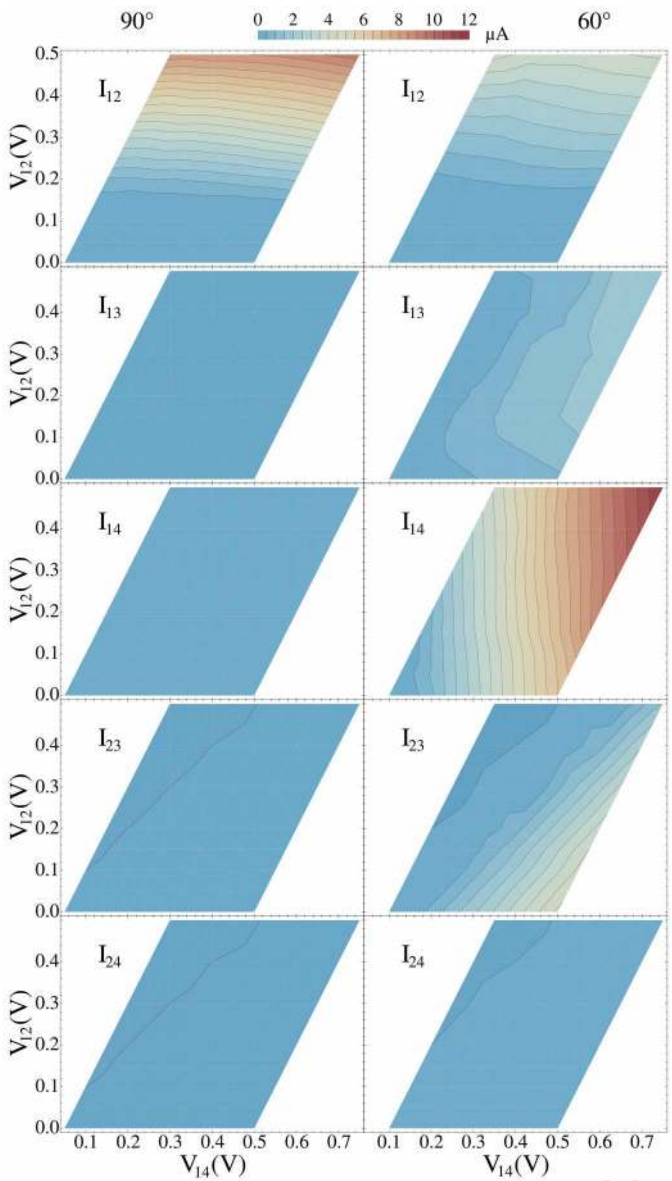
Finite bias effects





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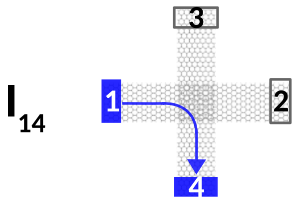
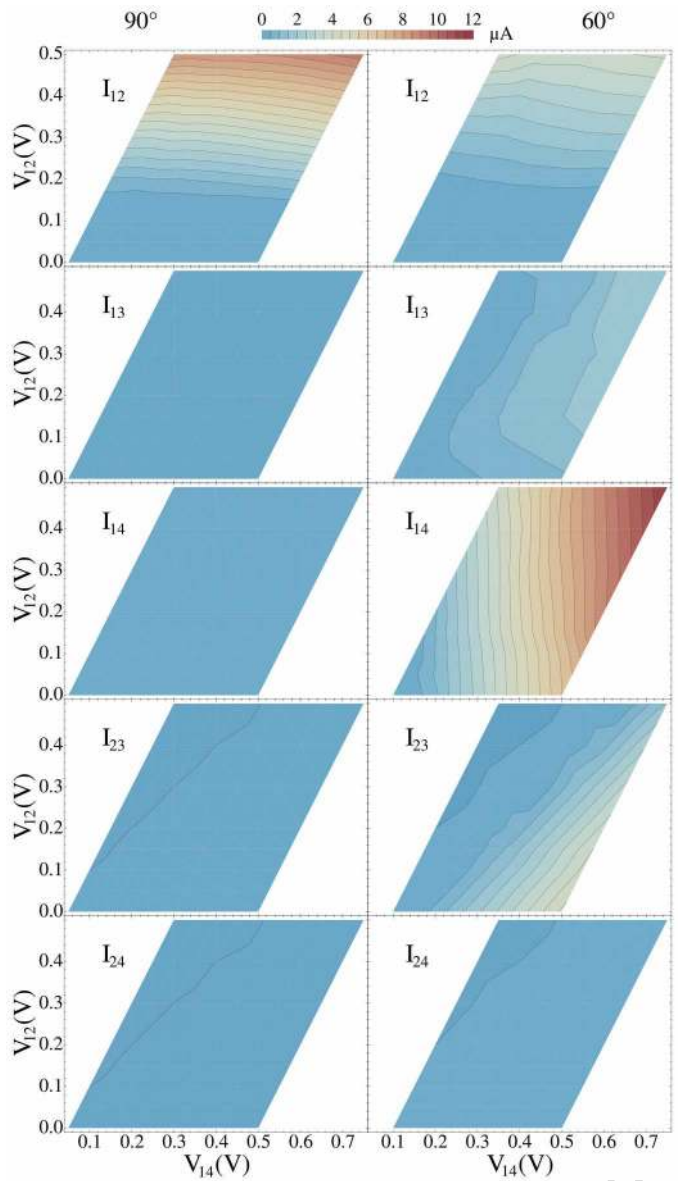
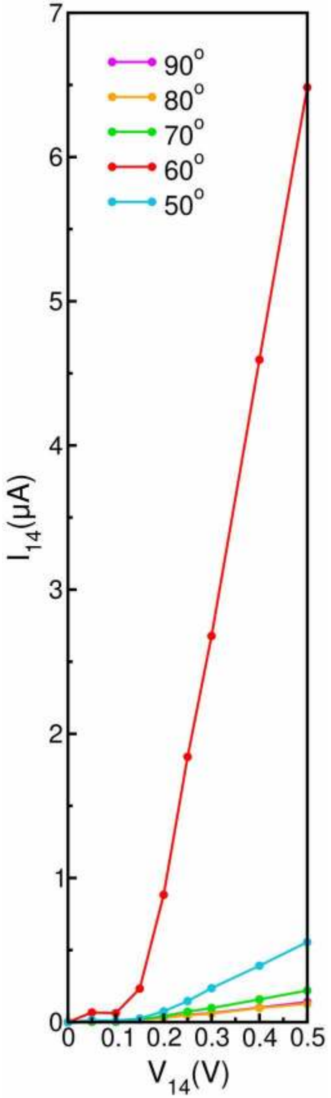
Finite bias effects



