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- Omics group has organised 500 conferences, workshops and national symposium across the major cities including SanFrancisco,Omaha,Orlado,Rayleigh,SantaClara,Chicago,Philadelphia,Unitedkingdom,Baltimore,SanAntanio,Dubai,Hyderabad,Bangaluru and Mumbai.

Quantum interference effects and molecular electronics

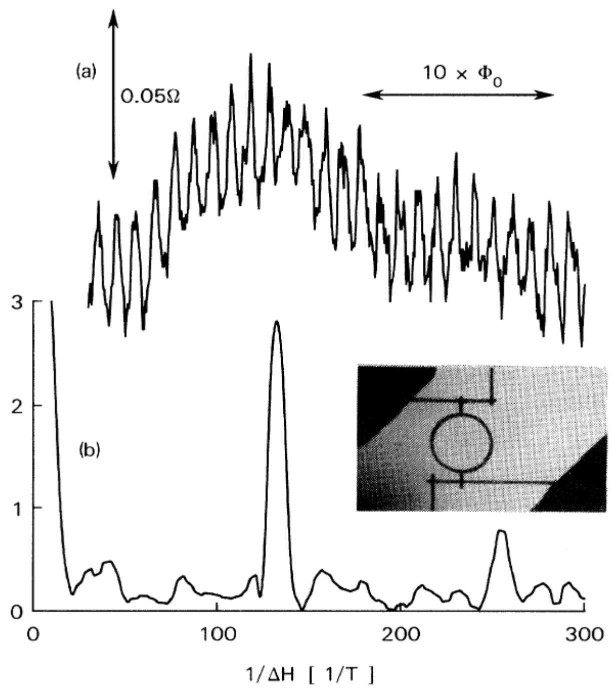
Philippe Lafarge

Université Paris Diderot, CNRS, Paris, France
philippe.lafarge@univ-paris-diderot.fr

Optics 2014 - sept. 10, 2014

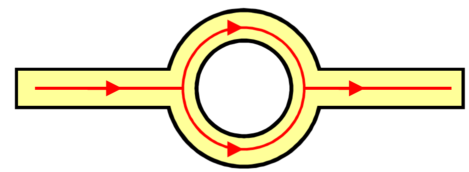
Quantum interference in mesoscopic systems

Aharonov-Bohm effect in a metal ring



R. A. Webb *et al*., Phys. Rev. Lett. **54**, 2696 (1985)

phase coherent transport



$$|\psi\rangle = c_1|\varphi_1\rangle + c_2|\varphi_2\rangle$$

$$P_{QM} = |A_1 + A_2|^2$$

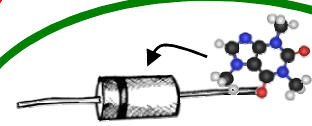
quantum interference

phase shift controlled by magnetic flux $= \pi\,\Phi/\Phi_0$

Molecular electronics

MOLECULES

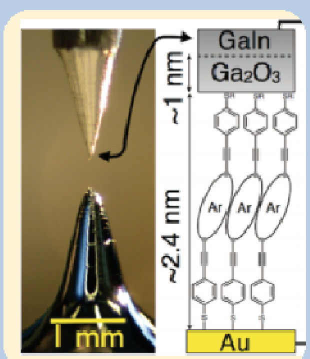
- **Nanoscale** structures
- **chemically active**
- **Cost-effective**



Electronic components made with molecules ?

Need to **probe the electronic properties** of molecules !

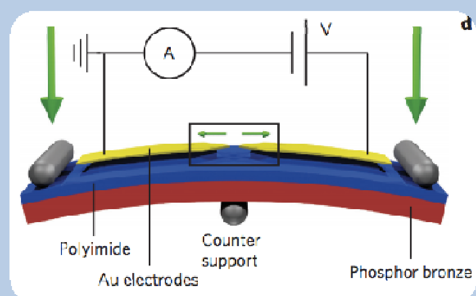
Molecular junctions



D. Fracasso et al. *J. Am. Chem. Soc.* **2011**,133, 9556-9563

Monolayer molecular junctions

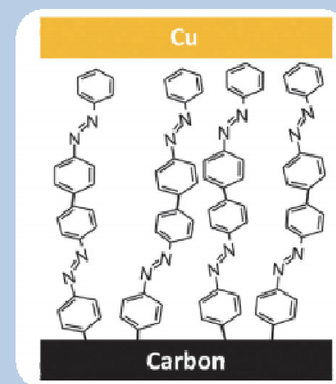
Based on self assembled monolayers (SAMs)



M. L. Perrin et al. *Nat Nano* **2013**, 8, 282-287

Mechanically controlled break-junctions

One or a few molecules connected



R. McCreery et al. *Phys. Chem. Chem. Phys.* **2013**, 15, 1065

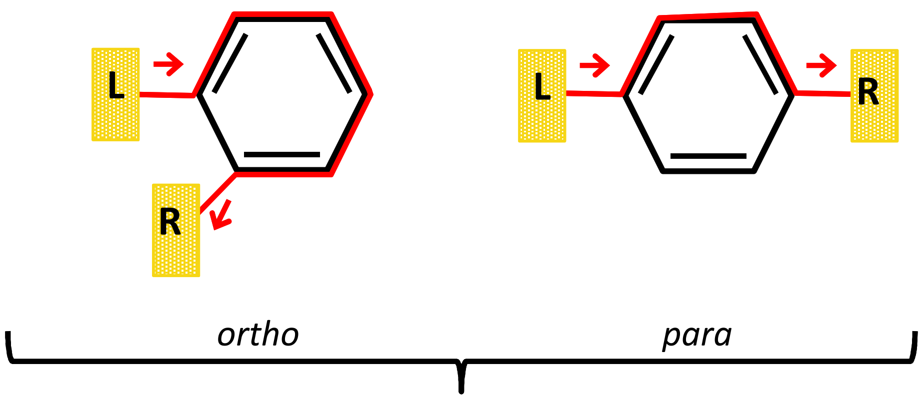
Solid state planar junction

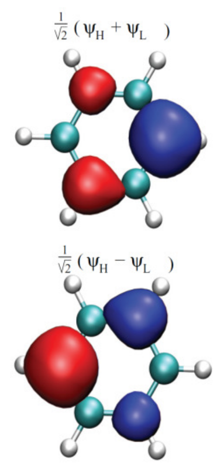
Millions of molecules are connected thanks to electrografting

