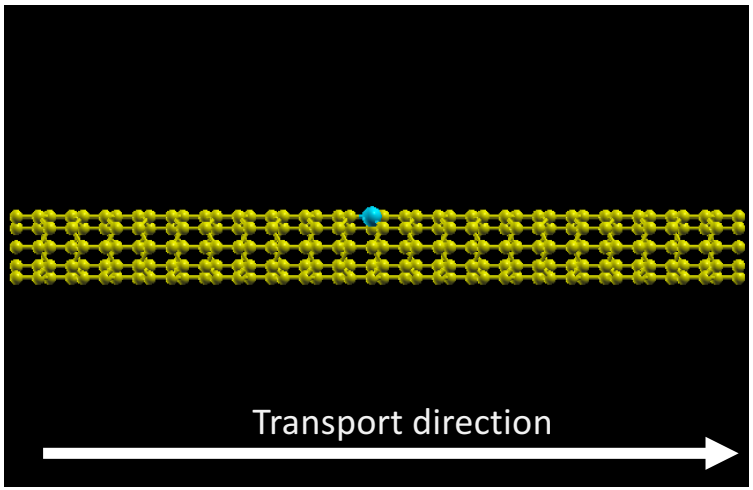
6.W90 - (5,0) Carbon nanotube

Objectives

- Simulate a quasi-one-dimensional (q1D) system with an impurity (atom of a different species, Si) and various channels.

- Calculate the transmission and other transport properties.



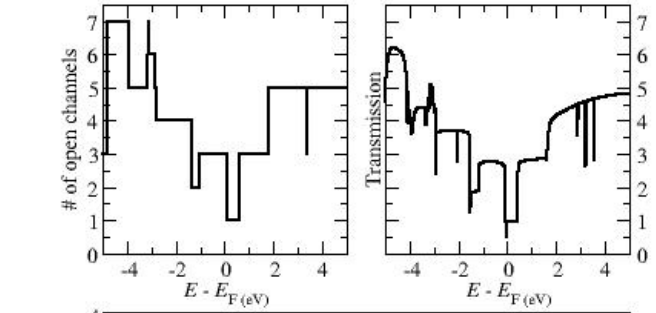
Results

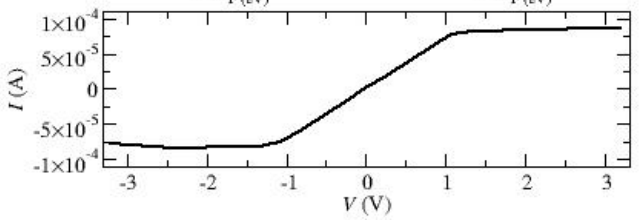
- The transmission is slightly smaller than the number of open channels due to scattering generated by the impurity. There are 4 Wanniers per atom (C or Si), which generate the s and p bands in the leads.

- The CNT is zigzag. It is metallic and has one channel at the Fermi level.

-The current linearly increases at low voltages (as expected, since it is equal to the integral of a positive function). It eventually saturates and slightly decreases (NDR) when it is partially destroyed by the bias voltage. Slight changes in the slope are due to the appearance or disappearance of new bands.

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.W90 - System description and parameters

Leads

- One CNT(5,0) unit cell made of four 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)

- 11 CNT(5,0) unit cells with the same transverse lattice vectors of the leads. 219 C atoms and 1 Si atom.
- The system is also periodic along the transport direction (*z*) to avoid finite size effects.

Ab-initio (QuantumEspresso-PW and Wannier90) parameters

- Basis set (PW) cutoff: ecutwfc = 60 (PW scf and nscf).
- LDA exchange and correlation functional. PZ parametrization (defined by the pseudopotential).
- Number of bands in the EM: nbnd = 1100 (PW nscf and W90). Number of Wanniers in the EM: num_wann = 550 (W90).
- 10 (PW scf and nscf and W90) *k*-points along *z* in the lead calculation. 1 *k*-point (Γ point) in the EM calculation and along the perpendicular directions.
- The number of Wannier functions is 2.5 times the number of atoms in both the leads, 50, and the extended molecule, 550; the number of Wannier groups is equal to 8 in the leads and 89 in the extended molecule.

* Files necessary to run the **leads** calculation: cnt.scf, cnt.nscf, cnt.pw2wan, cnt.win, C.pz-vbc.UPF
* Files necessary to run the **EM** calculation: cnt-p.scf, cnt-p.nscf, cnt-p.pw2wan, cnt-p.win, C.pz-vbc.UPF

Gollum parameters

- Transmission coefficients calculated between -5.0 eV and 5.0 eV in 2000 energy points.
- 2 principal layers on each electrode. Electronic structure obtained from the extended molecule (correct result) or from the leads calculation (incorrect result sometimes, depending on the Fortran compiler or QE version). Principal layer made of 1 unit cell of the leads (incorrect result due to second-nearest neighbours interactions) or 2 unit cells of the leads (correct result).
- No SAINT correction or Fermi level shift.
- Bias voltage between -3.2 V and 3.2 V calculated in 25 voltage points. The bias shift is applied at the beginning (Wannier group 32) and end (Wannier group 58) of the central part of the EM (4th column of the `atom` variable set to 1 or 2). This is an approximation since the voltage should not fall (or at least fall very slowly) in an almost perfect infinite system.