“Phenomenological Electronic Transport”:

= Quantitative theoretical predictions of quantum transport:
The DFT-NEGF method (incl. spin-orbit)

Mads Brandbyge

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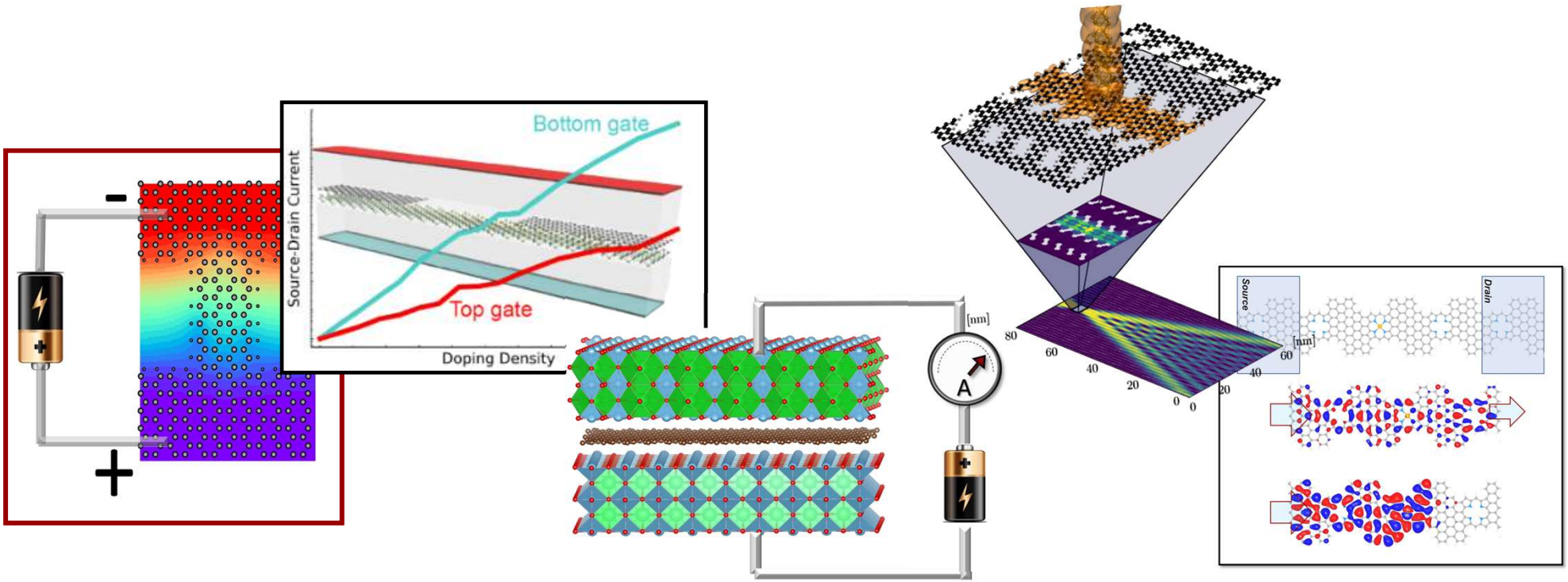

Thanks/Gracias/Eskerrik asko/Tak/Danke

Dr.
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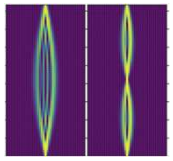

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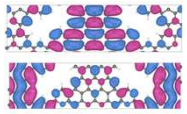

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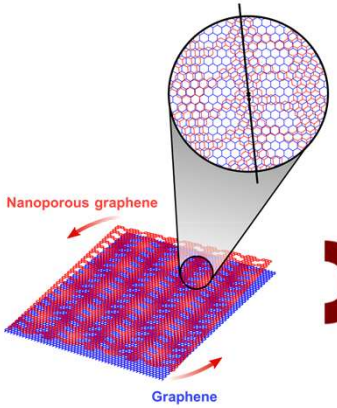

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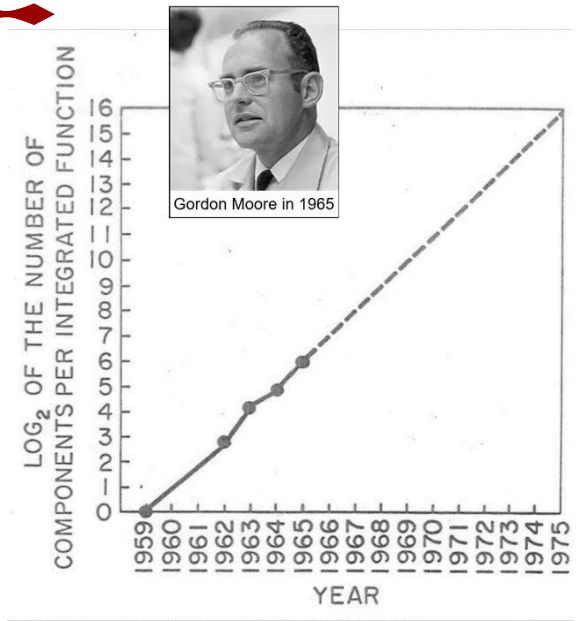
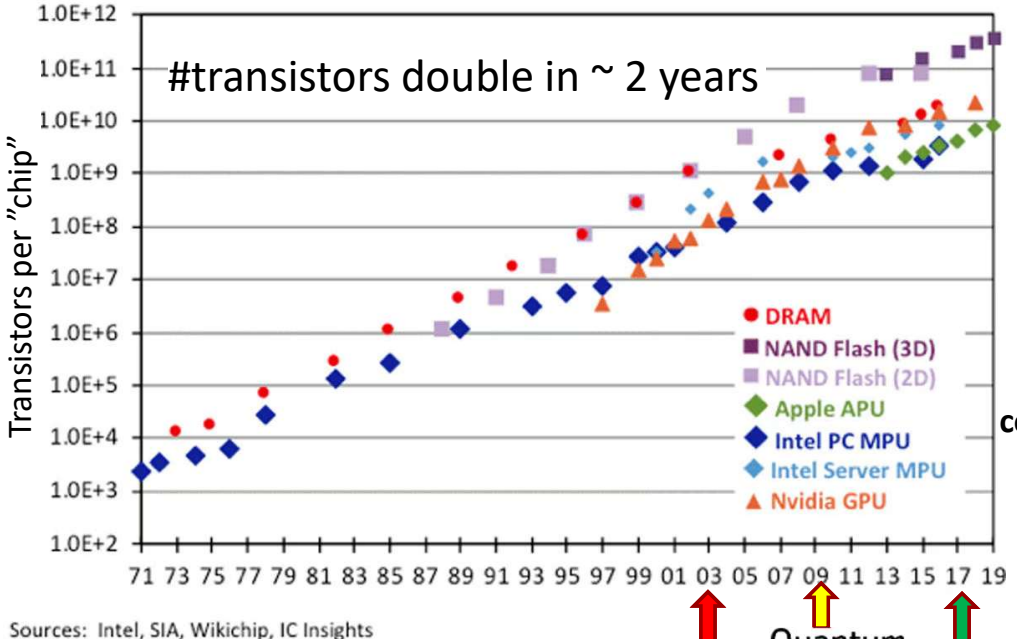
Outline

- **Motivation: “Quantum materials”/Landauer’s transport**
- **Theoretical methodology – a crash-course on DFT-NEGF**
- **Examples**
  - **Non-equilibrium & Gate effects in 2D devices**
  - **Current-only calculations**
  - **Large-scale systems: Nano-porous graphene**
  - **Spin-filtering in porphyrin-GNR hybrids**

Moore's "law"





DFT-NEGF in commercial software:

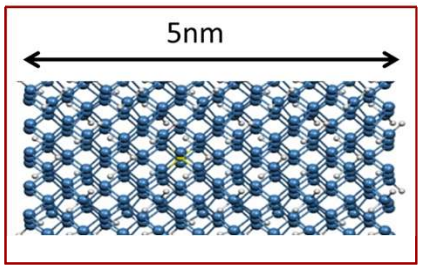
Dr. Kurt Stokbro

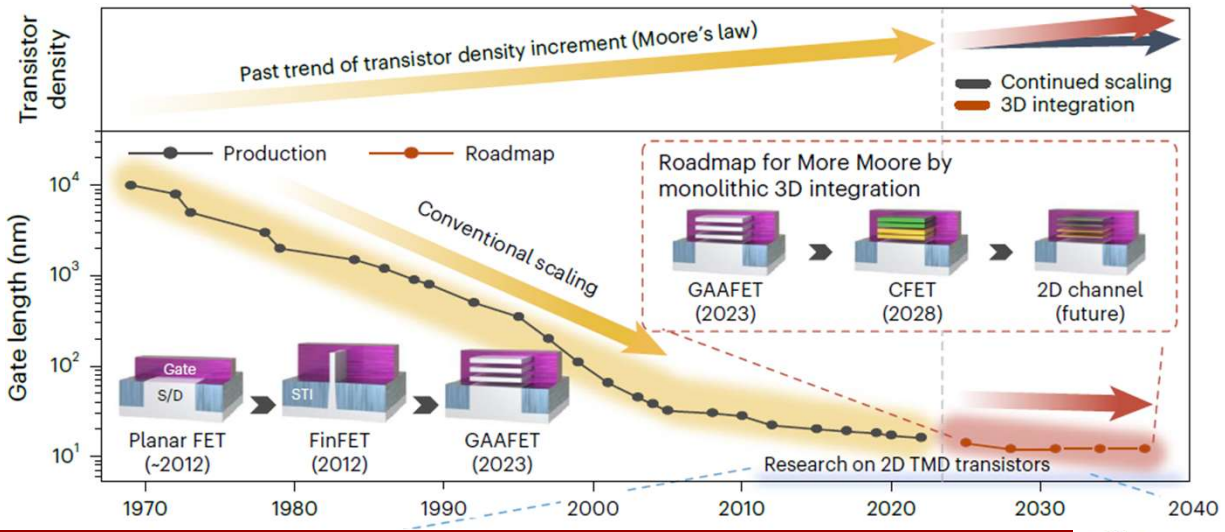
atomistix

Quantum Wise
When every atom matters

SYNOPSYS®
Silicon to Software™

- Scaling in transistor size stopped at ~ 10nm:





Nature Nano. 895, 19 (2024)

2DPHYS 2D MATERIALS ENGINEERING AND PHYSICS

”Quantum Materials”

what is the definition of a "quantum material"?

”Quantum Materials”

what is the definition of a "quantum material"?

Tænkte i et par sekunder ›

A **quantum material** is a material whose important properties are governed by **quantum-mechanical effects that remain visible at macroscopic or device-relevant scales**, rather than only at the atomic scale.

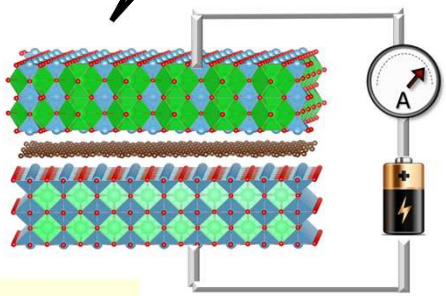
In practice, the term is used for materials where phenomena such as **electron spin, quantum coherence, entanglement, topology, strong electron–electron interactions, or superconductivity** determine how th material behaves.

Common examples include:

- **Superconductors**, where electrons form collective quantum states with zero resistance.
- **Topological insulators**, which conduct on their surfaces but not in their interiors.
- **Quantum magnets**, where spin interactions produce unusual magnetic states.
- **2D materials** such as graphene and moiré materials, where quantum effects can be tuned strongly.
- **Strongly correlated materials**, where electrons cannot be treated as mostly independent particles.

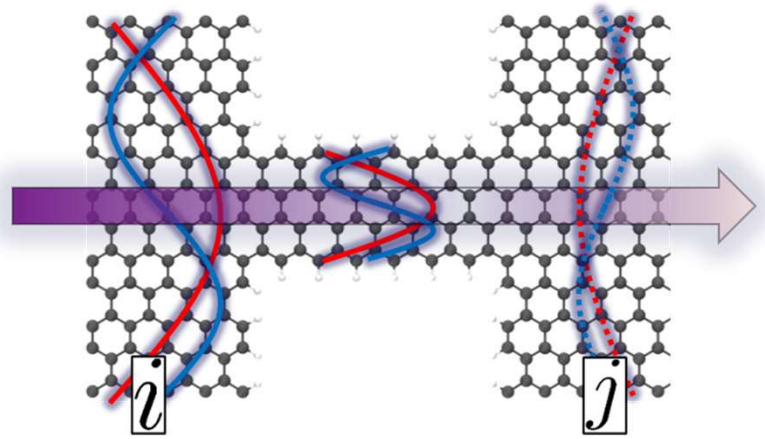
There is not one universally strict definition. In a broad sense, *all* materials obey quantum mechanics, but “quantum material” usually means a material where **nontrivial quantum effects are central to its useful or unusual properties**.

Device:
atomic in one direction
”Interface=Device”



Coherent waves: Landauer formula

Rolf Landauer (1927-99)



- Single particles
- Phase-coherence, energy (E) conservation
- Transmission amplitude matrix: $\mathbf{t}_{ij}$

$$T(E) = \mathrm{Tr}[\mathbf{t}^\dagger \mathbf{t}](E)$$

$$I(V) = G_0 \int_{\mu_L}^{\mu_R} dE\ T(E)$$

$$G_0 = \frac{2e^2}{h} \approx 77.5\mu S \approx 1/(12.9k\Omega)$$

$$G = G_0 T(E_F)$$

Quantum conductance = Quantum transmission

Ballistic transport at room temperature

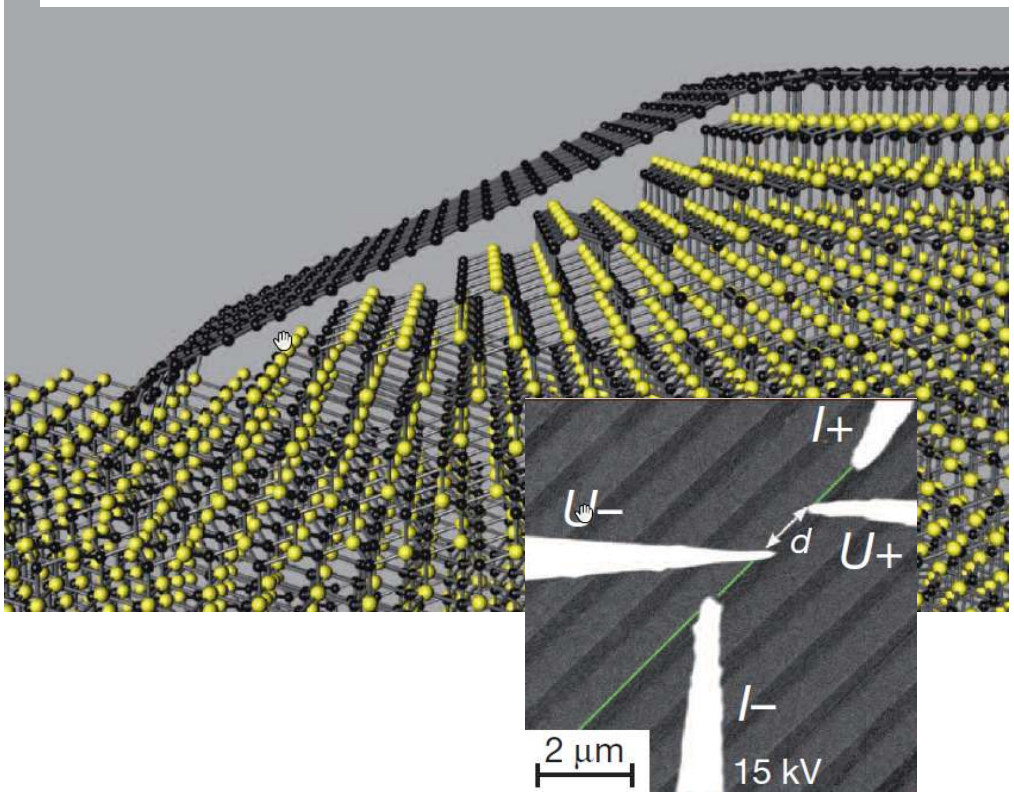
LETTER

doi:10.1038/nature12952

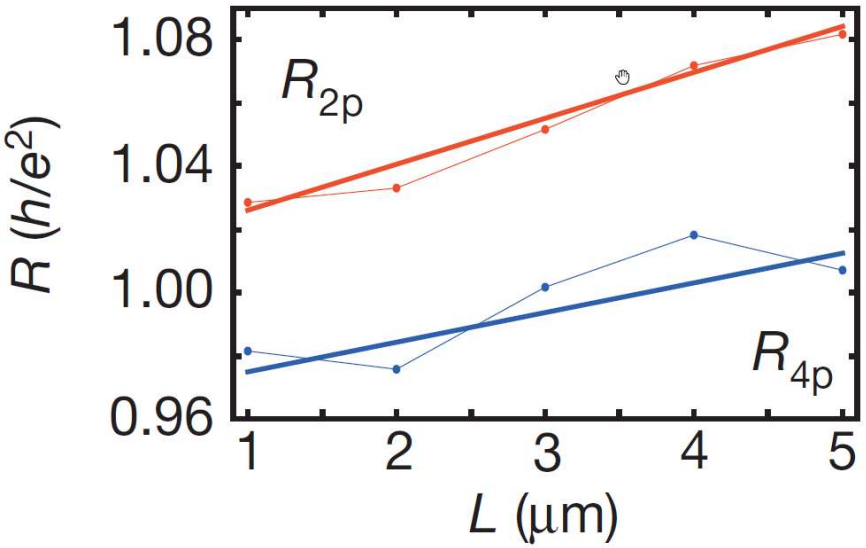
Exceptional ballistic transport in epitaxial graphene nanoribbons

2014 | VOL 506 | NATURE

Jens Baringhaus[1]*, Ming Ruan[2]*, Frederik Edler[1], Antonio Tejeda[3,4], Muriel Sicot[3], AminaTaleb-Ibrahimi[4], An-Ping Li[5], Zhigang Jiang[2], Edward H. Conrad[2], Claire Berger[2,6], Christoph Tegenkamp[1] & Walt A. de Heer[2]

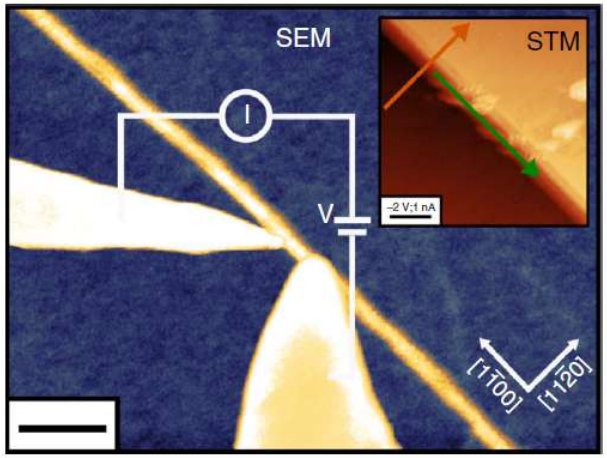


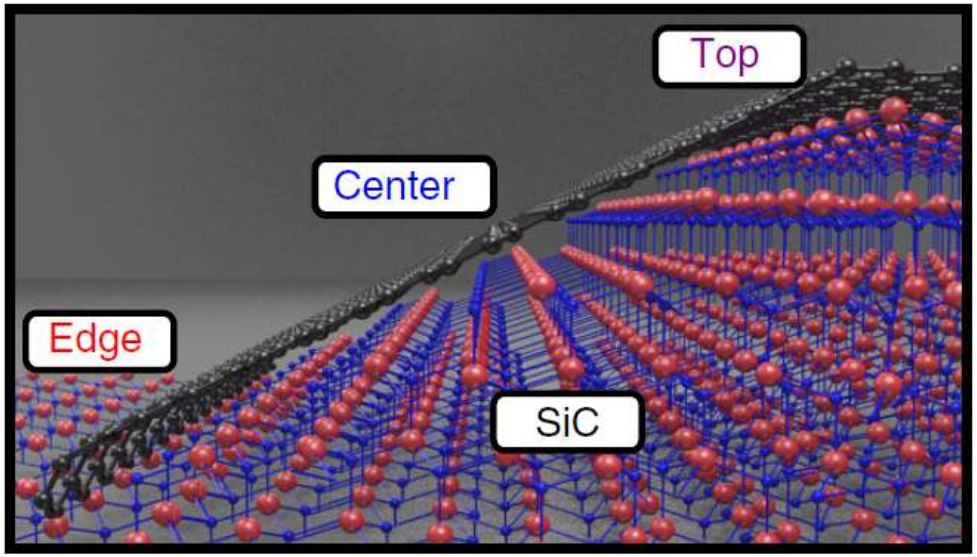
- Not Ohmic (scaling with length)
- Not depending much on sample length:

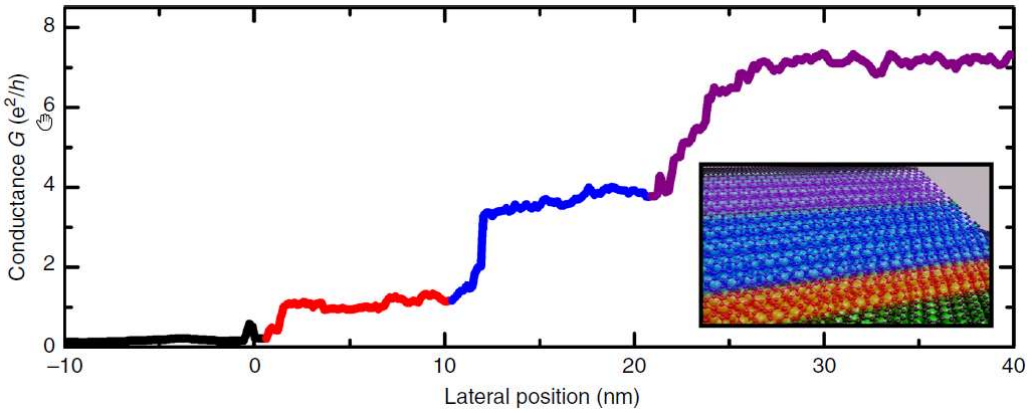


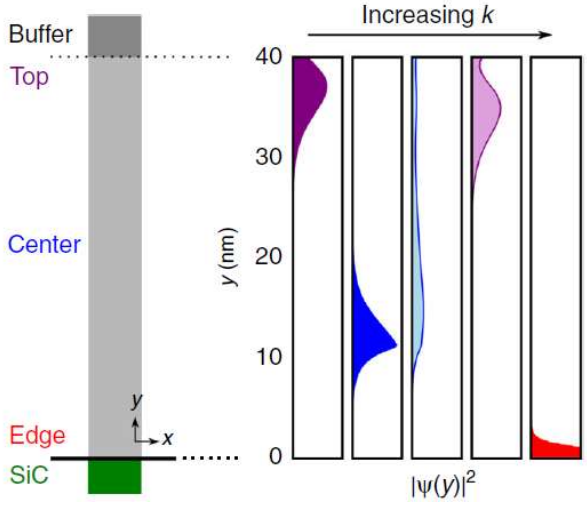
Probing the quantized conduction channels

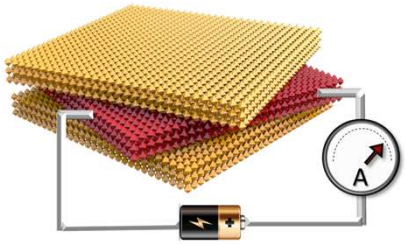
J. Apojanz et al. *Nature Comm.* **volume 9**, 4426 (2018)



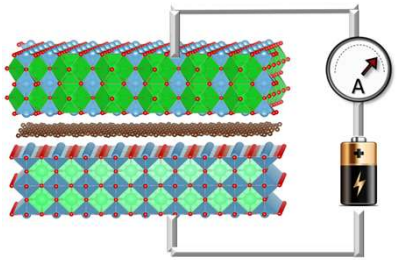








Challenges for theory



- Huge variety in materials *and* their combinations
- **Predictive** (no fitting parameters/*ab initio*)

→ Density Functional Theory (DFT)

- Devices under working conditions:

  Electrostatic gates, current/**nonequilibrium**

→ Nonequilibrium Greens Functions (NEGF)

- Combined effects: (defects + phonons + spins + ..)
- Device **size** and ”mixed” dimensions

→ ”Up-scaling” : DFT → ”model” Machine Learning

- Time-dependence: Small = Fast (THz operation..)

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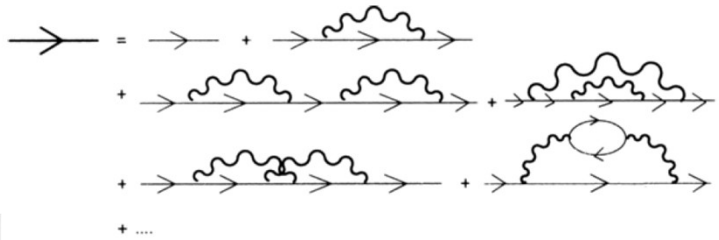
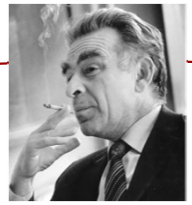
NEGF – why?

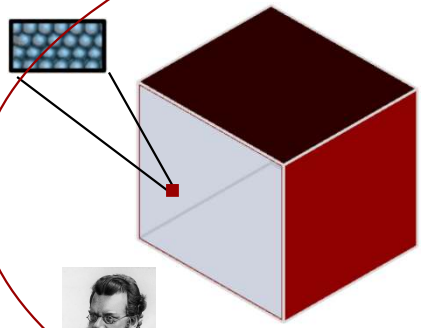
✓ Rigorously founded on Q.M.



✓ Bridging system scales



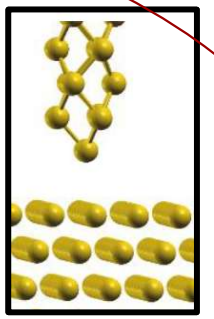
Keldysh
(1931-2016)



Boltzmann
(1844-1906)

Bulk
Diffusive

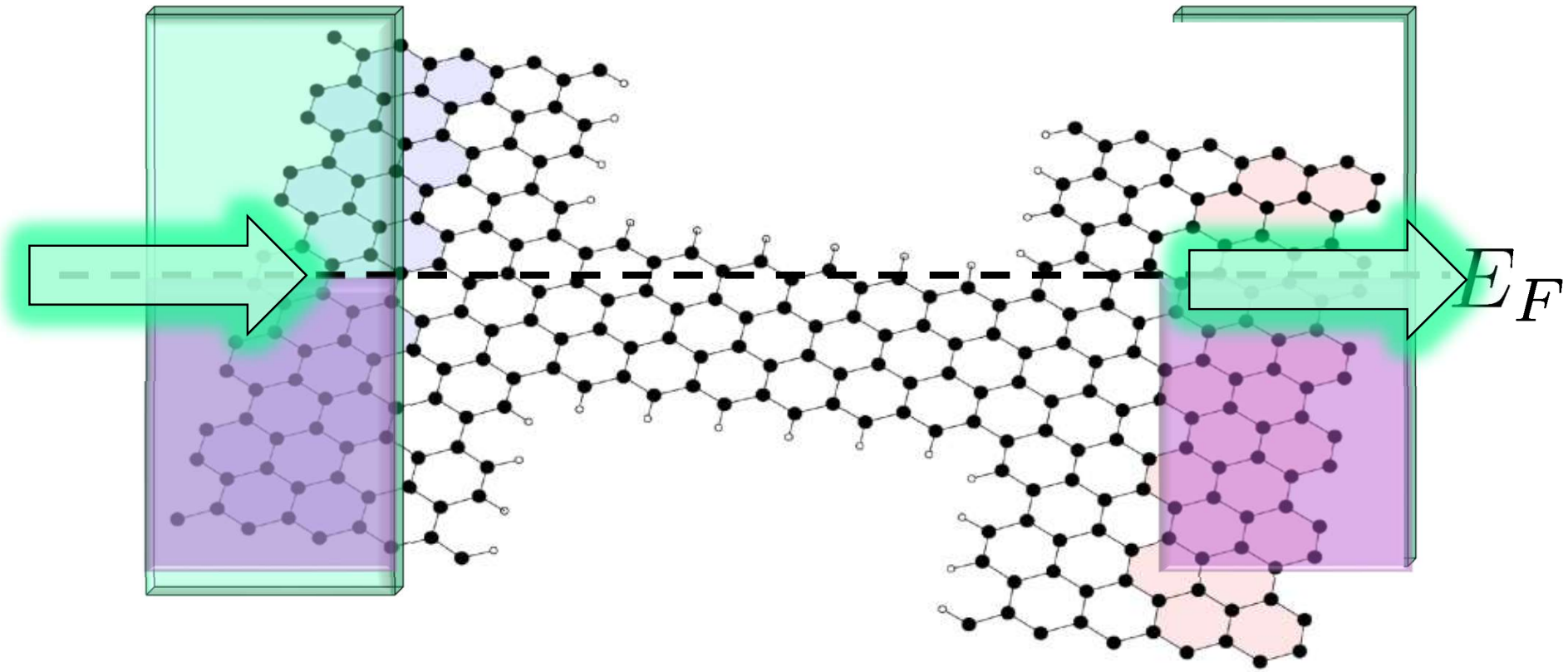
Atomic
Ballistic



Landauer
(1927-99)

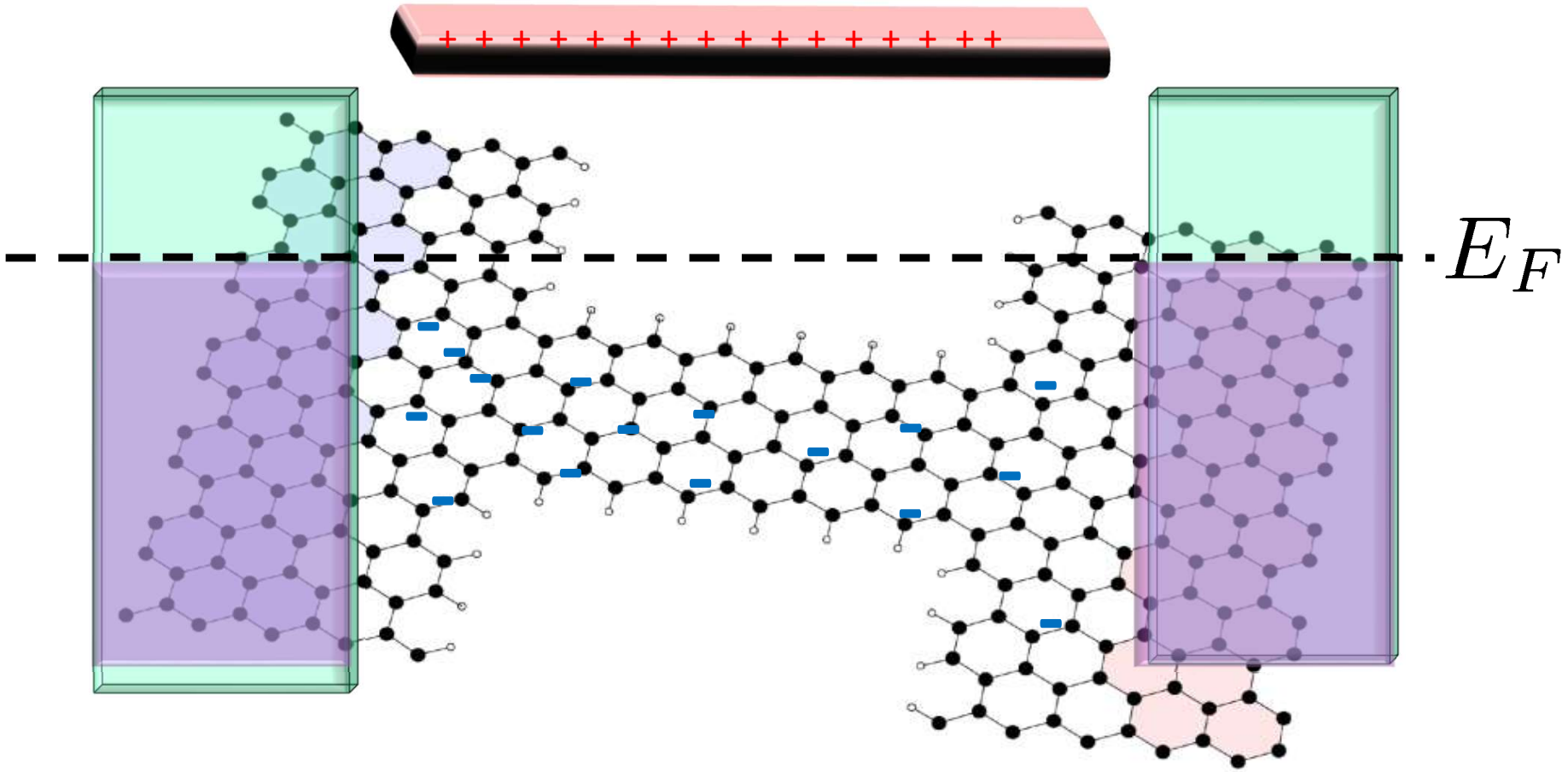
✓ **Non-equilibrium** beyond linear response: **Working conditions**!

Device modelling: Ingredients



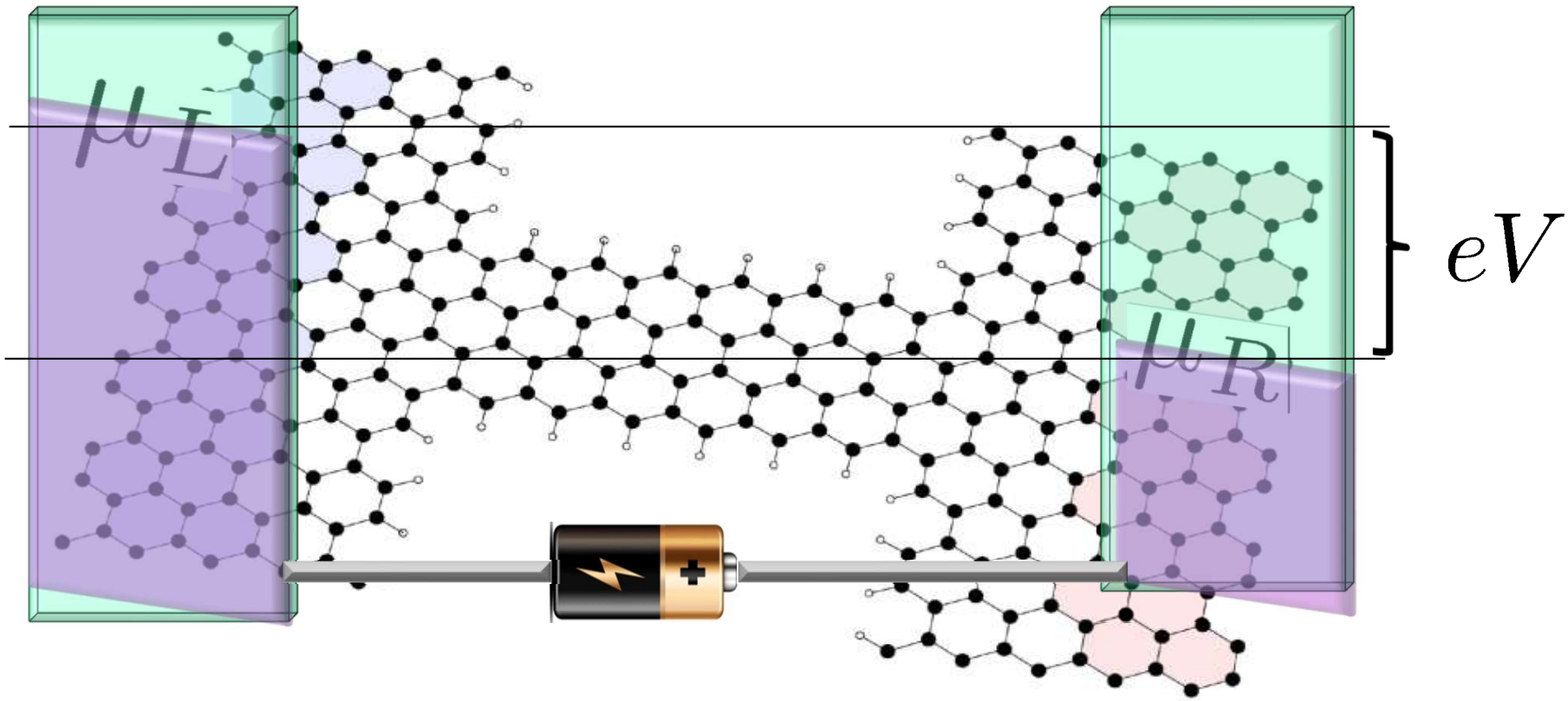
- Open quantum systems for transport (semi-infinite electrodes)

Device modelling: Ingredients



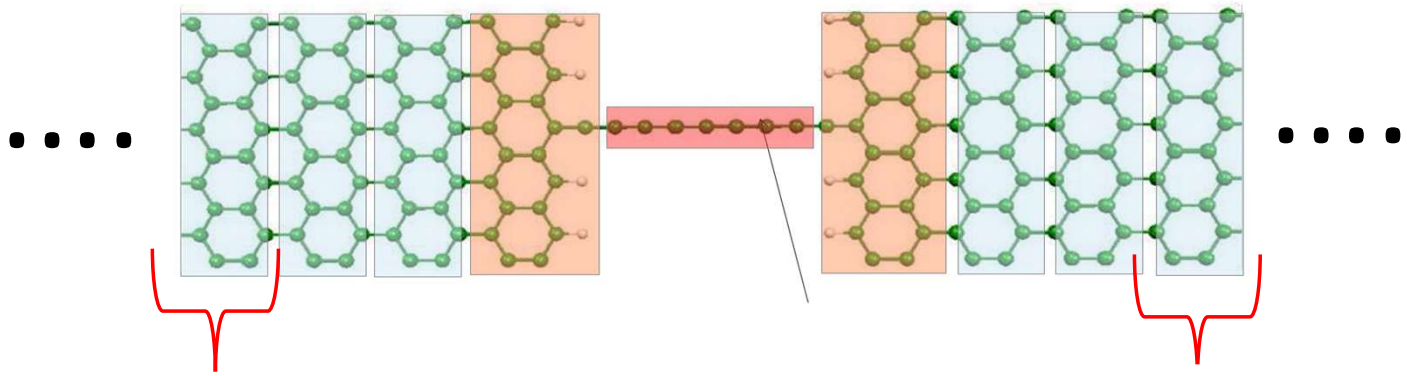
- Open quantum systems (semi-infinite electrodes)
- Environment: Electrostatic gates

Device modelling: Ingredients



- Open quantum systems (semi-infinite electrodes)
- Environment: Electrostatic gates (incapsulation)
- Non-equilibrium situation (Finite bias → two different chemical potentials)

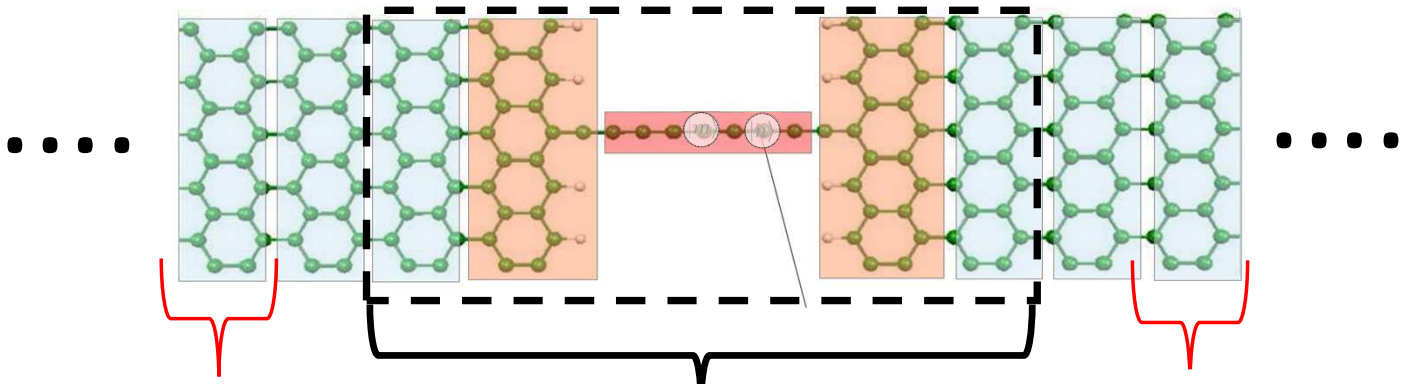
Open boundaries: Generic system



Semi-inifinitely repeated unit cell

Semi-inifinitely repeated unit cell

Open boundaries: Generic system



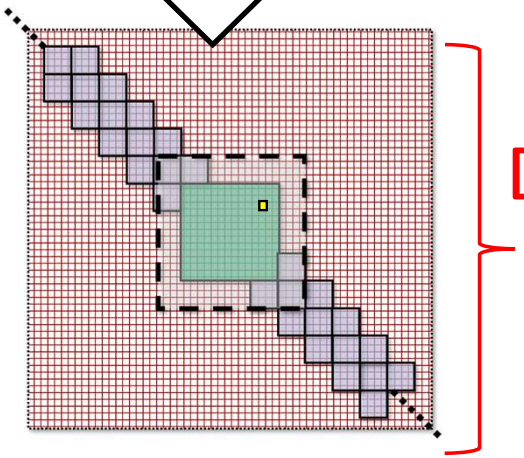
Semi-inifinitely repeated unit cell

Finite device region

Semi-inifinitely repeated unit cell

Atom-centered basis (LCAO, PAO, NAO,..)

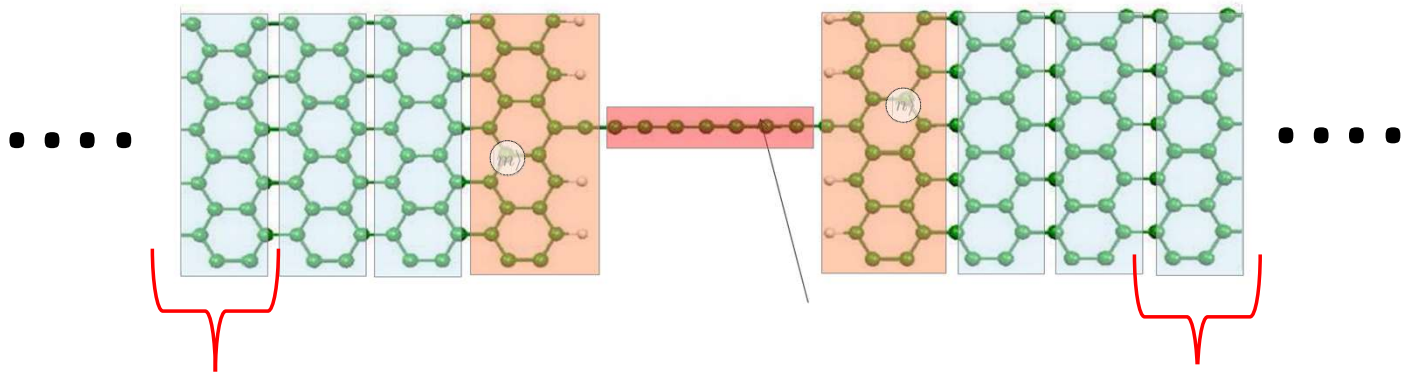
Hamiltonian matrix ($\boldsymbol{H}$)



DFT KS-Hamiltonian (!)

Open boundaries: Greens function

Also called: ”embedding” or ”electrode” self-energies



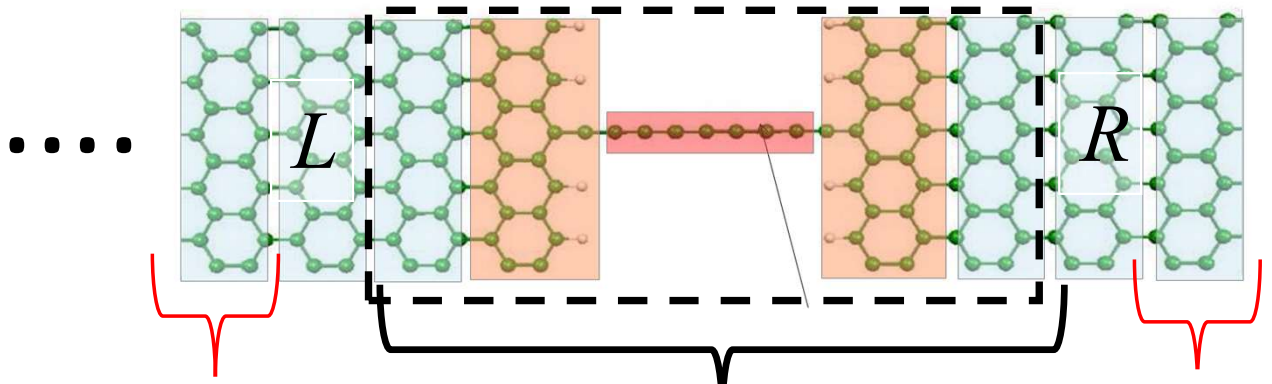
Semi-inifinitely repeated unit cell

Semi-inifinitely repeated unit cell

$$\mathbf{G}_{nm}(E) = \int_0^\infty e^{iEt/\hbar} \langle n|e^{-i\mathbf{H}t/\hbar}|m\rangle \, dt$$

Open boundaries: Greens function

Also called: ”embedding” or ”electrode” self-energies

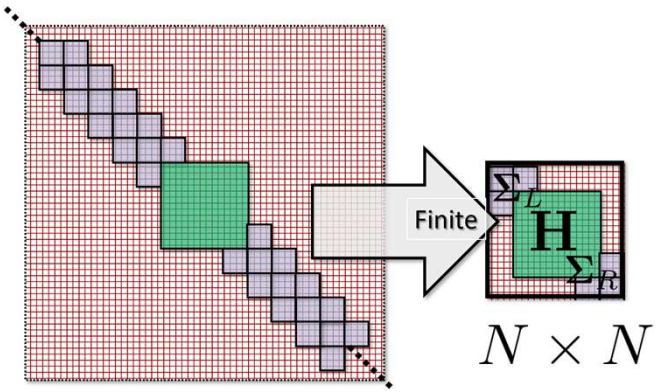


Semi-inifinitely repeated unit cell

Finite device region (N)

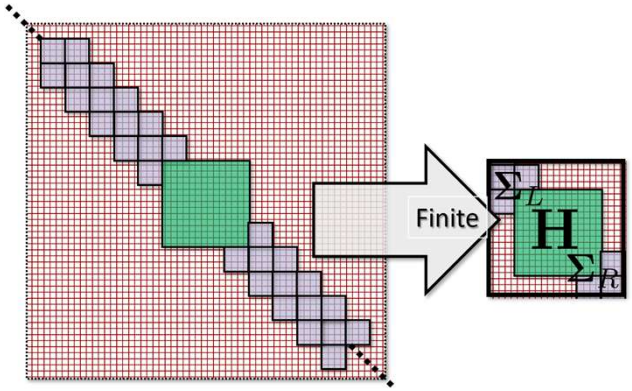
Semi-inifinitely repeated unit cell

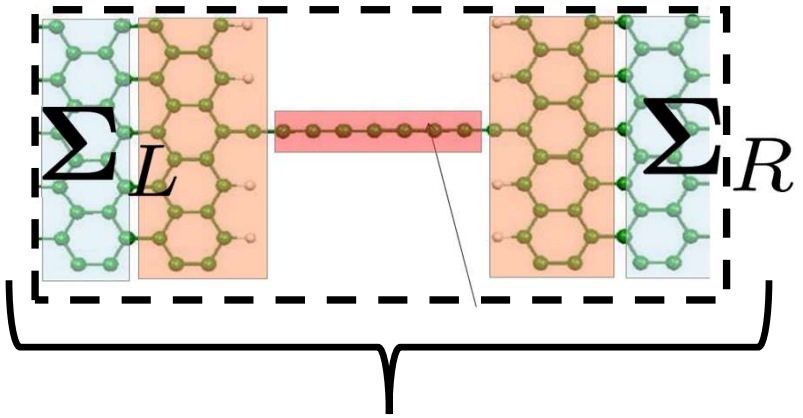
$$\mathbf{G}(E) = (\mathbf{1}E - \mathbf{H} - \mathbf{\Sigma}_L(E) - \mathbf{\Sigma}_R(E))^{-1}$$



Open boundaries: Self-energies (Σ)

Also called: ”embedding” or ”electrode” self-energies





Device region *D*

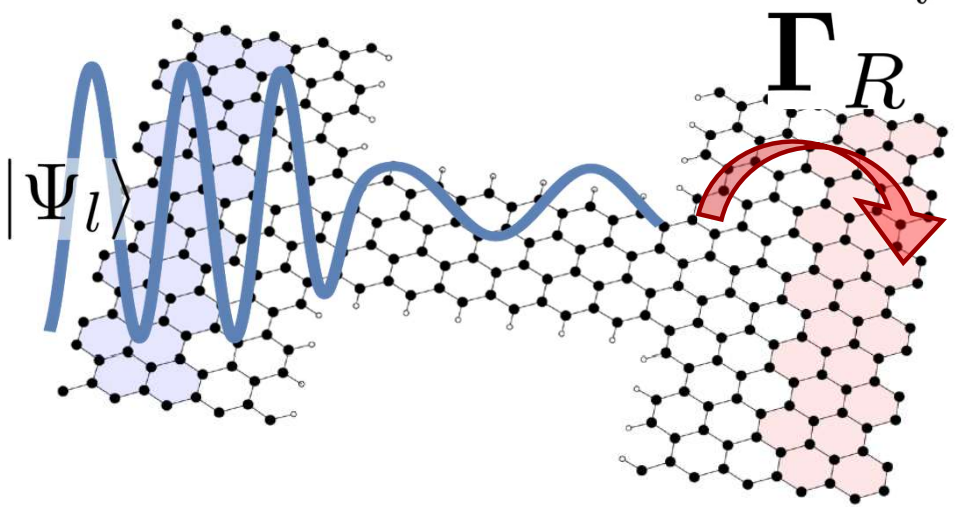
$$\mathbf{G}(E) = (\mathbf{1}E - \mathbf{H} - \mathbf{\Sigma}_L(E) - \mathbf{\Sigma}_R(E))^{-1}$$

Device level-broadening/”escape-rate” into electrode α

$$\mathbf{\Gamma}_\alpha = -2\mathrm{Im}[\mathbf{\Sigma}_\alpha] \quad \alpha = L, R$$

Landauer formula: Greens functions

Scattering state spectral density: $\mathbf{A}_L = \mathbf{G}\boldsymbol{\Gamma}_L\mathbf{G}^\dagger = \sum_l |\Psi_l\rangle\langle\Psi_l|\delta(E-\varepsilon_l)$



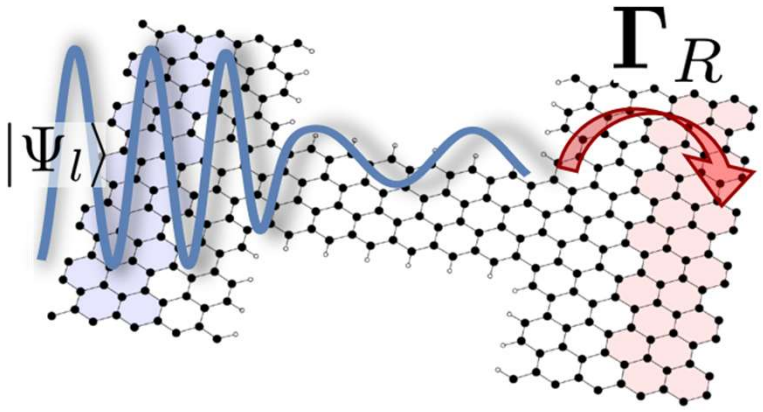
Elastic quantum transmission for electrons:

$$T(E) = \mathrm{Tr}[\boldsymbol{\Gamma}_R(E)\mathbf{A}_L(E)] = \mathrm{Tr}\left[\boldsymbol{\Gamma}_R(E)\mathbf{G}(E)\boldsymbol{\Gamma}_L(E)\mathbf{G}^\dagger(E)\right]$$

"Caroli formula": Caroli, C. et al. Direct calculation of the tunneling current. J. Phys. C: Solid State Phys. 4, 916 (1971).

Landauer formula: Greens functions

Scattering state spectral density: $\mathbf{A}_L = \mathbf{G}\mathbf{\Gamma}_L\mathbf{G}^\dagger = \sum_l |\Psi_l\rangle\langle\Psi_l|\delta(E-\varepsilon_l)$



"Fisher-Lee relation":

$$\mathbf{t}_{LR}(E) = \mathbf{\Gamma}_L^{1/2}(E)\mathbf{G}(E)\mathbf{\Gamma}_R^{1/2}(E)$$

"Caroli formula": Caroli, C. et al. Direct calculation of the tunneling current. J. Phys. C: Solid State Phys. 4, 916 (1971).
"Fisher-Lee relation": J. Wang, H. Guo, Phys. Rev. B 79, 045119 (2009)

Quantum conductance = Quantum transmission

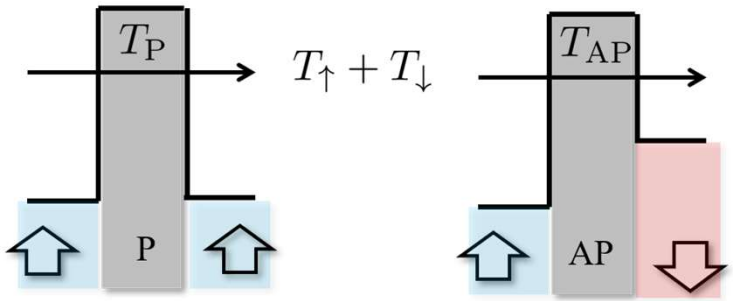
$$T(E) = \mathrm{Tr}\left[\mathbf{t}^\dagger\mathbf{t}\right](E)$$

$$I(V) = G_0 \int_{\mu_L}^{\mu_R} dE\; T(E,V)$$

Spin

- Collinear spin

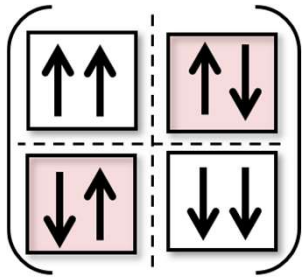
$$T_\sigma = \mathrm{Tr}\left[\mathbf{t}_\sigma^\dagger \mathbf{t}_\sigma\right] \quad \sigma = \uparrow, \downarrow$$



$$\mathrm{TMR} \equiv \frac{T_\mathrm{P} - T_\mathrm{AP}}{T_\mathrm{AP}}$$

Spin-transport (incl. SOC) lecture tomorrow!

- Non-collinear spin (e.g. SOC)



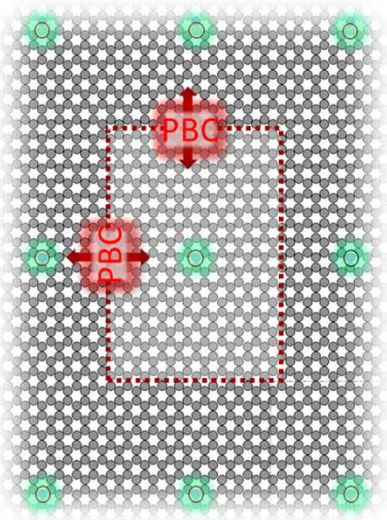
$$|\phi_\mu^\sigma\rangle = |\phi_\mu\rangle \otimes |\sigma\rangle \qquad \rho^{\sigma\sigma'}(\mathbf{r}) = \sum_{\mu\nu} \phi_\mu(\mathbf{r})\, \mathbf{D}_{\mu\nu}^{\sigma\sigma'}\, \phi_\nu(\mathbf{r})$$

$$(m_x, m_y, m_z)(\mathbf{r}) = \left(\rho^{\uparrow\downarrow} + \rho^{\downarrow\uparrow}, i(\rho^{\uparrow\downarrow} - \rho^{\downarrow\uparrow}), \rho^{\uparrow\uparrow} - \rho^{\downarrow\downarrow}\right)(\mathbf{r})$$

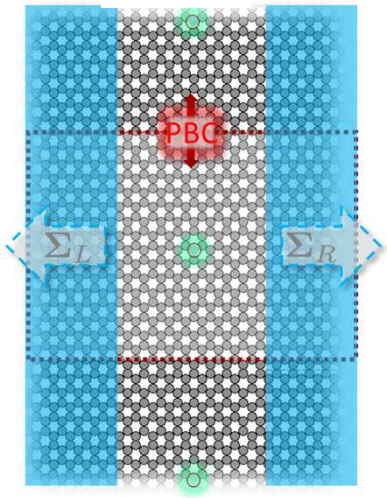
$$T = \mathrm{Tr}\left[\mathbf{t}^\dagger \mathbf{t}\right] = \mathrm{Tr}_\mathrm{orb}\left[\mathbf{t}_{\uparrow\uparrow}^\dagger \mathbf{t}_{\uparrow\uparrow} + \mathbf{t}_{\downarrow\downarrow}^\dagger \mathbf{t}_{\downarrow\downarrow}\right] + \underbrace{\mathrm{Tr}_\mathrm{orb}\left[\mathbf{t}_{\downarrow\uparrow}^\dagger \mathbf{t}_{\downarrow\uparrow} + \mathbf{t}_{\uparrow\downarrow}^\dagger \mathbf{t}_{\uparrow\downarrow}\right]}_{\text{Spin-flip}}$$

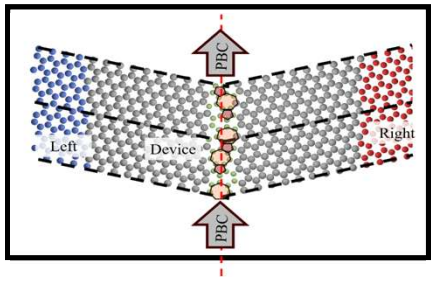
Boundary conditions

XYZ-periodic

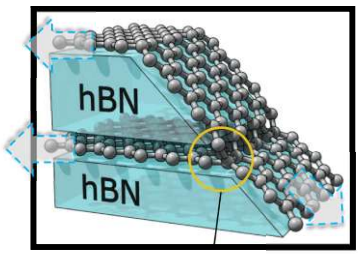


Mixed

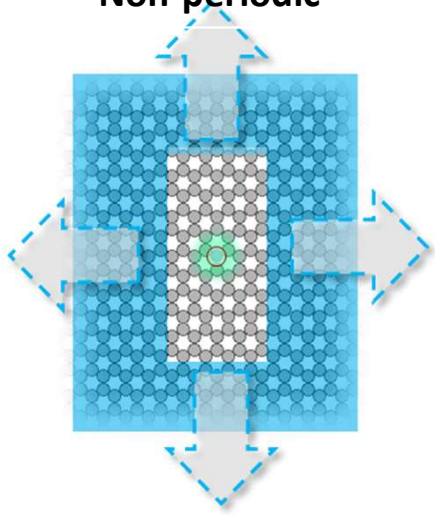




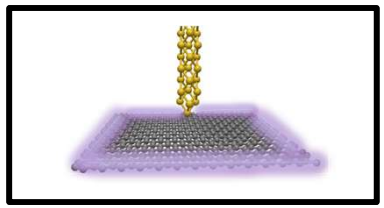
- Multi-electrode



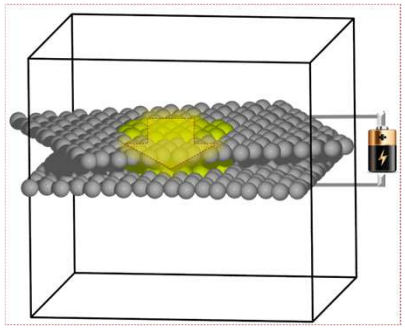
Non-periodic



- Single-point-injection

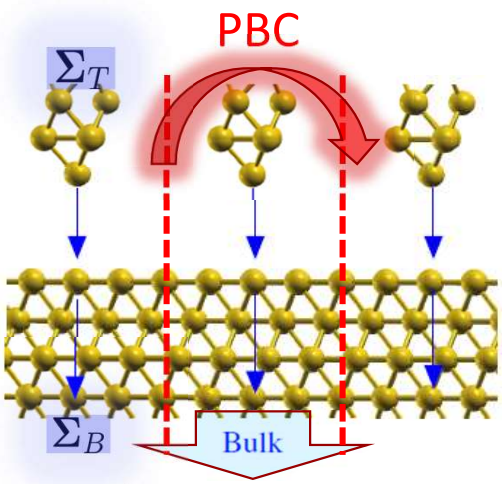


- 2D-to-2D tunnelling

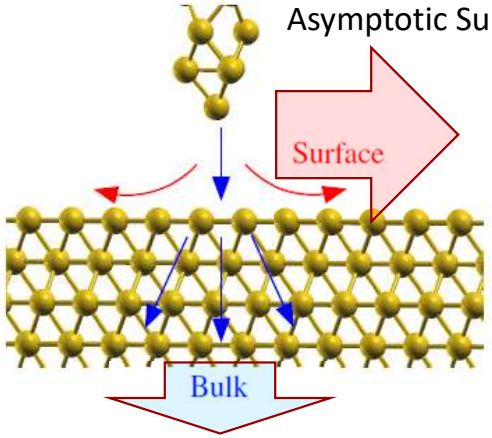


Beyond periodic boundary conditions

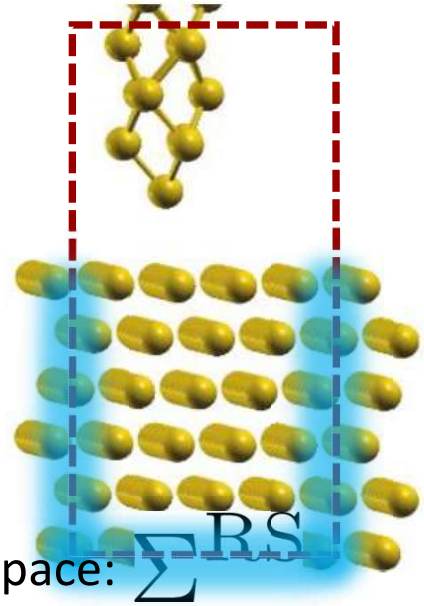
D. Li, J. L. Bertelsen, N. Papior, A. Smogunov, MB, Phys. Rev. Research **3**, 033017 (2021)



Asymptotic Bulk

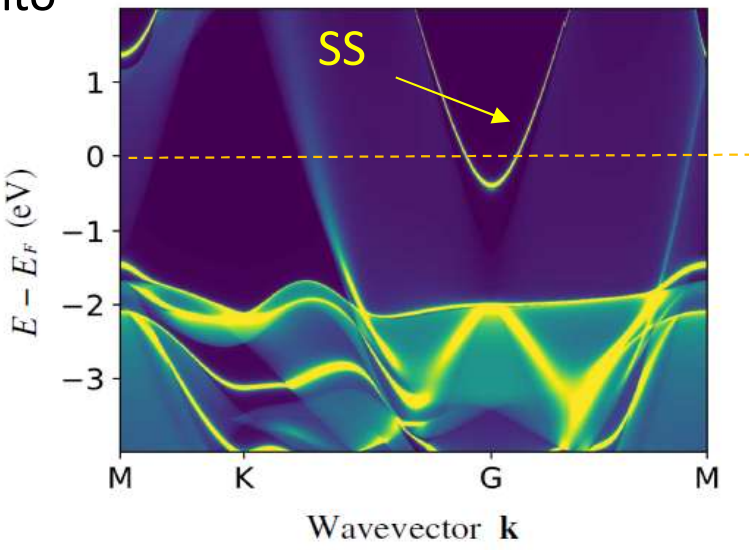


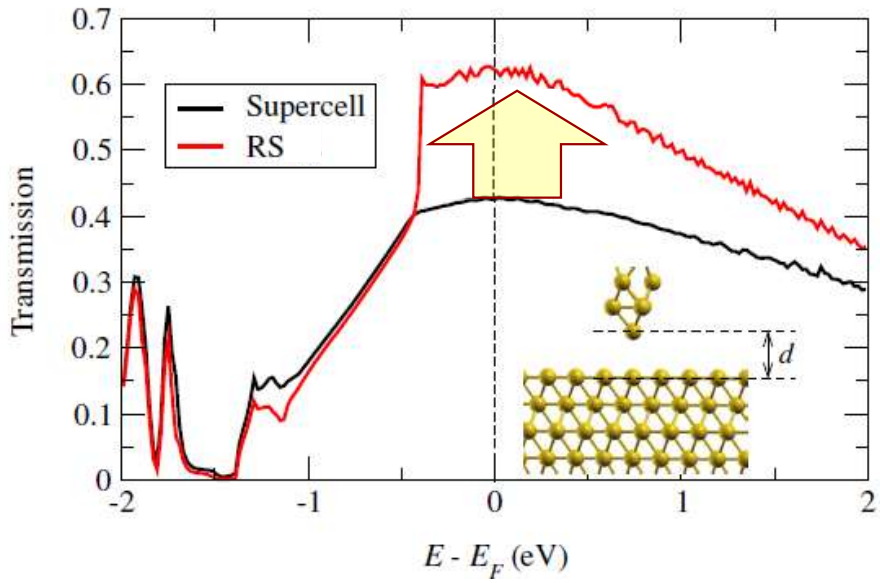
Asymptotic Bulk



Real-Space:

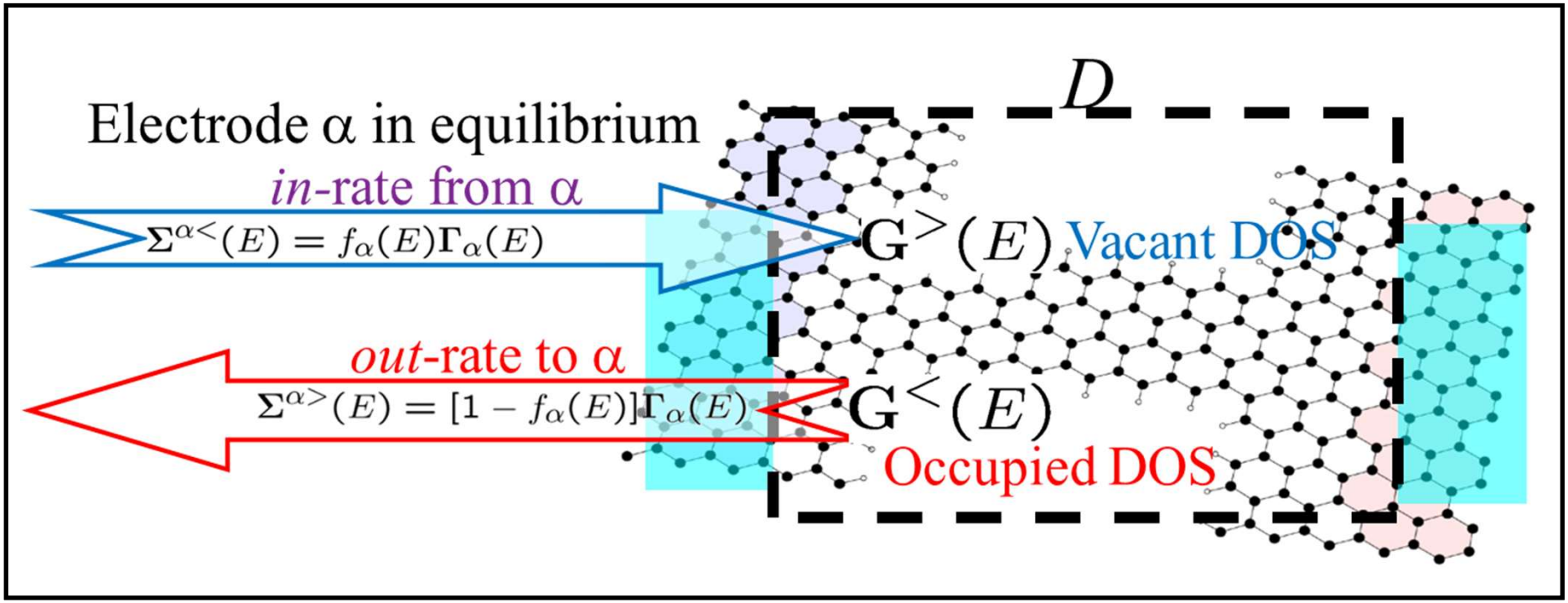
Tunnellig into Au(111)





Non-equilibrium Greens functions (NEGF)

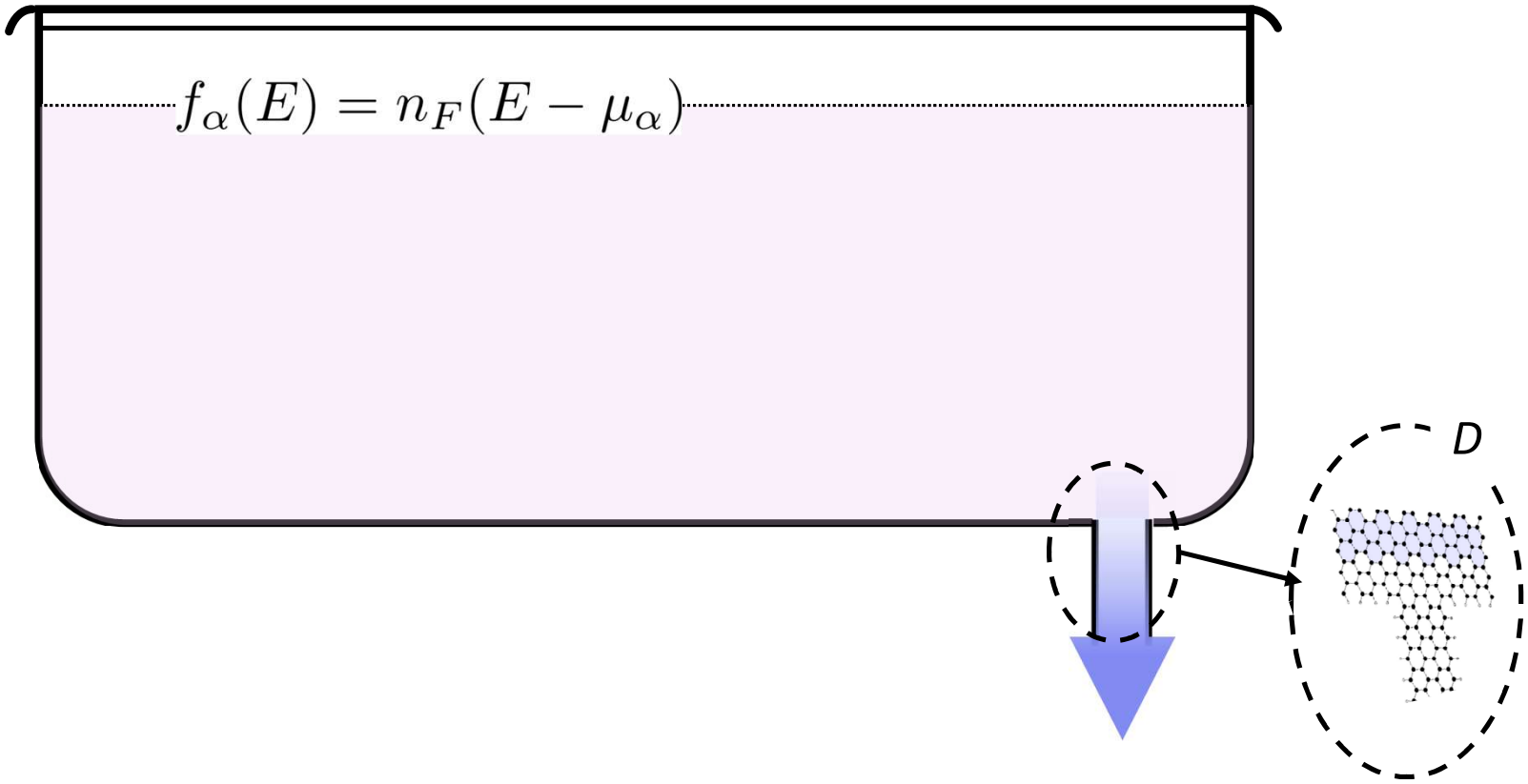
$$\mathbf{G}^r(E) = (\mathbf{1}E - \mathbf{H} - \mathbf{\Sigma}_L^r(E) - \mathbf{\Sigma}_R^r(E))^{-1}$$



Current from α: $J^\alpha = \int_{-\infty}^{\infty} dE\ \mathrm{Tr}\left[\mathbf{\Sigma}^{\alpha,<}(E)\mathbf{G}^>(E) - \mathbf{\Sigma}^{\alpha,>}(E)\mathbf{G}^<(E)\right]$

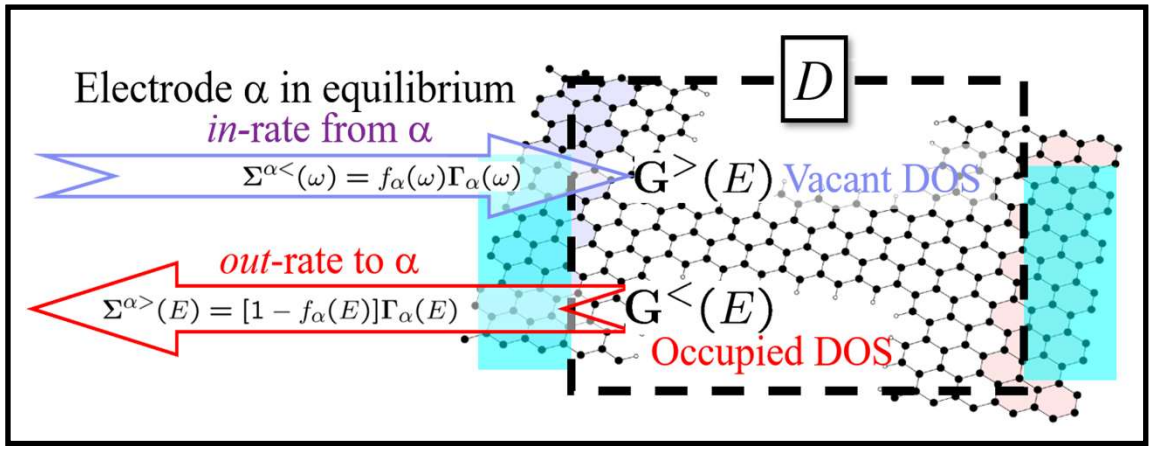
Mean-field single particles (DFT): Landauer formula!

Electrodes: The ”bath-tub” picture



NEGF + DFT

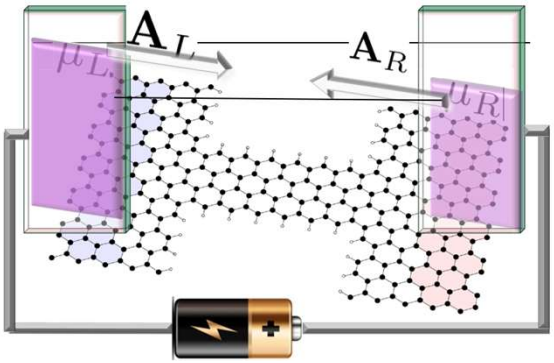
$$\mathbf{G}^r(E) = (\mathbf{1}E - \mathbf{H}_{KS} - \mathbf{\Sigma}_L^r(E) - \mathbf{\Sigma}_R^r(E))^{-1}$$

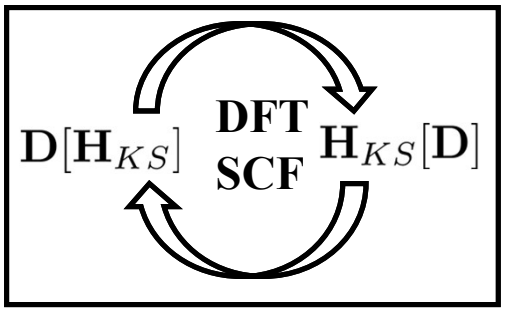


Non-equilibrium Density matrix

$$\mathbf{D} = \int_{-\infty}^{\infty} dE\ \mathbf{G}^<(E) = \int_{-\infty}^{\infty} dE\ \mathbf{A}_L(E) f_L(E) + \mathbf{A}_R(E) f_R(E)$$

$$\mathbf{A}_L = \mathbf{G}\mathbf{\Gamma}_L\mathbf{G}^\dagger = \sum_l |\Psi_l\rangle\langle\Psi_l|\delta(E - \varepsilon_l)$$





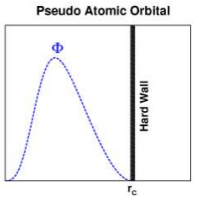
DFT-NEGF Implementation

Simulations of devices under working conditions without fitting parameters

Density Functional Theory

– Pseudopotentials

– Pseudo-AO basis set with *finite* range

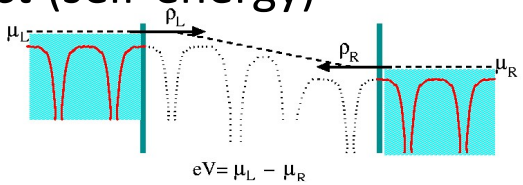


+

Non-equilibrium Greens functions (NEGF)

= Coupling to semi-infinite bulk treated *exact* (self-energy)

= Electron density at finite applied voltage



= transport calculations *incl.* many-body interactions in central region

=

TranSIESTA: Brandbyge *et al.*, MRS proc. 636 (2001); PRB 65, 165401 (2002);
N. Papior et al., Comp. Phys. Comm., **212**, 8, (2017)

siesta

N. Wittemeier, N. Papior, M. Brandbyge, Z. Zanolli, P. Ordejon, "Quantum transport with spin-orbit coupling: New developments in TranSIESTA", Comp. Phys. Comm. 109996, 320 (2026)

QuantumATK: Commercial www.synopsys.com
S. Smidstrup *et al.* , J. Phys. Cond. Mat. 32, 015901 (2020)

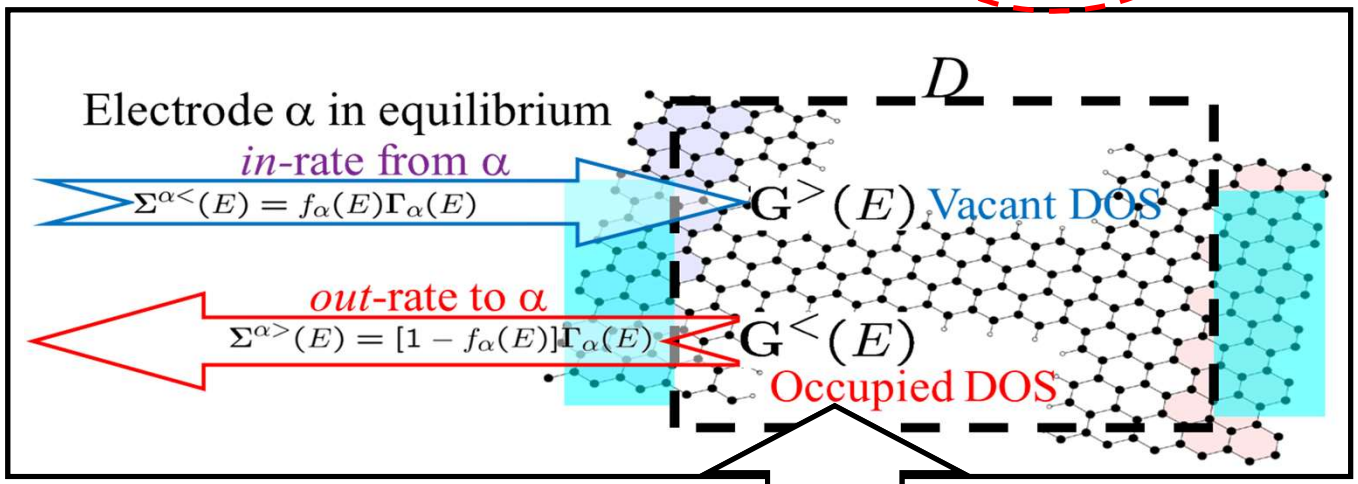
SYNOPSYS QUANTUMATK

Interactions with NEGF

Kadanoff-Baym equations

$$\mathbf{G}^r(E) = (\mathbf{1}E - \mathbf{H} - \mathbf{\Sigma}_e^r(E) - \mathbf{\Sigma}_i^r(E))^{-1}$$

$$\mathbf{G}^<(E) = \mathbf{G}^r(E)\left(\mathbf{\Sigma}_e^<(E) + \mathbf{\Sigma}_i^<(E)\right)\mathbf{G}^a(E)$$



Complication:

$$\mathbf{\Sigma}_i[\mathbf{G}]$$

Example Phonons:

in-rate due to local phonon (ω) in D: Self-consistent Born Approximation

$$\mathbf{\Sigma}^<_{\mathrm{ph}}(E) = \mathbf{M}_{\mathrm{eph}}\left[\underbrace{(n_p+1)\mathbf{G}^<(E+\hbar\omega)}_{\text{emission}} + \underbrace{n_p\mathbf{G}^<(E-\hbar\omega)}_{\text{absorbtion}}\right]\mathbf{M}_{\mathrm{eph}}$$

Electron-electron interaction beyond mean-field:

Y. Meir, N. S. Wingreen, PRL **68**, 2512 (1992)

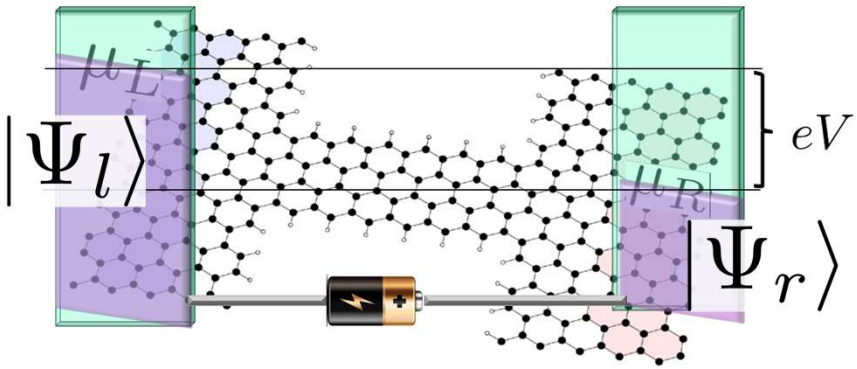
GW: K. S. Thygesen, A. Rubio, Phys. Rev. B **77**, 115333 (2008); L. Deuschle .. L. Mathieu, Phys. Rev. B 111, 195421 (2025)

DMFT: D. Nell .. A. Droghetti, Phys. Rev. B **113**, 155132 (2026)

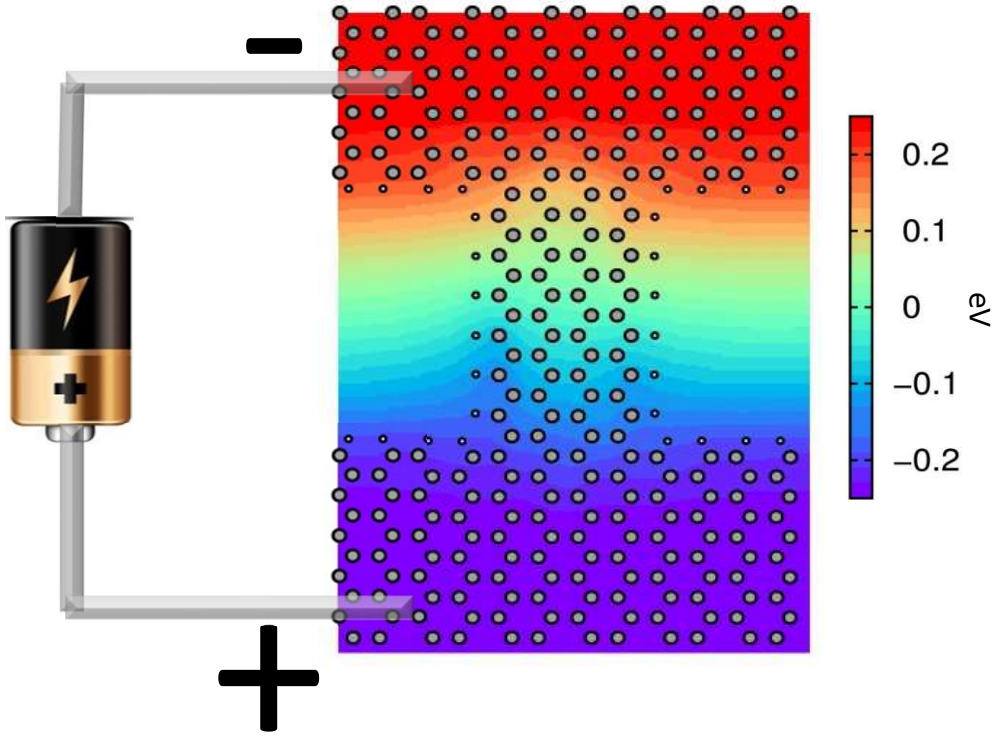
Outline

- **Motivation: “Quantum materials”/Landauer’s transport**
- **Theoretical methodology – a crash-course on DFT-NEGF**
- **Examples**
  - **Non-equilibrium & Gate effects in 2D devices**
  - Current-only calculations
  - Large-scale systems: Nano-porous graphene
  - Spin-filtering in porphyrin-GNR hybrids

Model system: Graphene nano-constriction

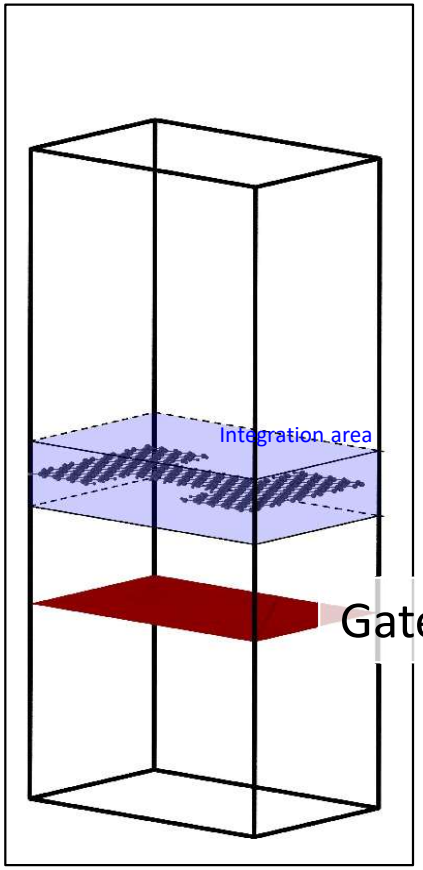


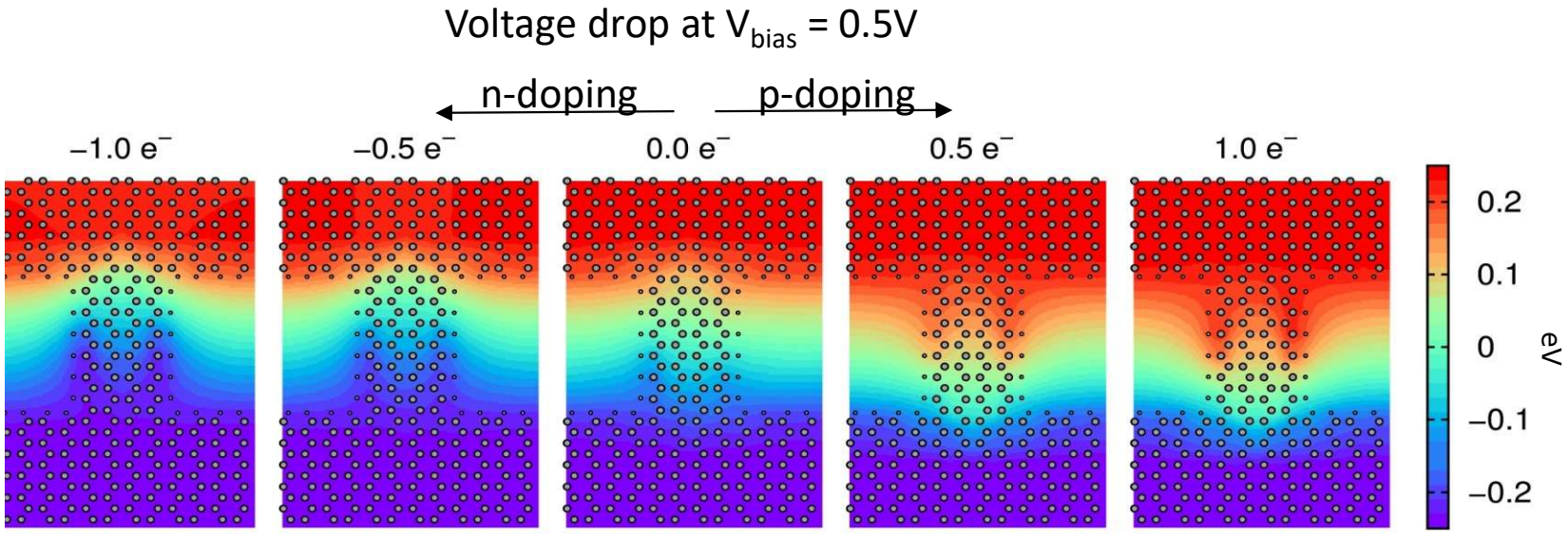
Voltage drop at V_{bias} = 0.5V



N. Papior, T. Gunst, D. Stradi, M. Brandbyge, Phys. Chem. Chem. Phys., 18, 1025-1031(2016)

Graphene Nano-constriction





Voltage drop: Can be controlled by gate

N. Papior, T. Gunst, D. Stradi, M. Brandbyge, Phys. Chem. Chem. Phys., **18**, 2025 (2016)

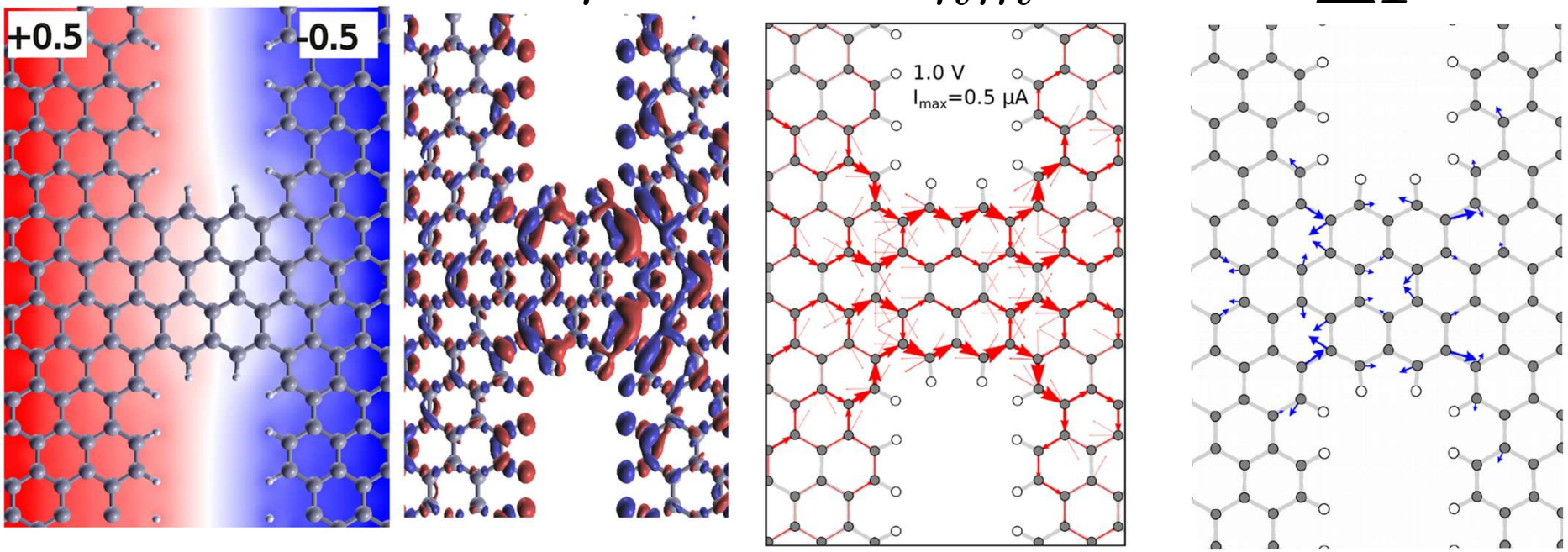
Potential drop, induced charge, bond currents, forces

S. Leitherer, N. Papior, MB, Phys. Rev. B 100, 035415 (2019)

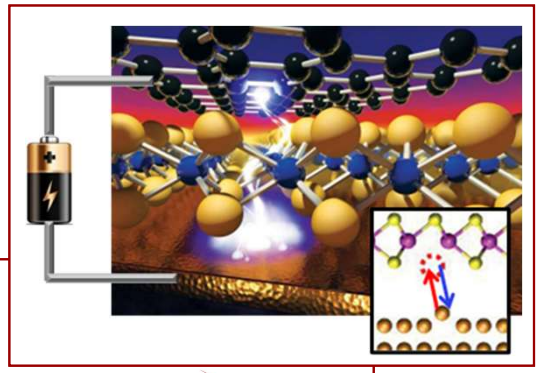
V=1.0 V
p-doping (2 10^{13} cm^{-2})

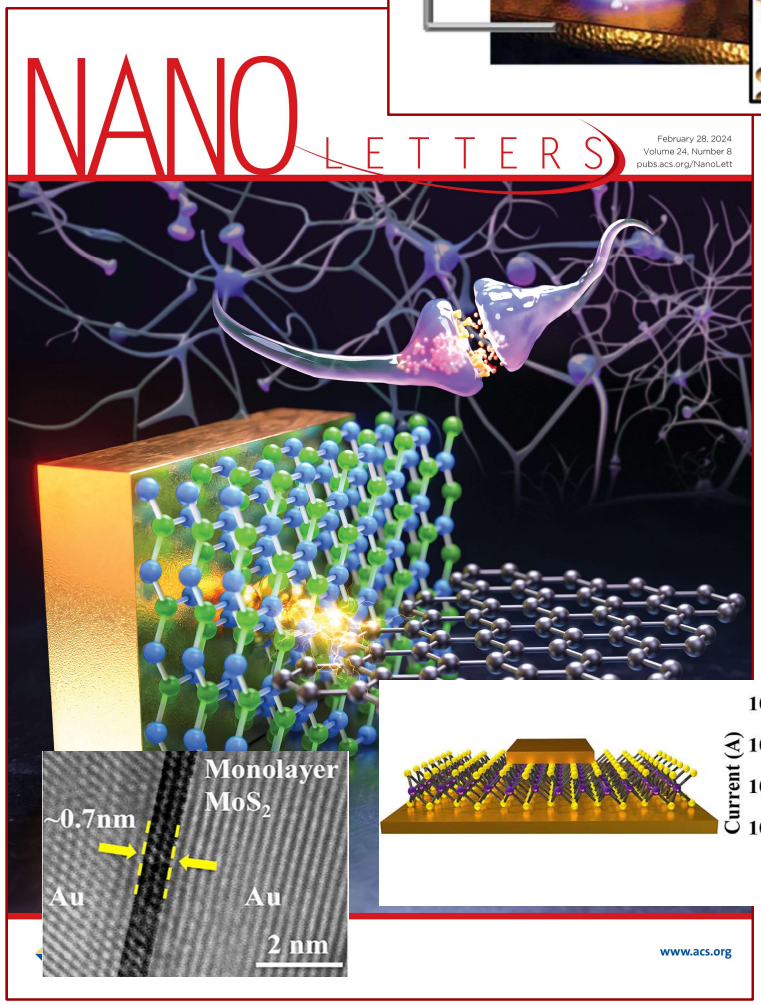
Bond currents

ΔV $\Delta \rho$ J_{nm} ΔF



2D mat-based memristors/"atomristors"





Neuromorphic/memcomputing

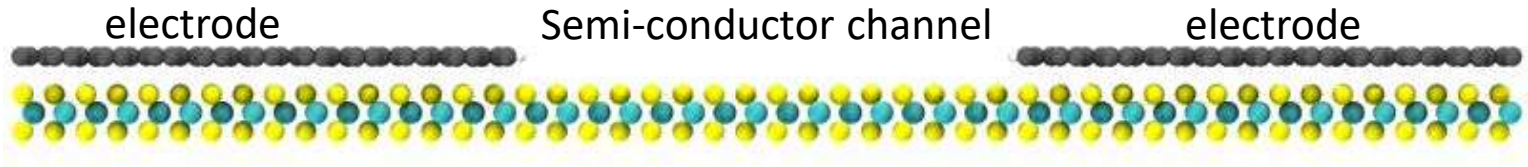
- ✓ Ultra-thin/flexible – **advanced architectures**
- ✓ **Integration**/Scalability
- ✓ **Atomic** or Ferro-magnetic/electric **mechanism**
- ✓ High on/off ratios
- ✓ Good retention (non-volatile)
- ✓ Fast switching speeds (up to THz)
- ✓ **Low power consumption**

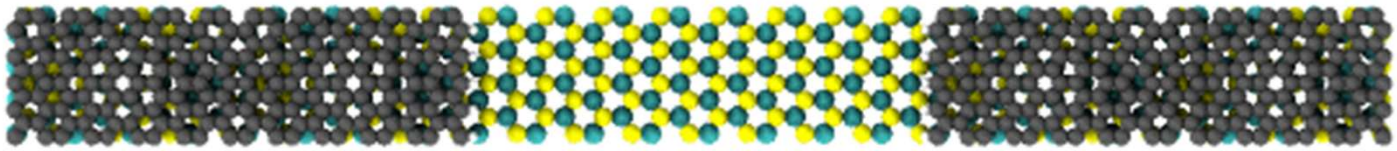
J. Xie *et al., Nano Lett.* 2473, **24** (2024)

R. Ge et al. & D. Akinwande, Nano Lett., 434 **18**,(2018); Adv. Mater., 2007792, **33**, (2021)
S. M. Huus et al., Nature Nano. 58, **16** (2021); *X.* Li *et al.* Adv. Mater. **36**, 2307951 (2024)

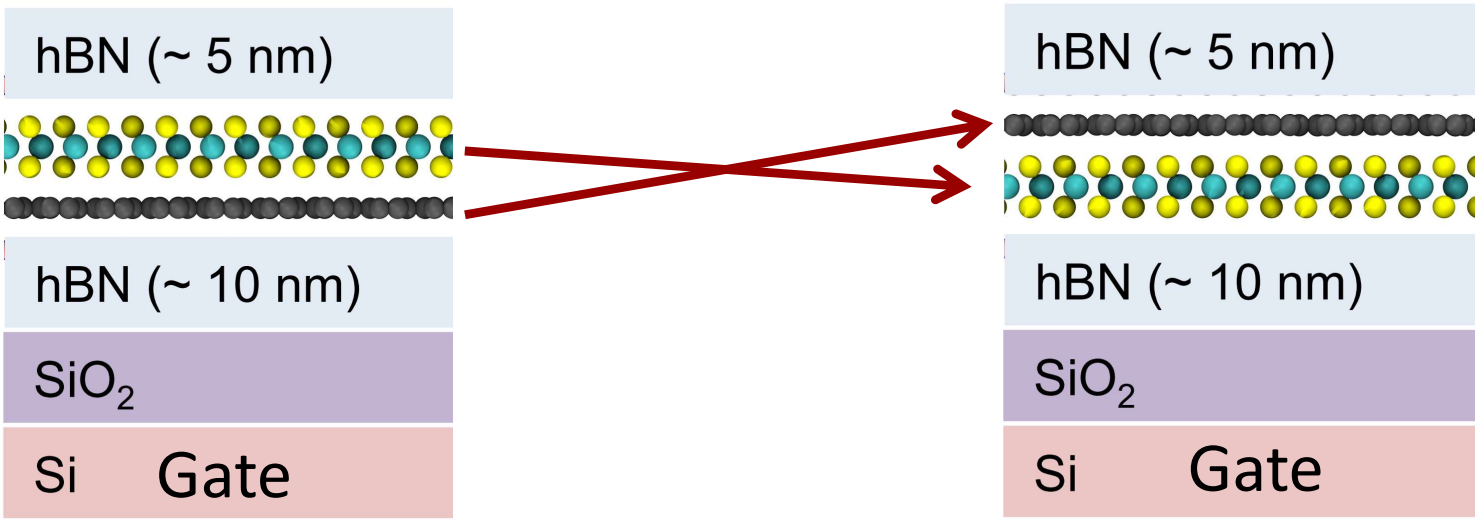
MoS_2 transistor with graphene electrodes

Experiments: *Vertical MoS_2 transistors with sub-1-nm gate lengths*, Fan Wu et al. & Tian-Ling Ren, Nature **603**, 259 (2022)



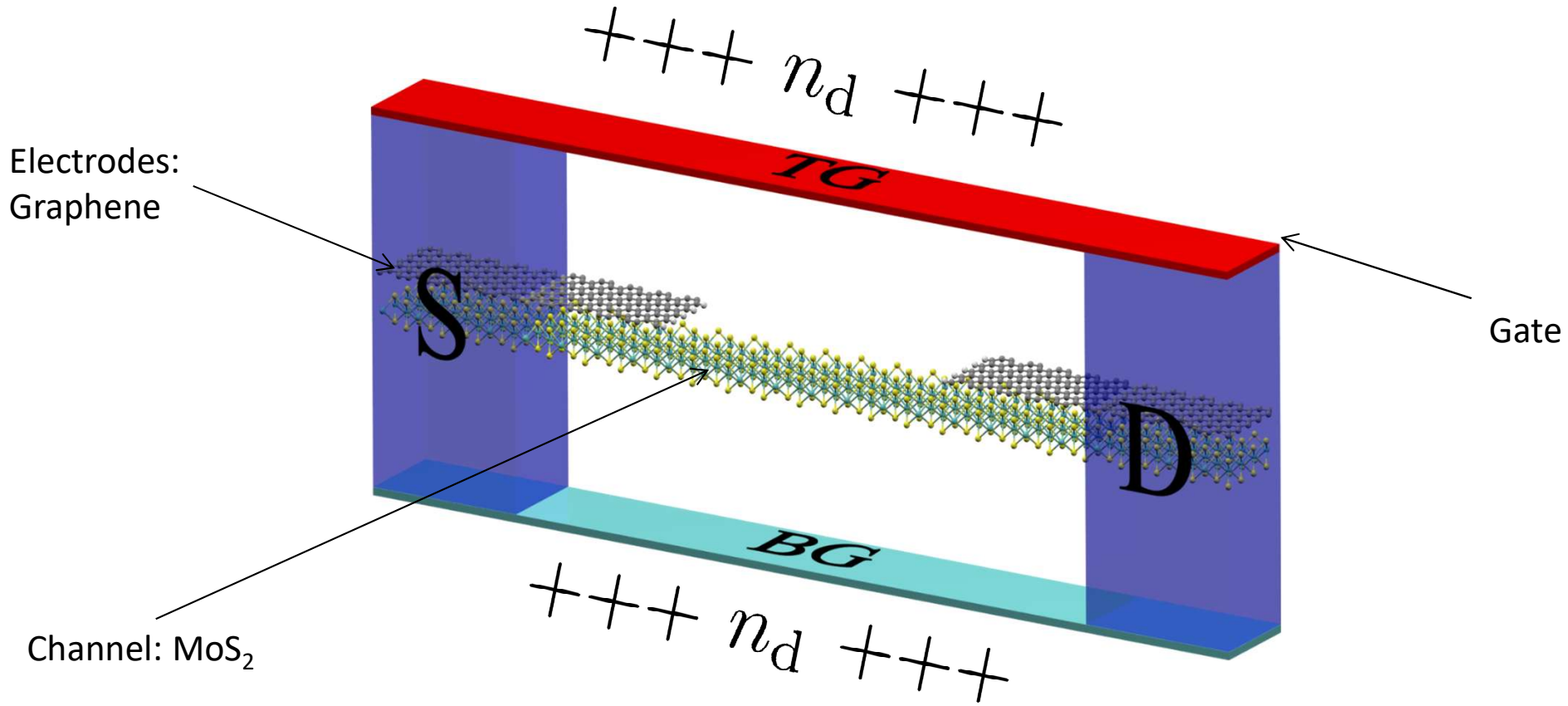


Does the stacking sequence matter?



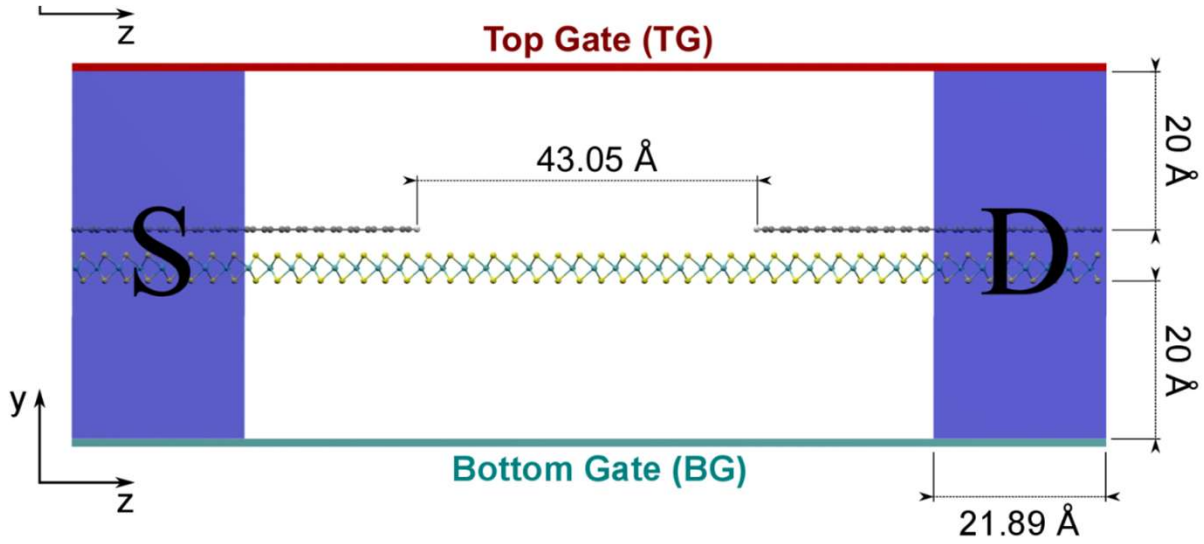
MoS_2-graphene transistor

Top-Gate versus Bottom-Gate

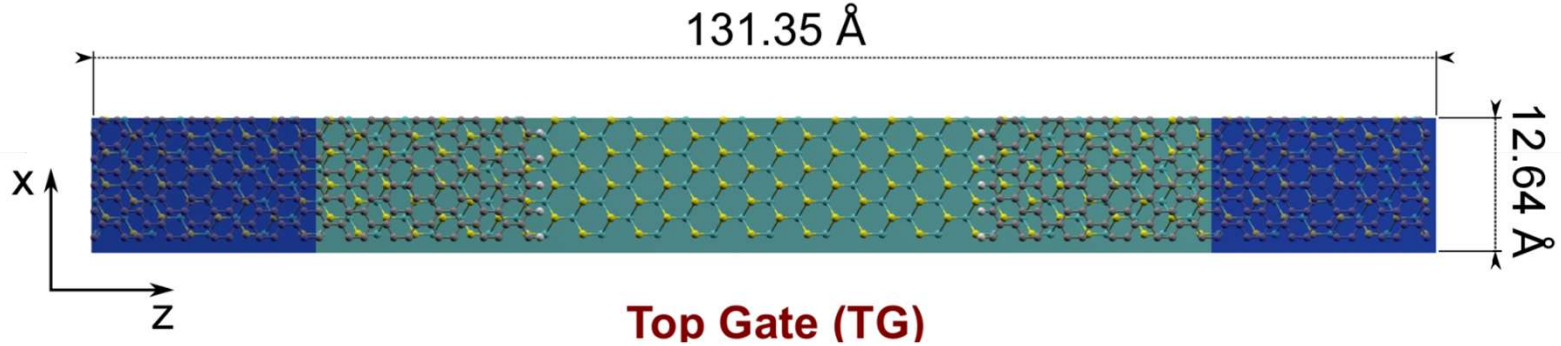


D. Stradi, N. R. Papior, O. Hansen, M. Brandbyge, Nano Lett. **17**, 2660 (2017)

Computational setup

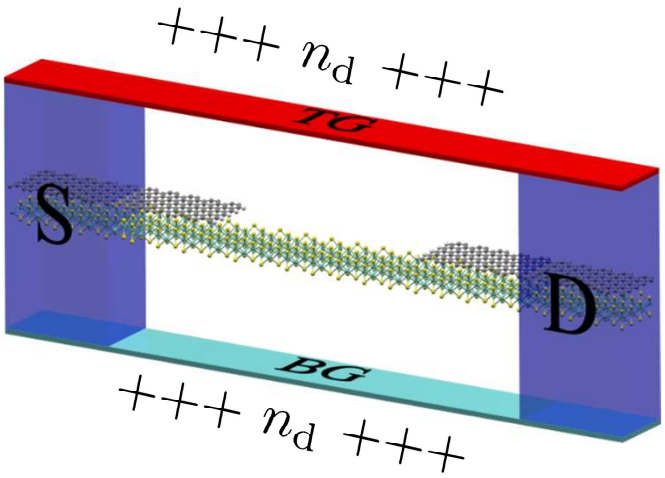


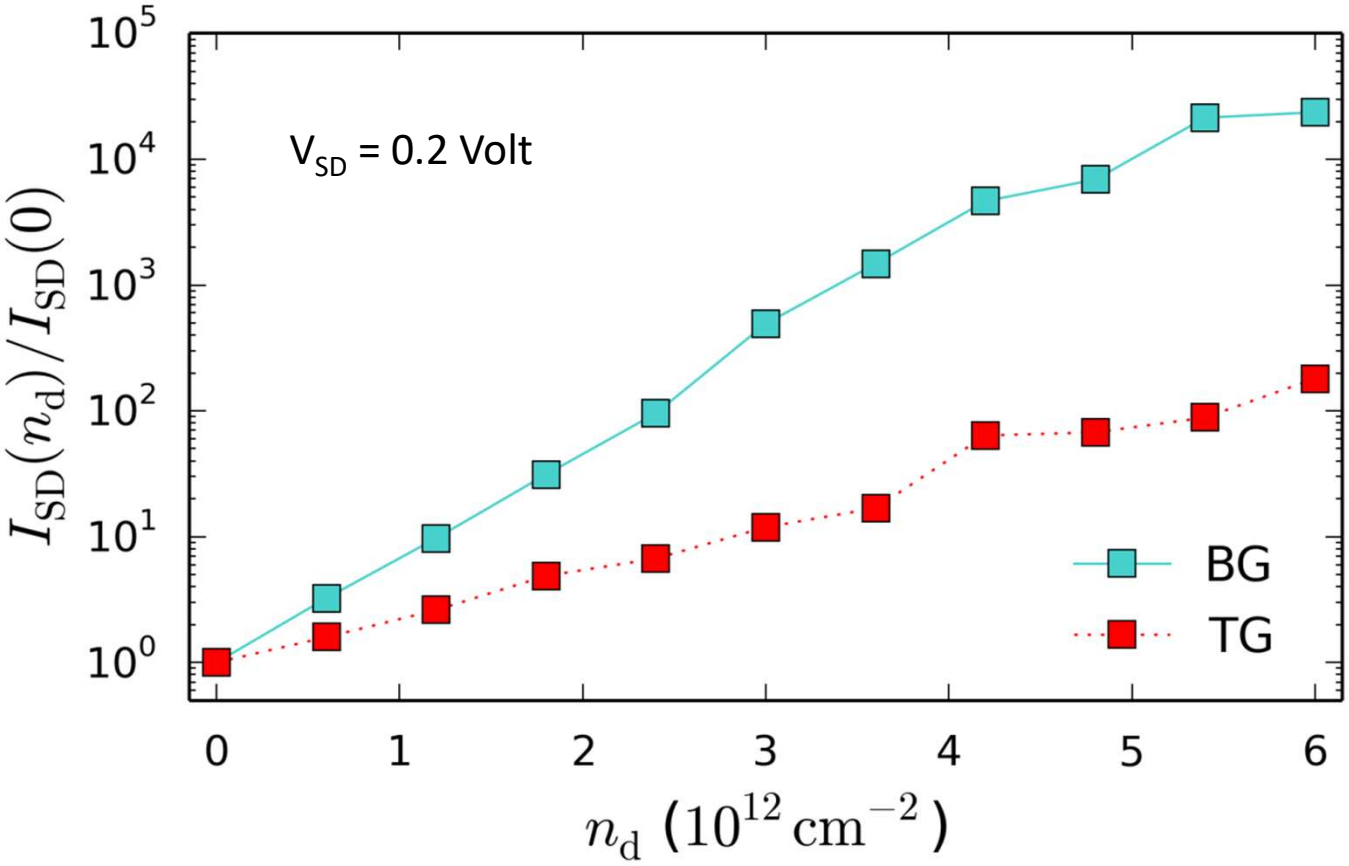
Transport direction: z (self-energies), x: PBC



D. Stradi, N. R. Papior, O. Hansen, M. Brandbyge, Nano Lett. **17**, 2660 (2017)

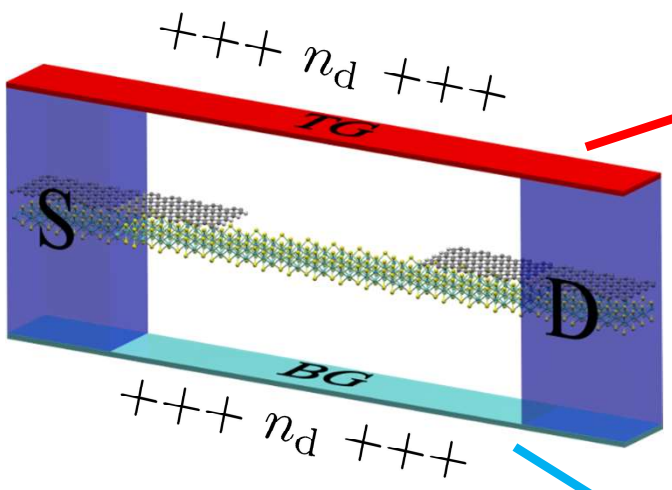
Current: Gate position matters!

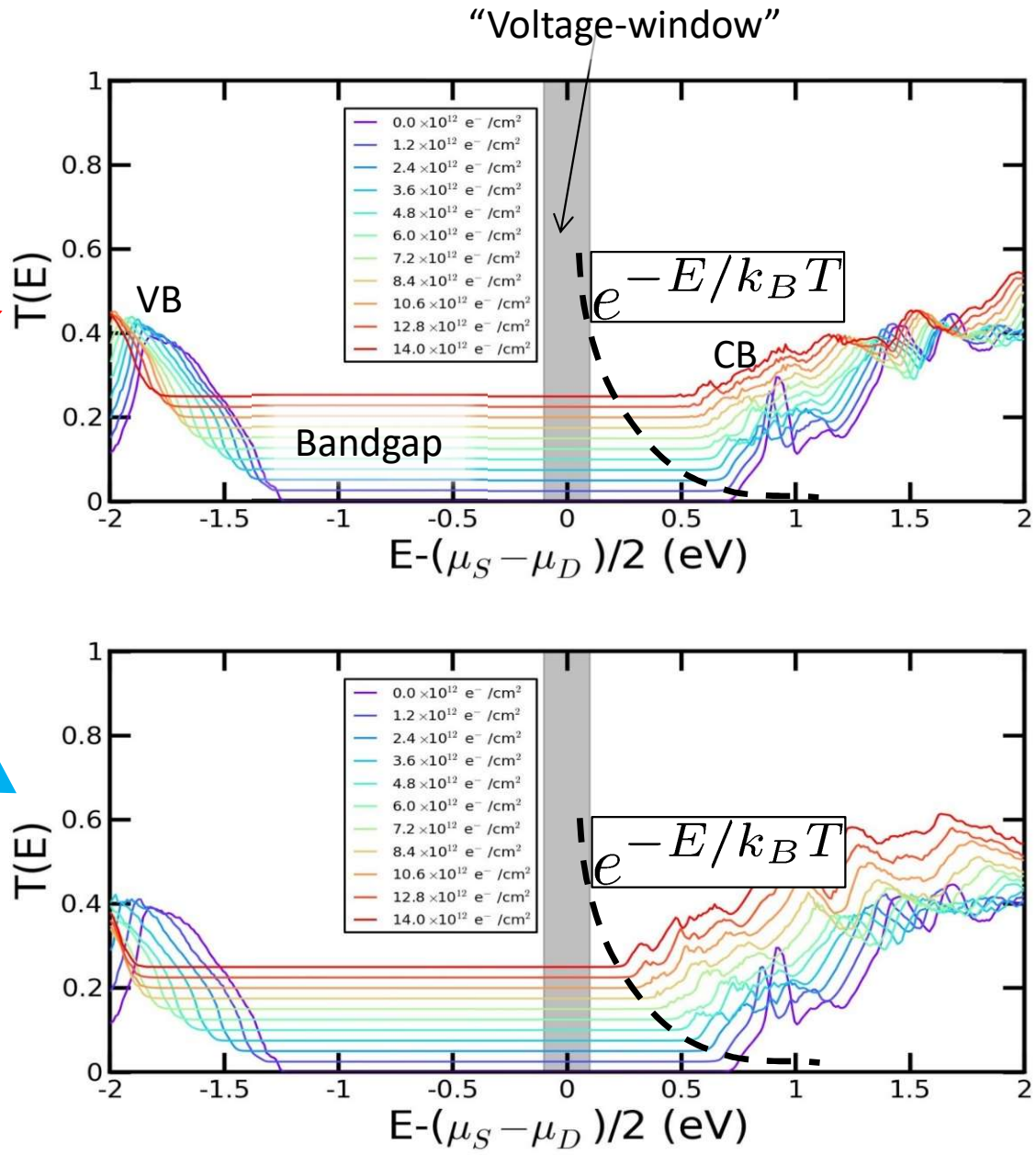




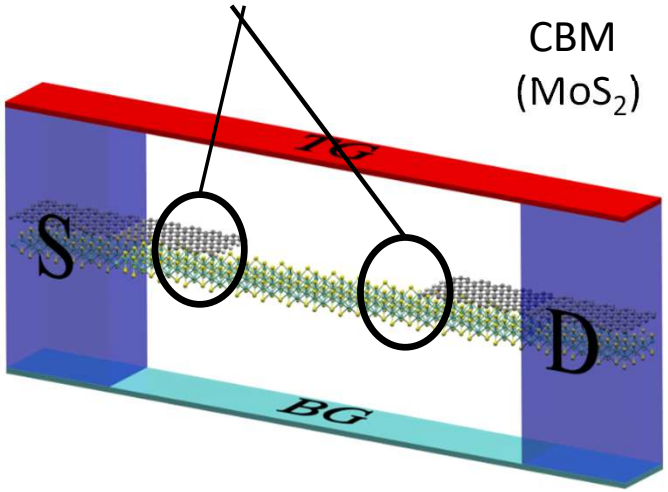
D. Stradi, N. R. Papior, O. Hansen, M. Brandbyge, Nano Lett. **17**, 2660 (2017)

Current: Thermionic emission

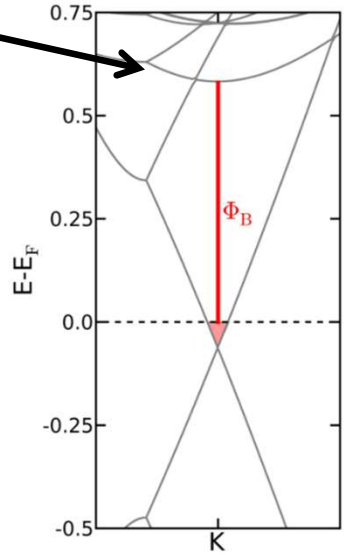




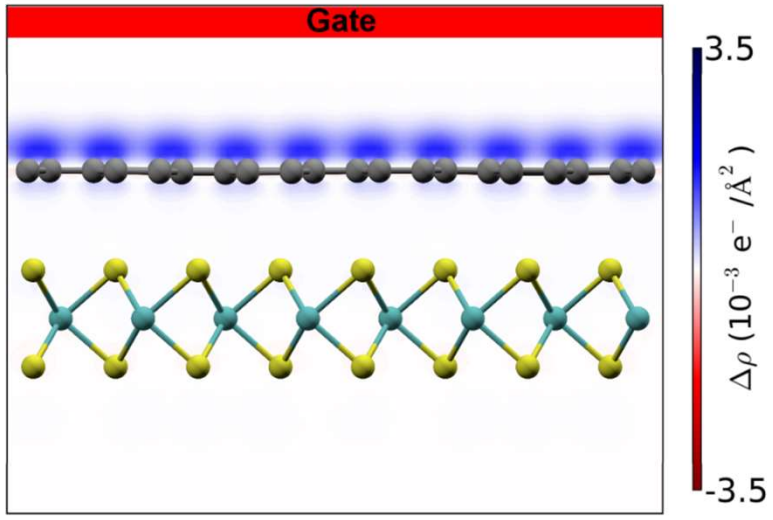
Simple picture: Screening & Schottky barrier



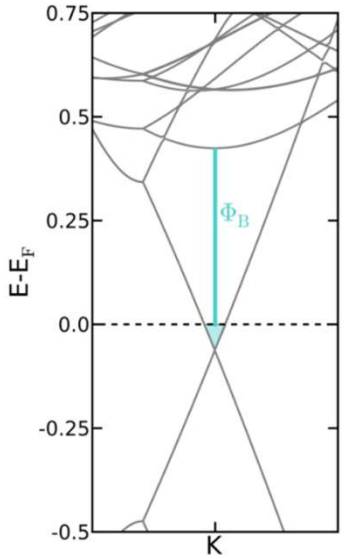
CBM (MoS_2)

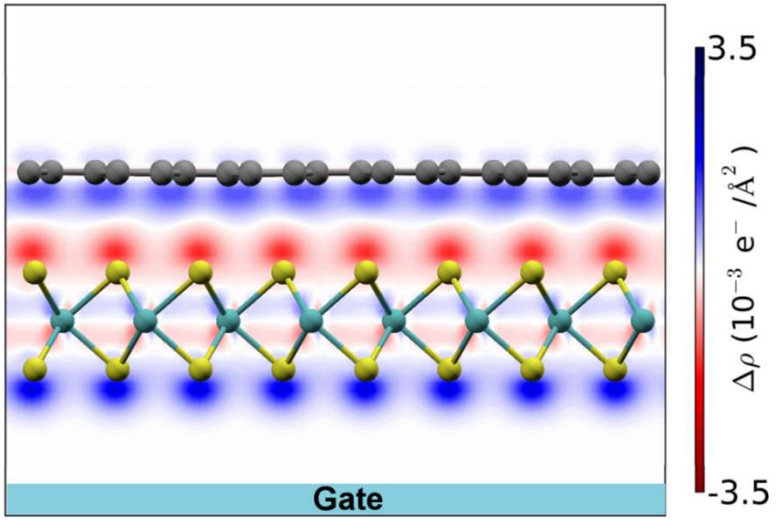


Graphene is screening the gate:



Stacking sequence matters!





D. Stradi, N. R. Papior, O. Hansen, M. Brandbyge, Nano Lett. **17**, 2660 (2017)

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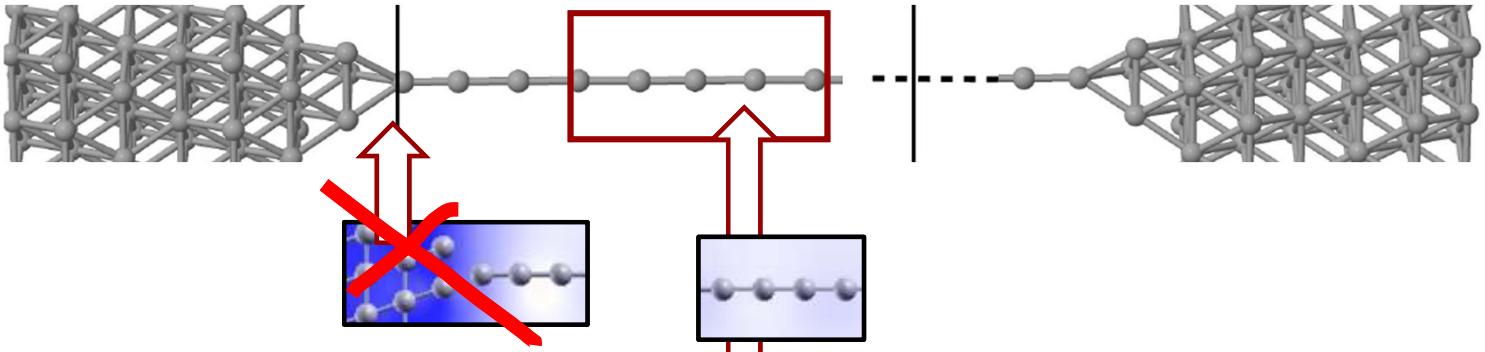
Simple approach: ”Bulk-bias”

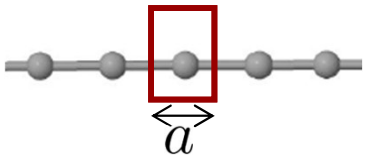
N. Papior, S. Leitherer, M. Brandbyge, Phys. Rev. B. **106**, 155401 (2022)


Dr. Nick Papior


Dr. Susanne Leitherer



Model: Chain with ballistic distribution function



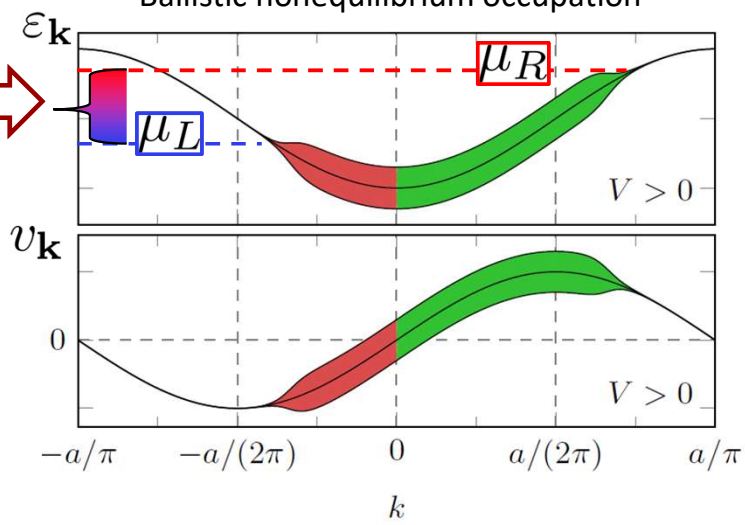
- Flat potential: **Periodic boundary conditions**
- Different chemical potential/filling of ”Left” and ”Right” movers μ_L/μ_R

$$p_{n\mathbf{k}} = -\hat{\mathbf{e}} \cdot \mathbf{v}_{nk}$$

$$\delta f(n\mathbf{k}) = \Theta(p_{n\mathbf{k}}) \left[n_F(\varepsilon_{n\mathbf{k}} - \mu_L) - n_F(\varepsilon_{n\mathbf{k}} - E_F) \right] + \Theta(-p_{n\mathbf{k}}) \left[n_F(\varepsilon_{n\mathbf{k}} - \mu_R) - n_F(\varepsilon_{n\mathbf{k}} - E_F) \right]$$

eV

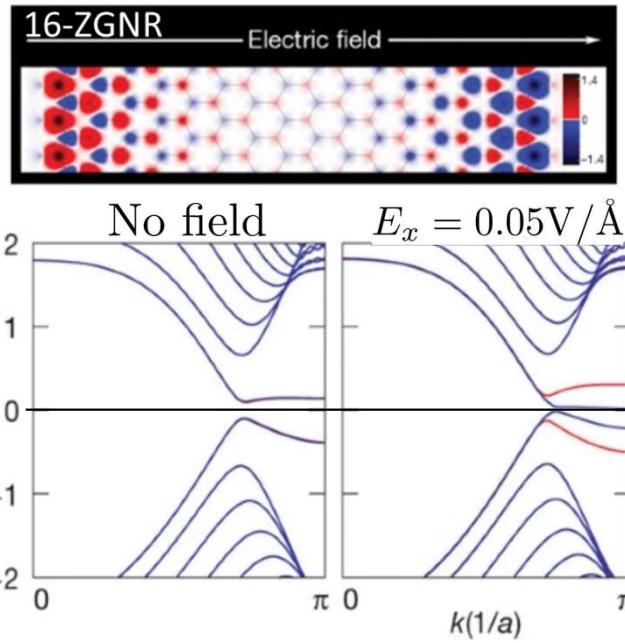
Ballistic nonequilibrium occupation



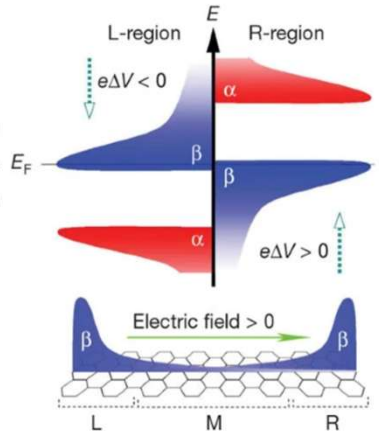
Magnetic graphene nanoribbons

Half-metallic graphene nanoribbons

Son, Y.-W., Cohen, M. L. & Louie, S. G.
Nature **444**, 347–349 (2006)

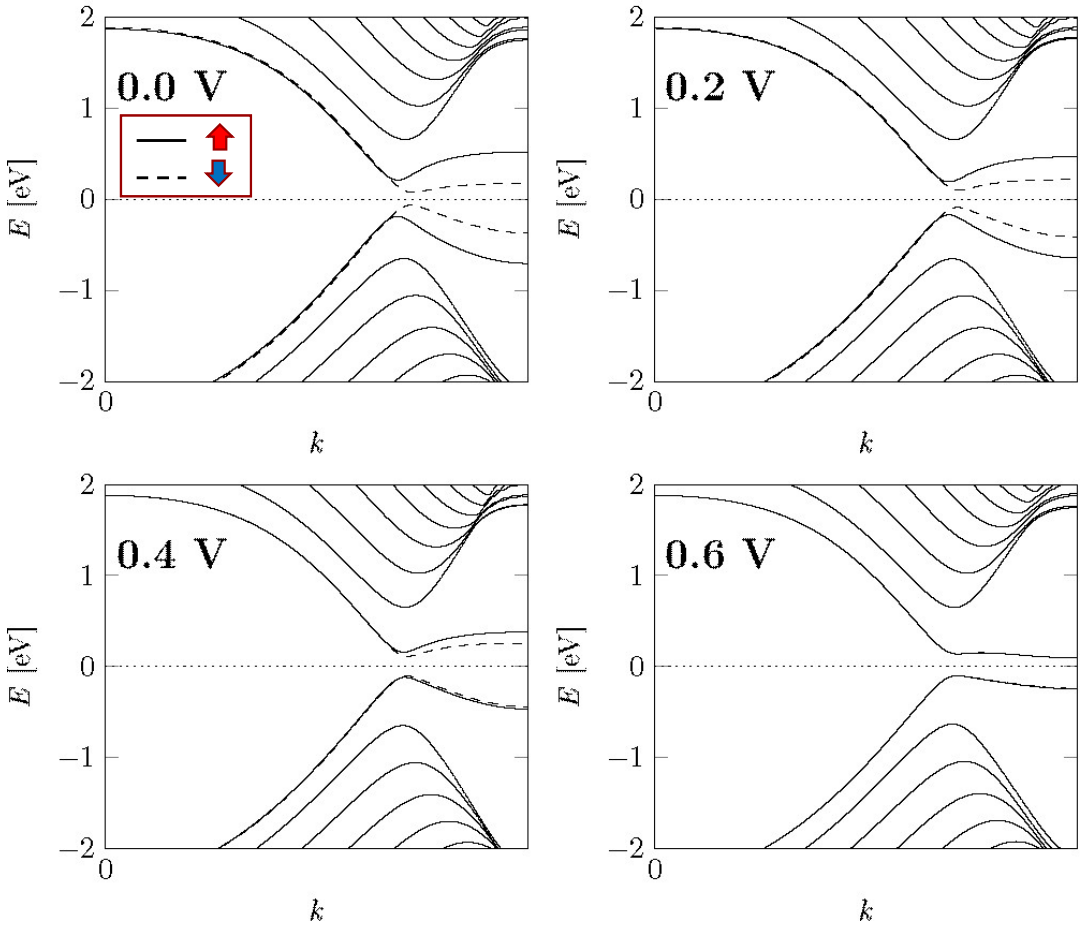


Conducting spin-polarized edge channel



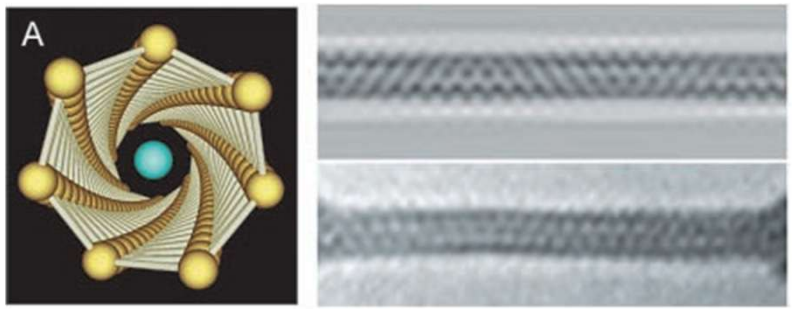
S. Leitherer, N. Papior, M. Brandbyge, "Strong current in carbon nanoconductors: Mechanical and magnetic stability", Carbon **232**, 119708 (2025),

$$E_x = 0.05\mathrm{V/Å}$$

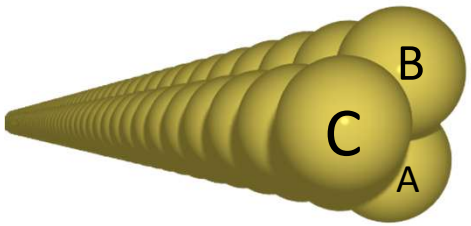


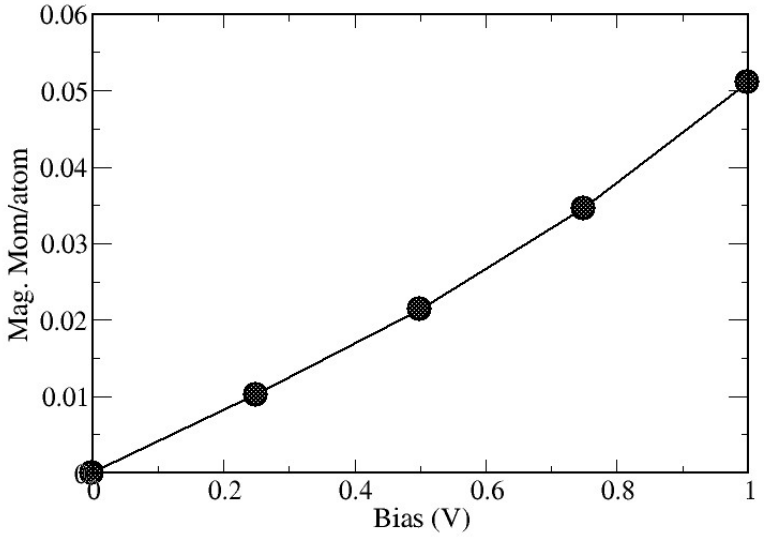
Au spiral chain & Spin-Orbit

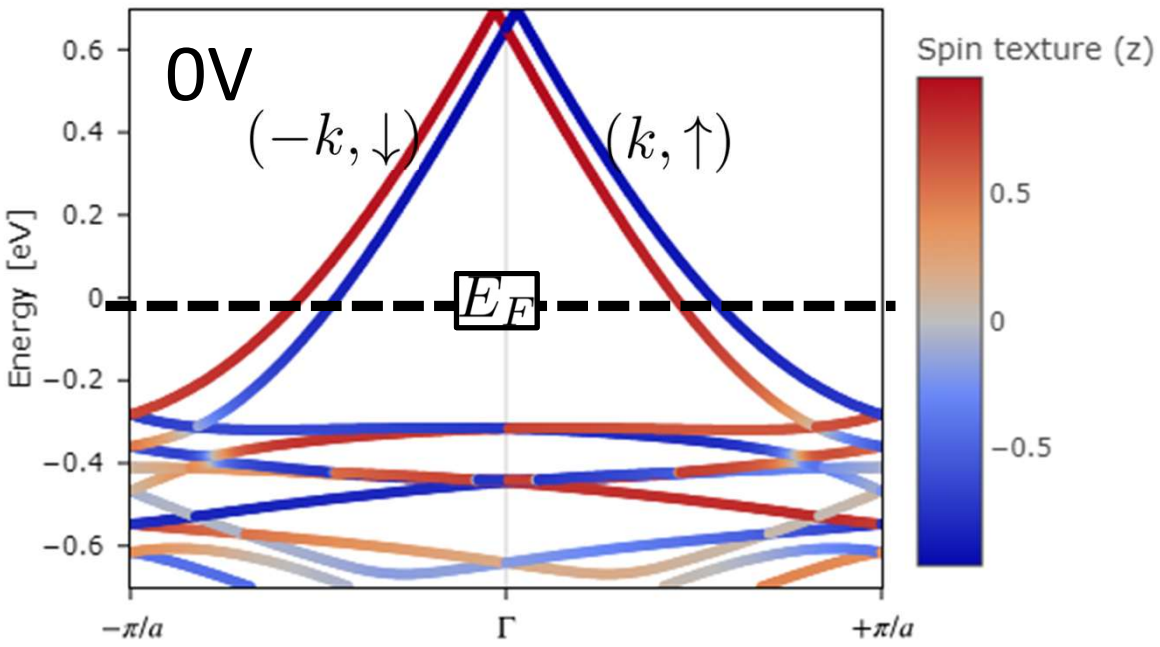
Helical Gold Nanowires

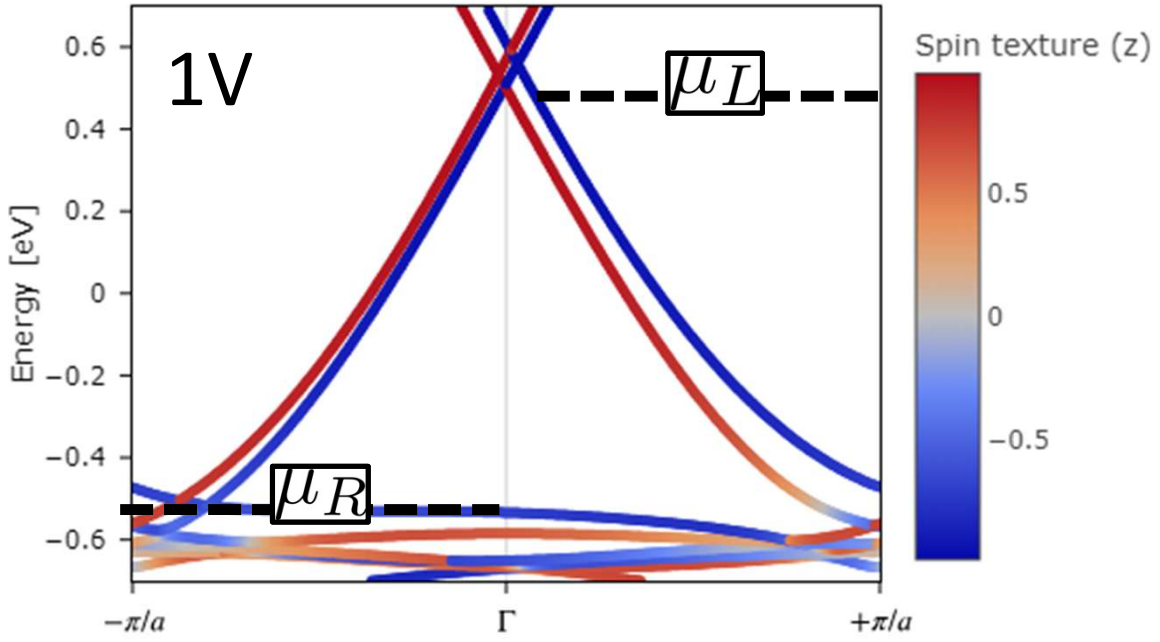


Y. Kondo, K. Takayanagi, SCIENCE 289, 606 (2000)







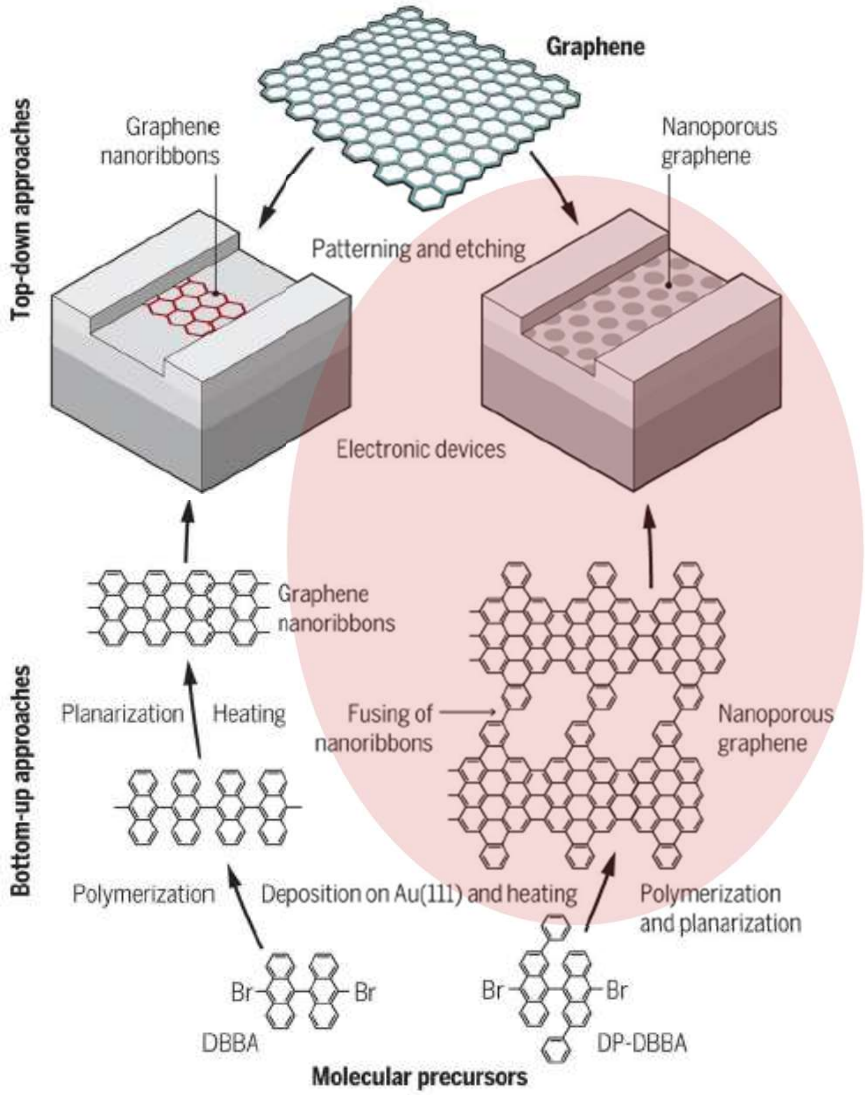


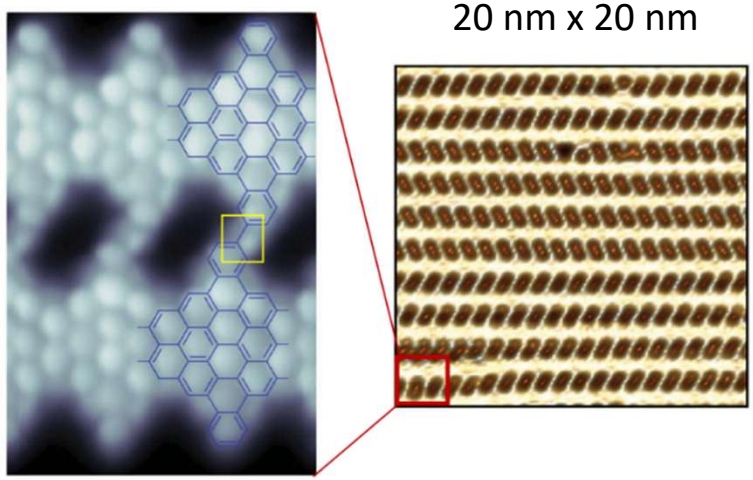
Outline

- **Motivation: “Quantum materials”/Landauer’s transport**
- **Theoretical methodology – a crash-course on DFT-NEGF**
- **Examples**
  - **Non-equilibrium & Gate effects in 2D devices**
  - **Current-only calculations**
  - **Large-scale systems: Nano-porous graphene**
  - Spin-filtering in porphyrin-GNR hybrids

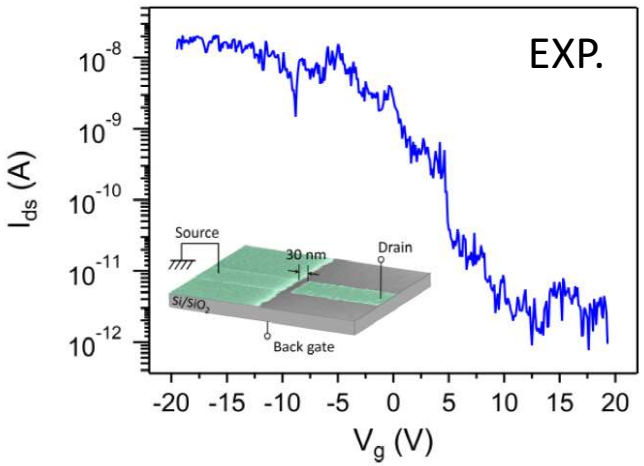
Nanoporous graphene (NPG)

Moreno et al., **"Bottom-up synthesis of multifunctional nanoporous graphene"**, Science, **360**, 199 (2018)





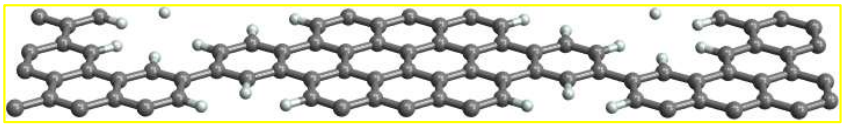
Band-gap



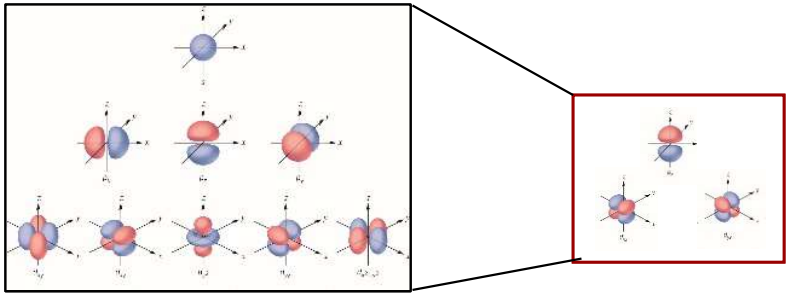
Multi-scale method: DFT to large-scale ”tight-binding”

[1] G. Calogero, N. R. Papior, M. Koleini, M.H.L. Larsen, M. Brandbyge, Nanoscale **11**, 6153 (2019)
[2] Software: Nick R. Papior, **SISL** (DOI:10.5281/zenodo.597181) **github.com/zerothi/sisl**

- **DFT**: ”Small” unit-cell (< 1000 atoms)
  SIESTA: NAO-basis, PBE-GGA



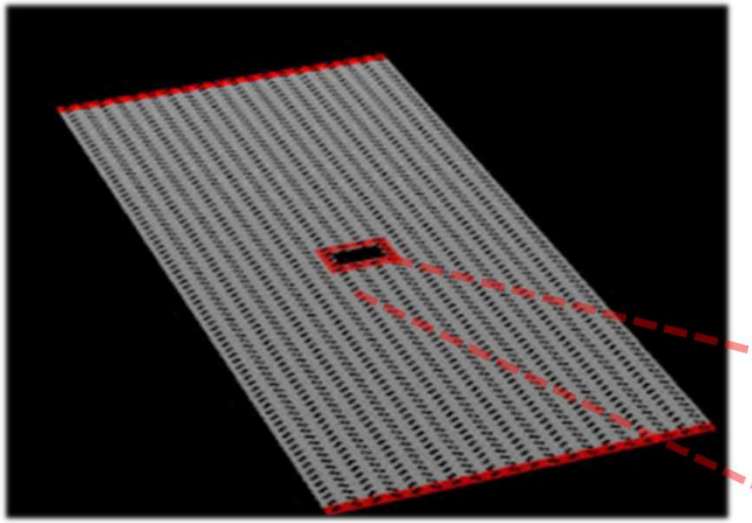
- **Project** to ”Tight-binding” [1,2]: ”TB”
  DFT-Hamiltonian to smaller basis (f.ex. pz-symm)

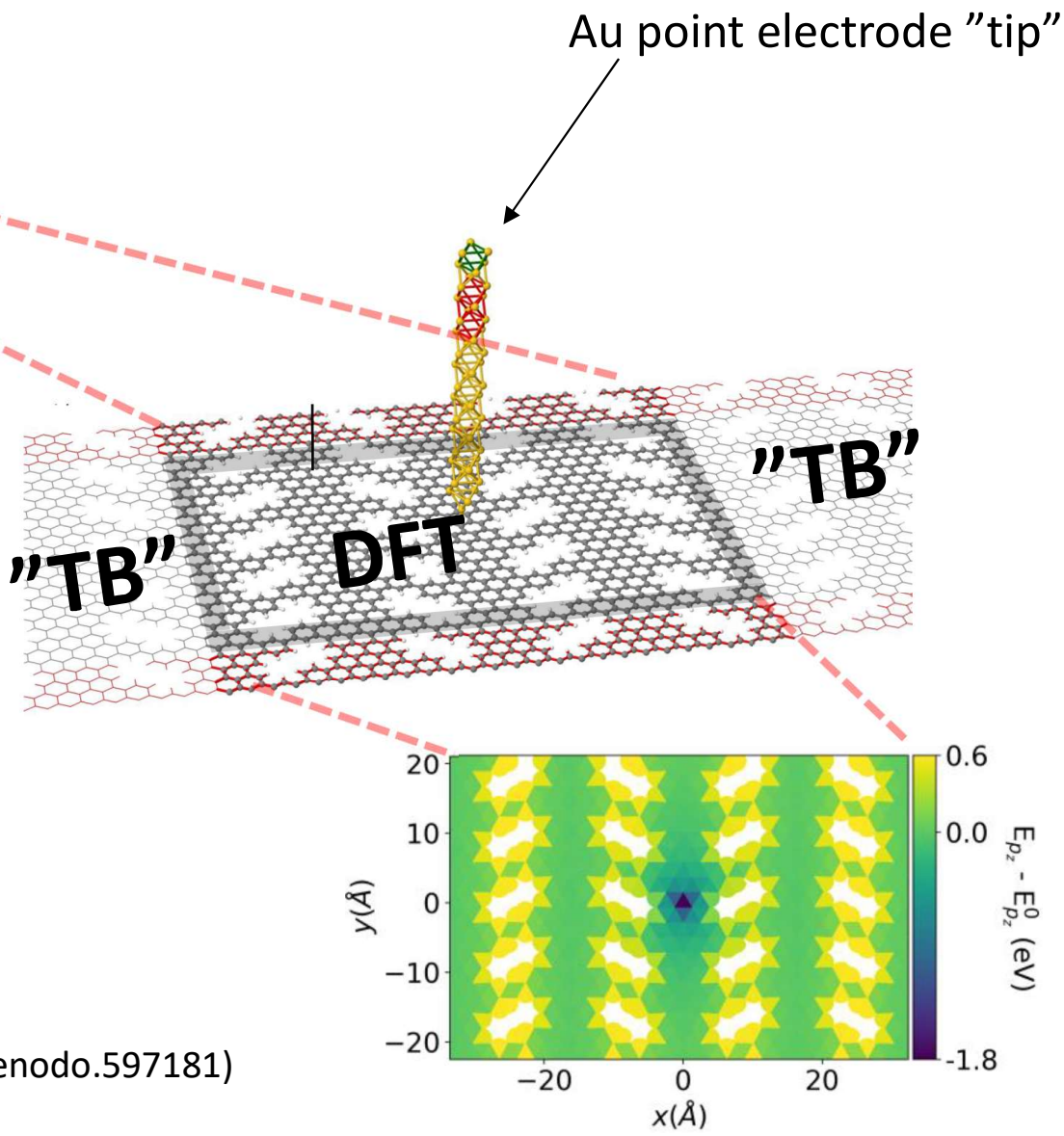


- **Tiling** [2] into 100-nm scale structure

- **Add semi-infinite electrodes** and complex absorbing potentials (CAP)

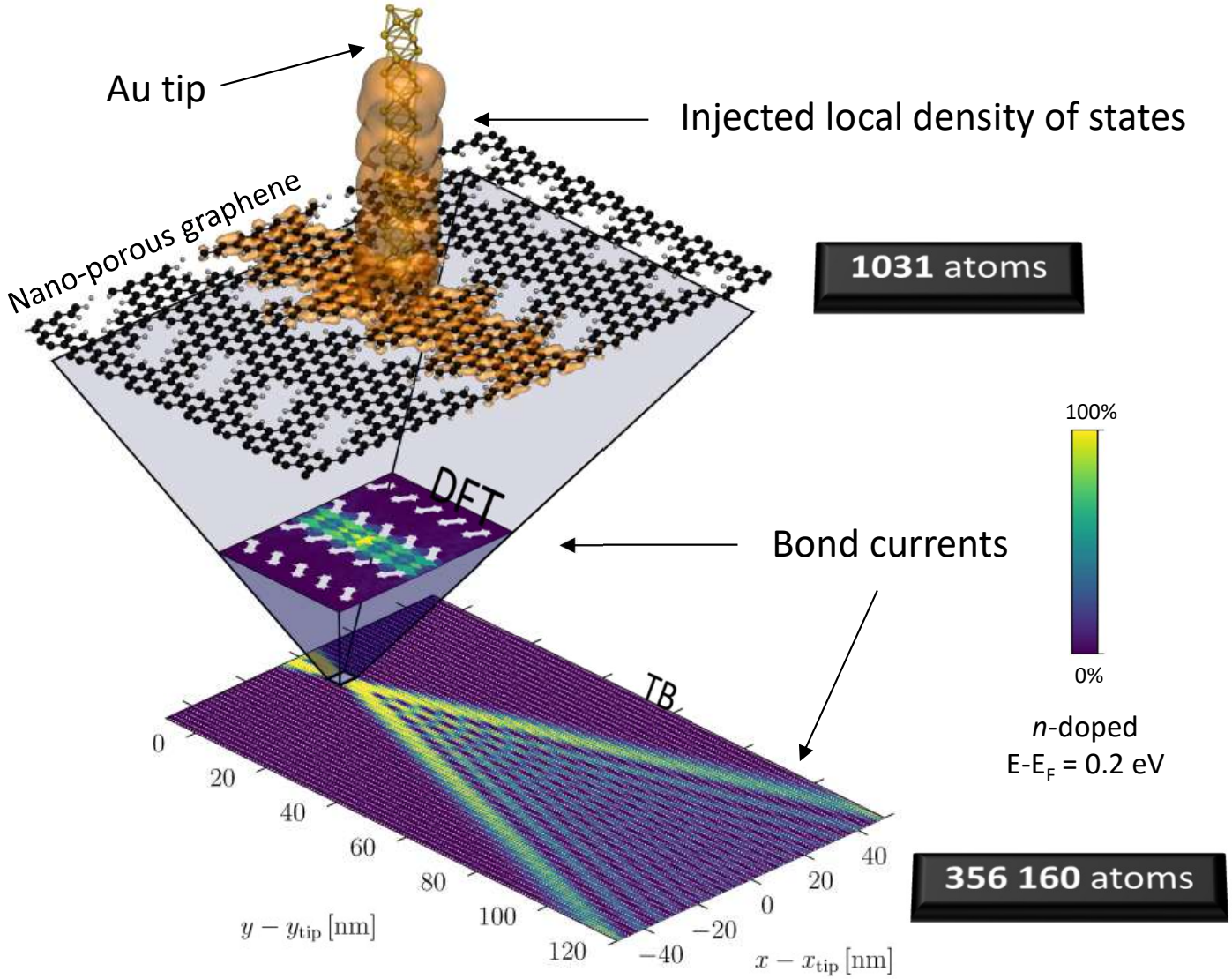
Seamless embedding DFT regions





Software: Nick R. Papior, **SISL** (DOI:10.5281/zenodo.597181)

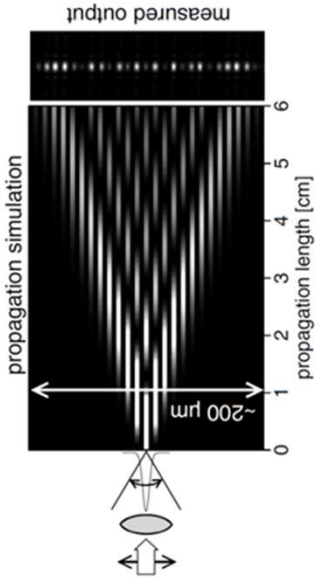
Point-injection from Au ”tip”

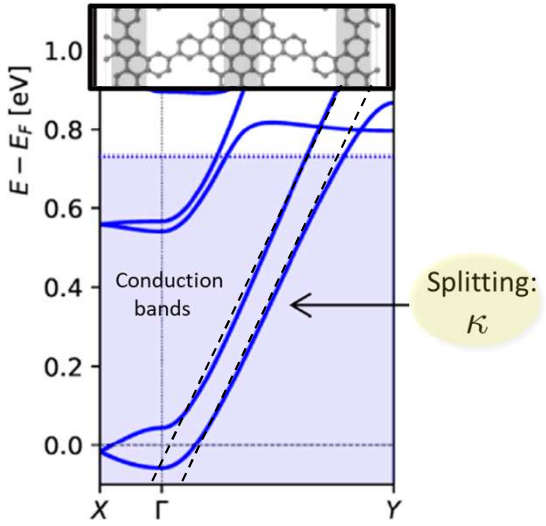


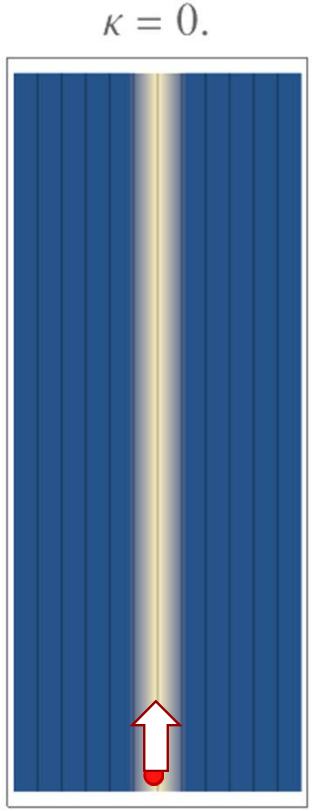
- G. Calogero, B. Kretz, N.R. Papior, A. Garcia-Lekue, T. Frederiksen, M.Brandbyge, **“Electron Transport in Nanoporous Graphene: Probing the Talbot Effect”**, Nano Letters, **19**, 576 (2019)

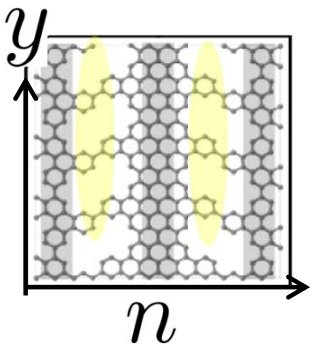
Light-like behaviour: Talbot effect

H.F. **Talbot**, *Phil. Mag.* 9, 401 (1836) *"LXXVI. Facts relating to **optical** science. no. IV"*









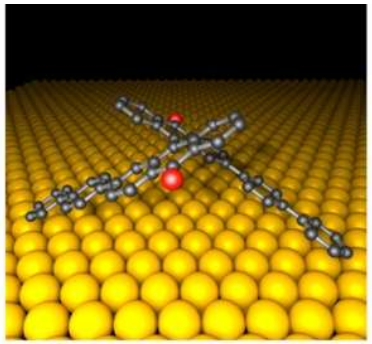
Wavefunction $\psi_n(y) = e^{iky}\psi_n$

$$i\frac{d\psi_n}{dy} - \kappa(\psi_{n-1} + \psi_{n+1}) = 0$$

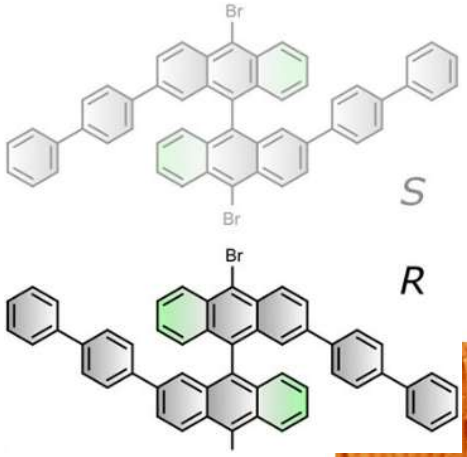
Injection: $\psi_0(0) = 1$ $\psi_n(y) \propto J_n(\kappa y)$

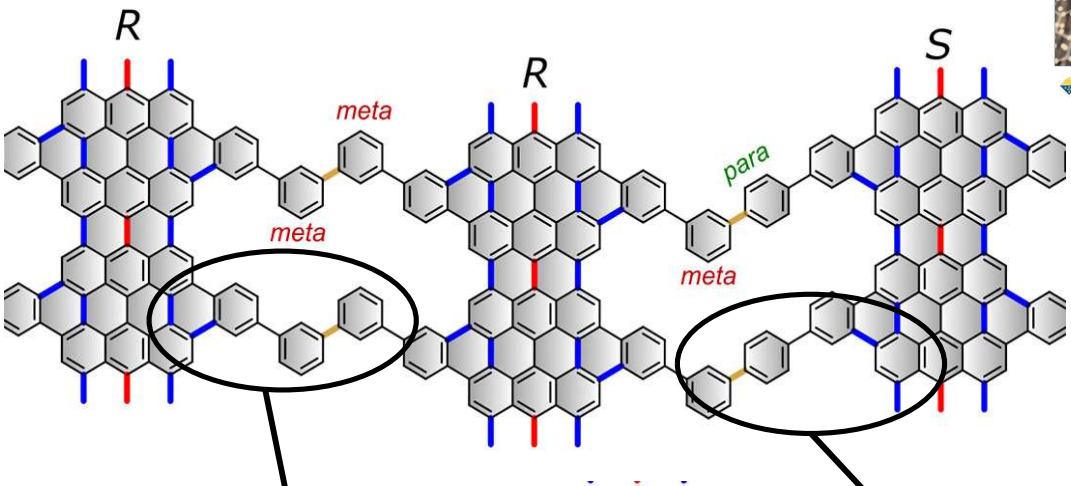
Bridge engineering

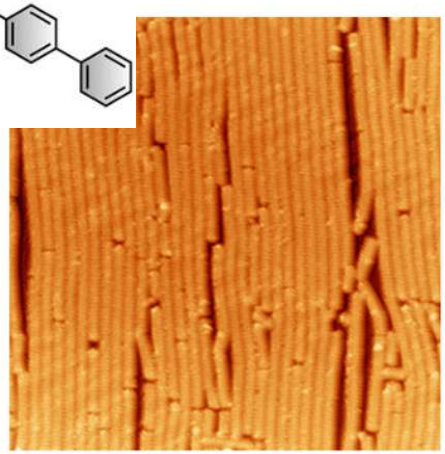
Moreno et al., J. Am. Chem. Soc., **145**, 8988 (2023)

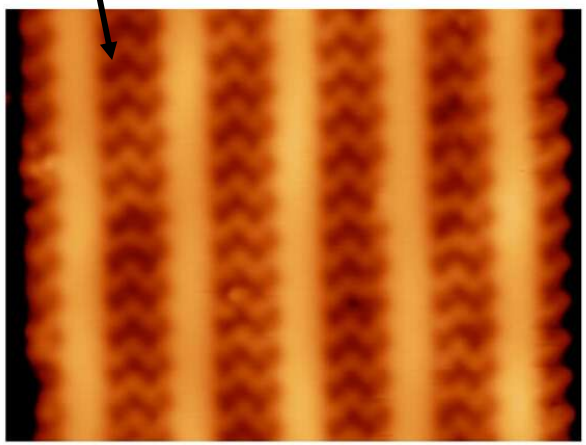


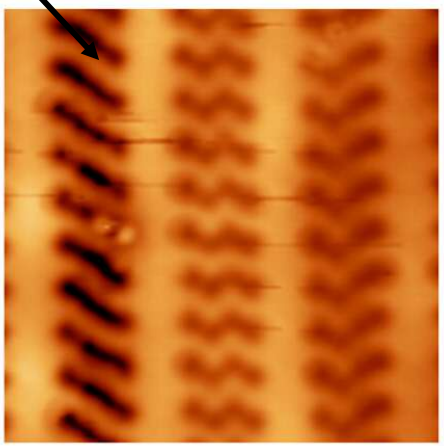
DBP-DBBA Monomer

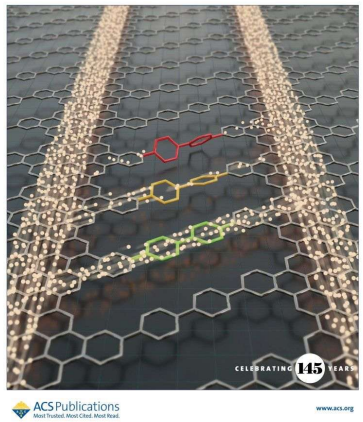








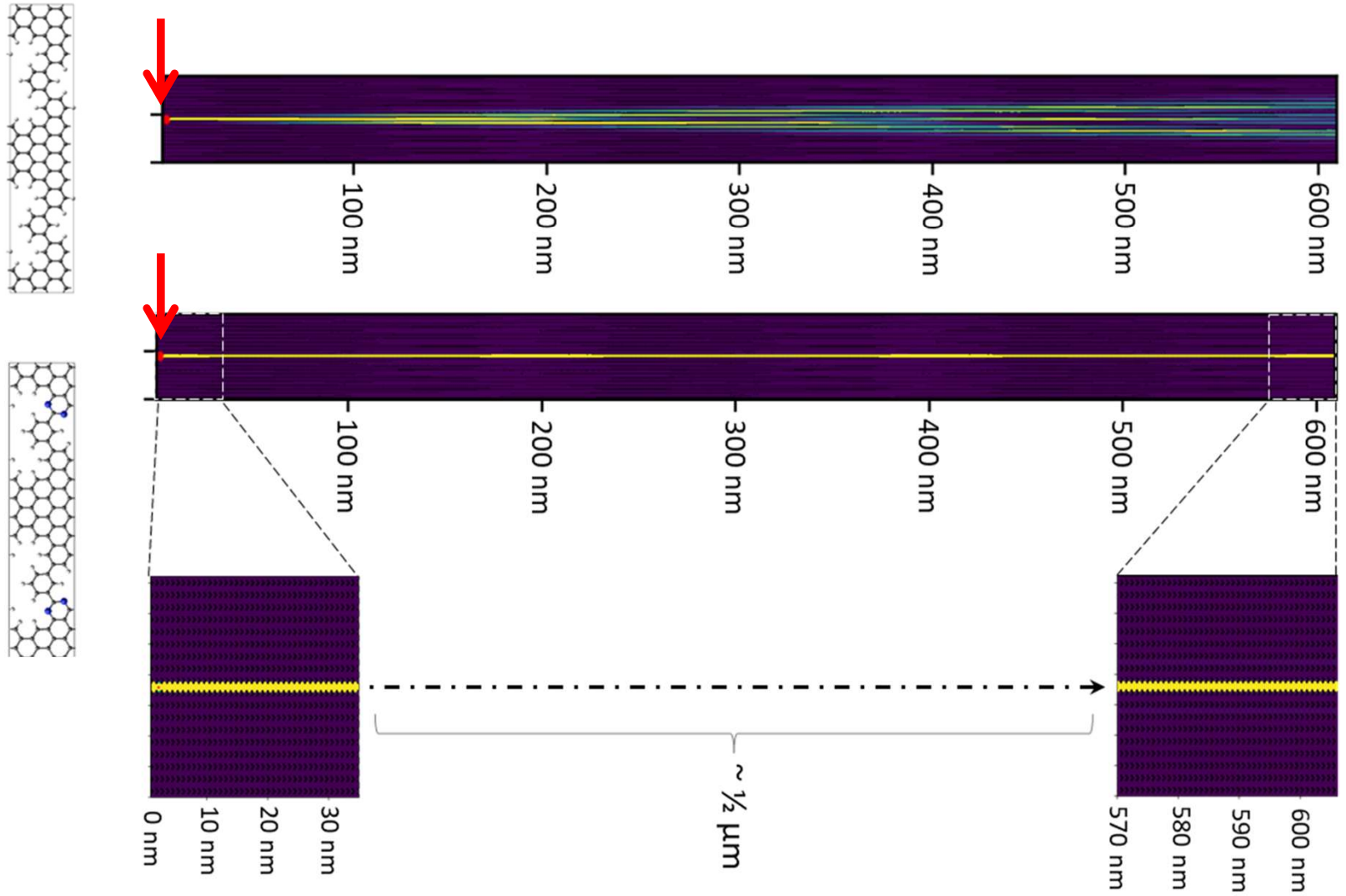




Isolation by ”bridge-engineering”

G. Calogero, I. Alcon, A. Morales, N. Papior, P. Febrer, A. W. Cummings, M. Pruneda, S. Roche, M. Brandbyge *Small* e08850 (2025)

- Meta
- hNPG + Meta



Calculated MFP [G. Calogero et al., Carbon **234,** 119950 (2025)]

Mean free path at 300 K along the two in-plane directions for each material, calculated using Eq. (6).

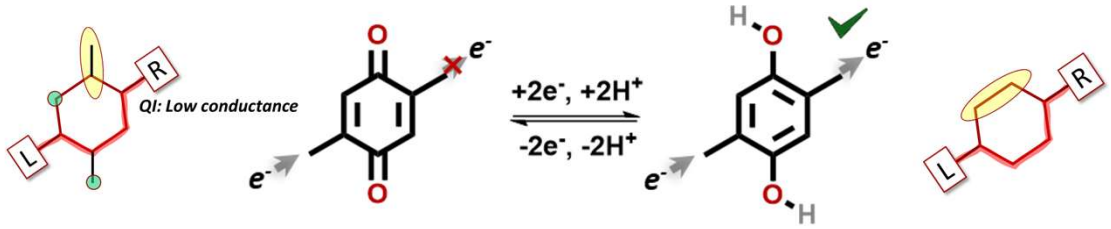
	Graphene	NPG	*para*-NPG	*meta*-NPG
$l^{\|}$ (nm)	772.6	277.8	317.4	318.4

Theoretical proposal: Switching bridges

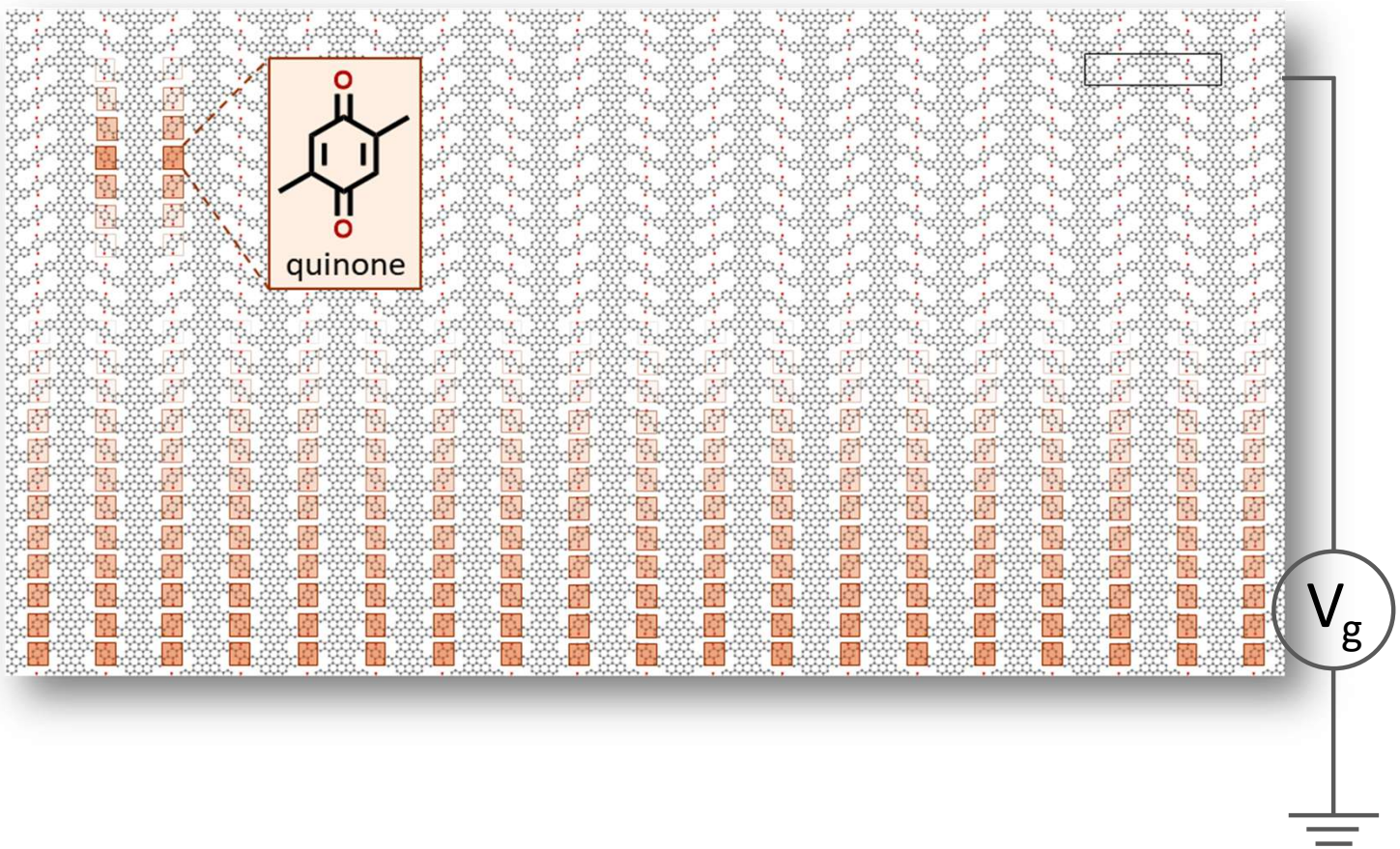
- Electrochemical control of charge current flow

I. Alcon, G. Calogero, N. Papior, M. Brandbyge, Adv. Funct. Mater. (2021) 31, 2104031

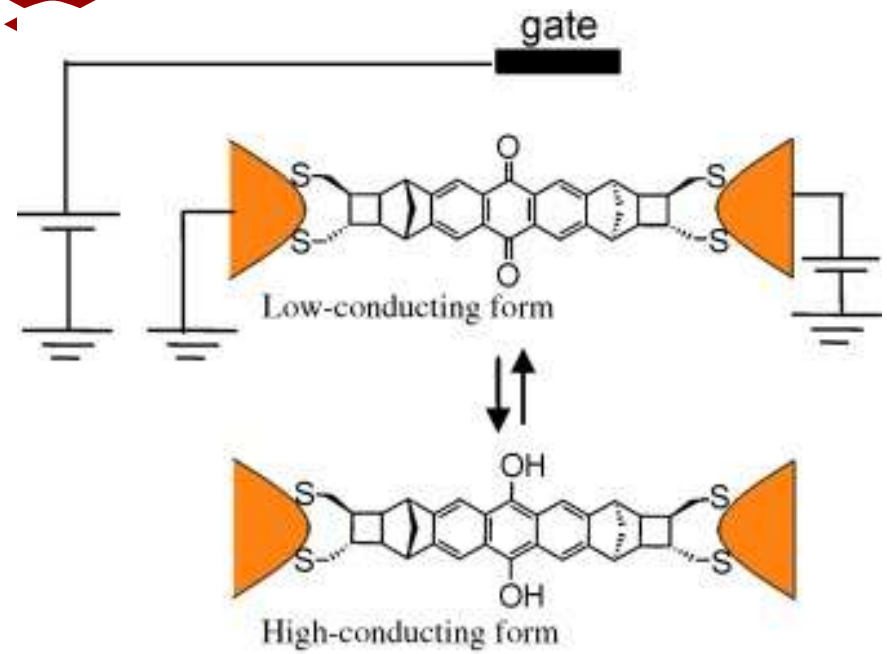
Dr.
Isaac Alcon
ICN2, Barcelona



”Quinone-NPG”

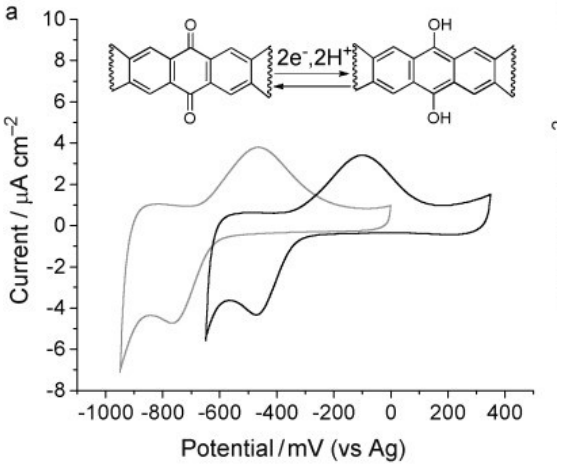


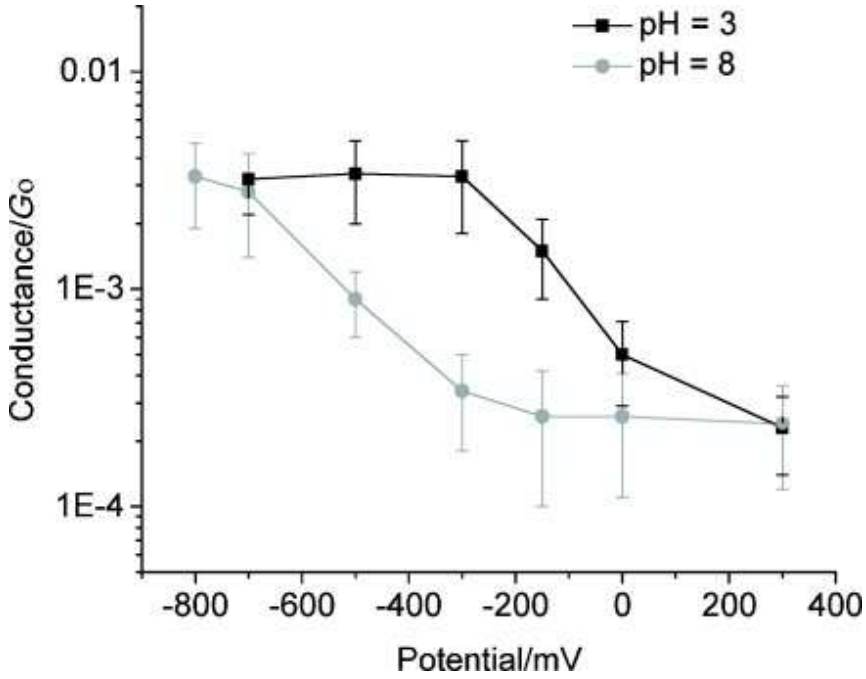
Electrochemical control of QI



Observation of **Electrochemically Controlled Quantum Interference** in a Single Anthraquinone-Based Norbornylogous Bridge Molecule

Angew. Chemie Int. Ed. **51**, 3203–3206 (2012)



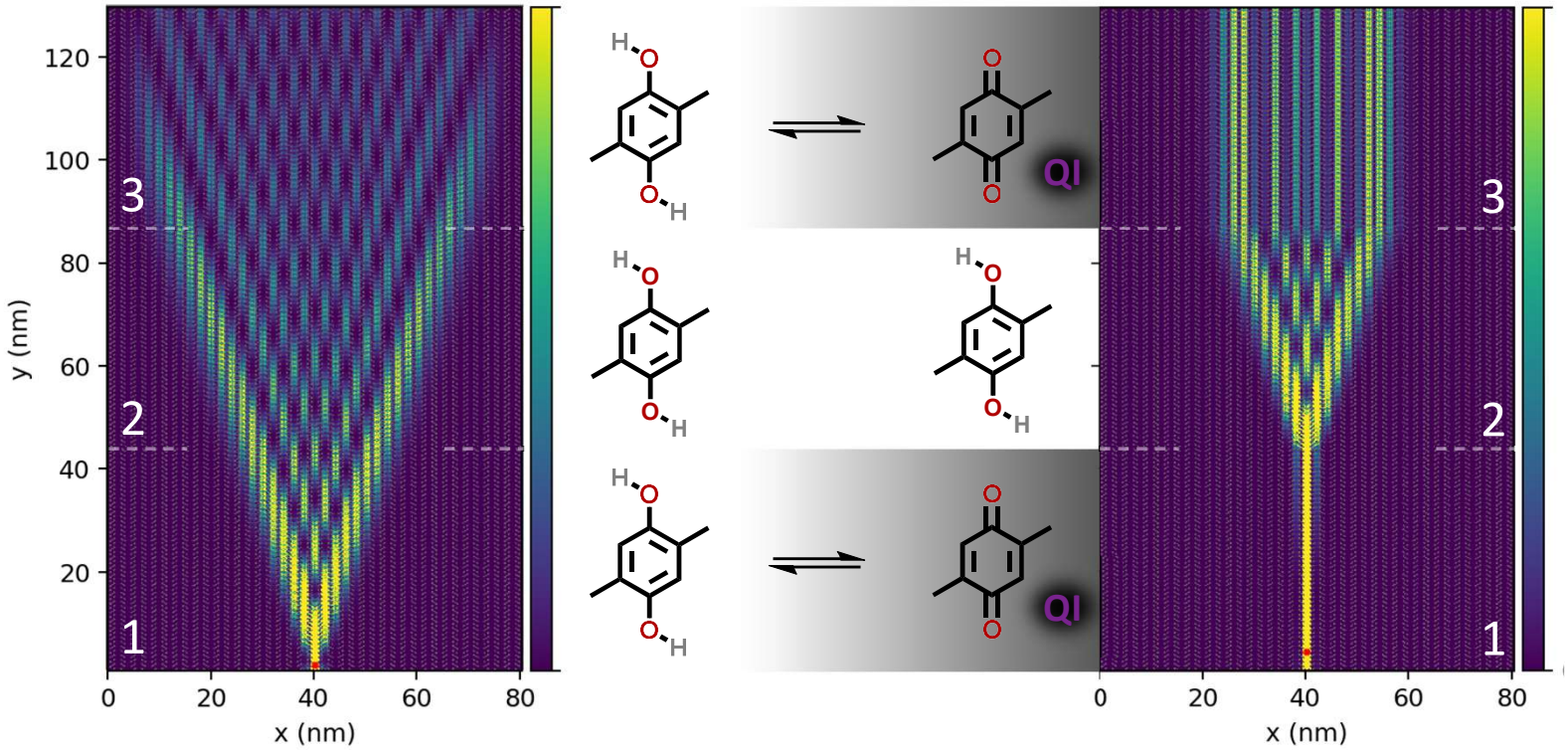


Local electro-chemical modifications

I. Alcon, G. Calogero, N. Papior, M. Brandbyge, Adv. Funct. Mater. (2021) 31, 2104031

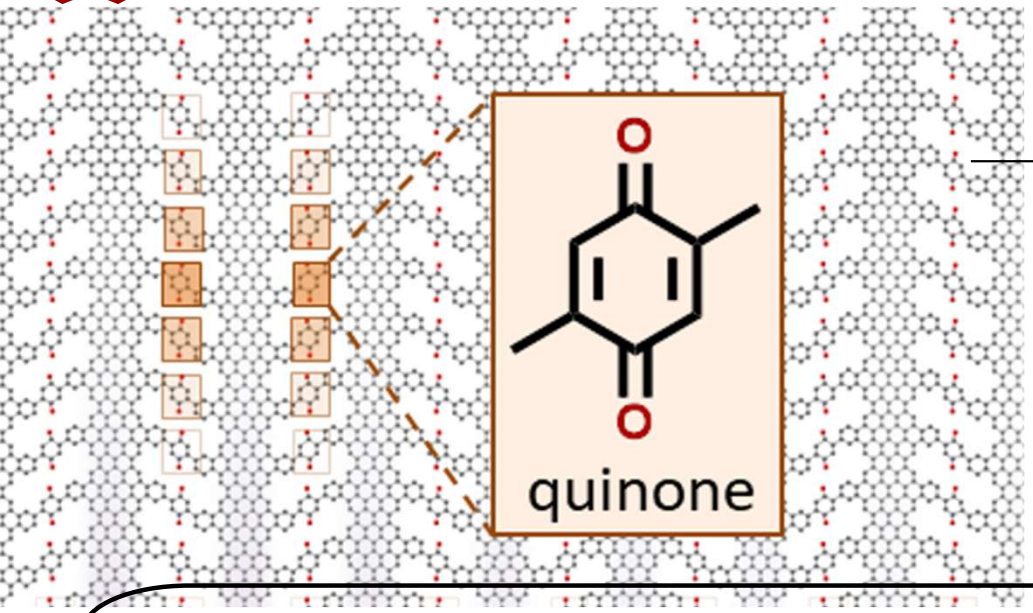
Model:

nn TB fitted to DFT Bond currents in valence bands@ E = -0.75 eV + E_F $\sim \frac{dI}{dV}(\vec{r}, -0.75V)$



Electron doping: Spin polarization

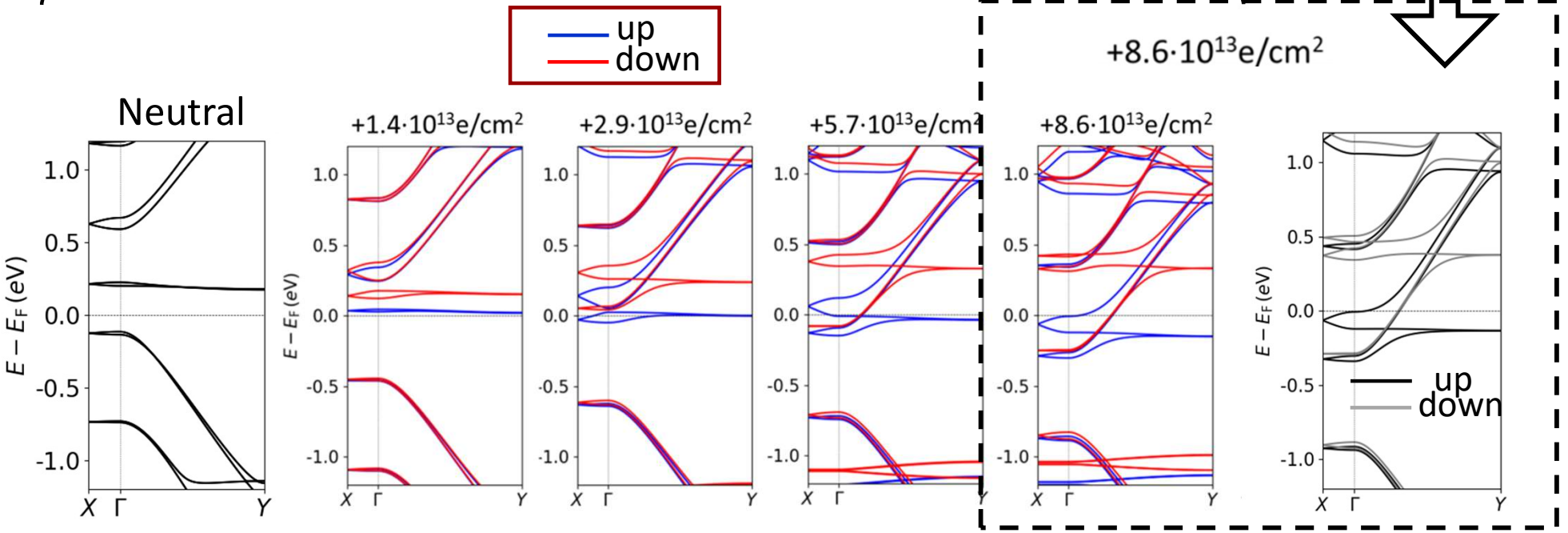
I. Alcon, G. Calogero, N. Papior, M. Brandbyge, Adv. Funct. Mater. (2021) 31, 2104031



V_g

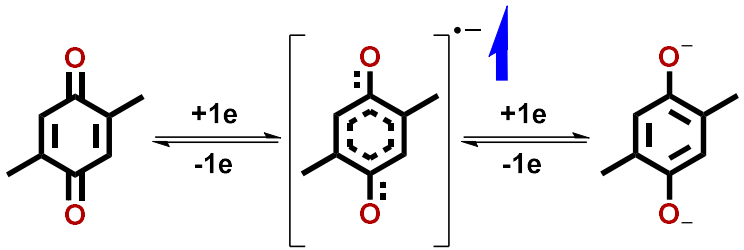
Gated DFT

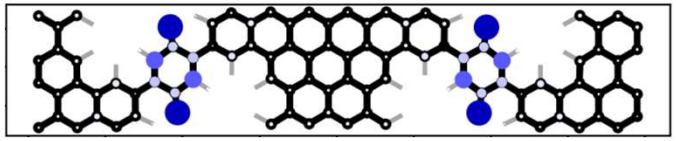
TB
C-p_z & O-p_z

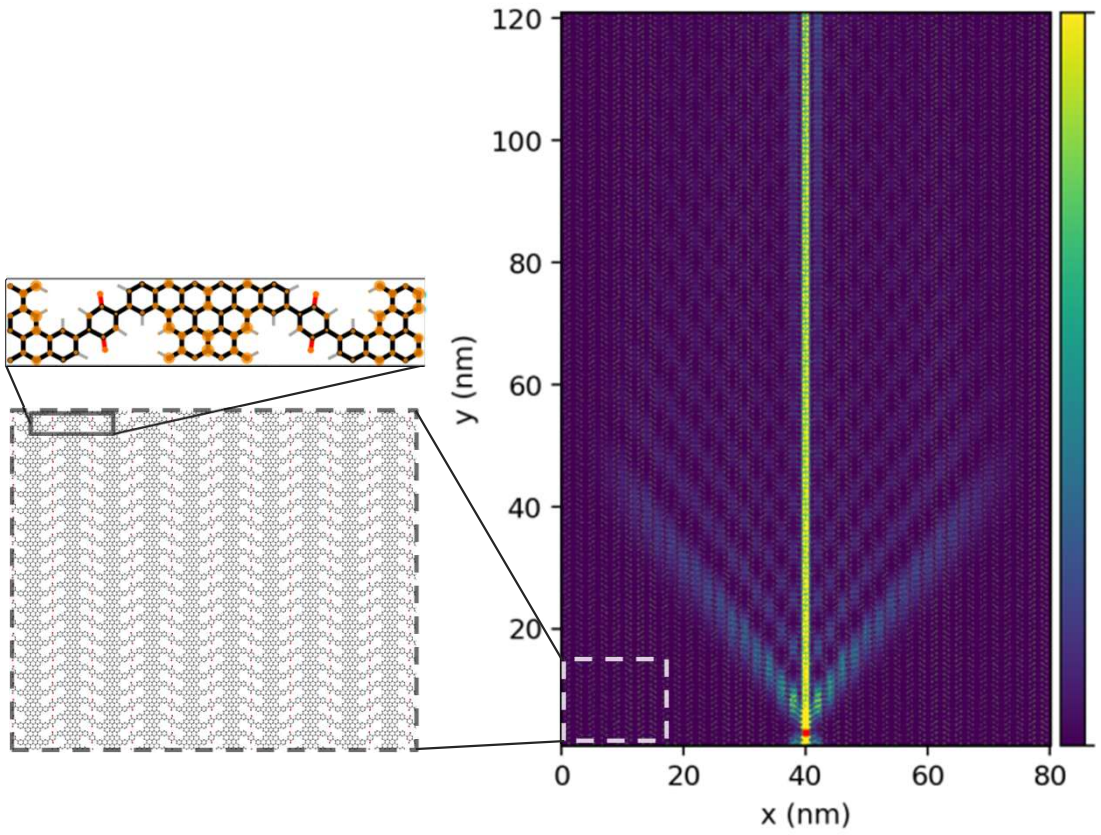


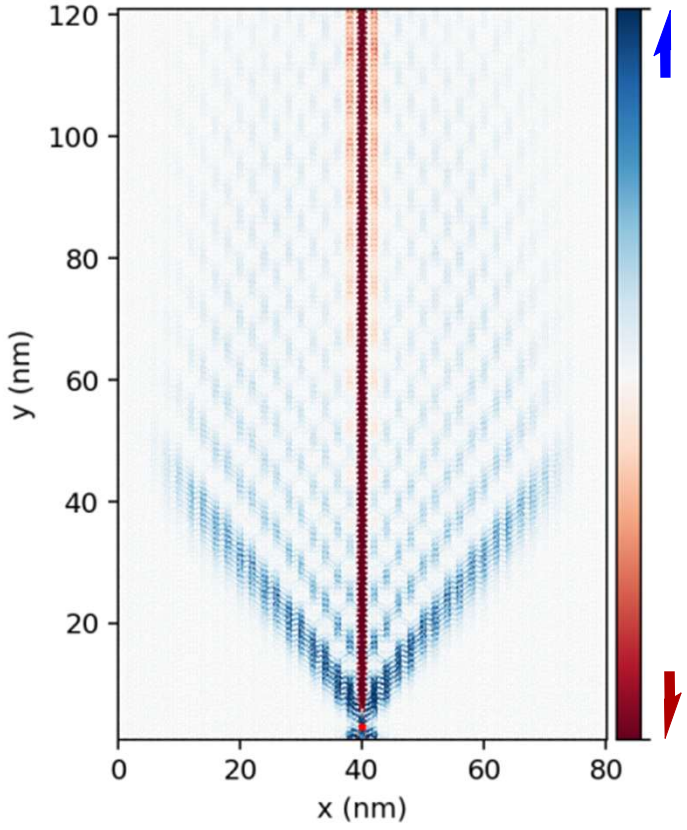
Electron doping: Spatial Spin filtering

I. Alcon, G. Calogero, N. Papior, M. Brandbyge, Adv. Funct. Mater. (2021) 31, 2104031









Take-home messages

Computational tools for complex quantum devices:

- DFT-NEGF: Calculations without fitting parameters under working conditions
- Inclusion of electrodes/open boundaries/gates in DFT
- Extension to multi-scale (> 100 nm's)

TranSIESTA School 2026

Technical University of Denmark, 9th - 13th November 2026

Topics covered (may be subject to changes):

- Usage of TranSIESTA/TBtrans and sisl.
- Correlated systems and the mean field Hubbard model.
- Single contacts by removal of periodic images.
- Modelling of extremely large systems with DFT precision.
- Manipulation of Hamiltonians by merging and creating real-space plots.

It will cost 250 EUR to participate, paid in advance. This will cover lunches, coffee breaks and the conference dinner. All other expenses are your own responsibility (accommodation, flights, etc.). One can sign up here.