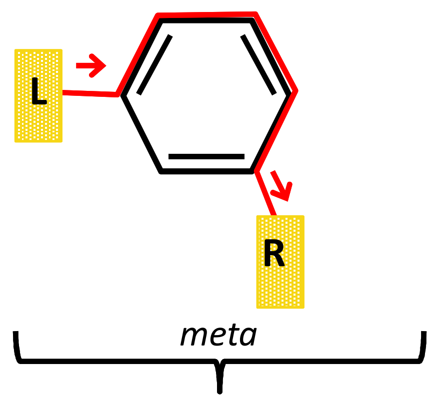
Quantum interference

- The **connection between the molecule and the electrodes influences the**
- **electronic properties** described by the electronic **transmission probability $T_{LR}(E)$**

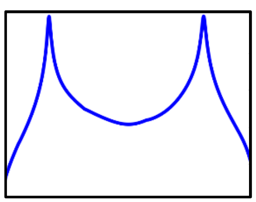
→ **Electron transport** through a **single benzene** molecule connected in **ortho**, **para** or **meta.**





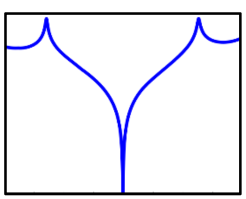


$T_{LR}(E_F) \neq 0$



No QI

$T_{LR}(E_F) = 0$



Destructive QI

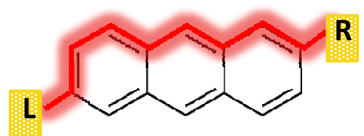
P. Sautet, C. Joachim, *Chem. Phys. Lett.*, **153**, 511 (1988)
T. Markussen et al. *Nano Lett.* **10**, 4260-4265 (2010)
C. R. Arroyo et al. *Ang.Chem.*, **125**, 3234-3237 (2013)

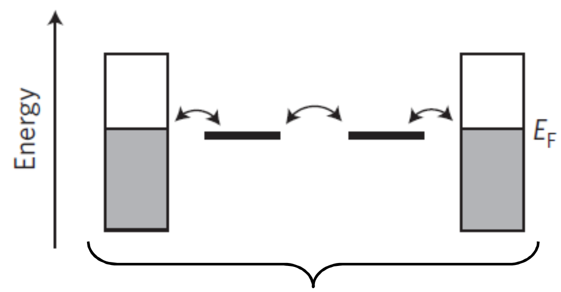
QI and molecular structure

para – MOLECULE – *para*

linearly conjugated

Anthracene (AC)





Only **1 path** allowed

Constant transmission function at E_f

No QI

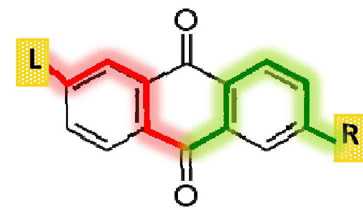
✓ **Molecular junctions**

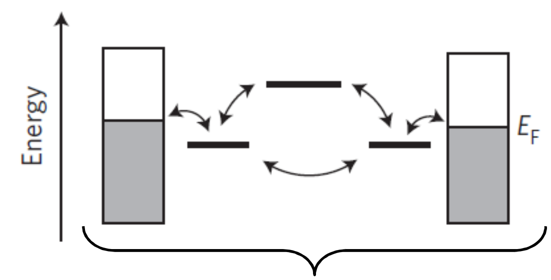
Energy diagrams

(Localized Molecular Orbitals)

cross conjugated

Anthraquinone (AQ)





2 phase-opposed electronic paths

Antiresonance in the transmission function

$T(E_f) = 0$

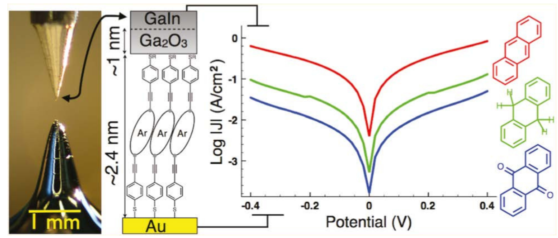
Destructive QI

G. Solomon et al. *ChemPhysChem*, **10**, 257-264 (2009)
C.M.Guédon et al. *Nat Nano.* **7**, 305-309 (2012)

First experimental evidences

- **In SAMs of AC and AQ arylethynylene thiolates** with eutectic Ga-In top contacts

  D. Fracasso *et al.*, JACS **133**, 9556 (2011)

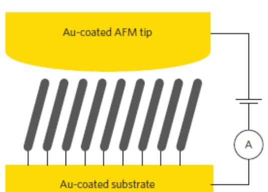


$I_{AQ}(V) < I_{AC}(V)$

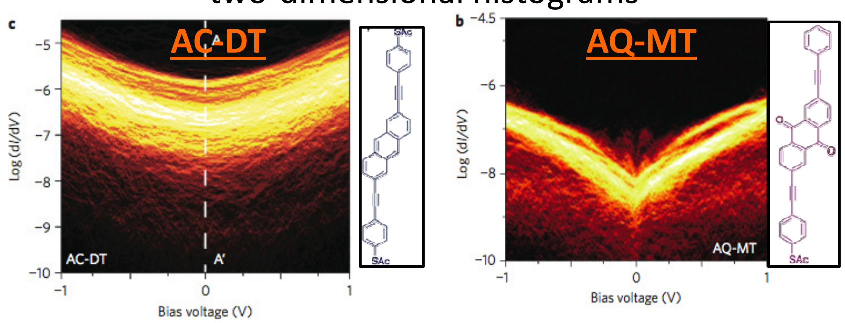
- From an **indirect measurement of AQ and AC based SAMs, statistical analysis**

  C.M.Guédon et al. Nat Nano. **7**, 305-309 (2012)

C-AFM



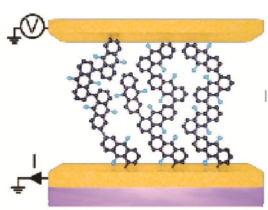
two-dimensional histograms

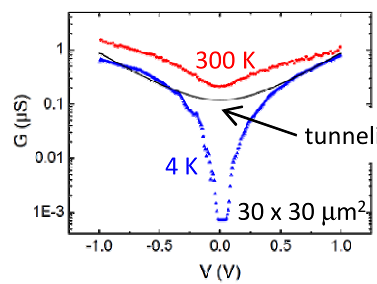


dI/dV vs V

- **In AQ based molecular junctions** from a **direct measurement** of the conductance curves