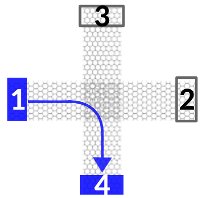


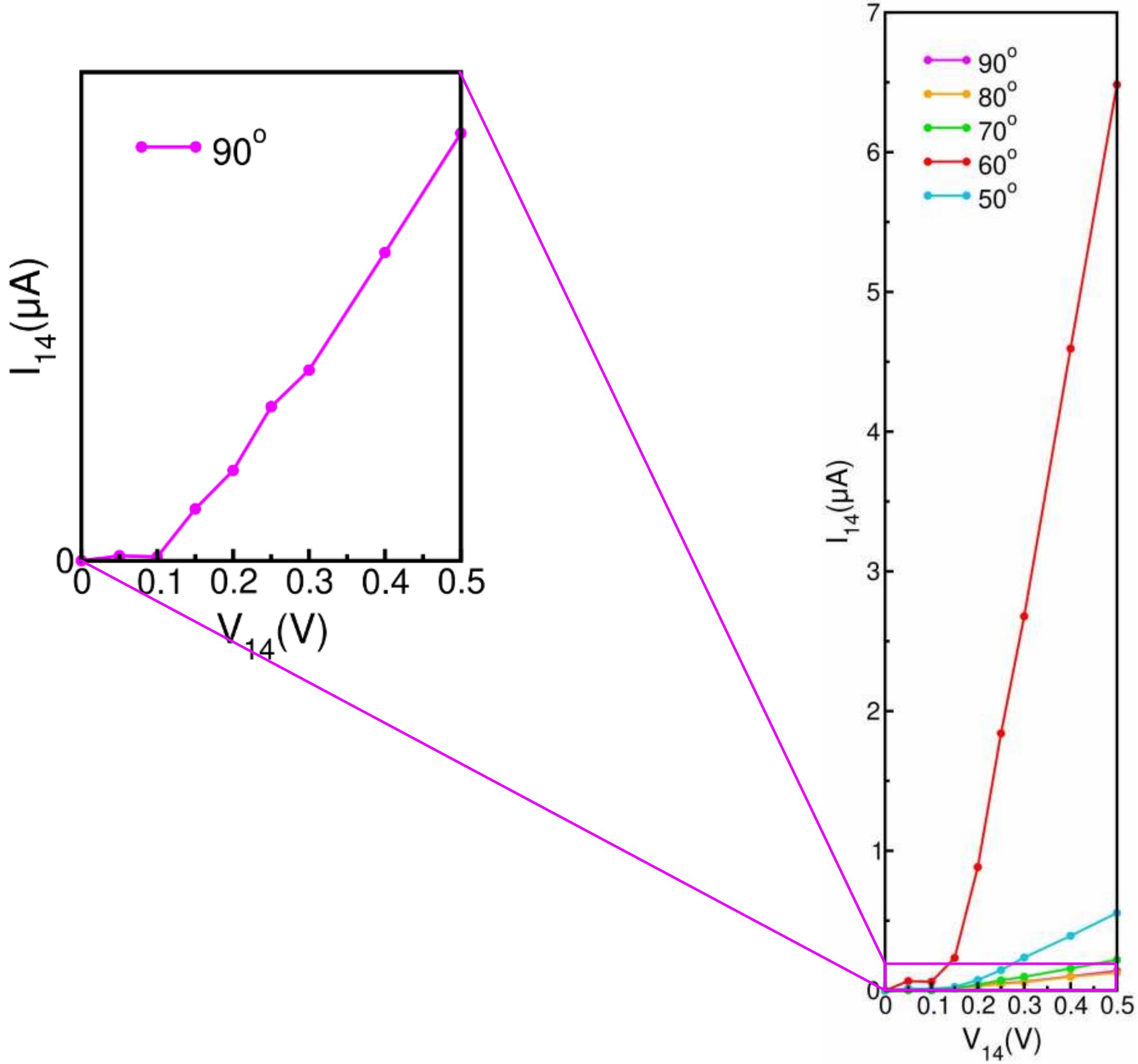


P. Brandimarte *et al*. *J. Chem. Phys.* **146**, 092318 (2017).

Finite bias effects

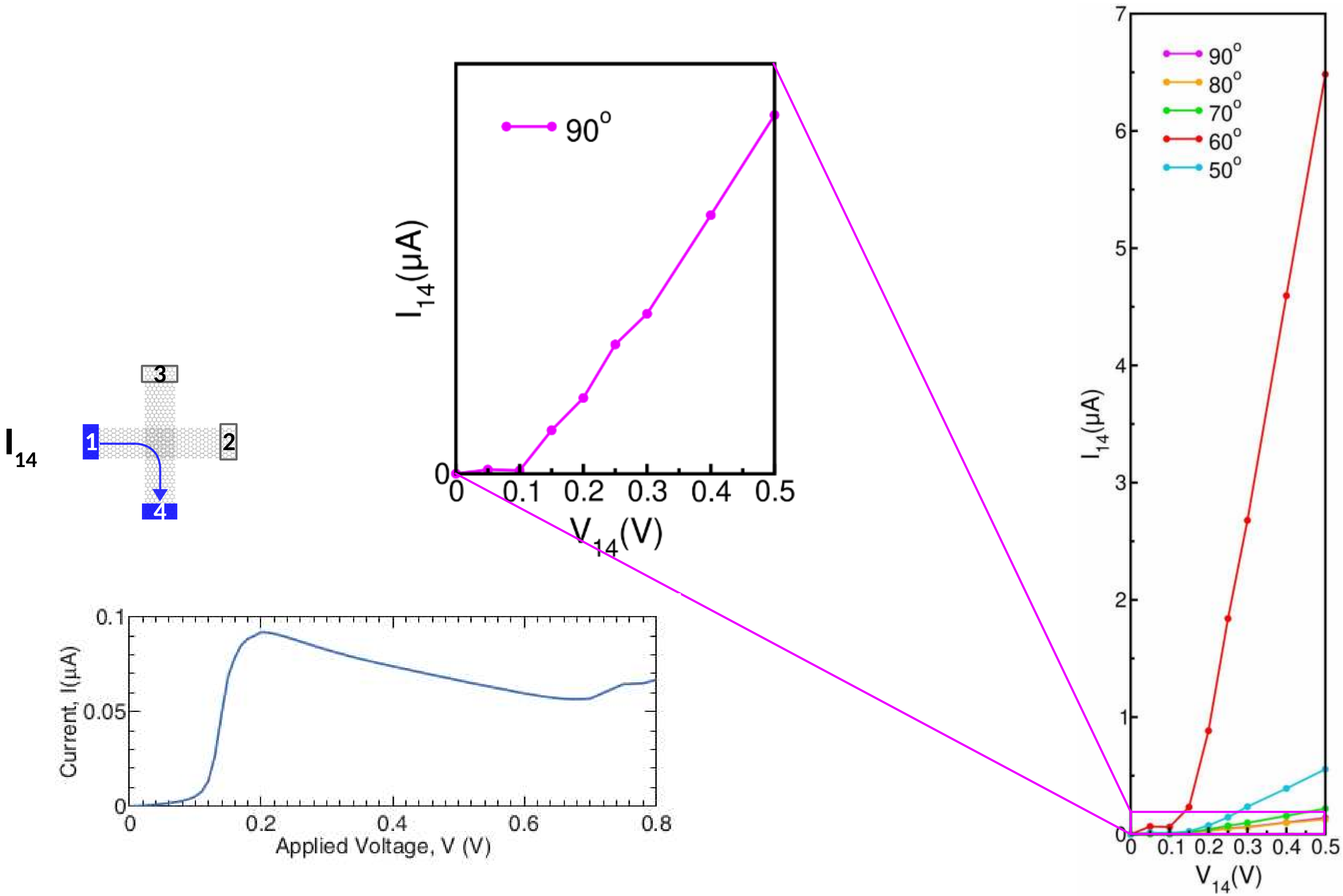
I_{14}





P. Brandimarte *et al*. *J. Chem. Phys.* **146**, 092318 (2017).

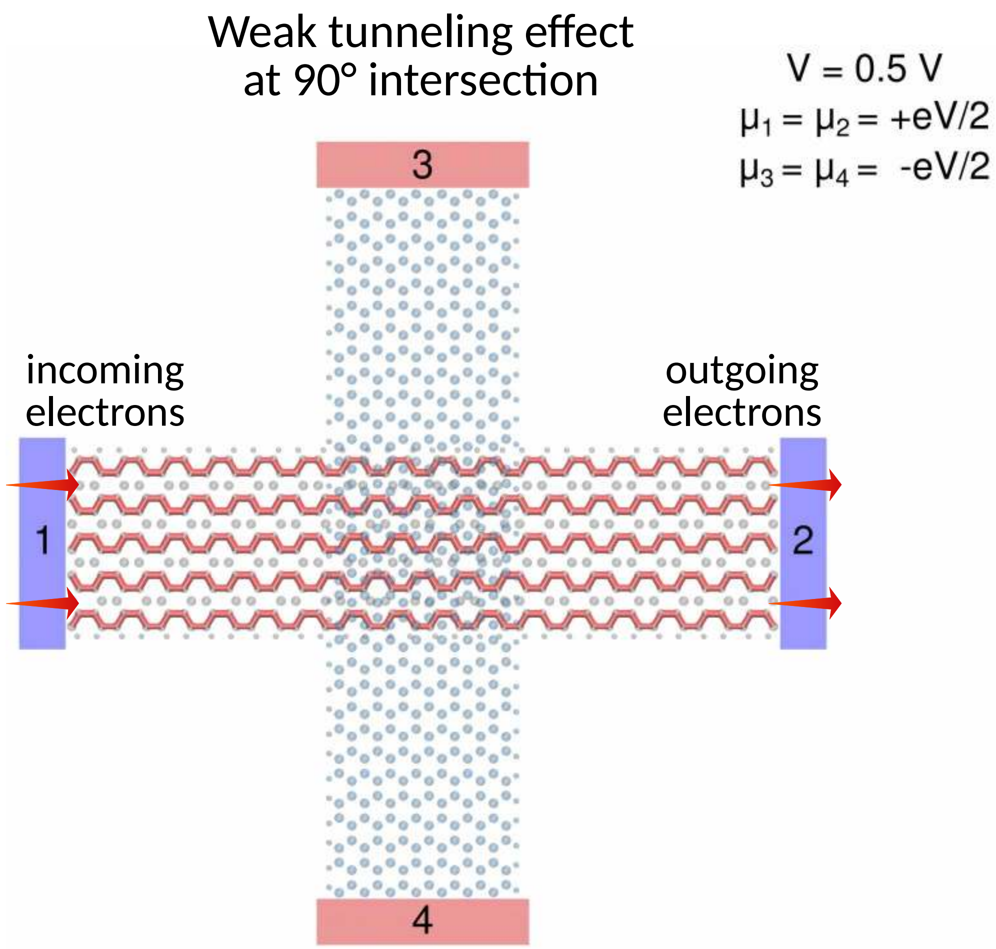
Finite bias effects



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

P. Brandimarte *et al*. *J. Chem. Phys.* **146**, 092318 (2017).

Bond currents



