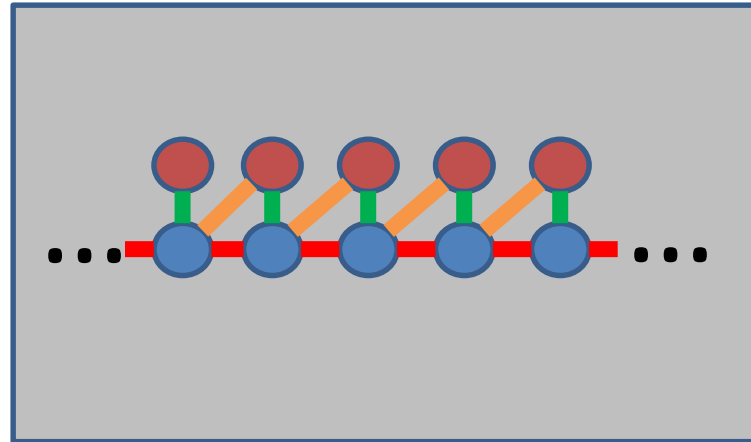


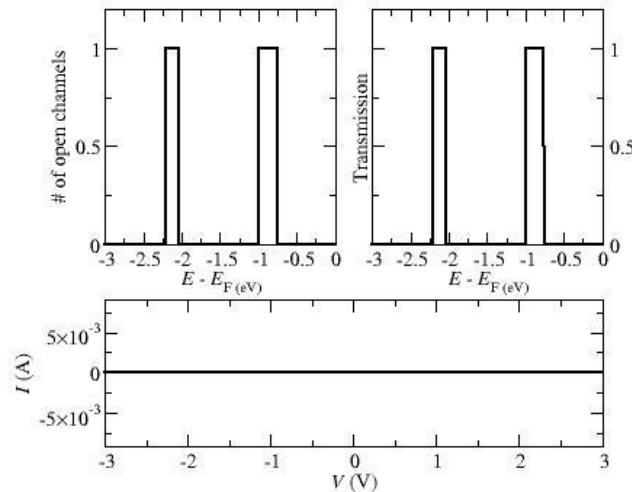
# Two-level chain

## Objectives

- Simulate one-dimensional (1D) system with different orbitals and perfect transmission (equal to the number of open channels or bands at a certain energy).
- Check that the transmission exactly coincides with the number of open channels.



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.

## Results

- The transmission has a step-like shape which corresponds to the number of open channels at a given energy.
- There are two separated bands whose center is located near the on-site energy of each type of orbital.
- The width and final position of the band depends on the couplings through the chain and between both types of orbitals.
- The current is zero because the bias window does not reach the nearest band at low voltages and the transmission is destroyed at large voltages.

# System description and parameters

## Leads

- Unit cell with just one atom. Two different orbitals per atom.
- Two-level chain with different couplings between orbitals in the same unit cell and orbitals in different unit cells.

## Extended molecule (EM)

- Five atoms in the calculation.
- Same parameters as in the leads

## Gollum parameters

- Transmission coefficients calculated between -3.0 eV and 0.0 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 -3.0 V and 3.0 V calculated in 20 voltage points. The bias shift is applied on the first terminating layer of the left and right electrodes only (4<sup>th</sup> 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): -2.0 eV and -1.0 eV for each type of orbital.
- Coupling between both types of orbitals: -3.0 eV.
- Coupling between orbitals in different unit cells:  $H_{11} = 0.1$  eV,  $H_{12} = -0.2$  eV,  $H_{21} = 0.0$  eV and  $H_{22} = 0.0$  eV.