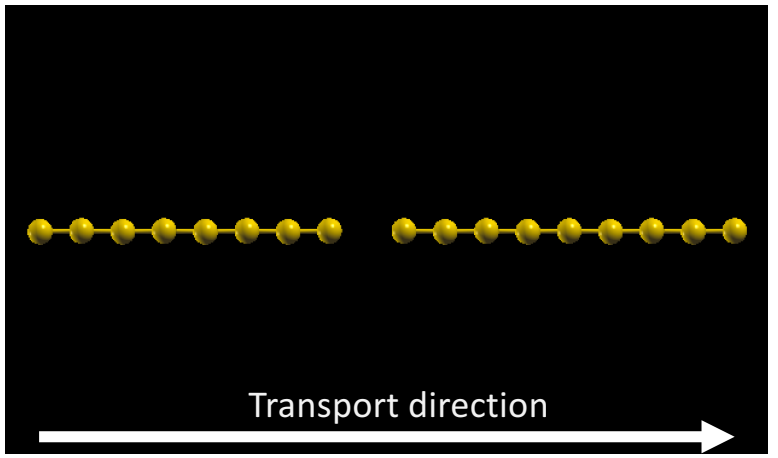
4.W90 - Gold almost-linear chain with a gap

Objectives

- Simulate a one-dimensional (1D) system (slightly zigzag to lift the degeneracy of the Wannier functions) with a defect (structural gap in the chain, i.e. two of the atoms have a large separation) and various channels.

- Calculate the transmission and accurately obtain the current at finite voltages.



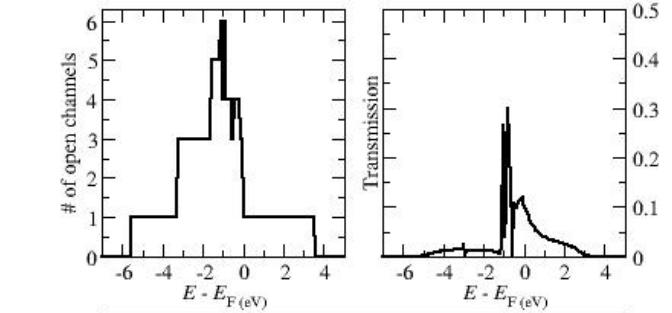
Results

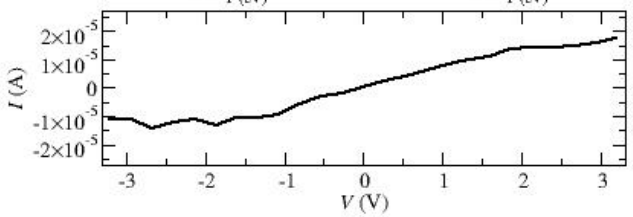
- The transmission is much smaller than one due to scattering at the gap. There are 6 Wanniers per atom of gold, which generate the s and d bands; the later provide more conduction channels and increase the transmission around the Fermi level.

- 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.

- The current is also slightly asymmetric because the positions of the Wannier functions on both sides of the gap are not exactly the same.

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.

4.W90 - System description and parameters

Leads

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

Extended molecule (EM)

- Two gold chains with 8 (2 unit cells of the electrodes) and 9 (2 unit cells + 1 Au) atoms separated 4.5 Å and with the same transverse lattice vectors of 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 = 101 (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 24 in the leads and 101 in the the extended molecule; the number of Wannier groups is 8 in the leads and 31 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 choice is accurate because the voltage should fall just in the gap.