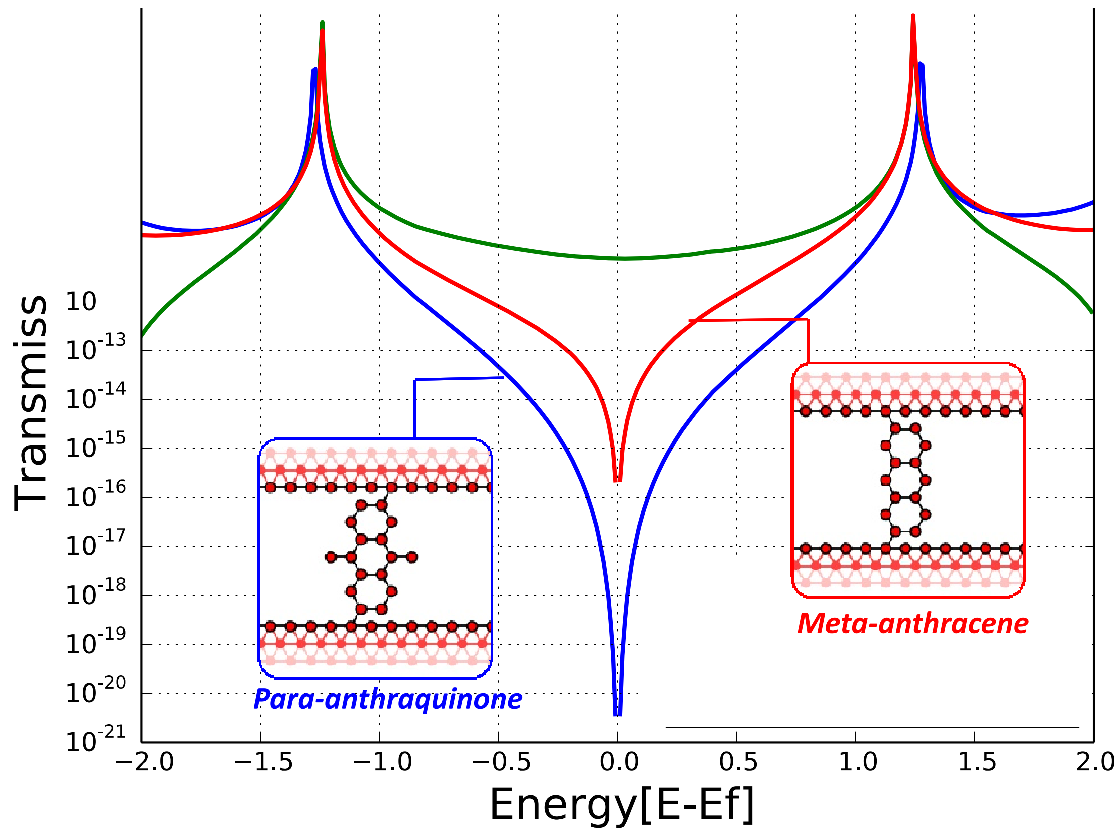
  Rabache *et al.*, JACS **135**, 10218 (2013)





Transmission function calculation

- **Tight binding approach** applied to charge transport (KWANT)
- Key role played by **the way the molecules are connected to the electrodes.**



Parameters

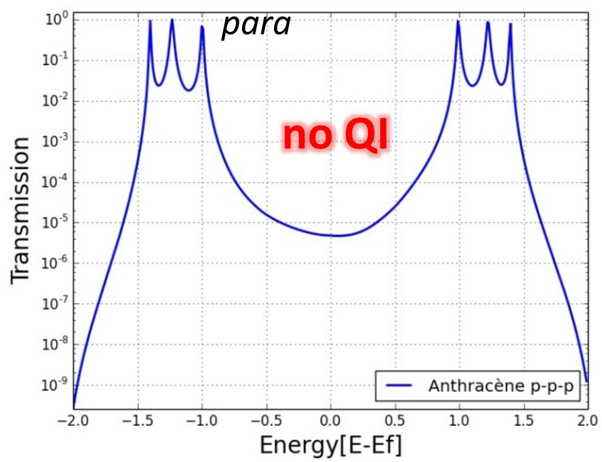
On site energies = 0eV / **Coupling energies** = -3eV / **Coupling to the electrodes** = -1eV

