MAX DRIVING THE EXASCALE TRANSITION

ICN2 Institut Català de Nanociència i Nanotecnologia

EXCELENCIA SEVERO OCHOA

Overview of the TranSIESTA module for transport simulations

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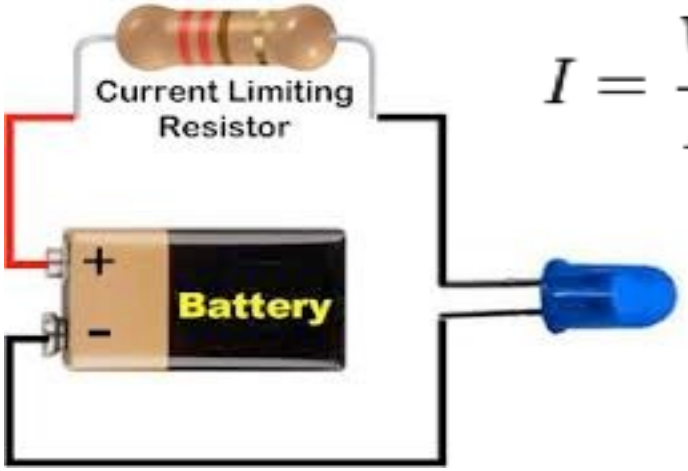
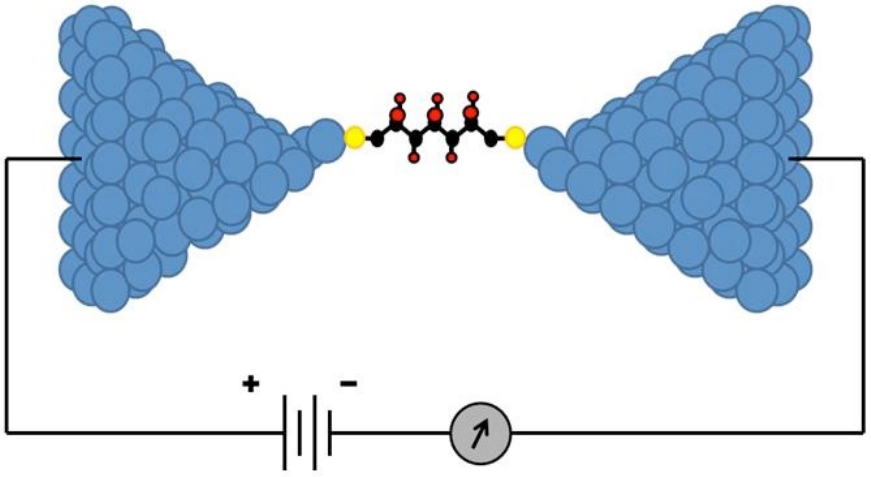
Challenge: Charge Transport at the Nanoscale



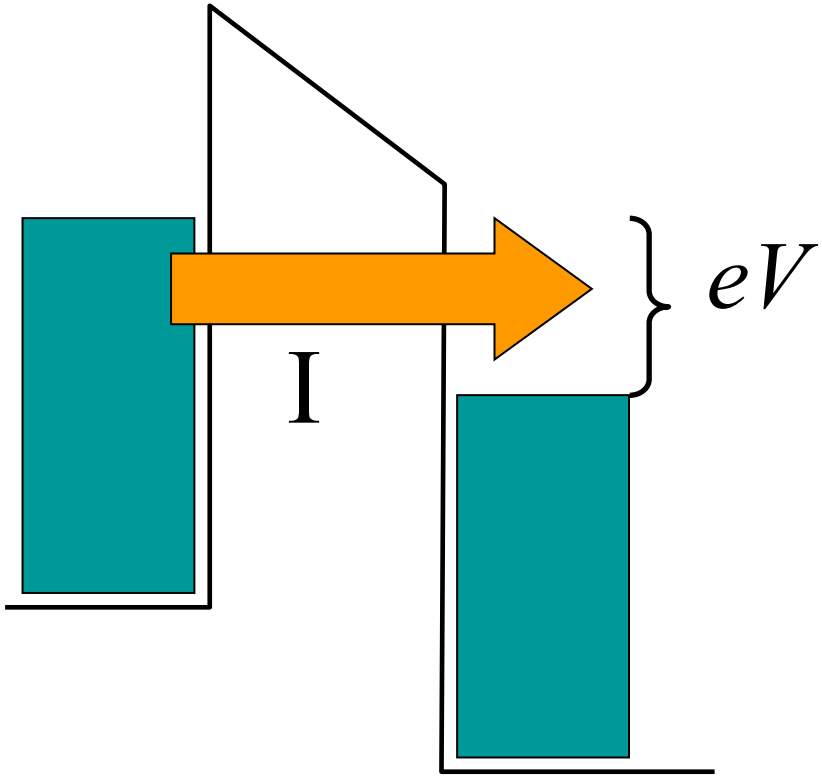
$$I = \frac{V}{R}$$

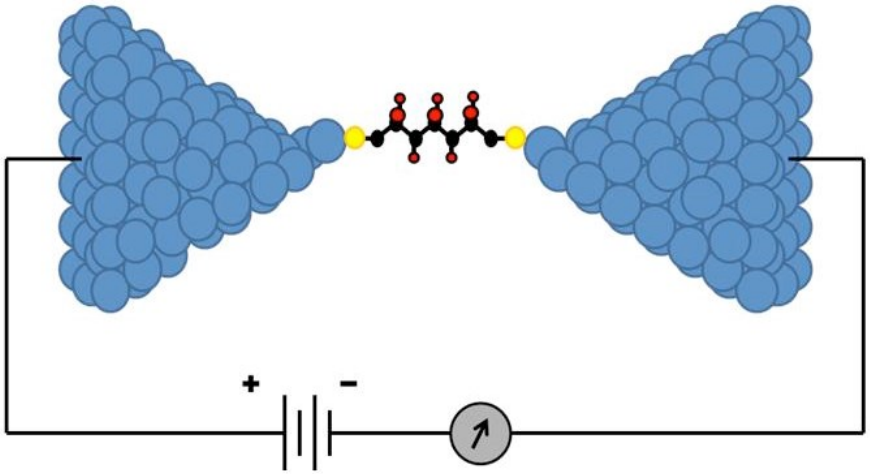


- Basic understanding of transport phenomena in nanoscale materials and devices
- Quantum effects are essential (quantum confinement; ballistic conduction; ...)
- Atomic detail
- “Ab-initio” (from first principles)
- TranSIESTA – module of SIESTA. Quantum Transport from Density Functional Theory
- Brandbyge et al., Phys. Rev. B 65, 165401 (2002)

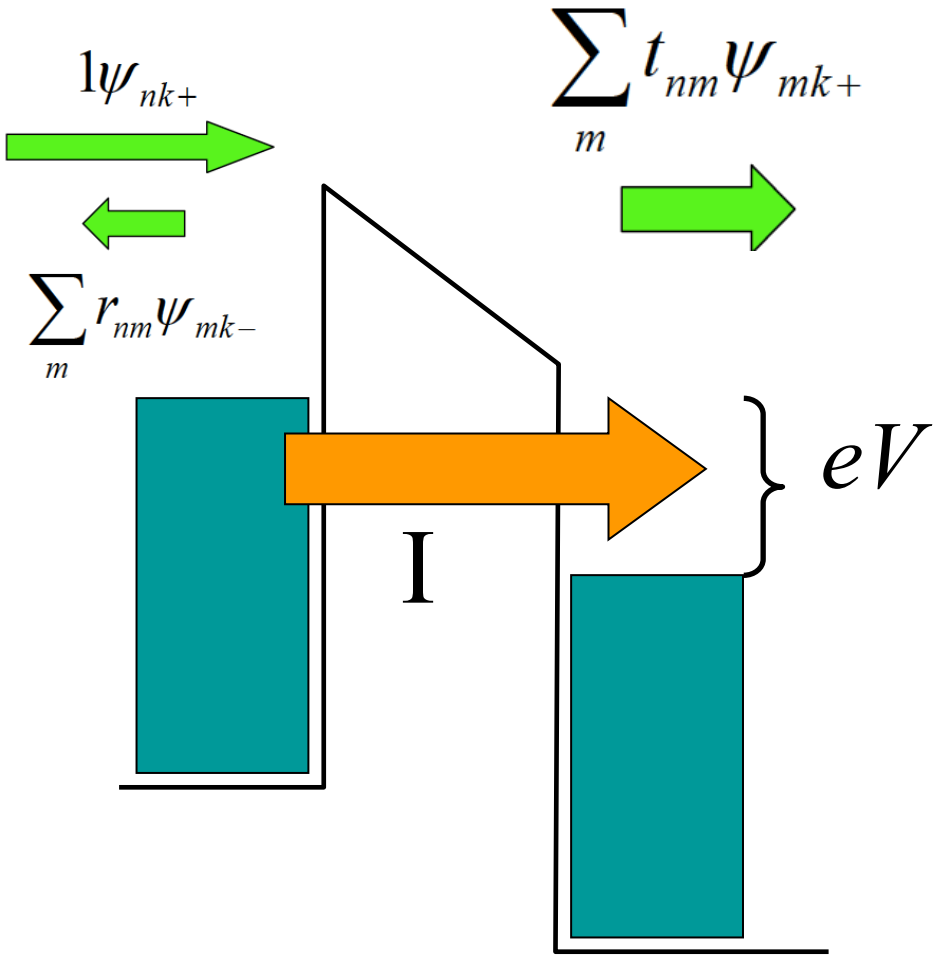
Electronic Transport: Conductance of a nanocontact

$$I = \frac{V}{R}$$





Electronic Transport: Conductance as scattering



transmission matrix and
transmission coefficient:

$$T(\varepsilon) = Tr\,[t^{+}t]\,(\varepsilon)$$

Current

$$I = \frac{2e}{h}\int d\varepsilon \left(f_L(\varepsilon) - f_R(\varepsilon)\right) T(\varepsilon)$$

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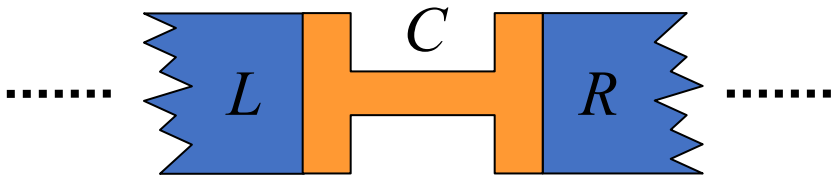
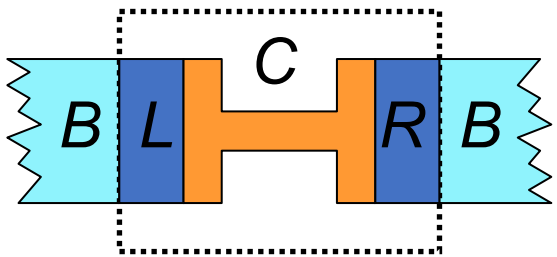
Green's Functions in an Open System



$$G(\varepsilon) = (\varepsilon - H)^{-1} = \begin{bmatrix} \ldots & -V_L^+ & & & \\ -V_L^- & \varepsilon - H_L & -V_{LC} & & \\ & -V_{CL} & \varepsilon - H_C & -V_{CR} & \\ & & -V_{RC} & \varepsilon - H_R & -V_R^+ \\ & & & -V_R^- & \ldots \end{bmatrix}^{-1}$$

Contact:

- Contains the molecule, and part of the Right and Left electrodes
- Sufficiently large to include the screening



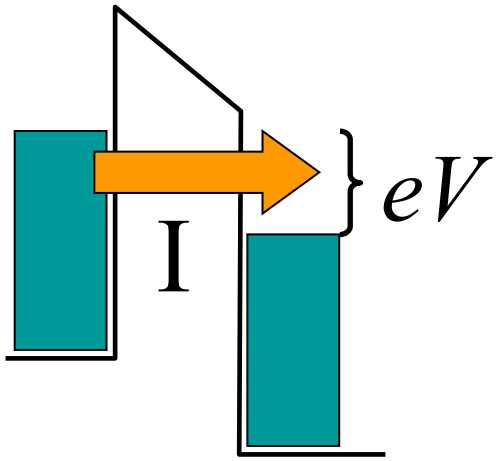
Solution in finite system:

$$G(\varepsilon) = \begin{bmatrix} \varepsilon - H_L - \Sigma_L & -V_{LC} & \\ -V_{CL} & \varepsilon - H_C & -V_{CR} \\ & -V_{RC} & \varepsilon - H_R - \Sigma_R \end{bmatrix}^{-1}$$

$\Sigma(\varepsilon)$ = Selfenergies. Can be obtained from the bulk Greens functions

Lopez-Sancho et al. J. Phys. F 14, 1205 (1984)

Transmission and Green's Functions



transmission matrix and transmission coefficient:

$$T(\varepsilon) = Tr\,[t^{+}t]\,(\varepsilon)$$

LANDAUER - BÜTTIKER

Current

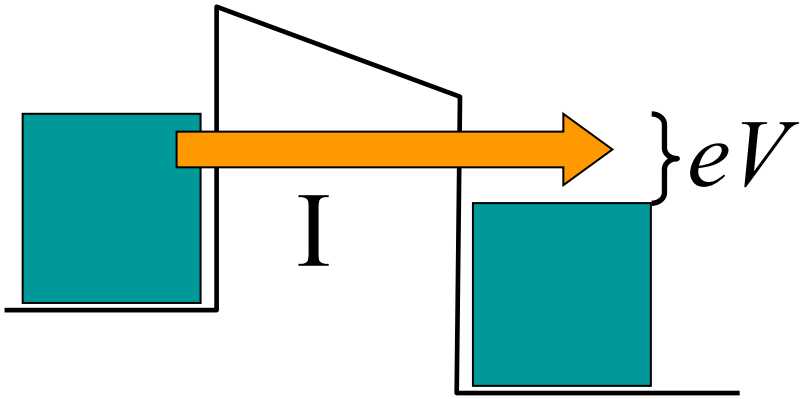
$$I = \frac{2e}{h} \int d\varepsilon \left(f_L(\varepsilon) - f_R(\varepsilon)\right) T(\varepsilon)$$

Transmission from Green's functions:

$$\mathbf{t}(\varepsilon) = [\mathbf{\Gamma}_R(\varepsilon)]^{1/2}\mathbf{G}(\varepsilon)[\mathbf{\Gamma}_L(\varepsilon)]^{1/2},$$

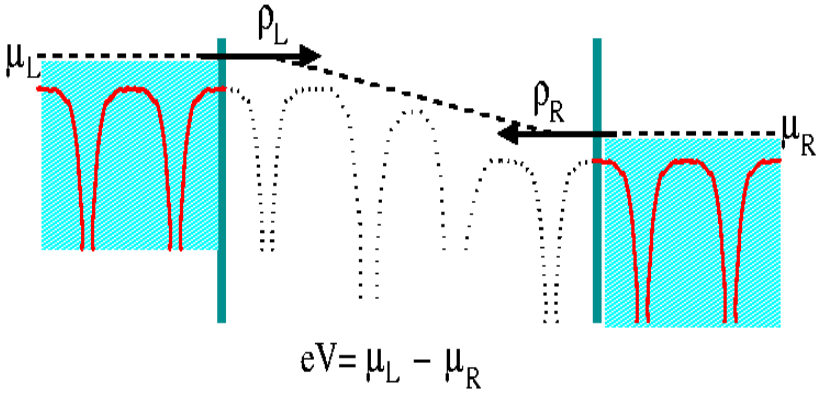
$$\mathbf{\Gamma}_L(z) \equiv i[\mathbf{\Sigma}_L(\varepsilon) - \mathbf{\Sigma}_L(\varepsilon)^{\dagger}]/2,$$

Handling Non-Equilibrium to compute the Density



How to compute the electron density if there is not a single Fermi level?

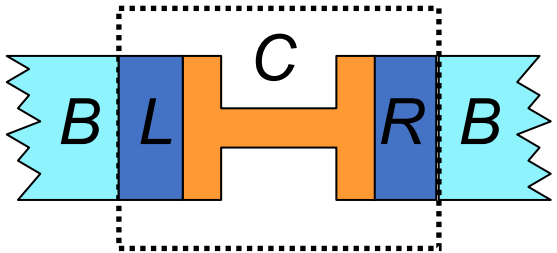
Non-equilibrium Green's Functions (Keldish formalism):

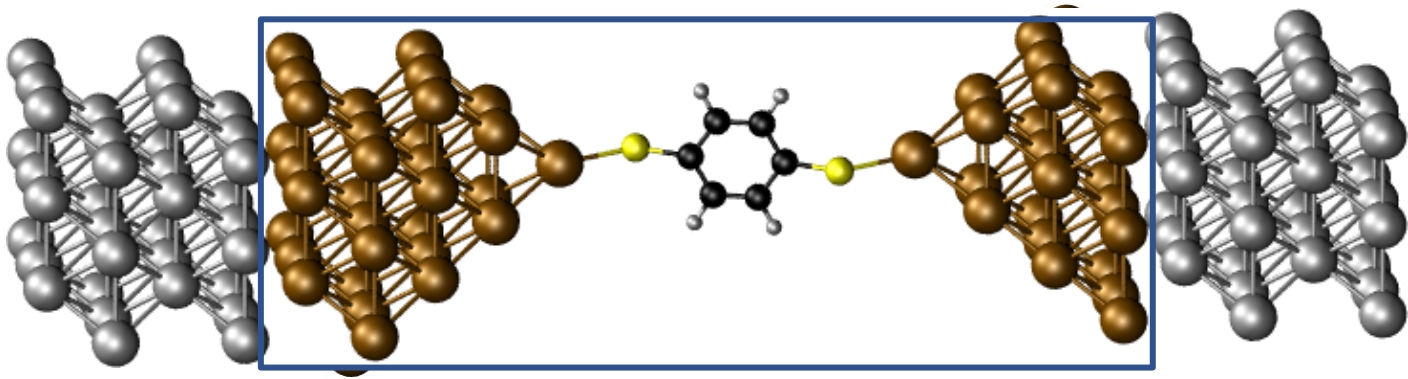


$$D_{\mu\nu} = \int_{-\infty}^{\infty} d\varepsilon \left[\rho^{L}_{\mu\nu}(\varepsilon)\, n_F(\varepsilon - \mu_L) + \rho^{R}_{\mu\nu}(\varepsilon)\, n_F(\varepsilon - \mu_R) \right]$$

$$\rho^{L}_{\mu\nu}(\varepsilon) = \frac{1}{\pi} \left(G(\varepsilon)\, Im\left[\Sigma_L(\varepsilon) \right] G^{t}(\varepsilon) \right)_{\mu\nu}$$

System setup



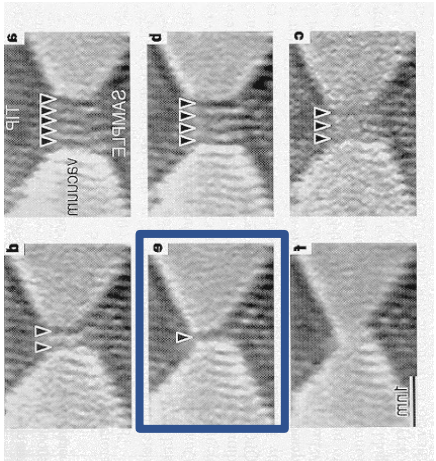


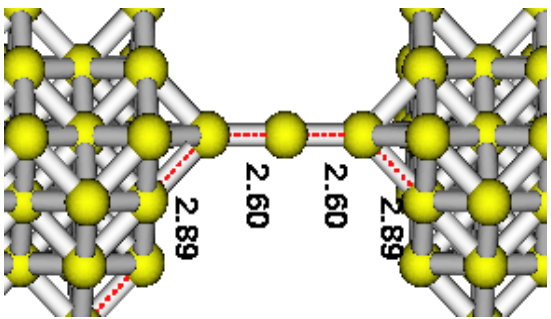
1. Define molecule or device
2. Attach connection to the molecule
3. Attach a few electrode layers
4. Effect of the bulk electrodes – via the Self-energies

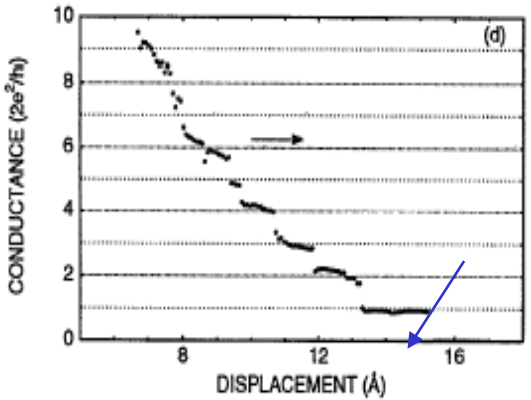
- Consider the molecule as a defect.
- The defect has a screening length in the electrode region (thus the extra electrode layers).
- Ensure that the electrodes behave as bulk electrodes (away from the defect).
- A previous SIESTA run for the bulk electrodes is needed, to compute the self-energies.
- The TranSIESTA calculation is done in the contact region
- Periodic Boundary Conditions perpendicular to transport

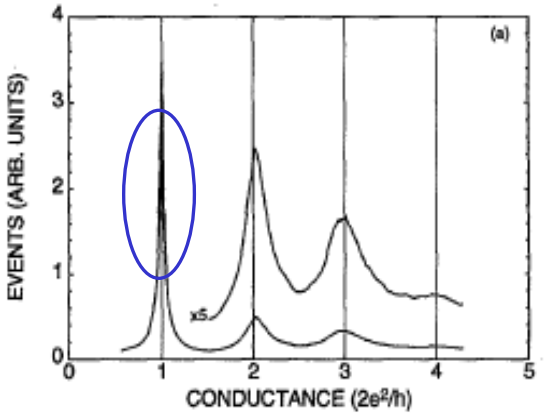
Some examples

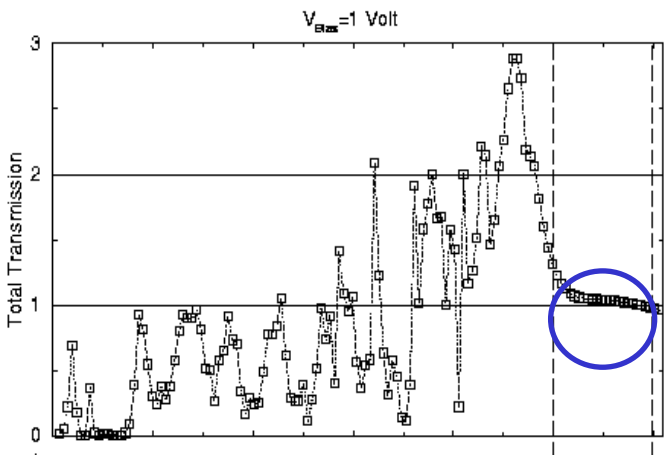
Monoatomic Gold wires

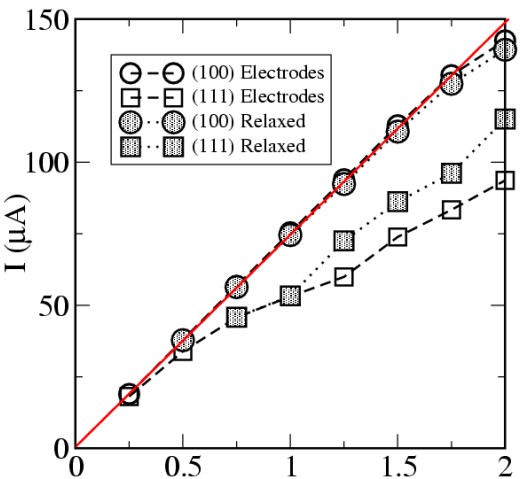








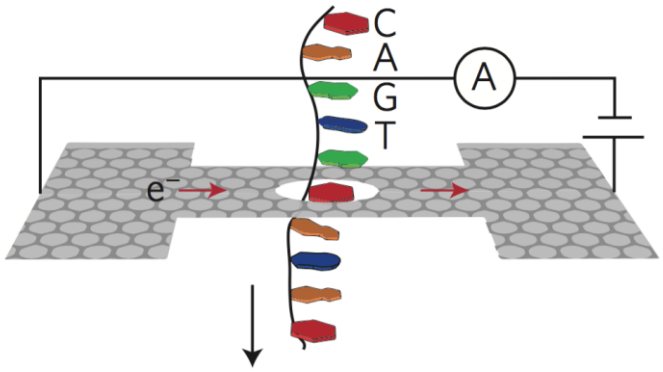


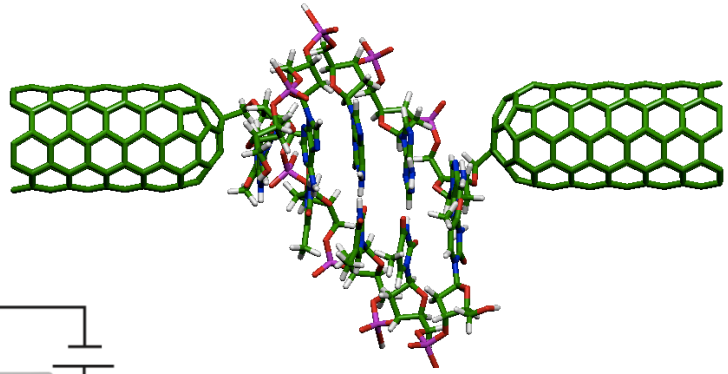


Stokbro, Taylor, Brandbyge, Mozos, Ordejón, Computational Materials Science 27 (2003) 151–160

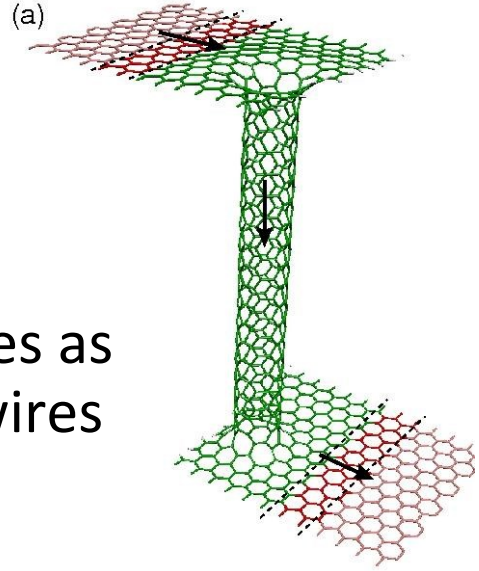
Some examples

DNA Sequencing

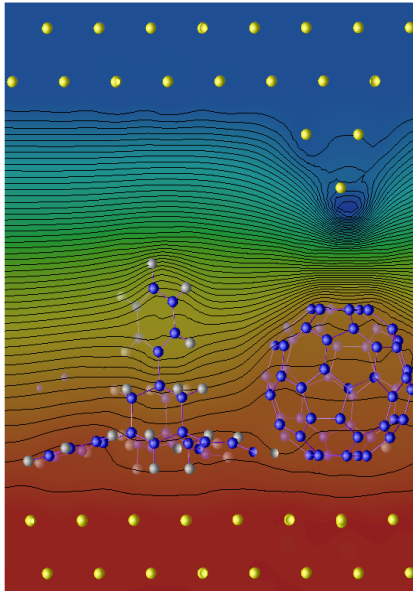




Nanotubes as electric wires



STM Imaging



Thank you!

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