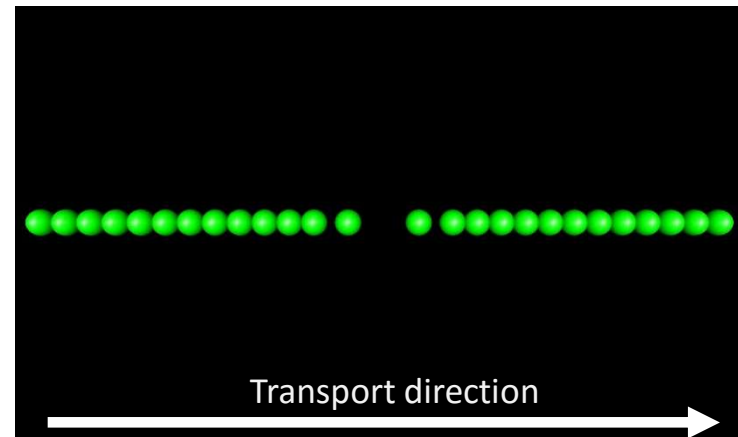


3.DFT - Carbon chain + gap. NDR

Objectives

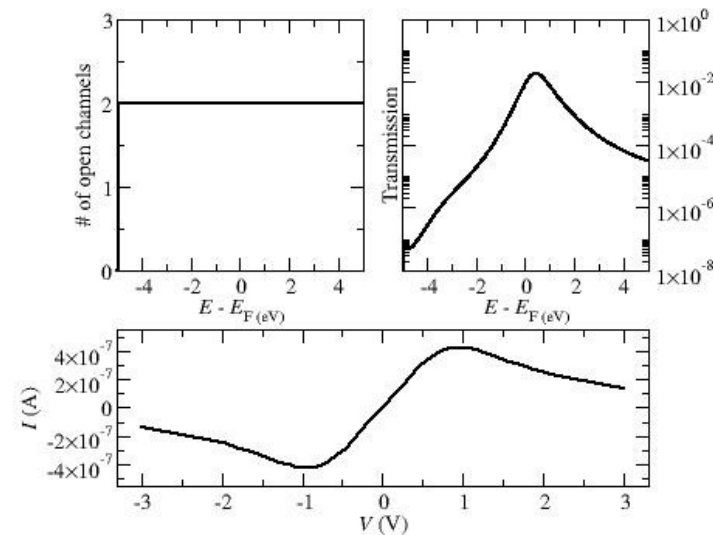
- Simulate a one-dimensional (1D) system with a vacuum gap to see the effect of including a bias voltage that falls in the middle.
- Check that the transmission is dramatically affected by the bias voltage and decreases as the bias increases.



Results

- The transmission has a peak slightly above the Fermi level with a height much lower than one, which means we are in the tunneling regime. The height decreases as the bias increases as a consequence of the misalignment of the levels on both surface atoms.
- The current linearly increases until it reaches a maximum at around 1 V and then decreases, giving rise to negative differential resistance (NDR).

Transmission and number of open channels as a function of energy. Calculated with **Mode 1** of Gollum.



Current as a function of voltage.
Calculated with **Mode 4** of Gollum.

3.DFT - System description and parameters

Leads

- C leads made of 4 C atoms to avoid second-nearest neighbour interactions.
- Lattice vectors long enough along the transverse directions to make sure the system is 1D.

Gollum parameters

- Transmission coefficients calculated between -10.0 eV and 10.0 eV in 1000 energy points.
- 3 principal layers on each electrode. The terminating principal layer is the second on each. Electronic structure obtained from the leads calculation.
- No SAINT correction or Fermi level shift.
- Bias voltage between -3.0 V and 3.0 V calculated in 60 voltage points. The bias shift is applied just in the middle of the chain (4th column of the `atom` variable set to different from 0).

Ab-initio (Siesta) parameters

- Basis set: Single- ζ (DZ); s and p orbitals included in the C valence.
- LDA exchange and correlation functional. CA parametrization.
- Mesh cut-off: 200 Ry.
- 100 k -points along z in the lead calculation. 1 k -point (Γ point) along the perpendicular directions. Γ point in the EM calculation.

Extended molecule (EM)

- 2 carbon chains of 12 atoms and a surface C atom each. 26 atoms in total. The surface atoms are slightly separated from the chain to increase the localization of their levels.
- Vacuum gap between the surface C's of 3.7 Å.
- The system is also periodic along the transport direction (z) to avoid finite size effects.

Files necessary to run the **leads** calculation: lead.fdf, C.psf

Files necessary to run the **EM** calculation: emol.fdf, C.psf