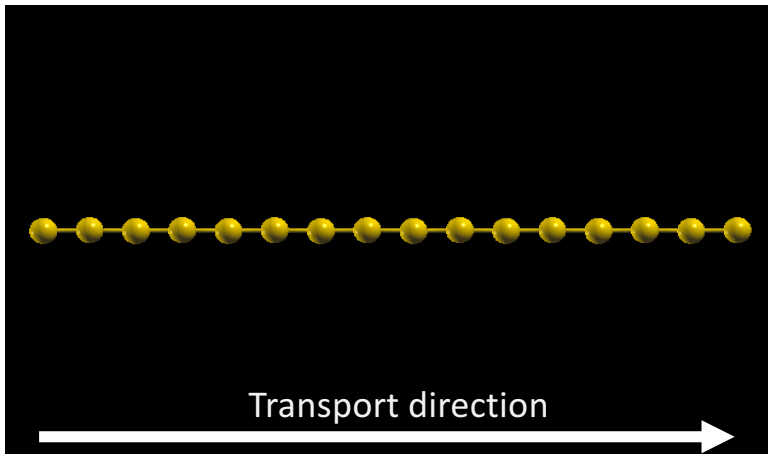
3.W90 - Gold almost-linear chain

Objectives

- Simulate a one-dimensional (1D) system (slightly zigzag to lift the degeneracy of the Wannier functions) 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.

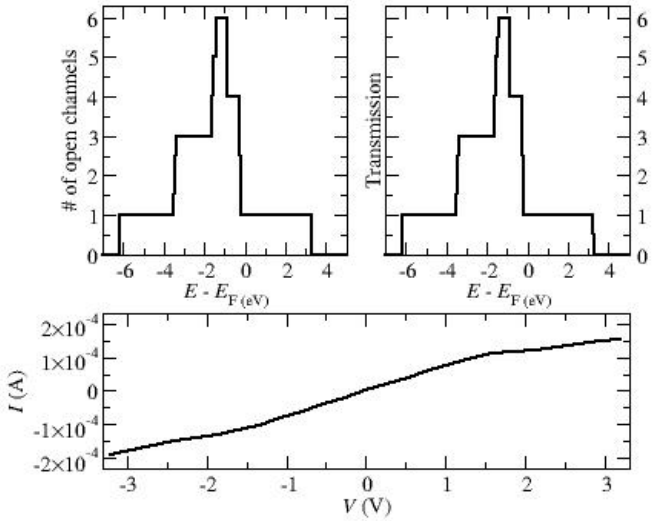


Results

- The transmission has a step-like shape whose plateaus coincide with the number of open channels. There are 6 Wanniers per atom of gold, which generate the s and the d bands. The s band is wider than the d bands.

- The current linearly increases (as expected, since it is equal to the integral of a positive function) until it slightly saturates. 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.

3.W90 - System description and parameters

Leads

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

Extended molecule (EM)

- Perfect gold chain made of 16 atoms (2 unit cells of the electrodes). Same transverse lattice vectors as in the leads.
- 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 = 30 (PW scf and nscf).
- LDA exchange and correlation functional. PZ parametrization (defined by the pseudopotential).
- Number of bands in the EM: nbnd = 112 (PW nscf and W90). Number of Wanniers in the EM: num_wann = 96 (W90).
- 2 (PW scf) and 4 (PW 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 6 times the number of atoms in both the leads, 24, and the extended molecule, 96; the number of Wannier groups is the number of Wanniers divided by 3: 8 in the leads and 32 in the extended molecule.

* Files necessary to run the **leads** calculation: Au.scf, Au.nscf, Au.pw2wan, Au.win, Au.pz-d-rrkjus.UPF
* Files necessary to run the **EM** calculation: Au_em.scf, Au_em.nscf, Au_em.pw2wan, Au_em.win, Au.pz-d-rrkjus.UPF

Gollum parameters

- Transmission coefficients calculated between -7.0 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 due to mismatches between the electronic structures of the leads and the extended molecule).
- 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 just in the middle of the chain (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 a perfect infinite system.