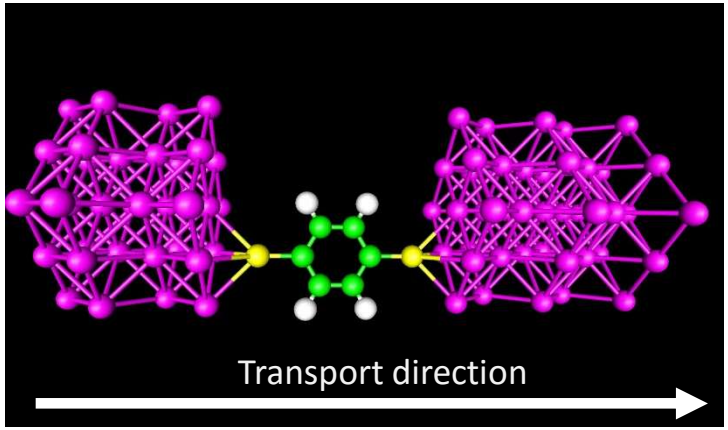
7.DFT - BDT molecule between (001) gold electrodes

Objectives

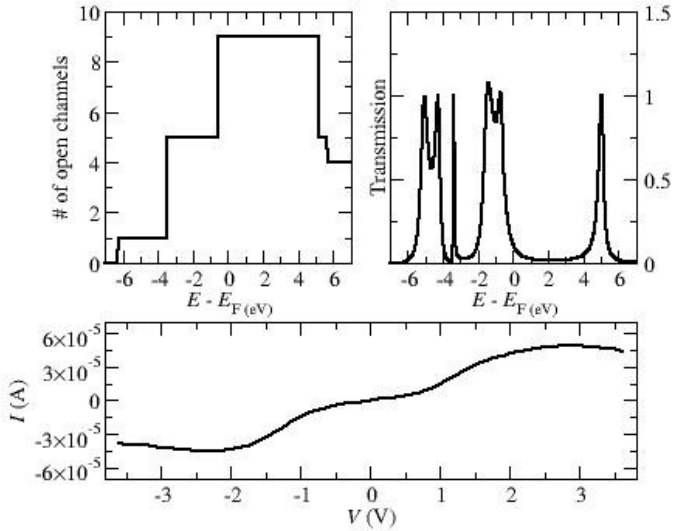
- Calculate the transport properties of a BDT (1,4-benzenedithiolate) molecule between gold electrodes.
- Correct the transport properties by applying a spectral adjustment (SAINT) to the occupied and unoccupied levels and shifting the Fermi level towards the HOMO.

Results

- The Fermi level is close to the HOMO orbital. After applying a SAINT correction of -1.0 eV and 1.0 eV to the occupied and unoccupied levels, respectively, the gap opens (~5 eV). After shifting the Fermi level 1.0 eV, it moves closer to the HOMO again.
- Under a bias voltage the HOMO slightly moves to lower energies and changes. The current remains initially low until the bias window starts covering the HOMO. A small asymmetry is observed due to the relaxation of the coordinates.



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.

7.DFT - System description and parameters

Leads

- Au leads grown along the (001) direction. AB stacking. 2 atomic layers with 9 atoms (3x3) per layer. 18 atoms in total.
- Perpendicular lattice vectors that replicate a fcc lattice along the transverse directions.

Extended molecule (EM)

- BDT coupled to both gold surfaces in a hollow configuration. 5 and 4 layers of gold on the left (ABAB) and right (BABAB), respectively. 93 atoms in total.
- Same perpendicular lattice vectors as in the leads. The systems is made periodic along z to avoid finite-size effects.

Gollum parameters

- Transmission coefficients calculated between -7.0 eV and 7.0 eV in 2000 energy points.
- 2 principal layers on each electrode. The terminating principal layer is the second on each electrode. Electronic structure obtainedfrom the leads calculation.
- Fermi energy shift of 1.0 eV.
- 42 electrons used to define the occupied and unoccupied states that move to lower and higher energies, respectively, under the SAINT correction. The orbitals where this correction is applied are those corresponding to the molecular atoms (between 37 and 48; 3rd column of the `atom` variable set to 0).
- Bias voltage between -3.6 V and 3.6 V calculated in 60 voltage points. The bias shift is applied on the left and right electrodes (4th column of the `atom` variable set to different from 0).

Ab-initio (Siesta) parameters

- Basis set: Single-ζ (SZ). Only s orbitals in the gold valence (d orbitals in the pseudopotential).
- GGA exchange and correlation functional. PBE parametrization.
- Mesh cut-off: 200 Ry.
- 90 *k*-points along *z* in the lead calculation. 1 *k*-point (Γ point) along the perpendicular directions. Γ point in the EM calculation.

Files necessary to run the **leads** calculation: lead.fdf, Au.psf
Files necessary to run the **EM** calculation: emol.fdf, coord.fdf, Au.psf, C.psf, H.psf, S.psf