

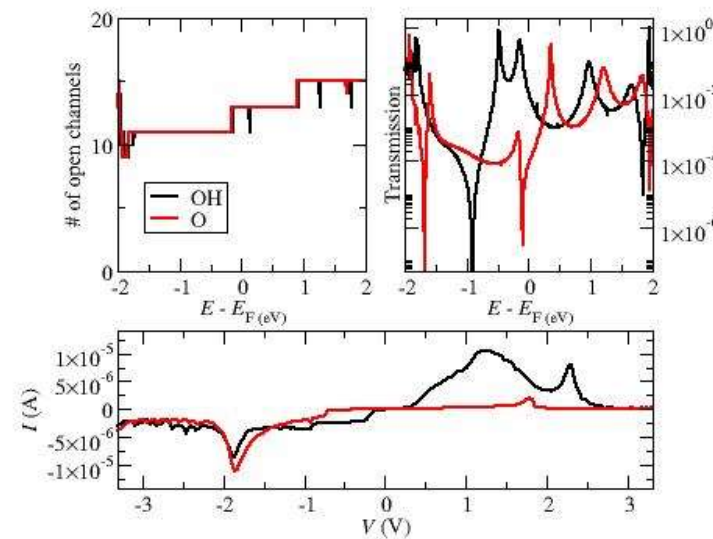
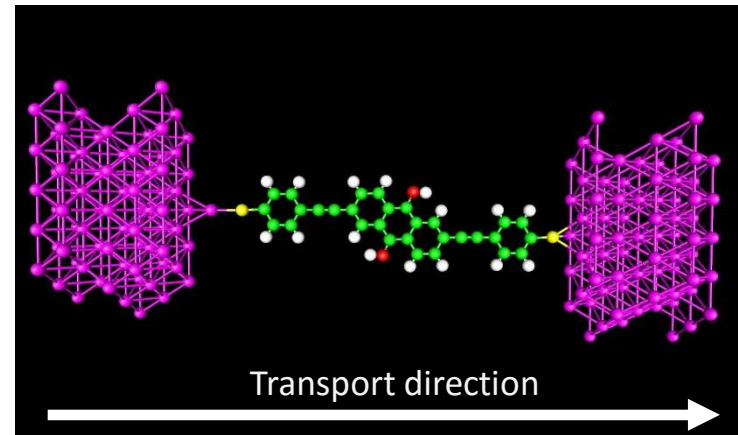
# 8.DFT - OPE molecule between (111) gold electrodes

## Objectives

- Calculate the transport properties of a OPE (oligo phenylene ethylene)-based molecule between gold electrodes.
- See an example of Fano resonance in the transmission coefficients. The position of such resonance can be changed by taking out the hydrogens attached to the oxygens.

## Results

- Fermi level very close to the HOMO orbital as a consequence the coupling configuration: the coupling of the sulphur on top of a gold adatom moves the HOMO towards the Fermi level due to a decrease of the charge transfer from the molecule to the leads.
- A clear Fano resonance is located below the Fermi level, at -1 eV. It can be moved to the Fermi level by removing the hydrogens from the oxygens.
- There is some rectification in the current due to the asymmetric coupling configuration.



Current as a function of voltage.  
Calculated with **Mode 4** of Gollum.

## 8.DFT - System description and parameters

### Leads

- Au leads grown along the (111) direction. ABC stacking. 3 atomic layers with 18 atoms (6x3) per layer. 54 atoms in total.
- Perpendicular lattice vectors that replicate a fcc lattice along the transverse directions.

### Gollum parameters

- Transmission coefficients calculated between -2.0 eV and 2.0 eV in 400 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 -3.6 V and 3.6 V calculated in 240 voltage points. The bias shift is applied on the left and right electrodes only (4<sup>th</sup> column of the `atom` variable set to different from 0). The adatom on the left is excluded from the bias shift.

### Ab-initio (Siesta) parameters

- Basis set: Single- $\zeta$  (SZ) in all atoms. The d orbitals are also included in the basis set of gold.
- LDA exchange and correlation functional. CA parametrization.
- Mesh cut-off: 200 Ry.
- 60 *k*-points along *z* in the lead calculation. 1 *k*-point ( $\Gamma$  point) along the perpendicular directions.  $\Gamma$  point in the EM calculation.

### Extended molecule (EM)

- OPE coupled to the left surface on top of an adatom and to the right surface in a hollow configuration.
- 5 layers of gold on each electrode (ABCAB, left and BCABC, right). 231 atoms in total.
- Same perpendicular lattice vectors as in the leads. The systems is made periodic along *z* to avoid finite-size effects.

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

Files necessary to run the **EM** calculation: emol.fdf, coordEM.fdf, Au.psf, C.psf, H.psf, O.psf, S.psf