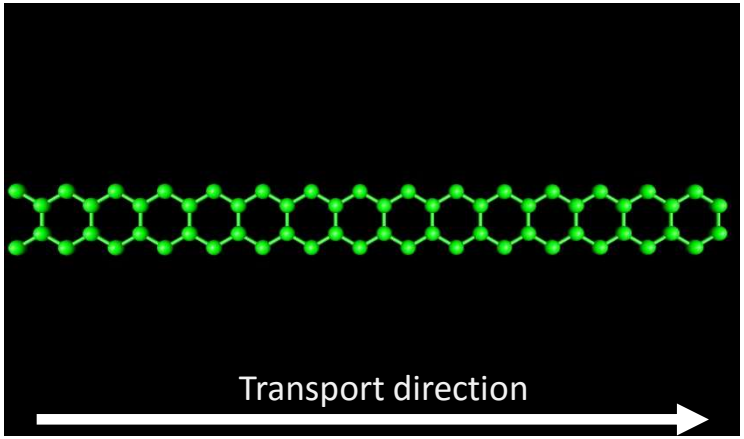
6.DFT - Graphene sheet

Objectives

- Simulate a perfect two-dimensional (2D) system (transverse periodic boundary conditions and *k*-points along *y*) 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 and tends to 0 at the Fermi level.



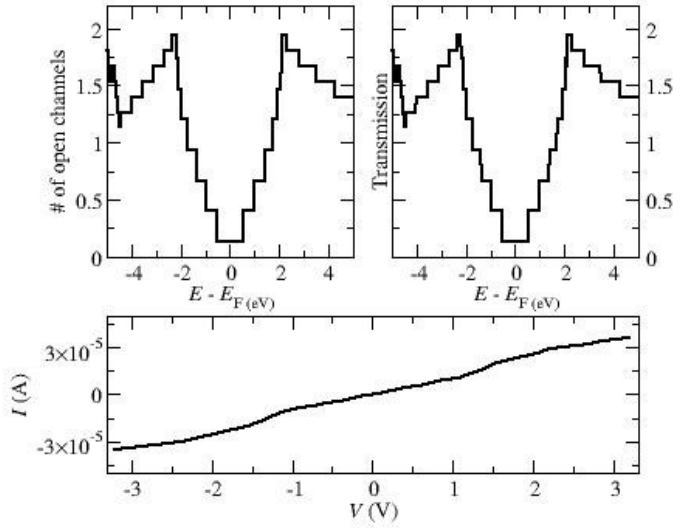
Results

-The transmission has V-shape which maps the electronic structure of the Dirac cones near the Fermi level

- The transmission becomes smoother and goes to zero at the Fermi level as the number of transverse *k*-points along *y* increases.

- The current linearly increases and does not seem to saturate on a large enough bias range. This is because the transmission does not seem to be destroyed but rather enhanced by the effect of the 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.

6.DFT - System description and parameters

Leads

- Leads made of 12 C atoms. 3 graphene unit cells along *z*.
- Lattice vectors that map a graphene sheet along *y* and long enough along *x* to make sure the system is 2D.

Extended molecule (EM)

- 60 C atoms. 15 graphene unit cells along *z*. Same transverse lattice vectors as in the leads calculation.
- 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 -3.2 V and 3.2 V calculated in 40 voltage points. The bias shift is applied on the first terminating layer of the left and right electrodes only (4^{th} 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 included in the C valence.
- LDA exchange and correlation functional. CA parametrization.
- Mesh cut-off: 200 Ry.
- 10 *k*-points along *z* in the lead calculation. 2 *k*-points in the EM calculation (to make sure the electronic structure exactly matches that of the leads). 1 *k*-point (Γ point) along *x* and 15 *k*-points along *y*.

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