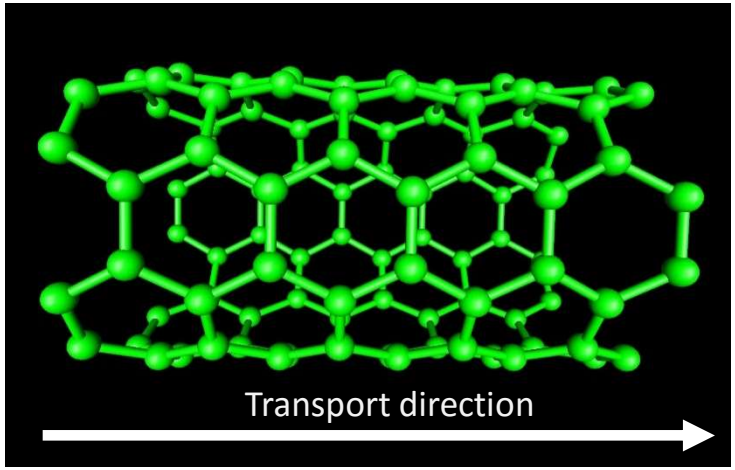
5.DFT - (5,5) Carbon nanotube

Objectives

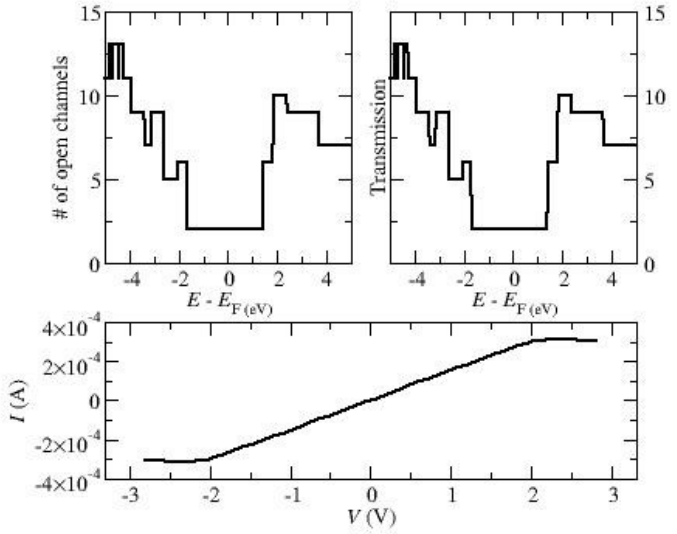
- Simulate a quasi-one-dimensional (q1D) system with perfect transmission (equal to the number of open channels or bands at a certain energy) and various channels.
- Check that the transmission exactly coincides with the number of open channels.



Results

- The transmission has a step-like shape which indicates the number of open channels. In this case we have s and p orbitasl in the valence of carbon.
- The CNT is armachair, so it is metallic and has two channels at the Fermi level.
-The current linearly increases at low voltages (as expected, since it is equal to the integral of a constant function). It eventually saturates because the transmission is partially destroyed by the bias voltage.

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.

5.DFT - System description and parameters

Leads

- One CNT(5,5) unit cell made of two layers of C atoms along *z*. 20 atoms.
- Lattice vectors long enough along the transverse directions to make sure the system is 1D.

Extended molecule (EM)

- 5 CNT(5,5) unit cells with the same transverse lattice vectors of the leads. 100 atoms.
- The system is also periodic along the transport direction (*z*) to avoid finite size effects.

Gollum parameters

- Transmission coefficients calculated between -5.0 eV and 5.0 eV in 1000 energy points.
- 2 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 -2.8 V and 2.8 V calculated in 60 voltage points. The bias shift is applied on the first terminating layer of the left and right electrodes only (4th column of the `atom` variable set to different from 0). This is an approximation since the voltage should not fall (or at least fall very slowly) on a perfect infinite system.

Ab-initio (Siesta) parameters

- Basis set: Single-ζ (SZ); s and p orbitals included in the C valence.
- GGA exchange and correlation functional. PBE parametrization.
- Mesh cut-off: 100 Ry.
- 50 *k*-points along *z* in the lead calculation. 10 *k*-points in the EM calculation (to make sure the electronic structure exactly matches that of the leads). 1 *k*-point (Γ point) along the perpendicular directions.

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