C.W. Groth et al. a software package for quantum transport, arXiv: 1309.2926

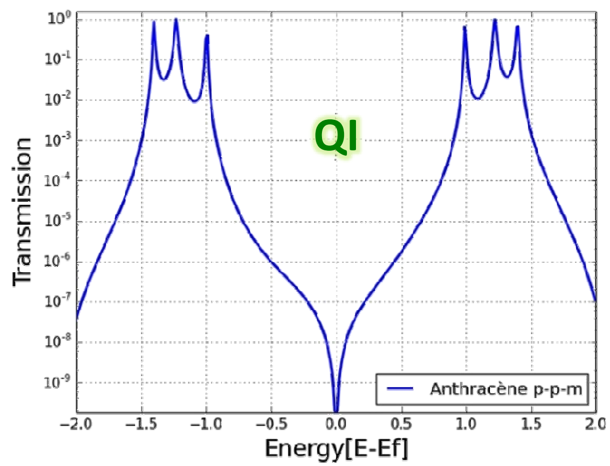
Simulations for anthracene

- **One meta connection** in a chain is enough to make **QI occur**

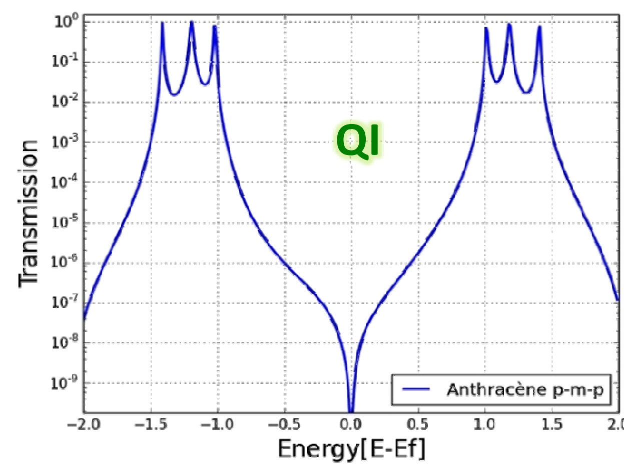
para-para-para

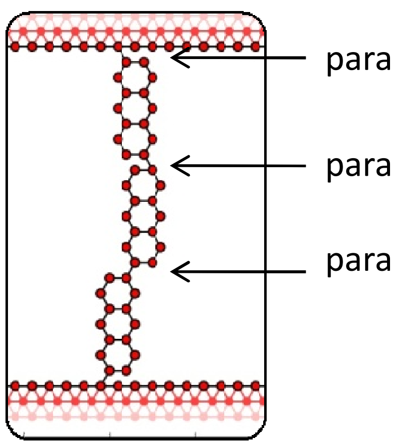


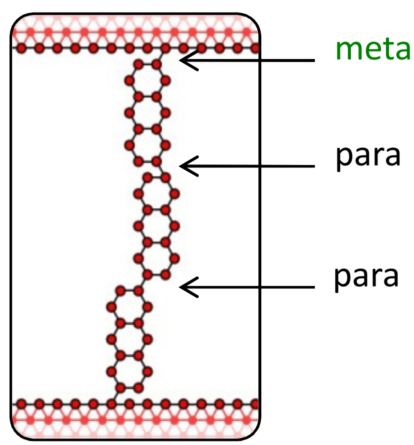
para-para-meta

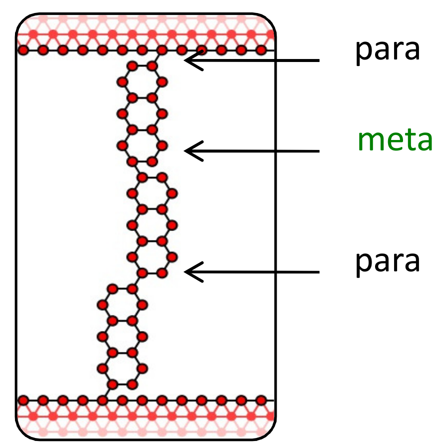


para-meta-para





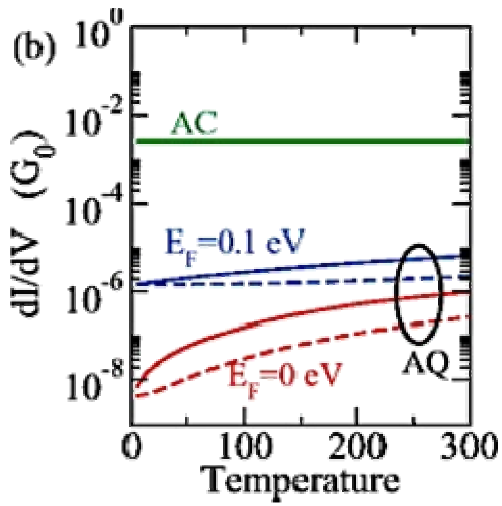




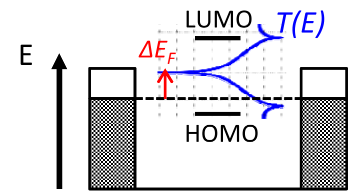
C.W. Groth et al. a software package for quantum transport, arXiv: 1309.2926

Recent theoretical predictions

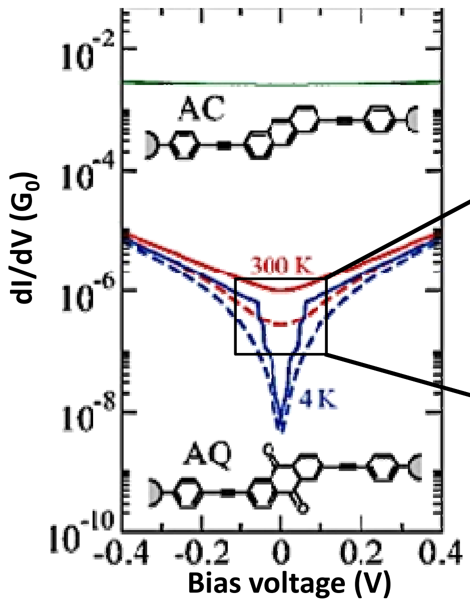
- **Influence of the temperature on QI effects**

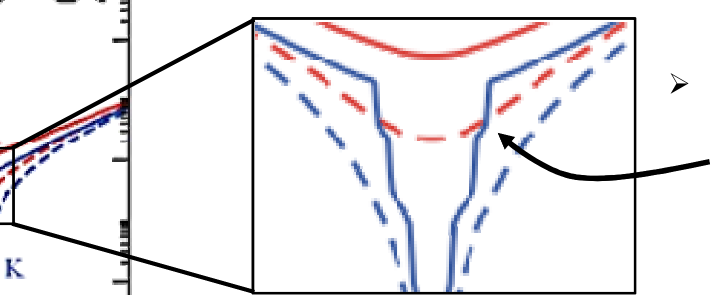


- ➢ **No thermal activation**
- ➢ Dependence on the **alignment of the transmission node** and **the Fermi level** (blue and red lines)
- ➢ **el-ph interactions (solid lines)**



- **Structures in the dI/dV curves**



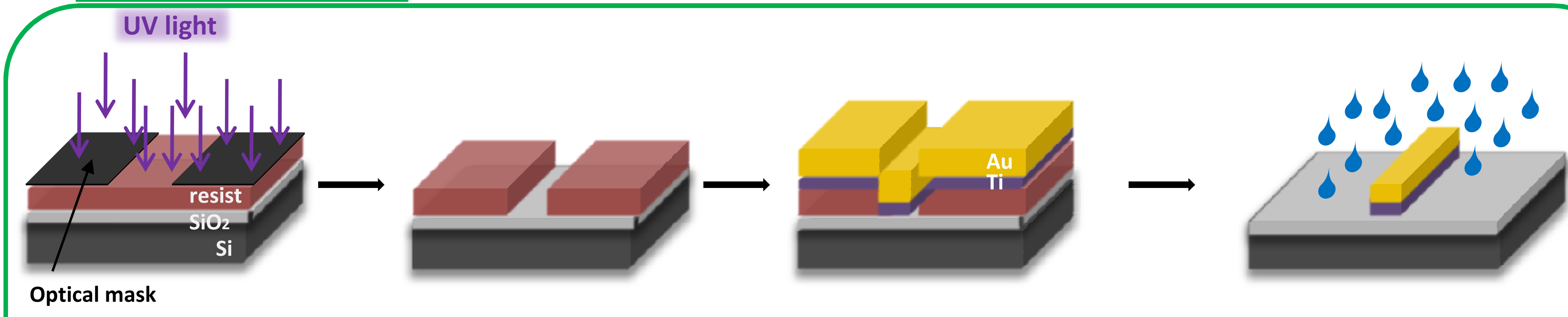


- ➢ **Steps visible a low T with el-ph interactions** (solid blue line), **not visible at RT** (solid red line)