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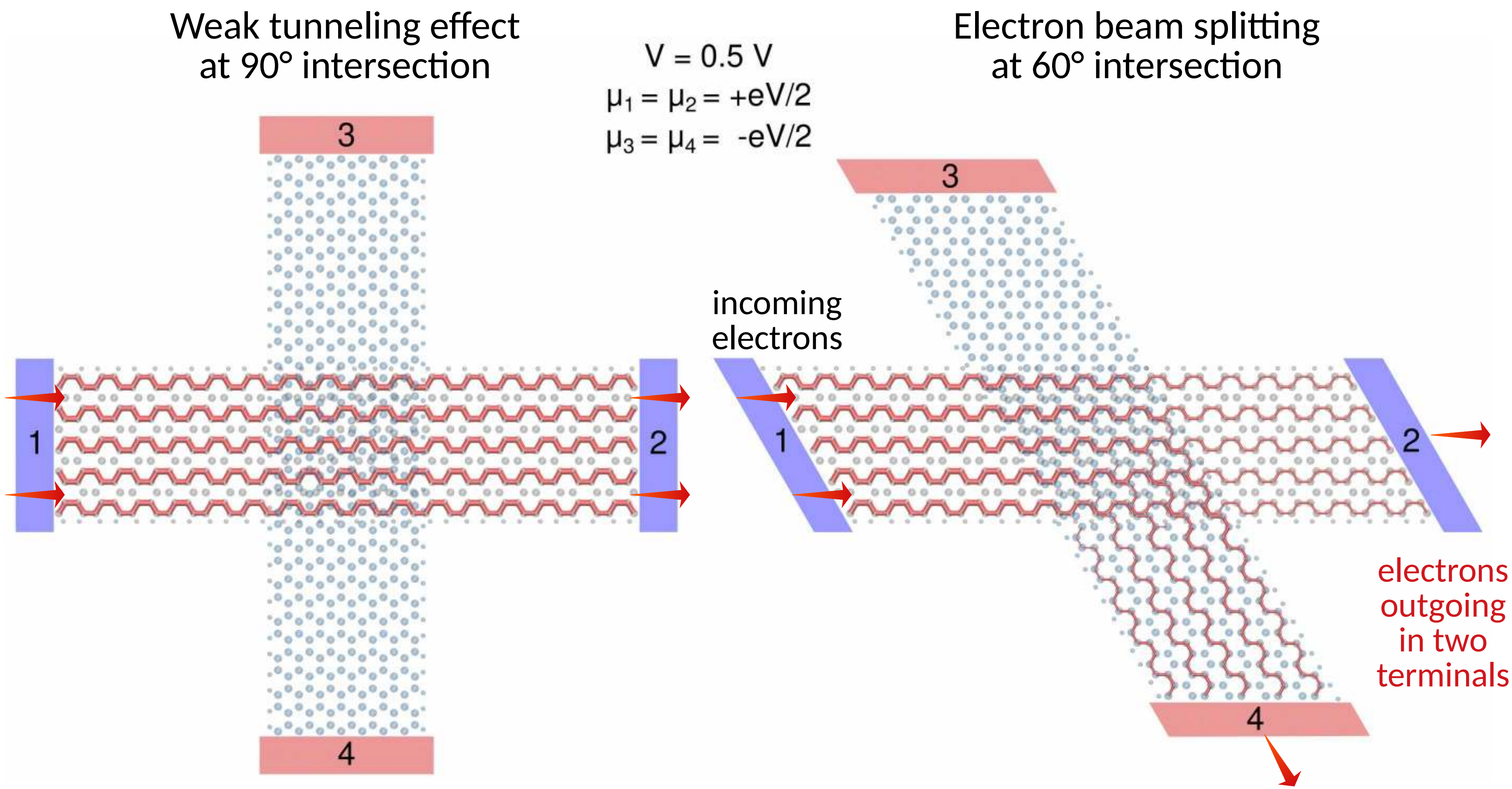
Bond currents



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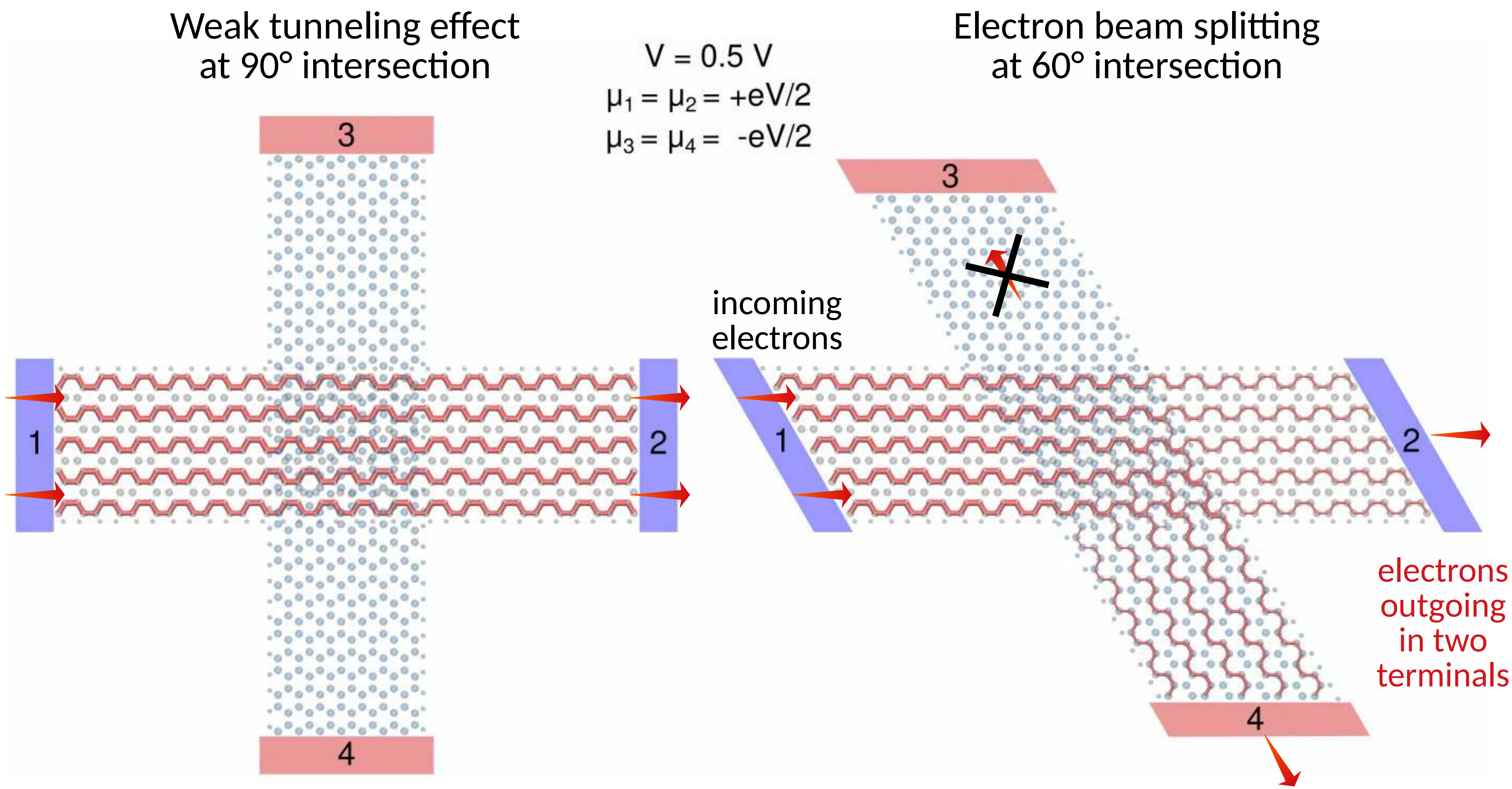
Bond currents



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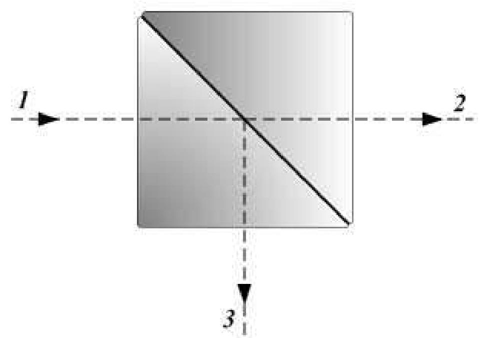
Bond currents

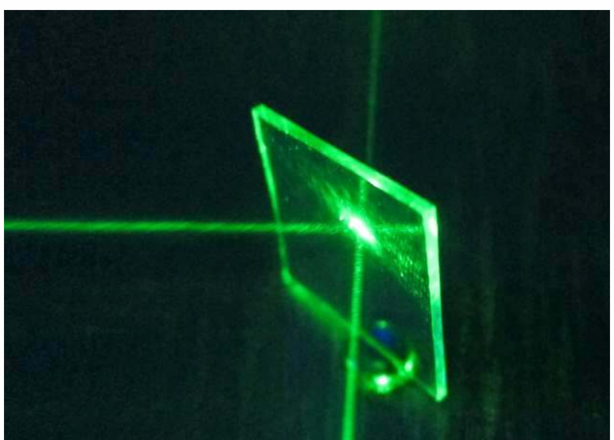
Beam splitter in optics

incident light



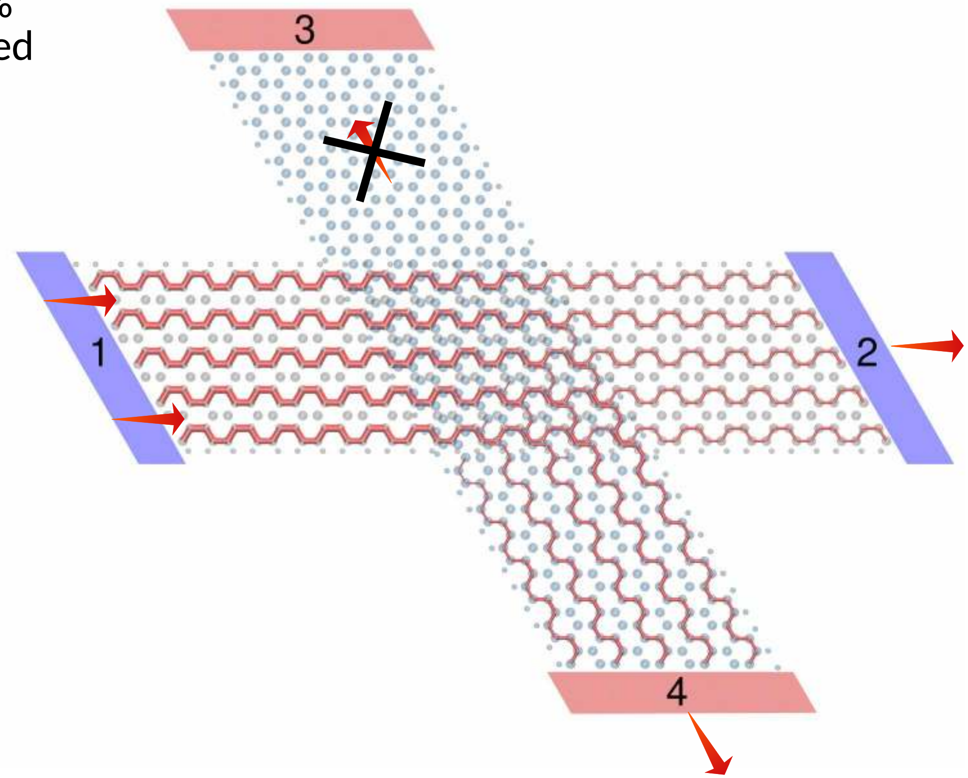
light 50% transmitted

light 50% reflected



(images: Wikipedia Commons)

