

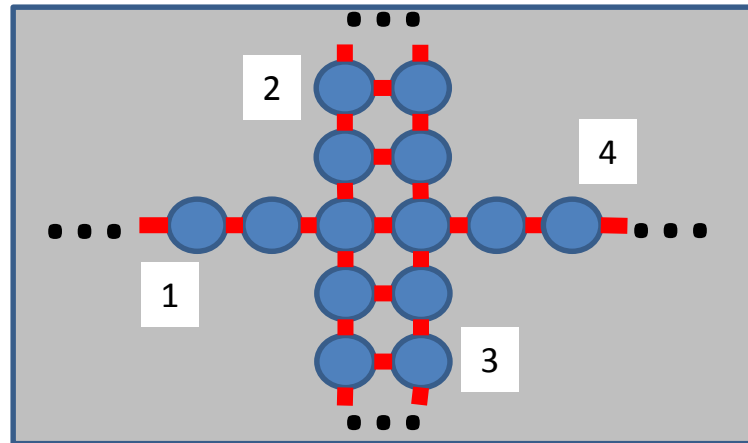
Four-probe system

Objectives

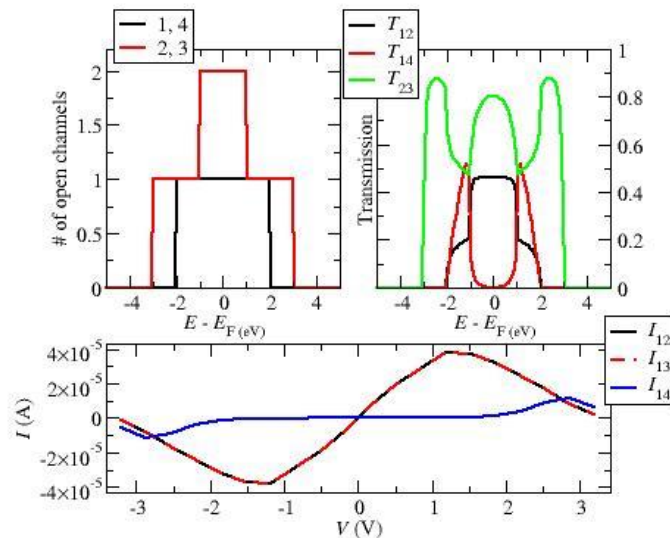
- Simulate a four-probe system with two types of electrodes.
- Calculate the transmissions from one to other electrodes.
- See the effect of including a bias voltage on one of the electrodes. Calculate the currents.

Results

- There is one open channel in electrodes 1 and 4 and a maximum of two in electrodes 2 and 3.
- The transmission between electrodes 1 and 4, T_{14} , is not perfect because the presence of the other electrodes (part of the probability is diverted towards them). The same for T_{23} .
- $T_{12} = T_{13} = T_{24} = T_{34}$.
- The voltage is ramped up only in the first electrode. The current towards electrodes 2 and 3 is much larger than that towards electrode 4 because the transmission in 2 and 3 is larger.
- NDR appears because the transmission is dramatically affected by 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.

System description and parameters

Leads

- 1 and 4: unit cell with just one atom. 2 and 3: unit cell with two atoms. One orbital per atom.
- Single-atom (1 and 4) and two-atom (2 and 3) chains connected in the middle of the EM.

Extended molecule (EM)

- 14 atoms in the calculation.
- Same parameters as in the leads (correspondingly).

Gollum parameters

- Transmission coefficients calculated between -5.0 eV and 5.0 eV in 100 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 20 voltage points. The bias shift is applied on the first terminating layer of each electrode 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.

Tight-binding parameters

- Orthogonal basis set (overlap matrix = identity matrix).
- On-site matrix elements (both leads and EM): 0.0 eV.
- Coupling between atoms (everywhere): 1.0 eV.