T. Markussen et al. *Phys.Rev.B*, **89**, 085420 (2014)

Fabrication of the junctions

Bottom electrode



Optical lithography
Postive resist with a positive mask

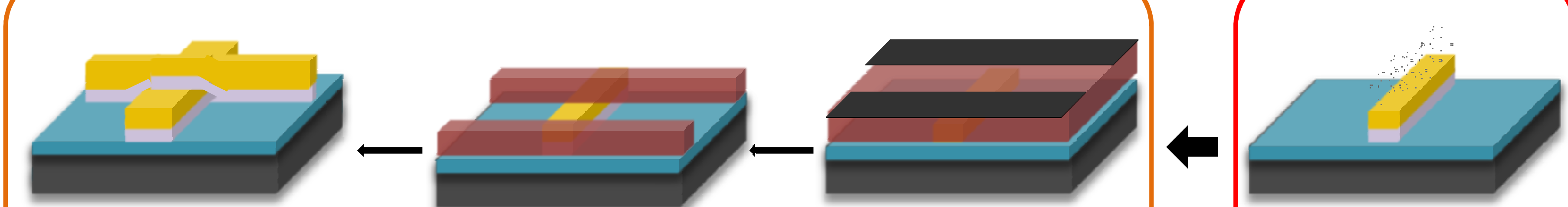
Development
To carve the design of the electrode

Metallic deposition
Au ~ 50nm
Ti ~ 2-3nm

Lift off
Aceton bath

electrografting

Top electrode



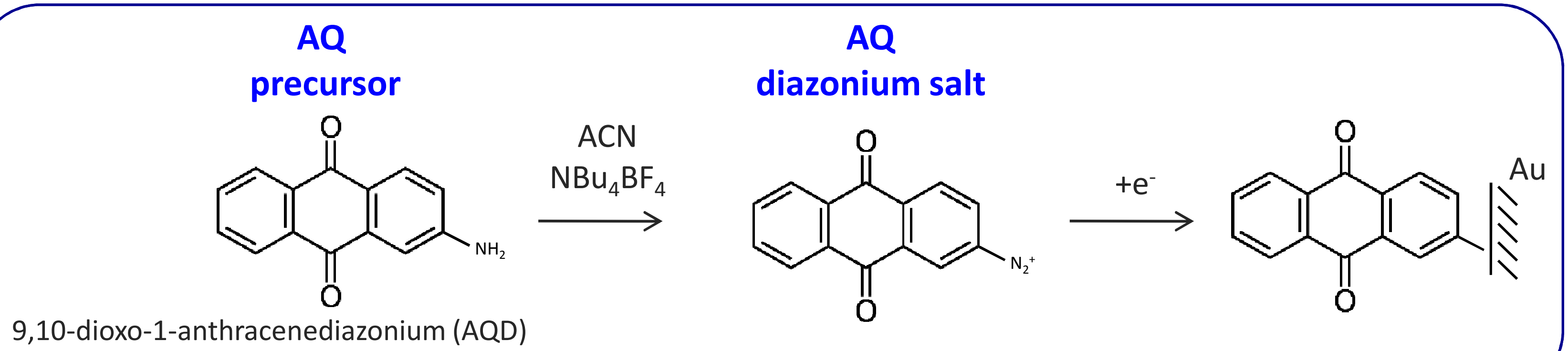
Metallic deposition + lift off

Development

Optical lithography

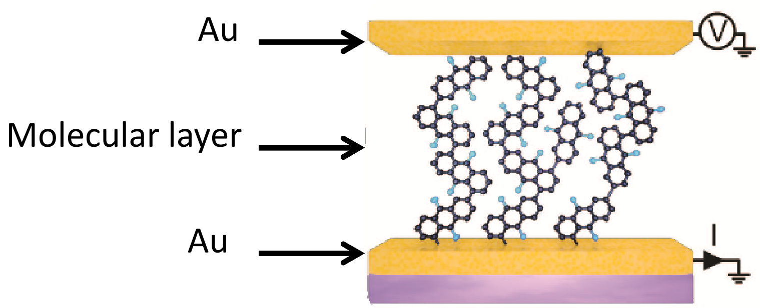
Fabrication of the junctions

➡ Formation of organic film by **reduction of diazonium salt**

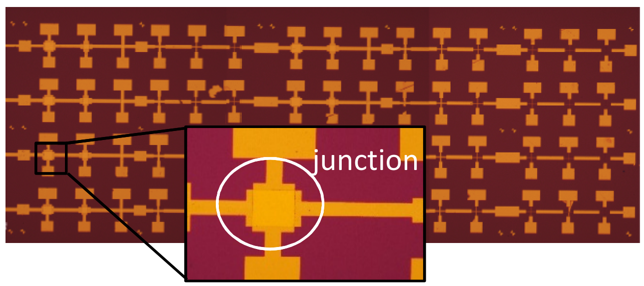


P. Martin, J.-C. Lacroix, ITODYS lab, Paris Diderot University

➡ **Final solid state planar junctions** (cross bar geometry)