Electron beam splitting at 60° intersection



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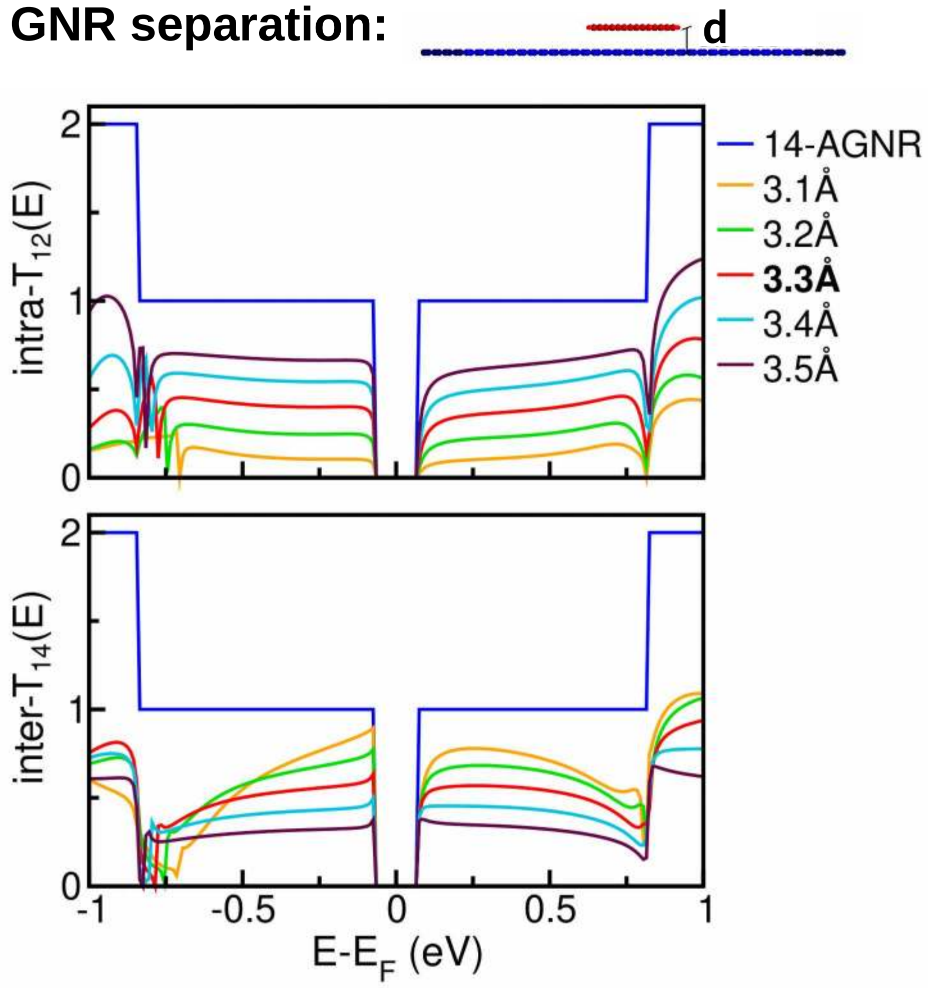
A tunable electron beam splitter at θ=60°

GNR separation:



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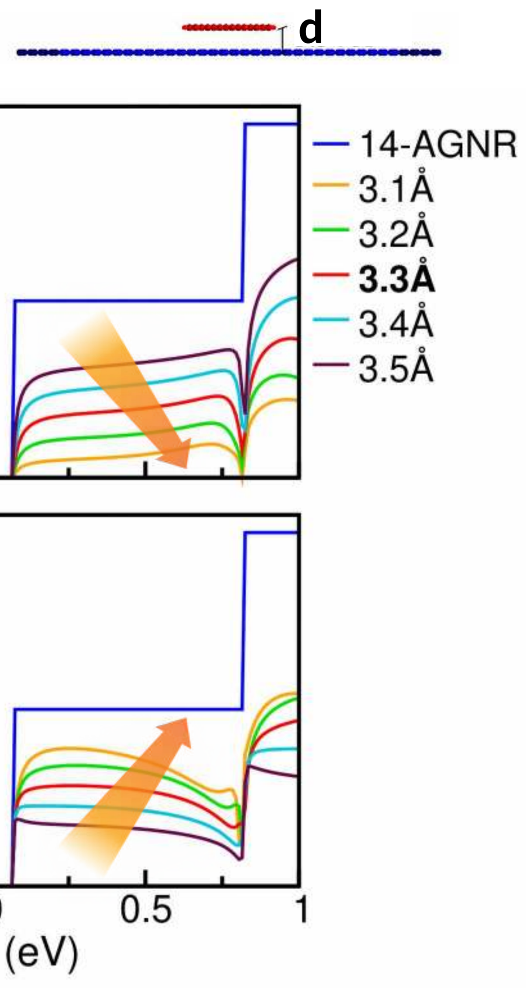
A tunable electron beam splitter at θ=60°

GNR separation:



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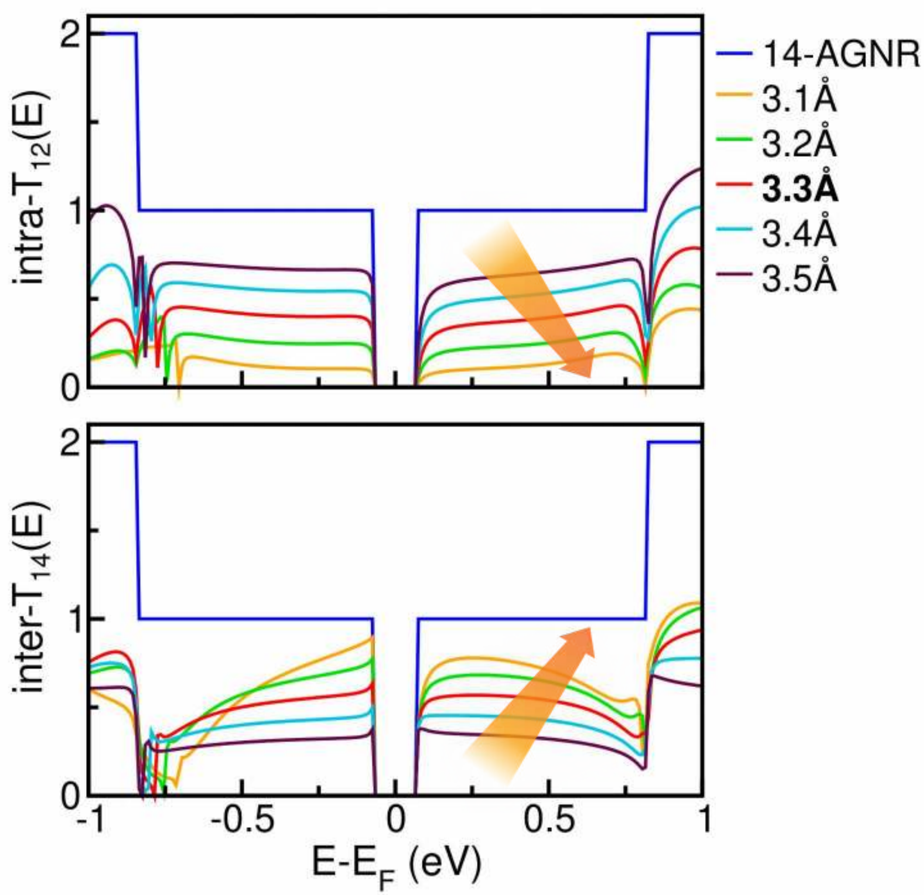
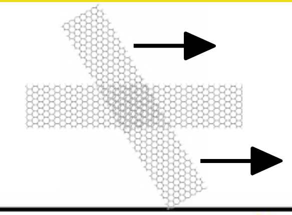
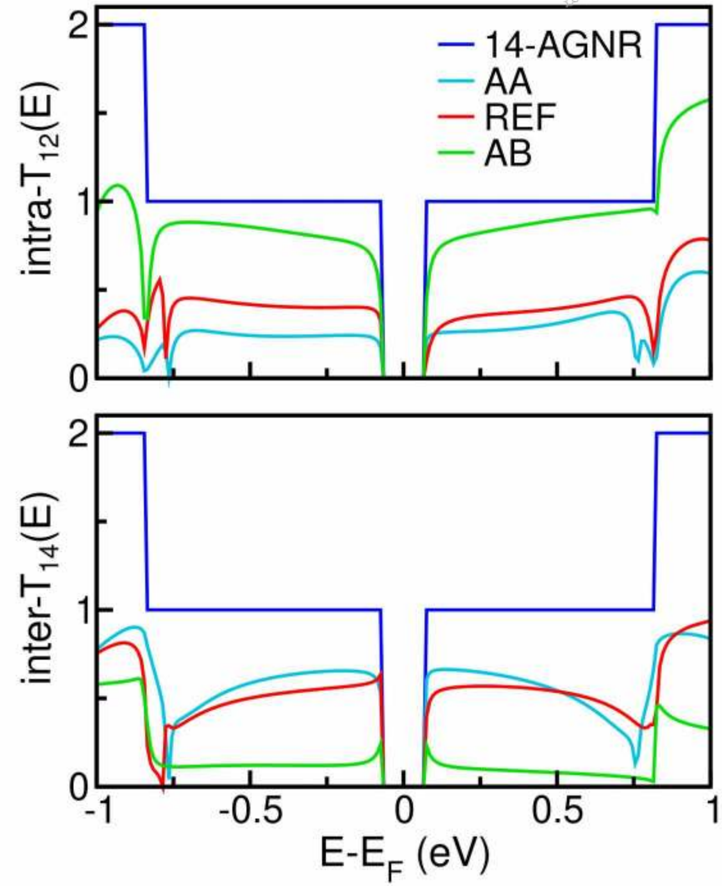
GNR separation:



GNR stacking:





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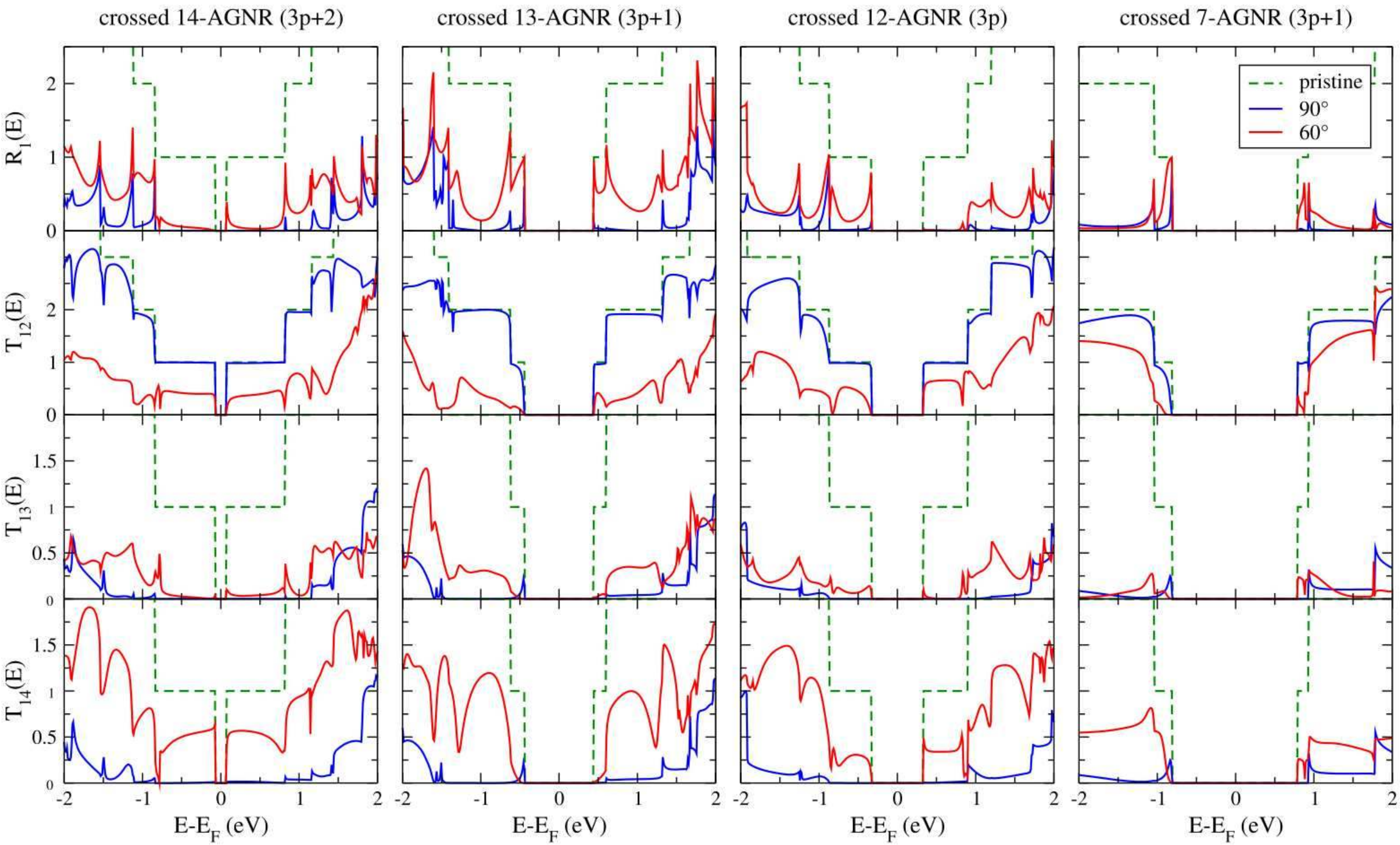
Role of GNR width



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Simple picture for the angle effect

Tunneling probability in perturbation theory:

$$T_{\mathrm{inter}} \propto \left|\langle \Psi_{\tilde{\mathbf{k}}_{\parallel},\tilde{\mathbf{k}}_{\perp}} | \Psi_{\mathbf{k}_{\parallel},\mathbf{k}_{\perp}} \rangle\right|^2$$

J. Bardeen. *Phys. Rev. Lett.* **6**, 57 (1961).

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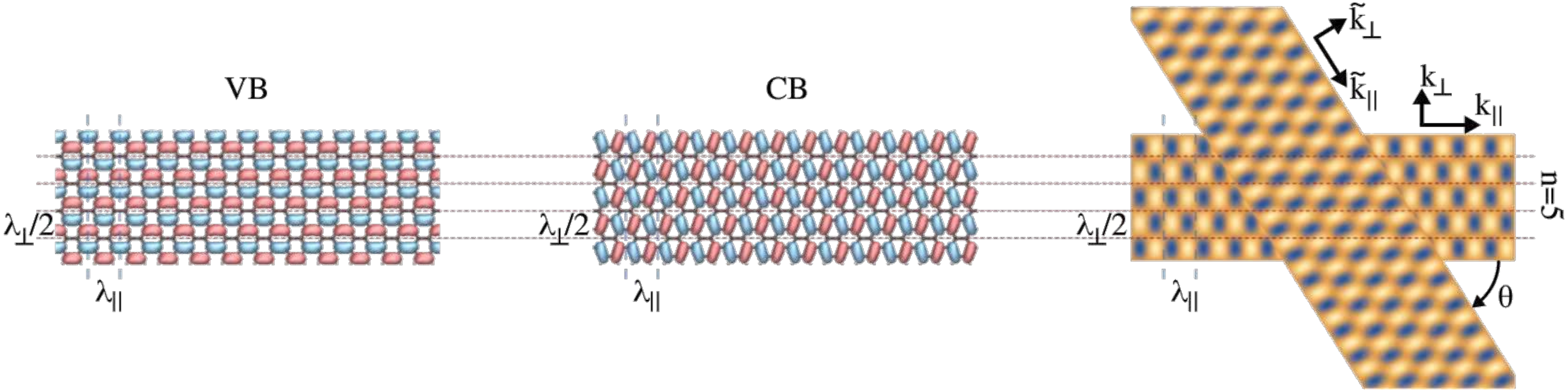
J. Bardeen. *Phys. Rev. Lett.* **6**, 57 (1961).

$$\langle \mathbf{r} | \Psi_{\mathbf{k}_{\parallel},\mathbf{k}_{\perp}} \rangle = \begin{cases} e^{-i\mathbf{k}_{\parallel}\cdot\mathbf{r}}\left(e^{-i\mathbf{k}_{\perp}\cdot\mathbf{r}} - e^{i\mathbf{k}_{\perp}\cdot\mathbf{r}}\right), & \mathbf{r} \in \mathrm{GNR} \\ 0, & \mathrm{elsewhere} \end{cases}$$



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J. Bardeen. *Phys. Rev. Lett.* **6**, 57 (1961).

$$\mathbf{k}_{\parallel} + \mathbf{k}_{\perp} = \tilde{\mathbf{k}}_{\parallel} \pm \tilde{\mathbf{k}}_{\perp} \longrightarrow \cos\theta^* = \frac{k_{\parallel}\tilde{k}_{\parallel} - k_{\perp}\tilde{k}_{\perp}}{k_{\parallel}^2 + k_{\perp}^2}$$

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Simple picture for the angle effect

Tunneling probability in perturbation theory: $T_{\text{inter}} \propto \left| \langle \Psi_{\tilde{\mathbf{k}}_{||},\tilde{\mathbf{k}}_{\perp}} | \Psi_{\mathbf{k}_{||},\mathbf{k}_{\perp}} \rangle \right|^2$

