

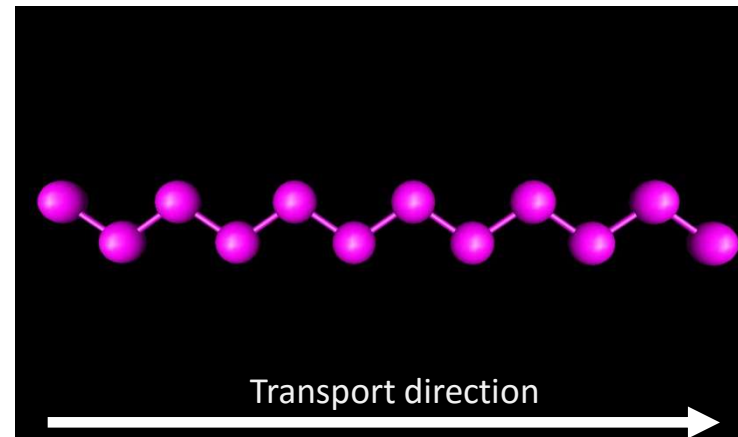
2.DFT- Iridium zigzag chain. Non-collinear magnetism

Objectives

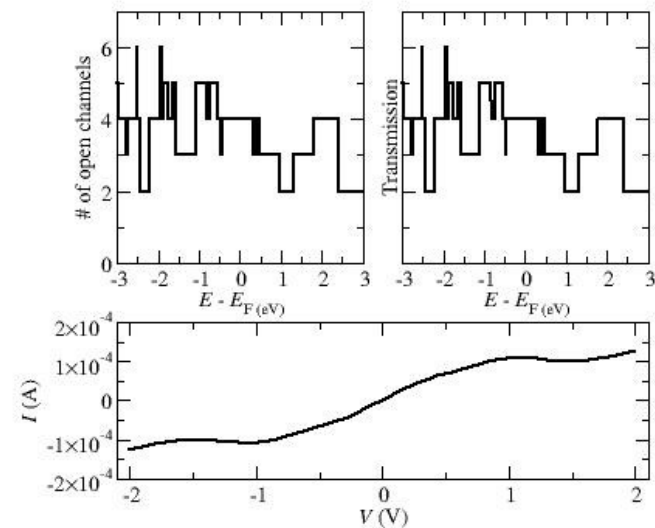
- Simulate a one-dimensional (1D) system with perfect transmission (equal to the number of open channels or bands at a certain energy), various channels and a non-collinear magnetic configuration.
- Check that the transmission exactly coincides with the number of open channels.

Results

- The transmission has a step-like shape which indicates the number of open channels. In this case we have s, p and d orbitals in the valence of iridium. The s band is more extended than the d bands. The p bands are above the Fermi level. The system is magnetic and the spins are oriented along the y axis.
- The current linearly increases (as expected, since it is equal to the integral of a constant 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.

2.DFT - System description and parameters

Leads

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

Extended molecule (EM)

- Perfect iridium chain made of 12 atoms (3 unit cells of the electrodes). Same transverse lattice vectors as the leads.
- The system is also periodic along the transport direction (z) to avoid finite size effects.

Gollum parameters

- Transmission coefficients calculated between -3.0 eV and 3.0 eV in 5000 energy points.
- 1 principal layer on each electrode. Electronic structure obtained from the leads calculation.
- No SAINT correction or Fermi level shift.
- Bias voltage between -2.0 V and 2.0 V calculated in 50 voltage points. The bias shift is applied just in the middle of the chain (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.

Ab-initio (Siesta) parameters

- Basis set: Single- ζ (SZ); s, p and d orbitals included in the Ir valence.
- LDA exchange and correlation functional. CA parametrization.
- Mesh cut-off: 300 Ry.
- 90 *k*-points along z in the lead calculation. 30 *k*-points in the EM calculation (to make sure the electronic structure exactly matches that of the leads). 1 *k*-point (Γ point) along the perpendicular directions.
- Non-collinear magnetism. Spins pointing towards the y direction. It is not possible to distinguish between spin-up and spin-down electrons (as in a spin-polarized calculation where spins are projected along z).

Files necessary to run the **leads** calculation: lead.fdf, Ir.psf

Files necessary to run the **EM** calculation: emol.fdf, Ir.psf