Profile view *(schematic)*

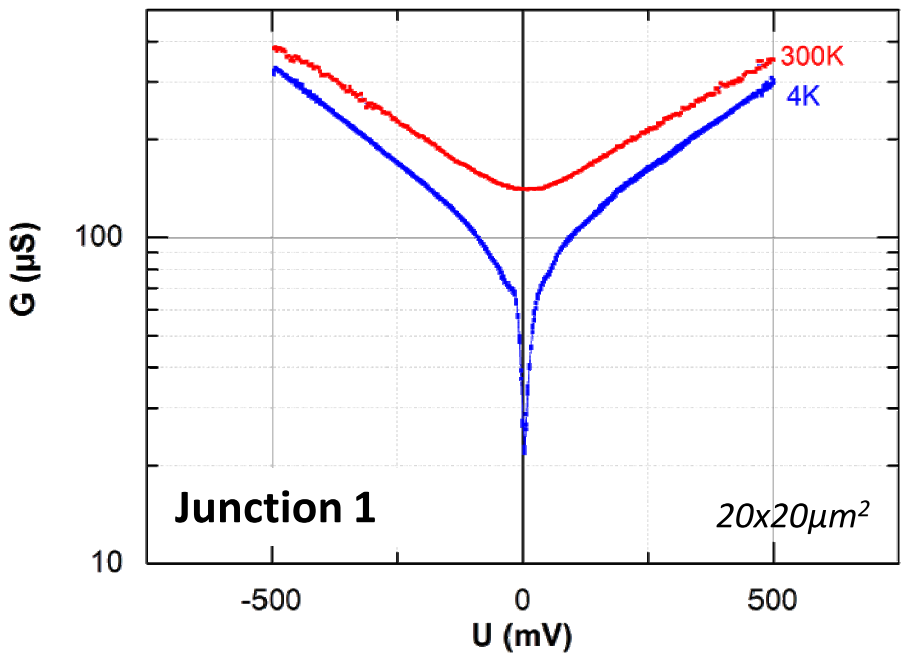


Crossed bar geometry junctions *(optical image x 20)*
Samples made with 24 junctions of 20x20µm²

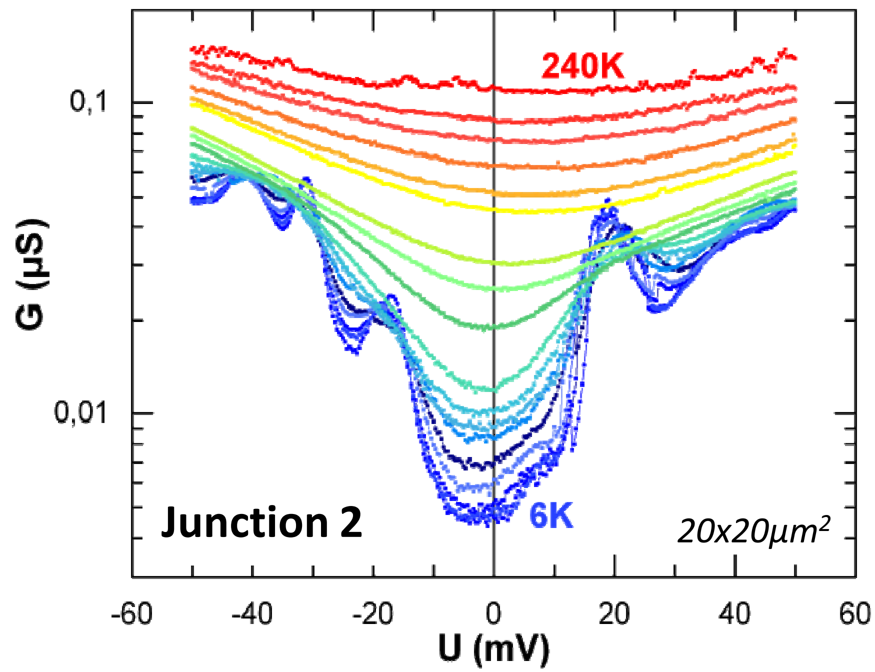
Conductance measurements

- **Au/ AQ /Au** junctions

G (V) vs bias voltage



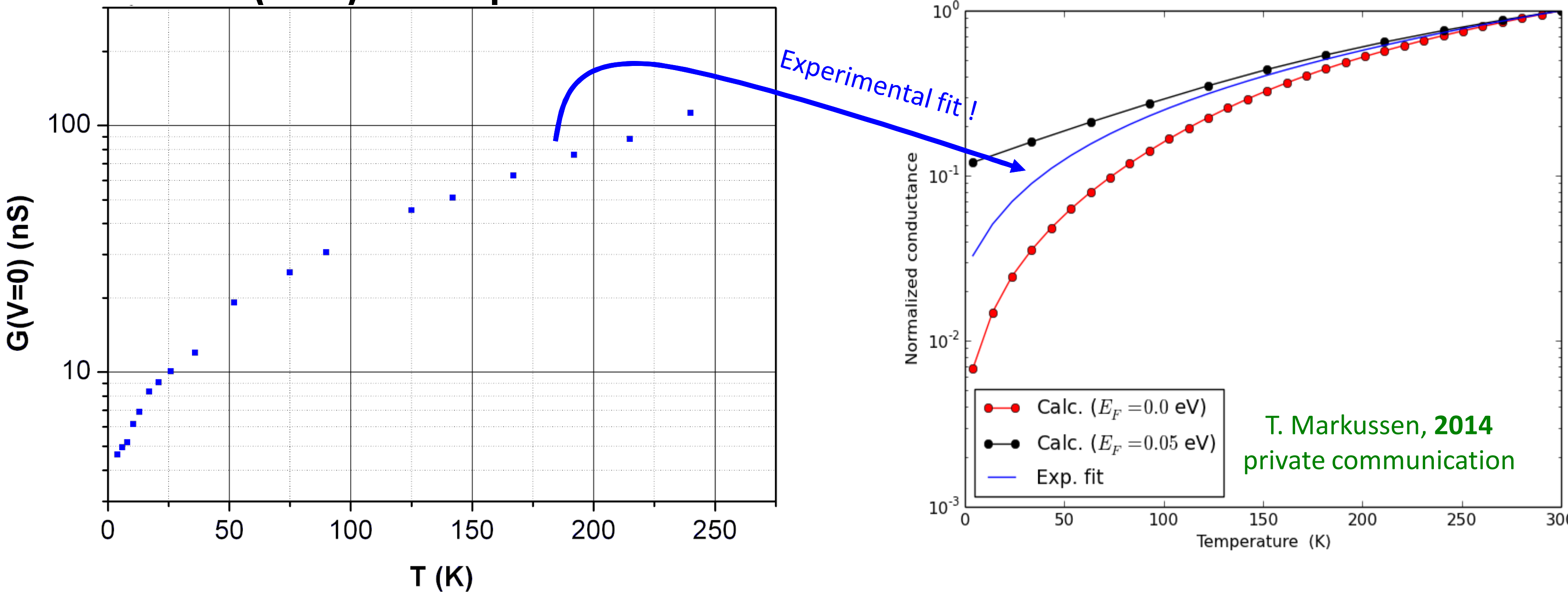
G (V = 0) vs bias voltage



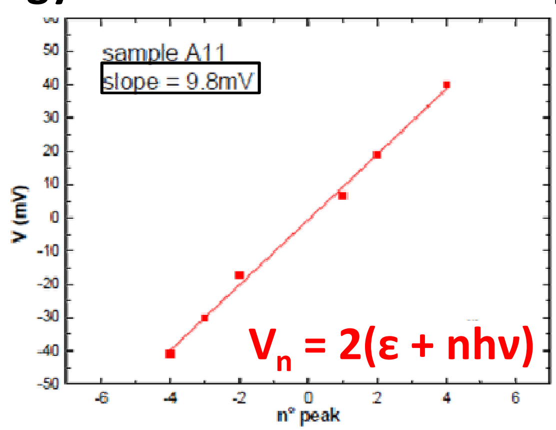
- **Antiresonance dip at 4K**, lower visibility at 300K
- **Temperature dependent structures at low T**