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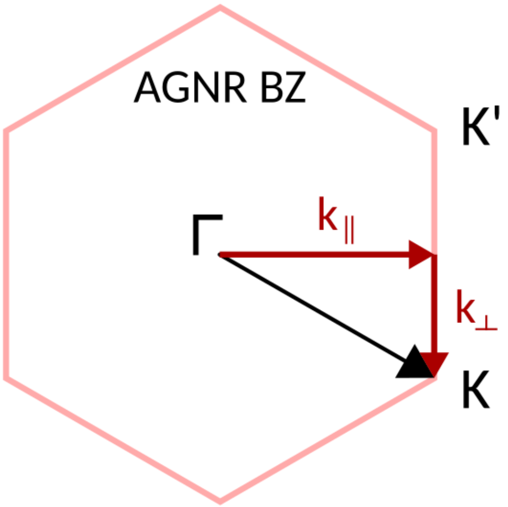

$$\frac{k_{||}}{k_{\perp}} = \sqrt{3} \longrightarrow \theta^* = 60^\circ$$

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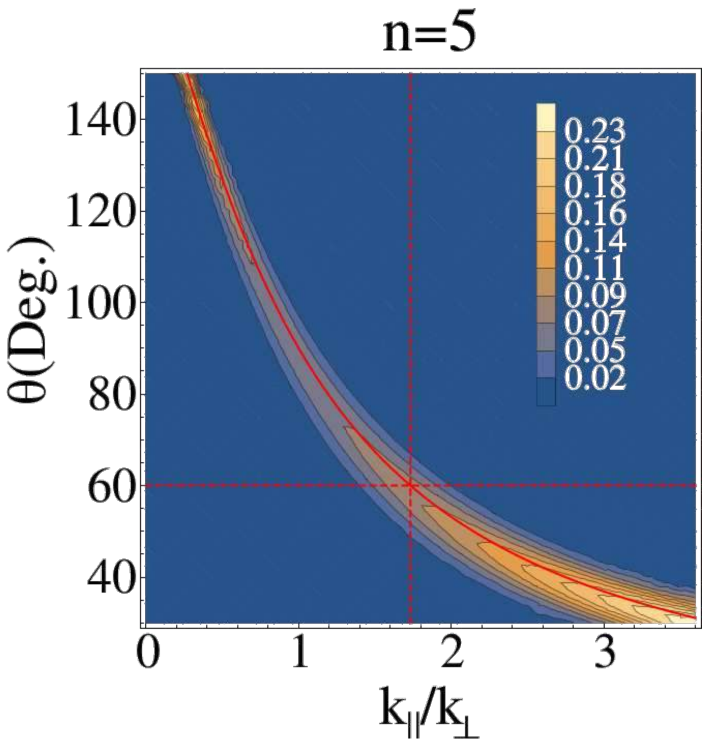
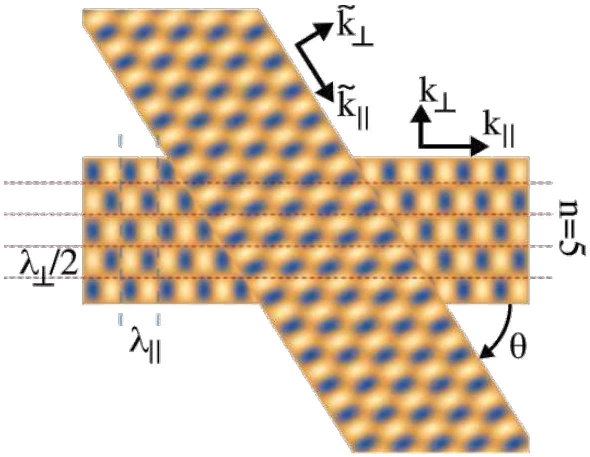
Simple picture for the angle effect

Tunneling probability in perturbation theory: $$T_{\text{inter}} \propto \left| \langle \Psi_{\tilde{\mathbf{k}}_{||},\tilde{\mathbf{k}}_{\perp}} | \Psi_{\mathbf{k}_{||},\mathbf{k}_{\perp}} \rangle \right|^2$$

J. Bardeen. *Phys. Rev. Lett.* **6**, 57 (1961).

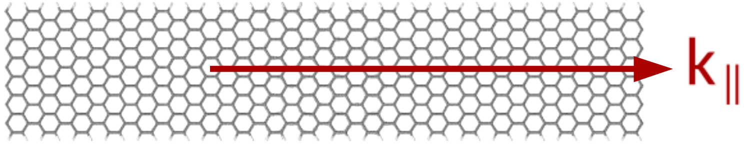


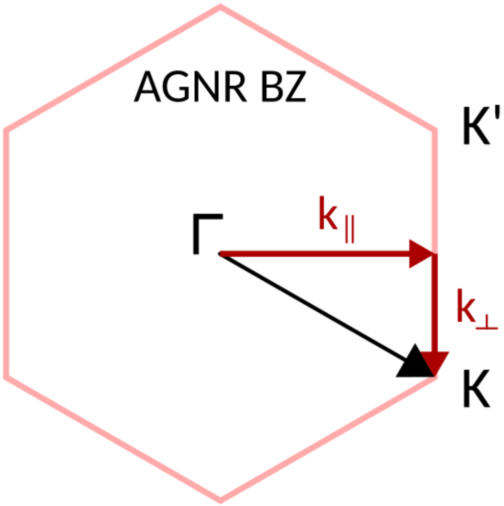


P. Brandimarte *et al*. *J. Chem. Phys.* **146**, 092318 (2017).

Pedro Brandimarte (brandimarte@pm.me)

Simple picture for the angle effect





P. Brandimarte *et al*. *J. Chem. Phys.* **146**, 092318 (2017).

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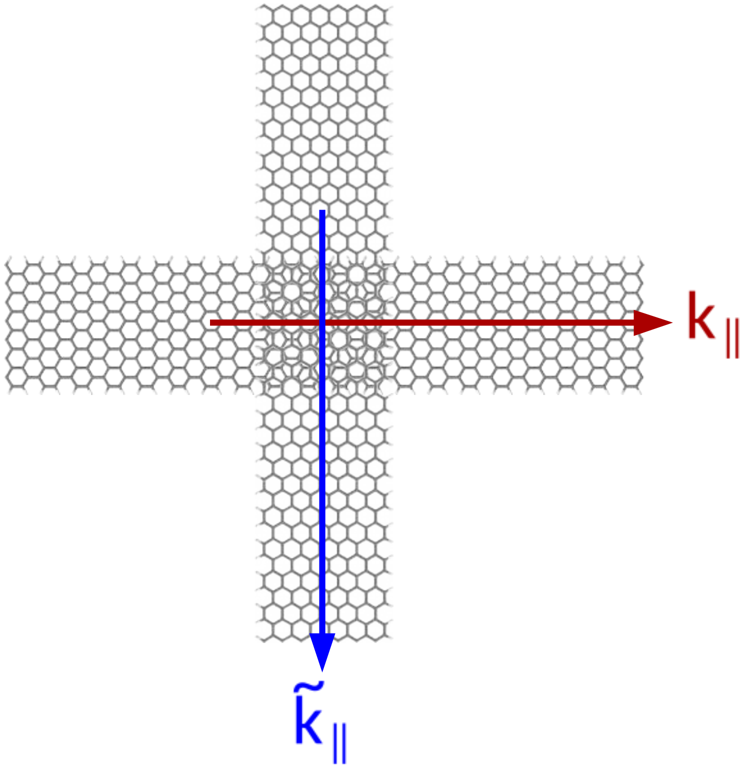

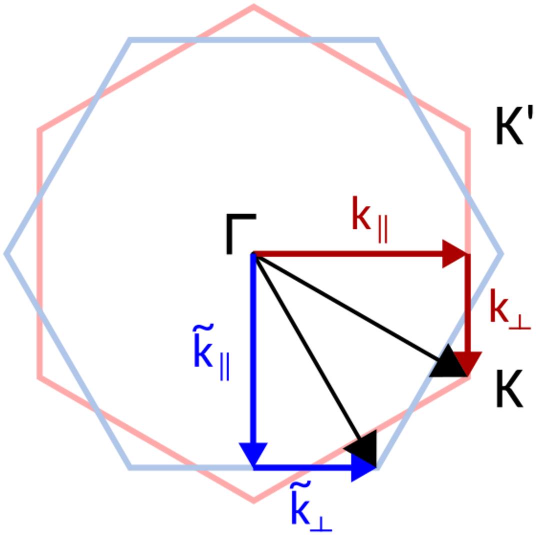

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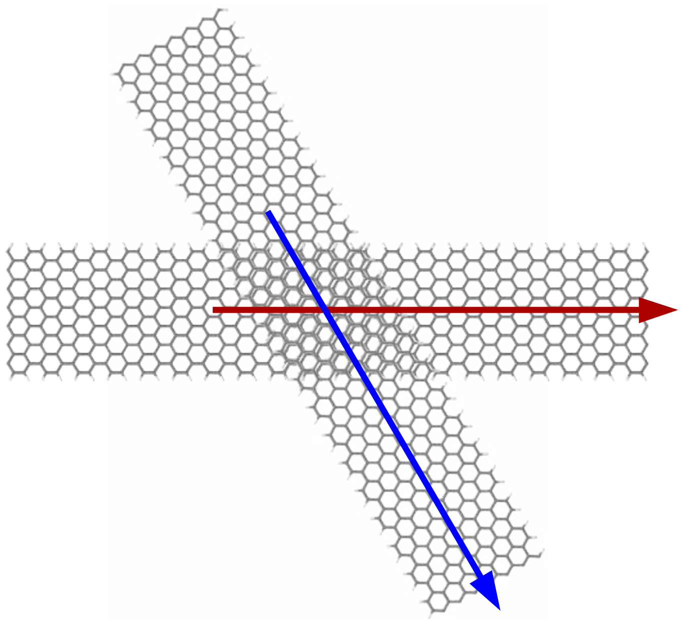
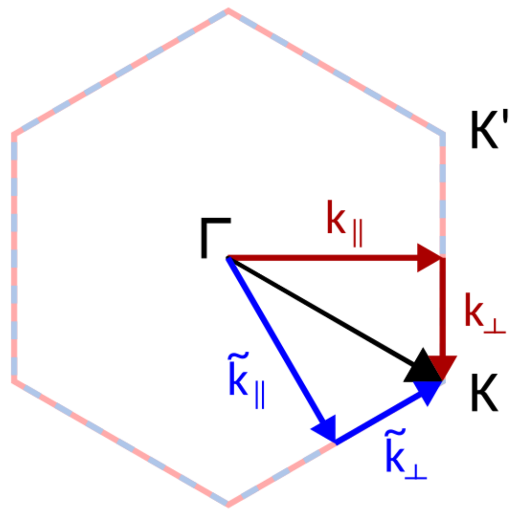
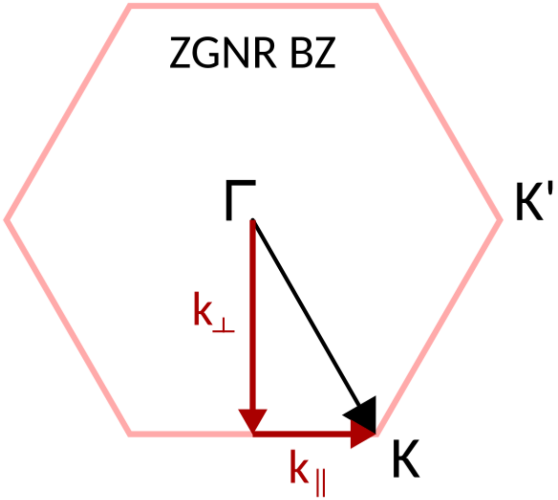


