

Optical properties of single-molecule junctions

H. Bulou

IPCMS/DSI, Strasbourg, France

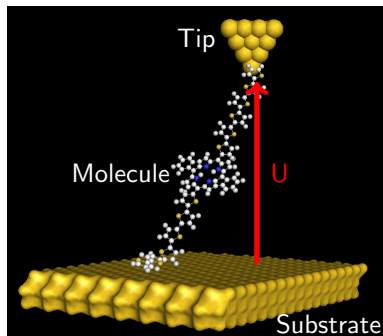
September 28, 2016

Office: 1034

email: herve.bulou@ipcms.unistra.fr

Single-molecule junctions

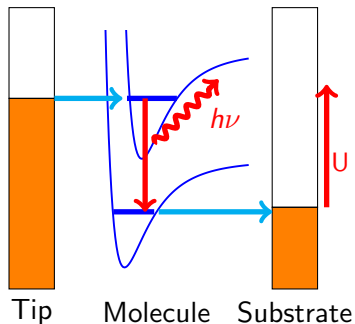
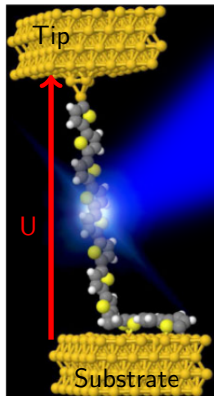
Description



- ▶ Three main parts:
 - ▶ two metallic electrodes
 - ▶ a molecule
- ▶ Bias between the electrodes
 - electron current crossing the molecule
 - Different physical and chemical processes are induced in the molecule

Single-molecule junctions

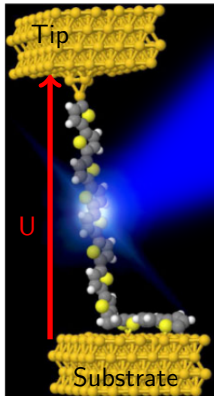
A light emitting single molecule junction



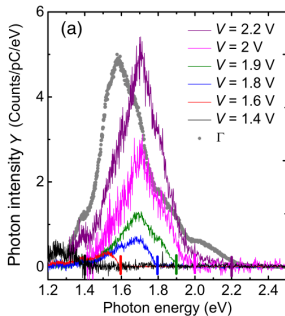
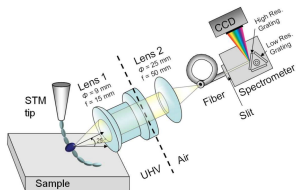
Reecht et al, Phys. Rev. Lett.
112, 047403 (2014)

Single-molecule junctions

A light emitting single molecule junction



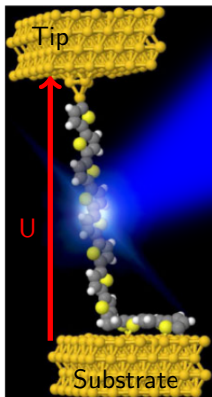
Reecht et al, Phys. Rev. Lett.
112, 047403 (2014)



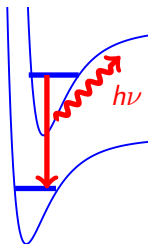
Single-molecule junctions

A light emitting single molecule junction

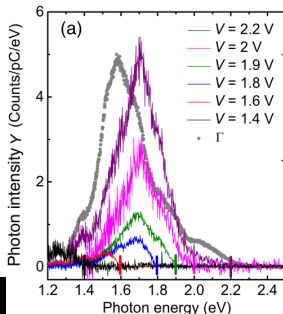
Optical transition: change of the electron distribution ground state \leftrightarrow excited state



Reecht et al, Phys. Rev. Lett.
112, 047403 (2014)



1. Building of the molecule
2. Geometry optimization of the molecule (DFT)
3. Computing of the ground state of the molecule (DFT)
4. Computing of the excited states of the molecule (TD-DFT/Linear response formalism)



- ▶ Ground state: DFT
- ▶ Excited states:
 - ▶ Time-dependent DFT (TD-DFT)
 - ▶ Linear response formalism
- ▶ PBE exchange-correlation functional
- ▶ Plane-wave basis set
- ▶ Recursive Davidson algorithm for TD-DFT
- ▶ QUANTUM ESPRESSO CODE
- ▶ P. GIANNOZZI et al.
J.PHYS.:CONDENS.MATTER 21, 395502 (2009).



- ▶ Hervé Bulou
- ▶ Office: 1034
- ▶ email: herve.bulou@ipcms.unistra.fr