Conductance vs temperature

G (V= 0) vs temperature



Energy of the structures vs the position

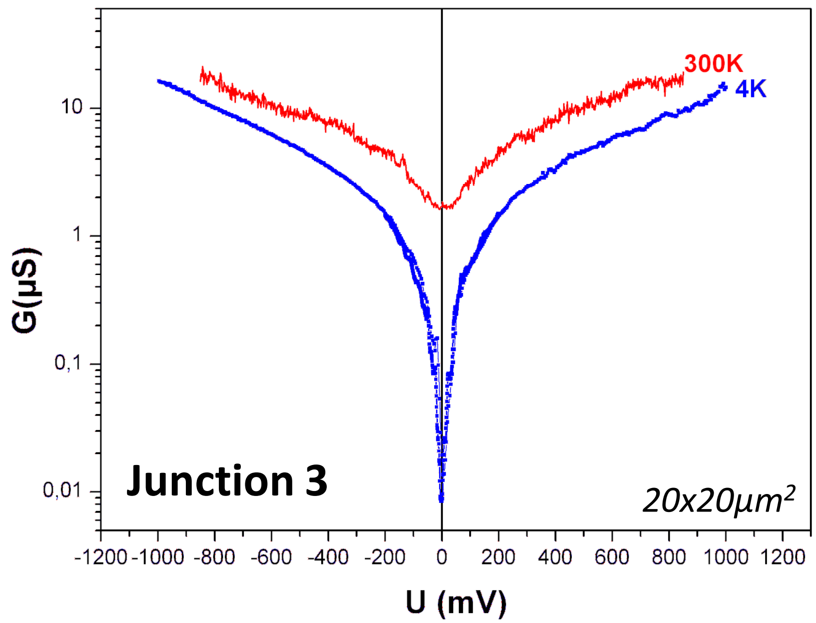


- **Experimental behaviour** (blue line) **similar to the one predicted** for single molecule **junctions** with el-ph interactions (red line)
- Decoherence by **electron phonon coupling** ?

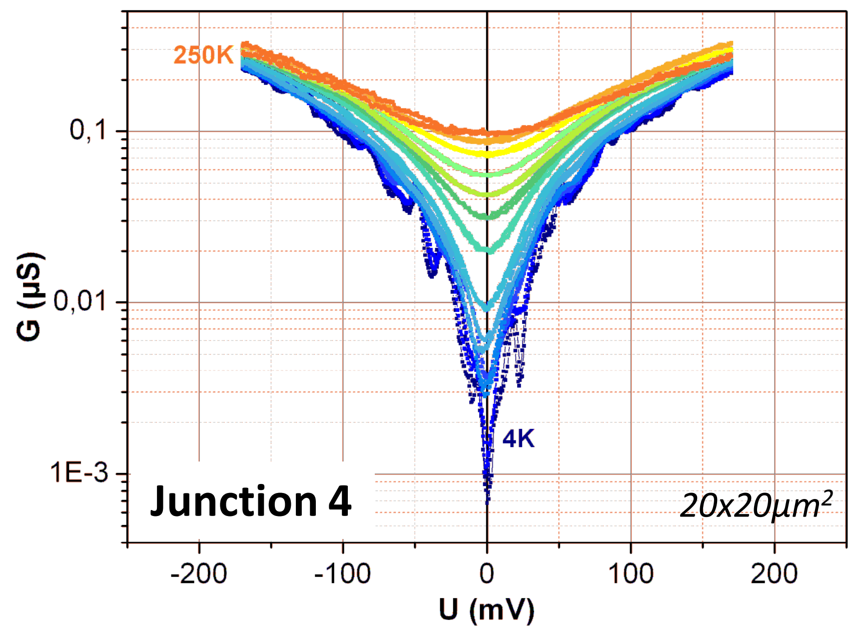
Anthracene based junctions

- **Au / AC /Au based junctions**

G (V) vs bias voltage



G (V = 0) vs bias voltage

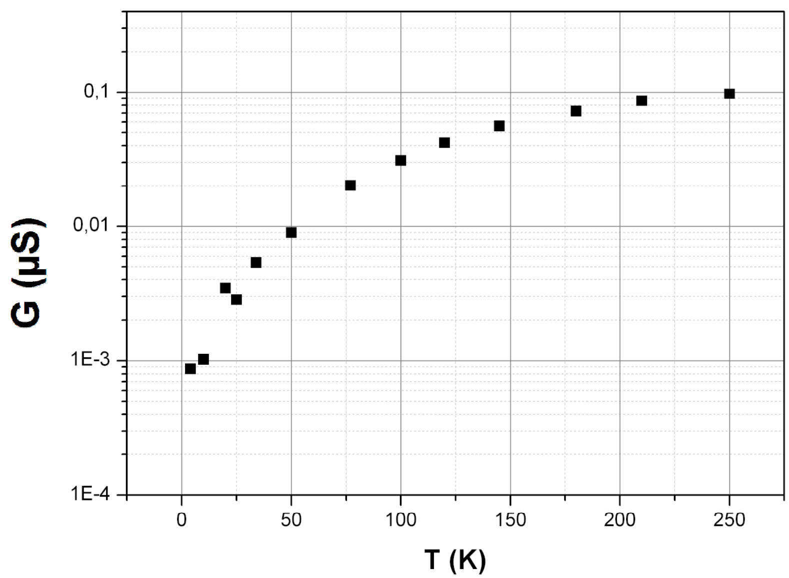


➢ **Antiresonance dip at 4K**, lower visibility at 300K as for the AQ-based junctions