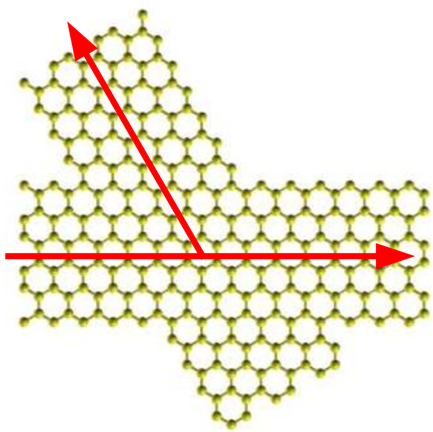


P. Brandimarte *et al*. *J. Chem. Phys.* **146**, 092318 (2017).

Does this applies to Zigzag GNRs?



$$\frac{k_{\parallel}}{k_{\perp}} = \frac{1}{\sqrt{3}} \longrightarrow \theta^* = 120^\circ$$



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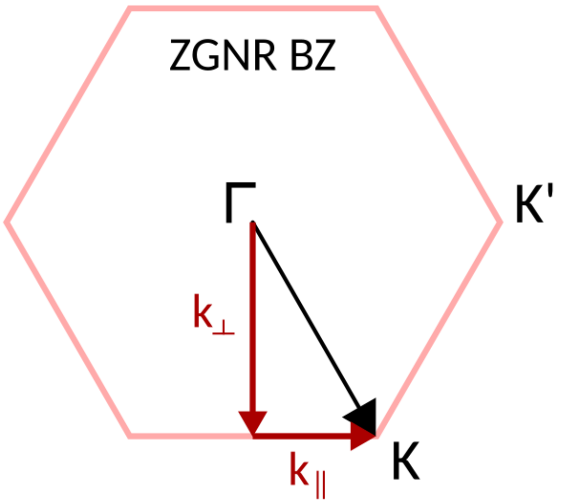
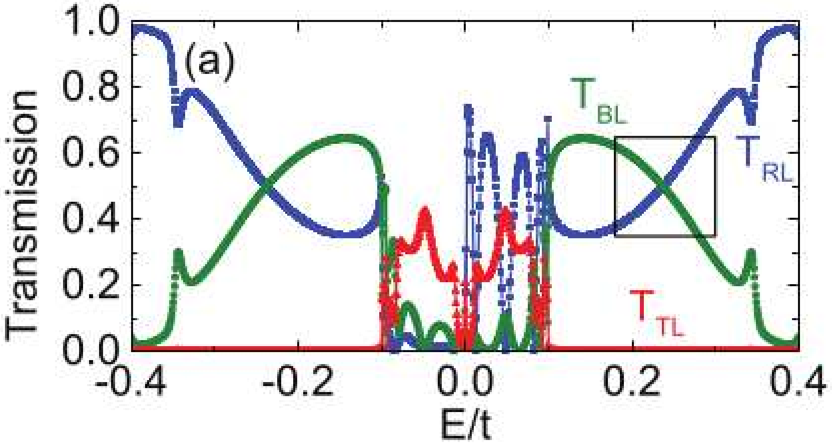


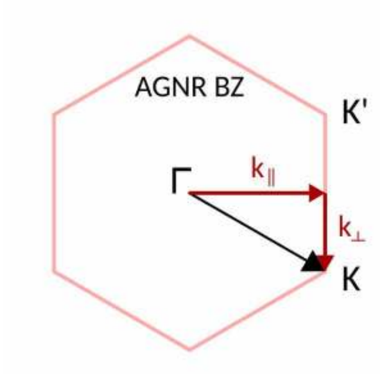
$$\frac{k_{\parallel}}{k_{\perp}} = \frac{1}{\sqrt{3}} \longrightarrow \theta^* = 120^\circ$$

In agreement with results based on a π tight-binding model by L. Lima *et al.* *J. Phys.: Cond. Matter* **28**, 505303 (2016).

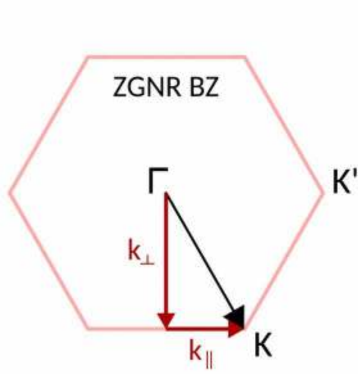


P. Brandimarte *et al.* *J. Chem. Phys.* **146**, 092318 (2017).

Now a homework!



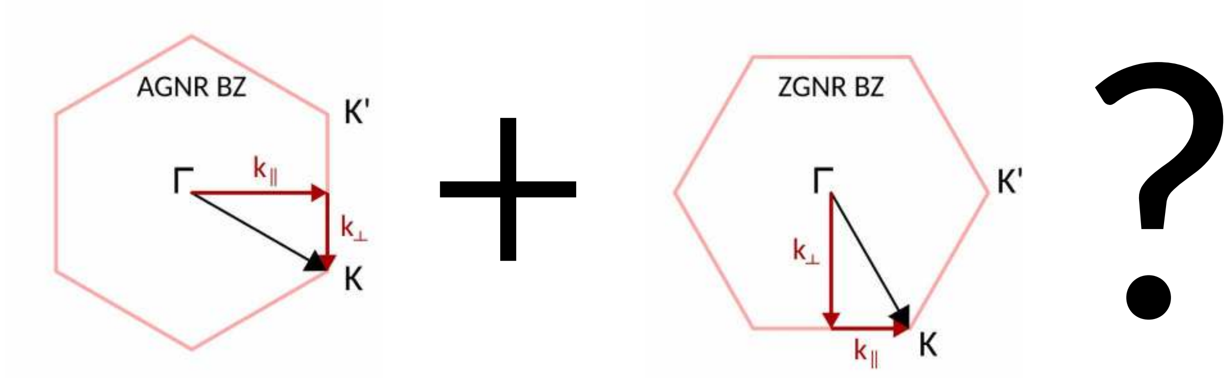
+



?

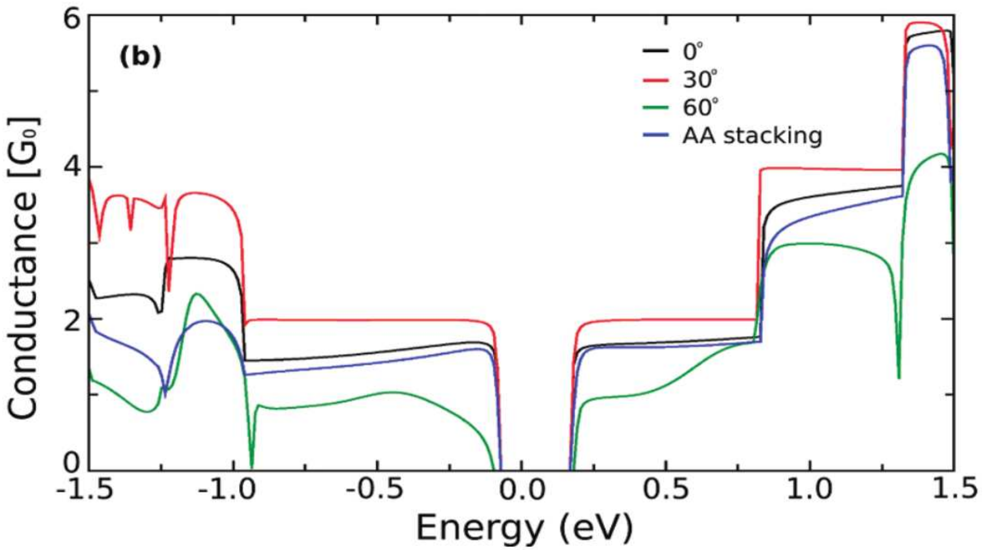
P. Brandimarte *et al*. *J. Chem. Phys.* **146**, 092318 (2017).

Now a homework!



!! 30° and 90° !!

In agreement with results from A. Botello-Méndez *et al*. *Nano Lett*. **11**, 3058 (2011).



P. Brandimarte *et al*. *J. Chem. Phys.* **146**, 092318 (2017).

Tight-binding model

Can we capture the beam splitting effect with two parameters?

$$H = t_0 \sum_{\mathrm{n.n}} (c_i^\dagger c_j + \mathrm{h.c.}) + t_\perp \sum_{\mathrm{n.n}} (c_{H,i}^\dagger c_{V,j} + \mathrm{h.c.})$$

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sisl

build passing | DOI 10.5281/zenodo.597181 | License LGPL v3 | chat on gitter

pypi package 0.9.2 | Anaconda Cloud 0.9.2 | codecov 85% | codacy A | Donate PayPal

The API documentation can be found here.

The sisl toolbox provides a simple API for manipulating, constructing and creating tight-binding matrices in a standard and uniform way.
Secondly, it provides easy interfaces for creating and calculating band-structures of simple tight-binding models as well as interfacing to more advanced DFT utilities.

sisl may also be used together with the ASE environment.