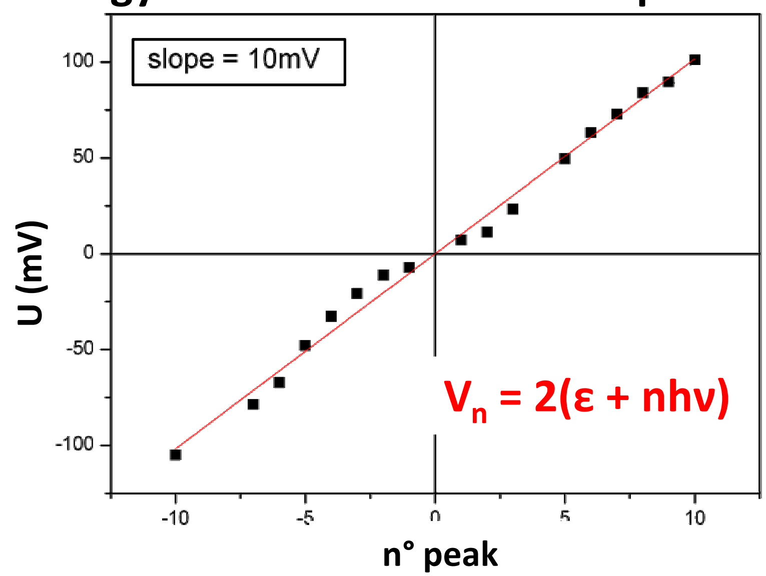
➢ **Temperature dependent structures at low T**

Temperature dependence

G (V= 0) vs temperature



Energy of the structures vs the position

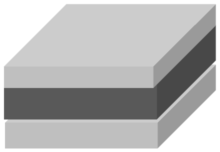


- **Experimental behaviour** similar **to the one predicted for single and AQ based junctions**
- Decoherence by **electron phonon coupling** ?
- **Same vibrational modes as for the AQ** excited

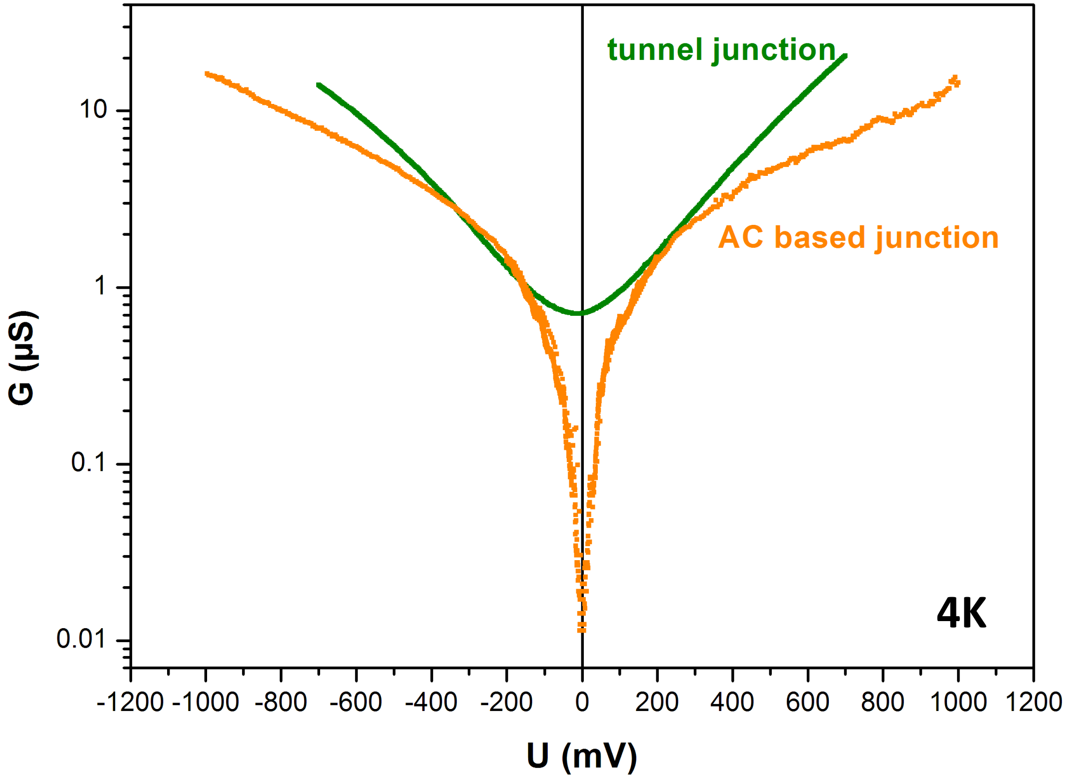
Molecular junction and tunneling

- **QI vs tunnel behaviour**

➡ **Metallic tunnel junctions** Al / Al_2O_3 /Al

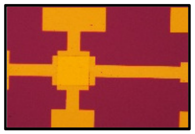


➡ **Different shapes at low T**

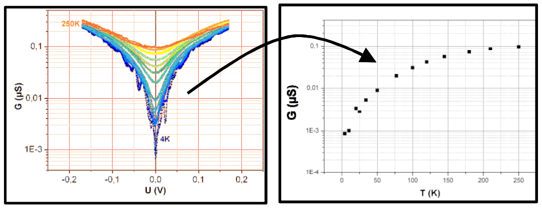


Conclusions and perspectives

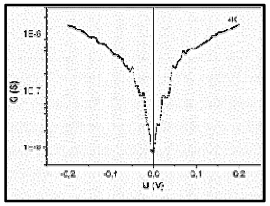
- **Large area solid state molecules based junctions** (with AQ, AC, oxides…)



- **Direct measurement of large antiresonance dip** in dI/dV curves with a **strong temperature dependence**.

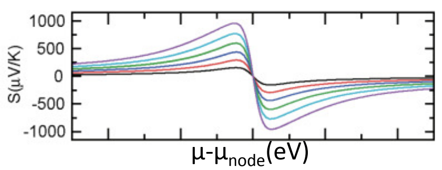


- **Additional structures at low T** that could be the **signatures of vibrational modes of the organic layer**.



- **Giant thermoelectric effect** predicted in molecular junctions where QI occur…

J.P. Bergfield and C.A. Stafford, NanoLett. 9, 3072 (2009)
J.P. Bergfield, M.A. Solis and C.A. Stafford, ACS Nano 4, 5314 (2010)



Thank you

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Maria Luisa Della Rocca, Clément Barraud, Charlotte Bessis, Julien Chaste, Philippe Petit

ITODYS, Paris Diderot University
Pascal Martin, Jean-Christophe Lacroix

University of Alberta
Richard L. McCreery

Copenhagen, Quantum Wise
Troels Markussen

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