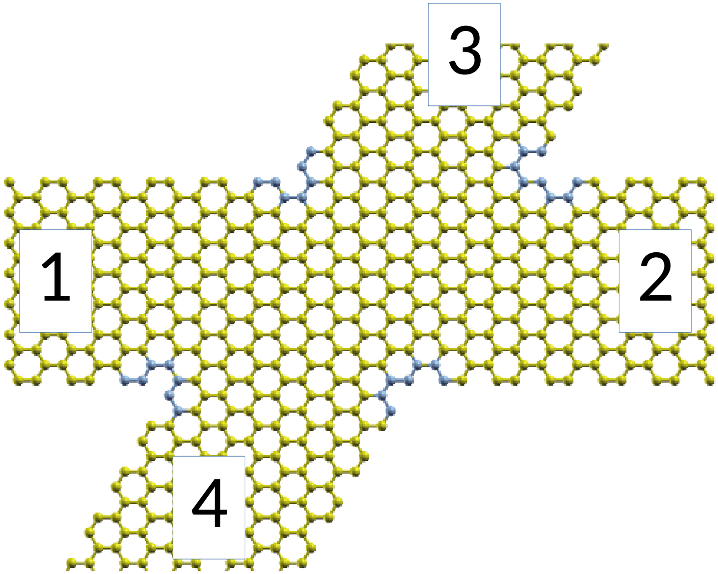
sisl provides an interface to TBtrans and enables the calculation of transport using the non-equilibrium Green function method and easily allows calculation of tight-binding systems of millions of atoms.

Nick Papior, https://github.com/zerothi/sisl .

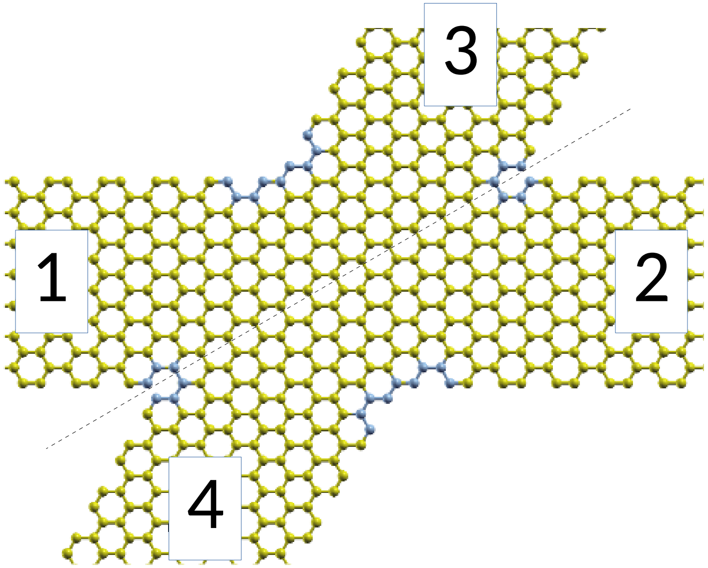
Tight-binding model

Two AA stackings:

asymmetric



symmetric



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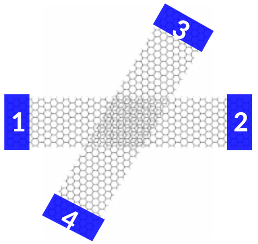
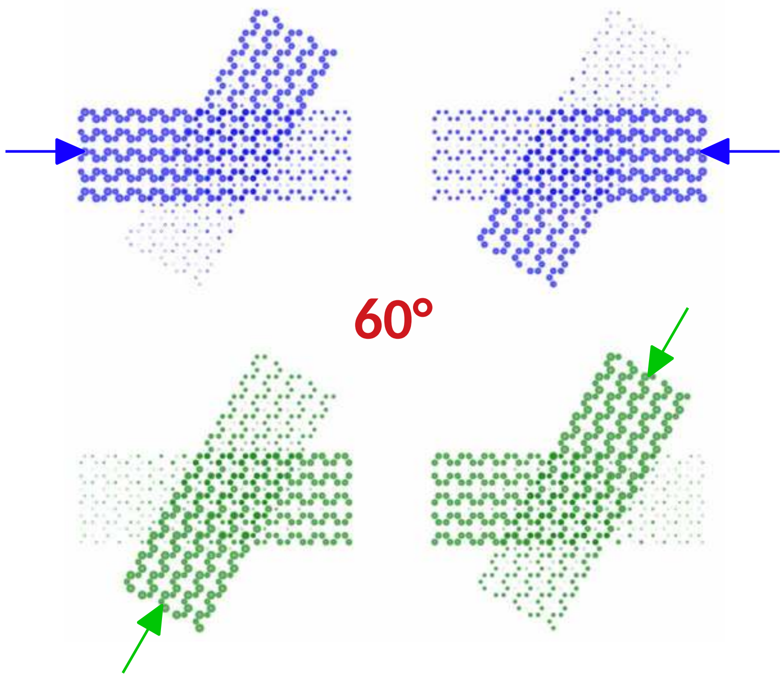
Tight-binding model

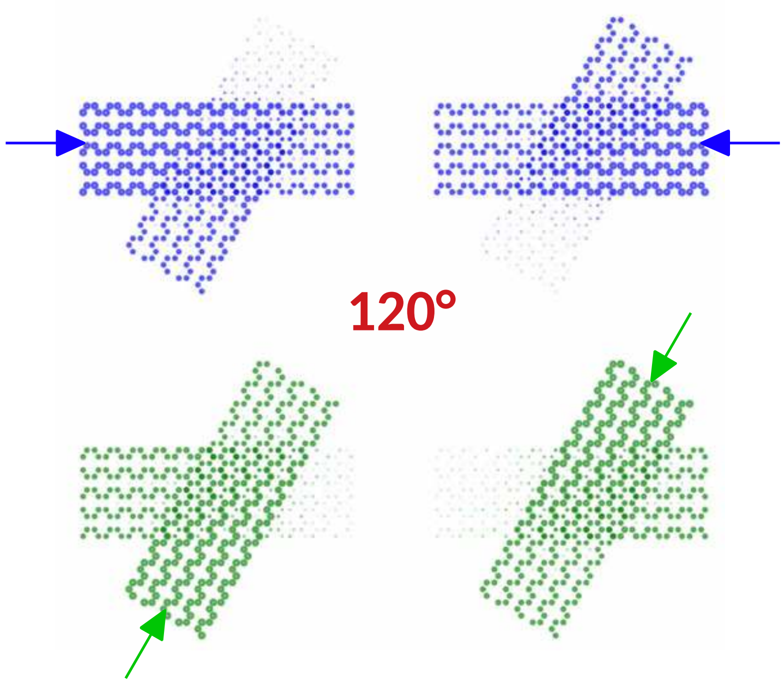
Spatially resolved electrode-induced DOS: $\mathbf{A}_i = \mathbf{G}\mathbf{\Gamma}_i\mathbf{G}^\dagger$



asymmetric



symmetric



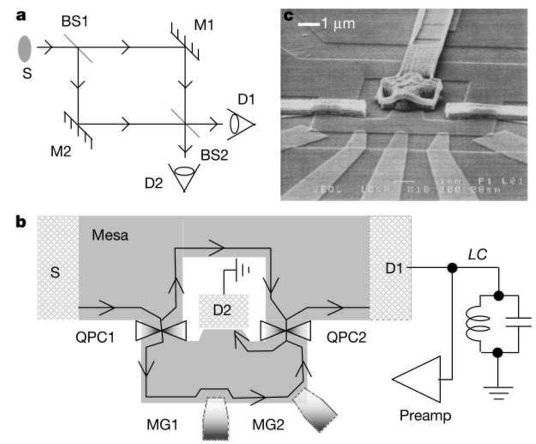
Conclusions

- Crossing GNRs can act as **electron beam splitter**
  - ✗ **50-50 splitting** of incident waves to outgoing terminals
  - ✗ **negligible** back-reflection
  - ✗ **tunable** devices (pressure/translation)
  - ✗ similar effects with **other GNRs**

What’s next?

An electronic Mach–Zehnder interferometer

Yang Ji, Yunchul Chung, D. Sprinzak, M. Heiblum, D. Mahalu & Hadas Shtrikman

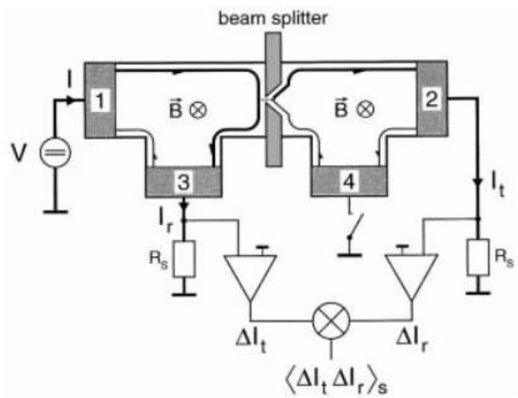


J. Yang *et al*. *Nature* **422**, 415 (2003).

The Fermionic Hanbury Brown and Twiss Experiment

M. Henny,[1] S. Oberholzer,[1] C. Strunk,[1] T. Heinzel,[2] K. Ensslin,[2] M. Holland,[3] C. Schönenberger[1*]

A Hanbury Brown and Twiss experiment for a beam of electrons has been realized in a two-dimensional electron gas in the quantum Hall regime. A metallic split gate serves as a tunable beam splitter to partition the incident beam into transmitted and reflected partial beams. In the nonequilibrium case the fluctuations in the partial beams are shown to be fully anticorrelated, ...lude each other. In equilibrium, the cross-



M. Henny *et al*. *Science* **284**, 296 (1999).

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Thank you!

PAMS

SEVENTH FRAMEWORK PROGRAMME

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CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS