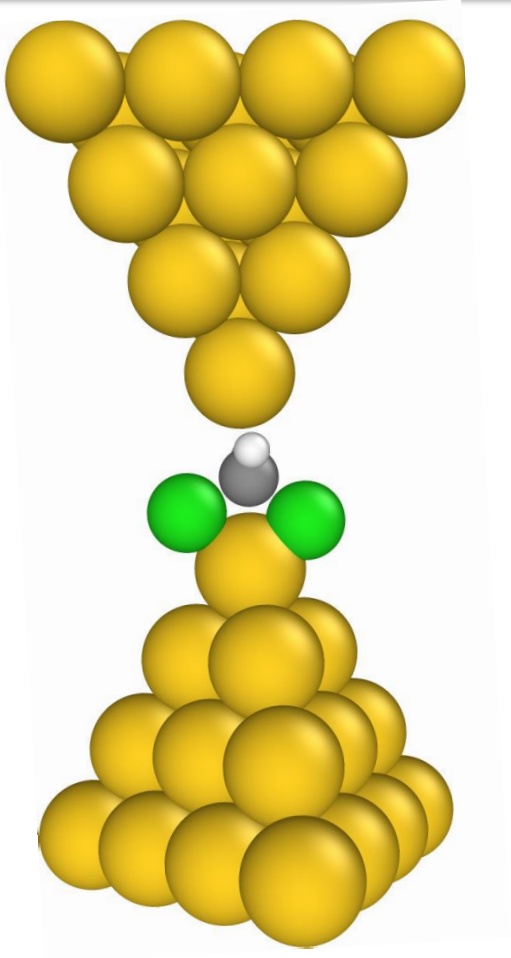
Molecular Electronics at Room Conditions and the Solvents' Role



QT-Lab

C. Sabater

LT lab nano

Prof. C. Untiedt

Universitat d'Alacant
Universidad de Alicante

Dr. Carlos Sabater

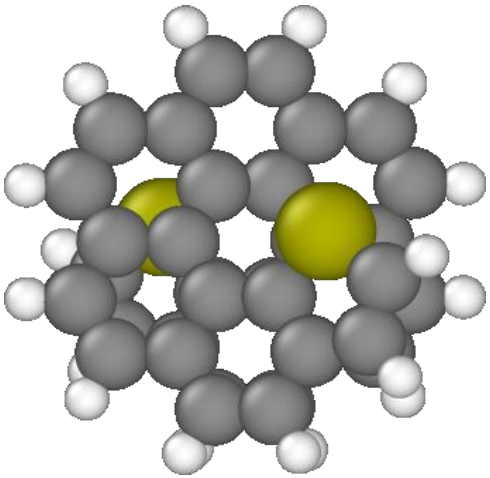
carlos.sabater@ua.es

18th European School on Molecular Nanoscience
(Santa Pola, Alicante)

ESMoINa 2025

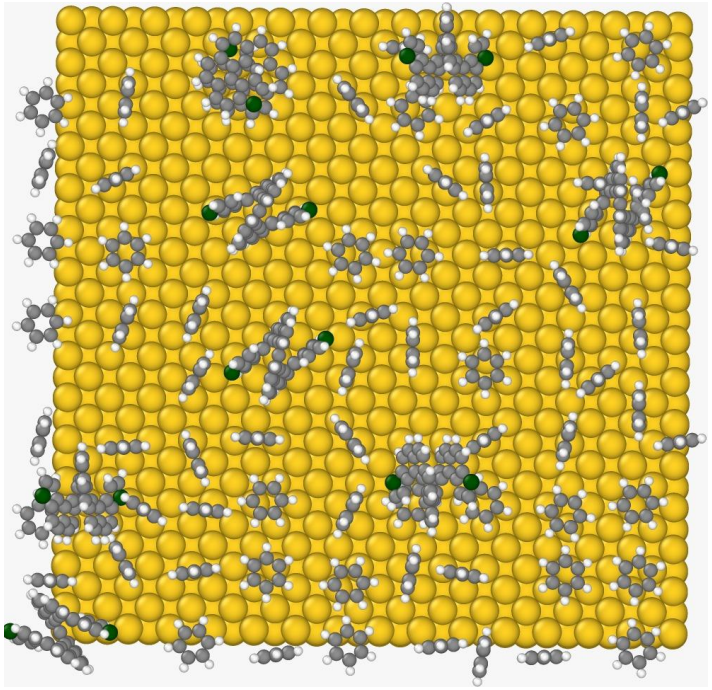
Motivation of the talk

Molecular solution



Dithiaelineces[n] + solvent

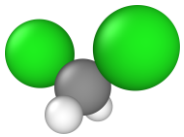
Exo-dithiaelineces[n] in bezene



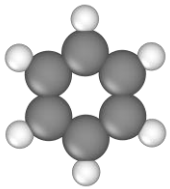
Are benzene fully evaporated?

Solvent used:

- Dichloromethane (DCM) & TCM



- Benzene, Toluene, Cyclohexane



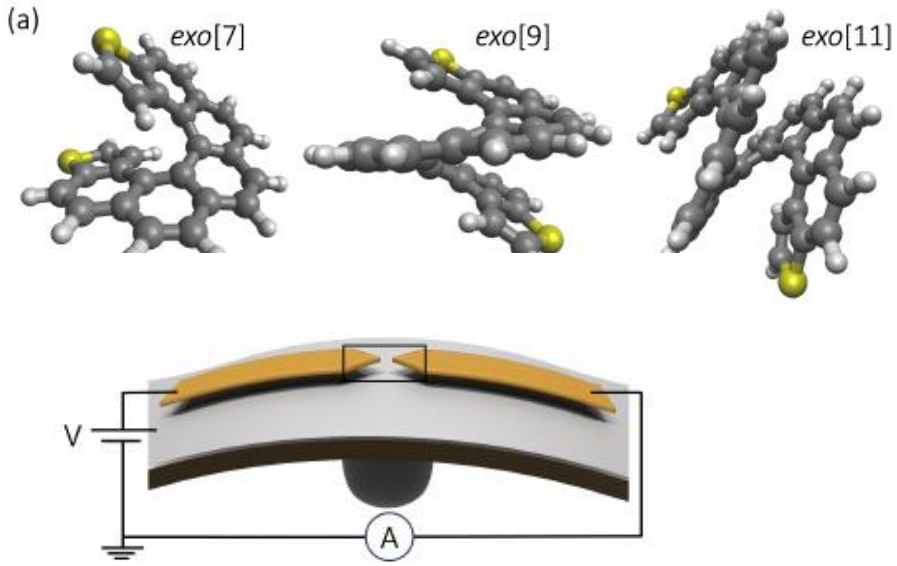
- Glycerol

Motivation of the talk

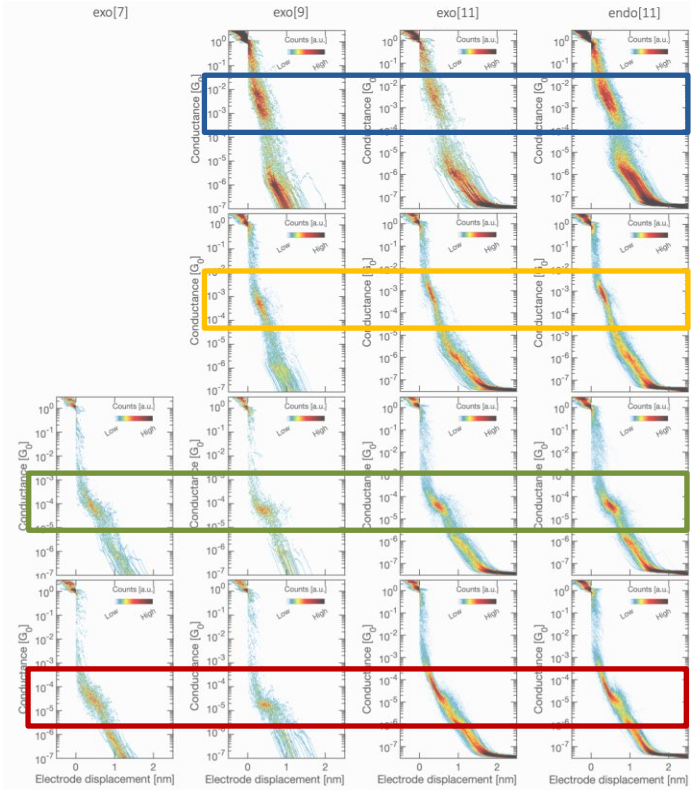
Helicenes in **DCM** solutions electronic transport experiments

van der Zant Lab TU Delft

Universitat d'Alacant
Universidad de Alicante



Clustering Machine Learning
K-mean



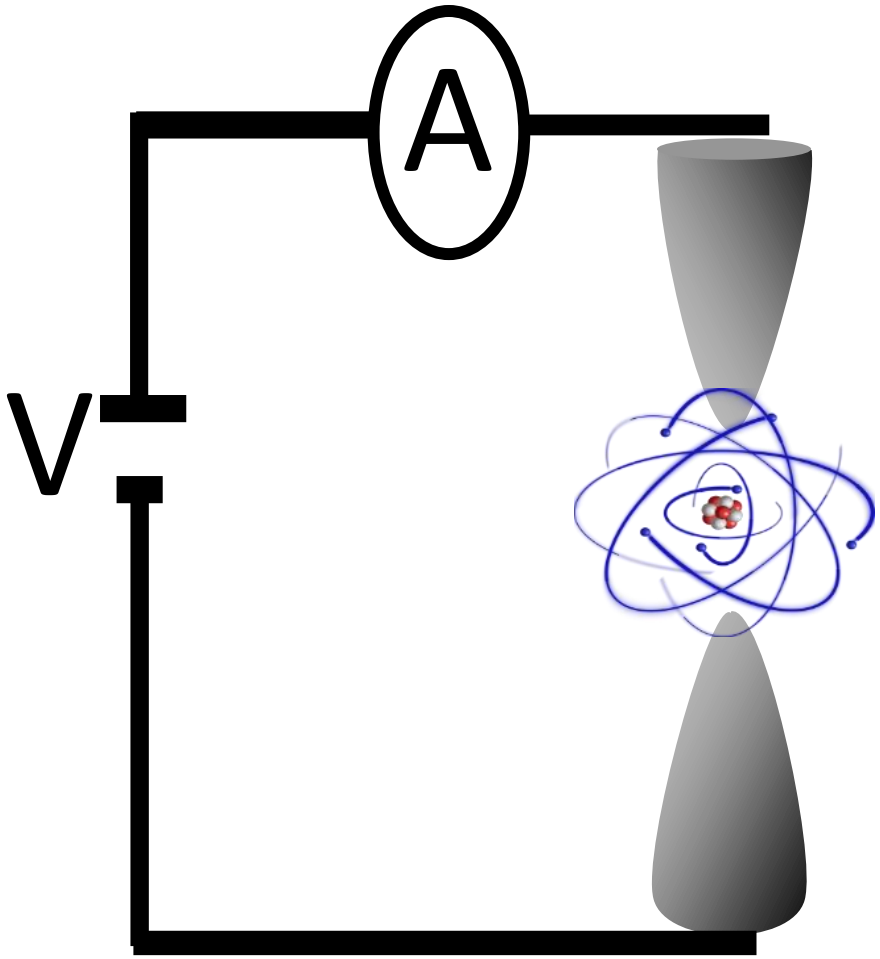
T. de Ara *et al. Phys. Chem. Lett.* ***15,*** *2024*

Questions to answer

- Are the solvents fully evaporated after the drop-casting deposition?
- Can we unmask the orientation of a single organic molecule captured between gold electrodes?

We need to solve it:		
Electronic Transport & STM experiments	Molecular Dynamics Simulations	DFT calculations

Electronic transport in atomic and molecular conductors



Ohm's law: $G = \frac{1}{R} = \frac{I}{V}$

Landauer formalism:

$$G = G_0 \sum_{i=1}^{n} T_i(E_F)$$

Quantum of conductance

$$G_0 \equiv \frac{2e^2}{h}$$

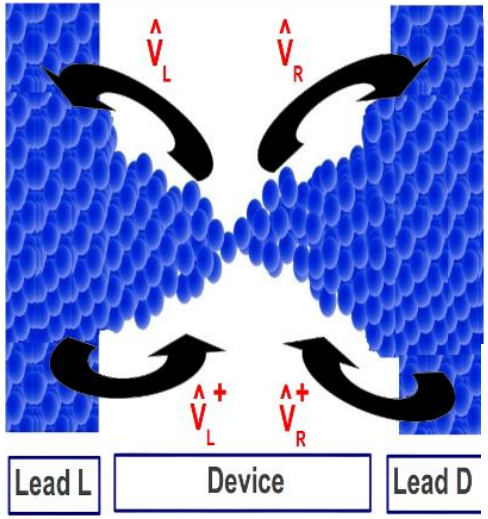
$$1G_0 \approx \frac{1}{13k\Omega}$$

Transport Calculations and Simulations

DFT-NEGF

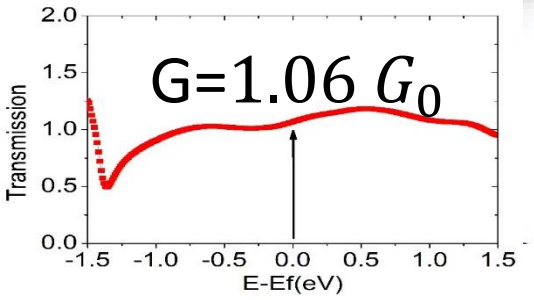
Landauer formalism:

$$G(E) = G_0 \sum_{i=1}^{n} T_i(E)$$



Green Functions Partitioning Method

$$T(E) = Tr\left[\hat{G}_D(E)\hat{\Gamma}_R(E)\hat{G}_D^{\dagger}(E)\hat{\Gamma}_L(E)\right]$$

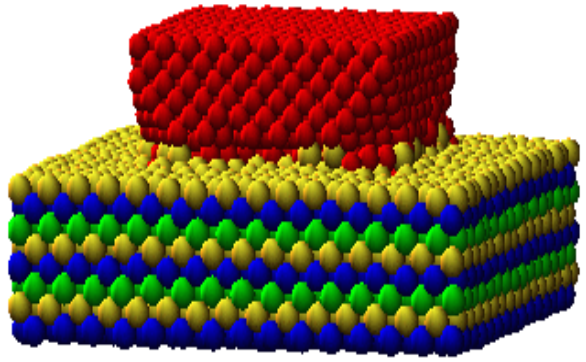


ANT.G

C. Sabater Ph.D. Dissertation (2013)

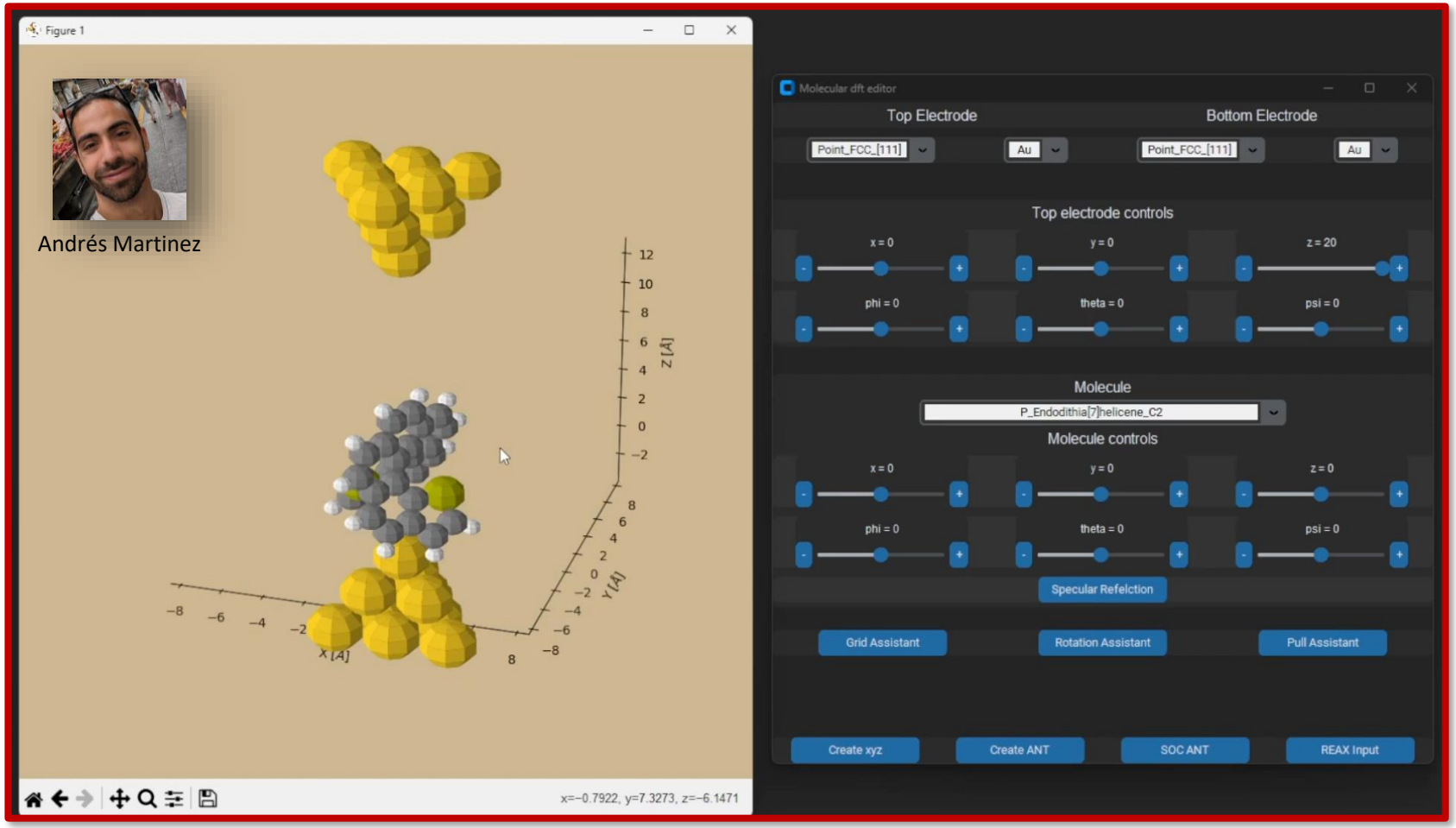
Molecular Dynamics Simulations

$$F = ma = -\nabla U$$



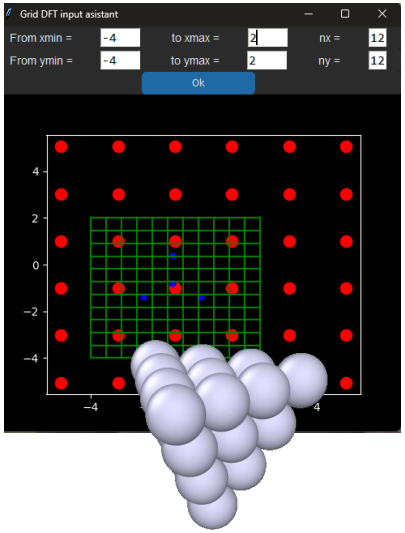
Uzi Landman *et al.* Science, **248** (1990)

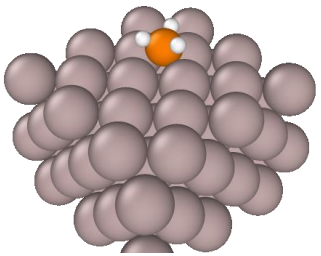
User Friendly Interface Input Generator For Molecular Dynamics and DFT



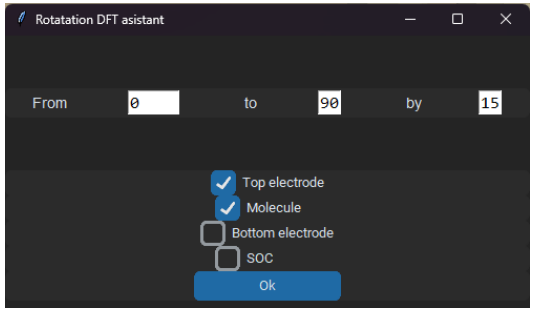
A. Martínez, C. Sabater (in preparation. 2025)

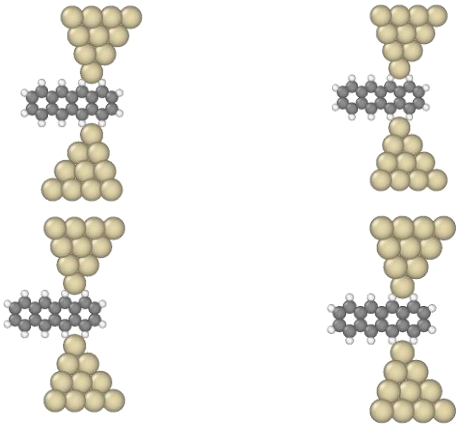
Scan



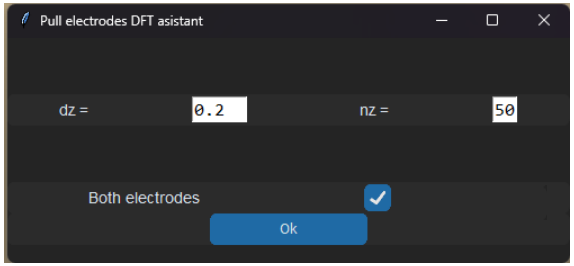


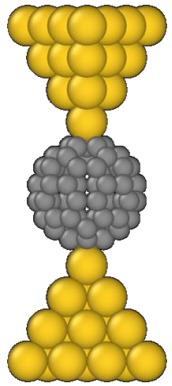
Rotate





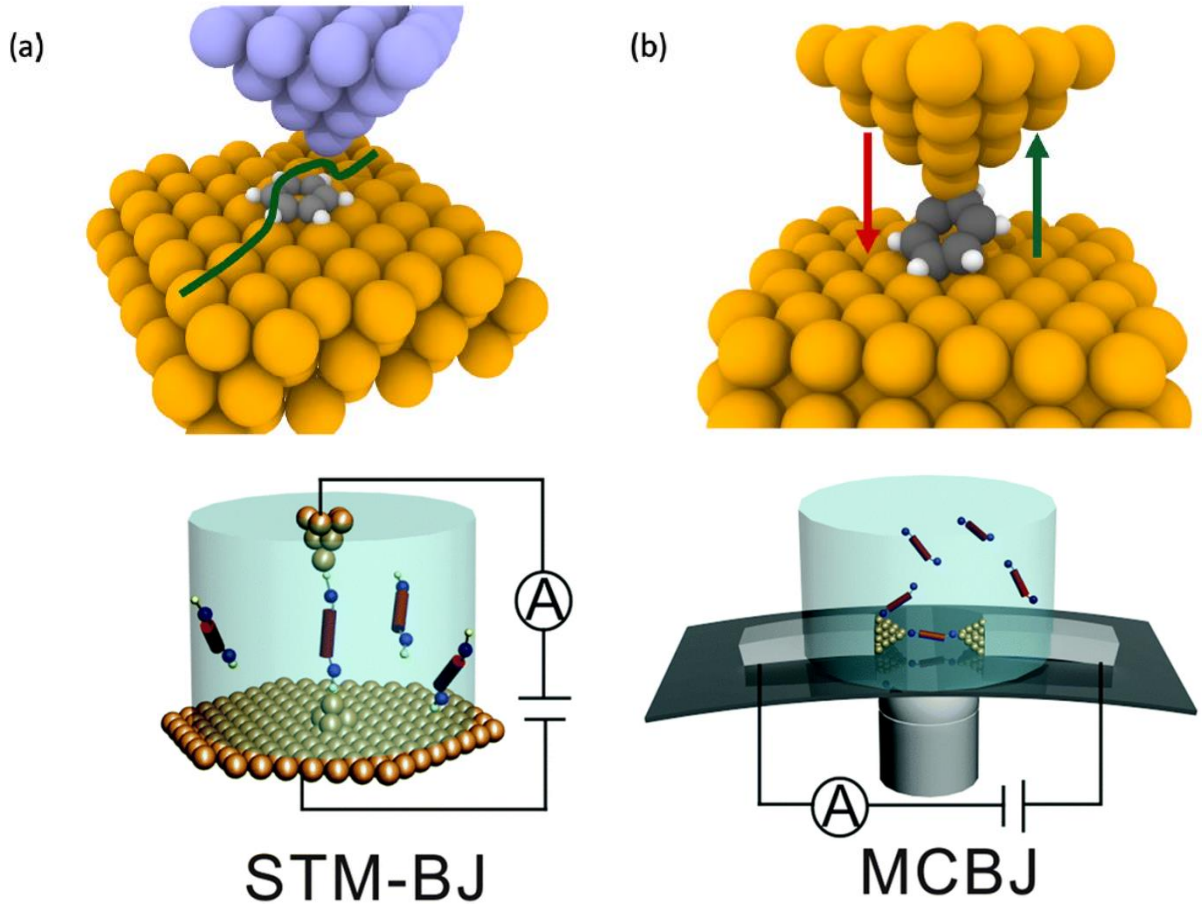
Pull





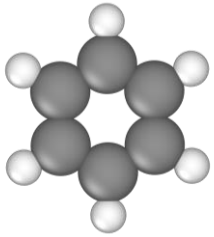
Experimental Techniques

STM & Break-Junctions (BJ)

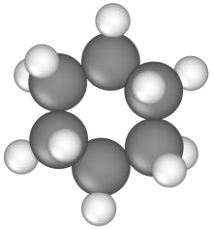


Veerabhadrarao Kaliginedi *et al* . Phys. Chem. Chem. Phys., 2014, **16**, 23529-23539

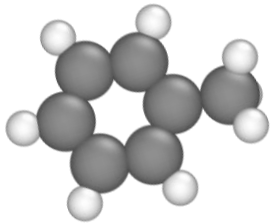
Solvent used in this work



Benzene



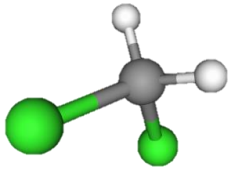
Cyclohexane



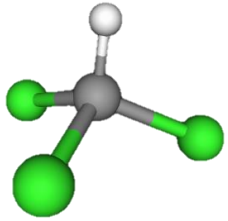
Toluene

T. de Ara *et al*. Materials Chemistry and Physics 291, 126645 (2022)

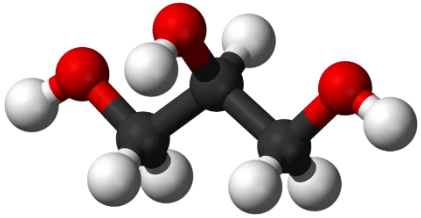
A. Martinez-Garcia *et al.* J. Phys. Chem. C, 127, 48, 23303 (2023)



Dichloromethane

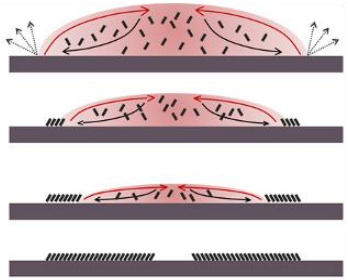


Trichloromethane

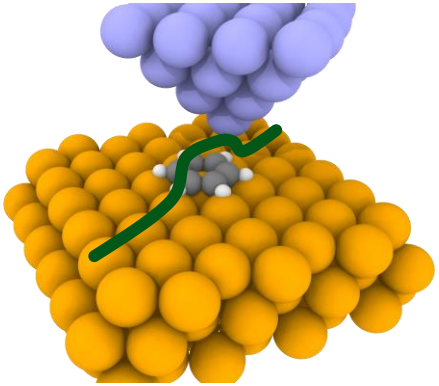


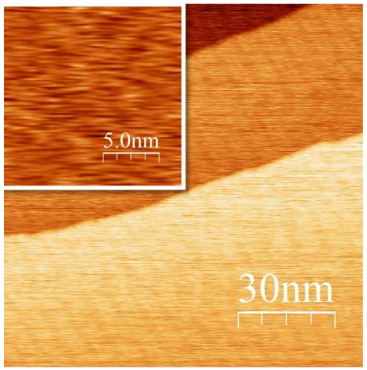
Glycerine

Drop Casting



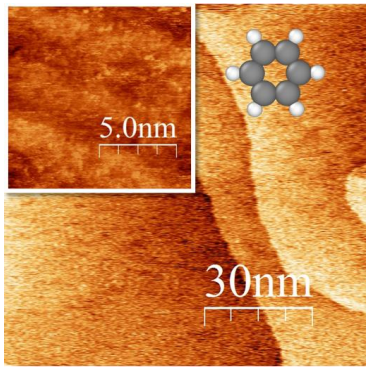
STM IMAGES OF ORGANIC MONOCICLYC SOLVENTS



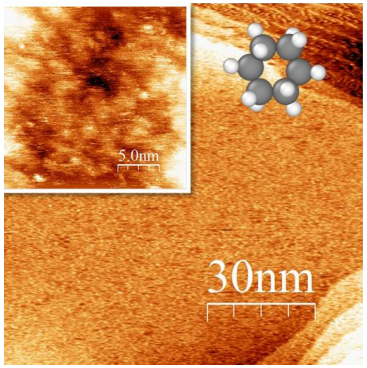


Au (111)

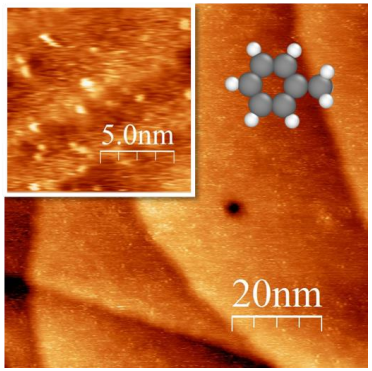
Molecule	$\emptyset_{exp}$ [nm]	$\emptyset_{lit}$ [nm]
Benzene	0.34 ± 0.01	0.28, 0.25, 0.38
Cyclohexane	0.40 ± 0.02	0.31, 0.49
Toluene	0.38 ± 0.01	0.42



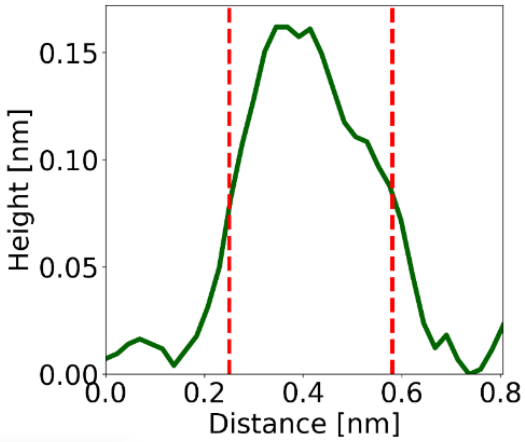
Benzene



Cyclohexane

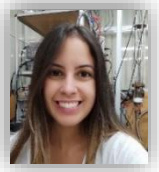


Toluene



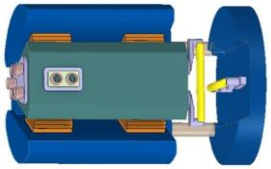
T. de Ara *et al*. Materials Chemistry and Physics 291, 126645 (2022)

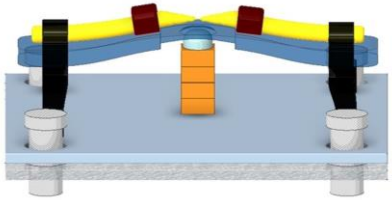
A. Martinez-Garcia *et al.* J. Phys. Chem. C, 127, 48, 23303 (2023)



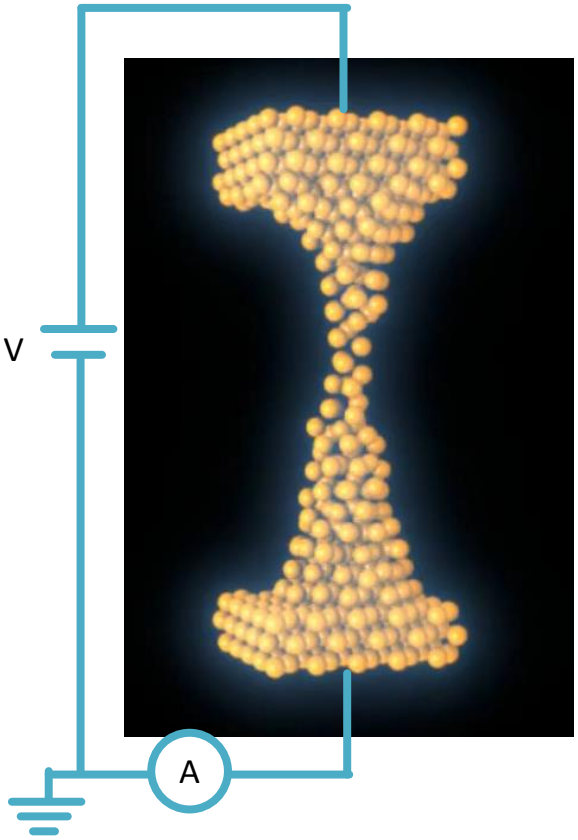
Dr. Tamara de Ara

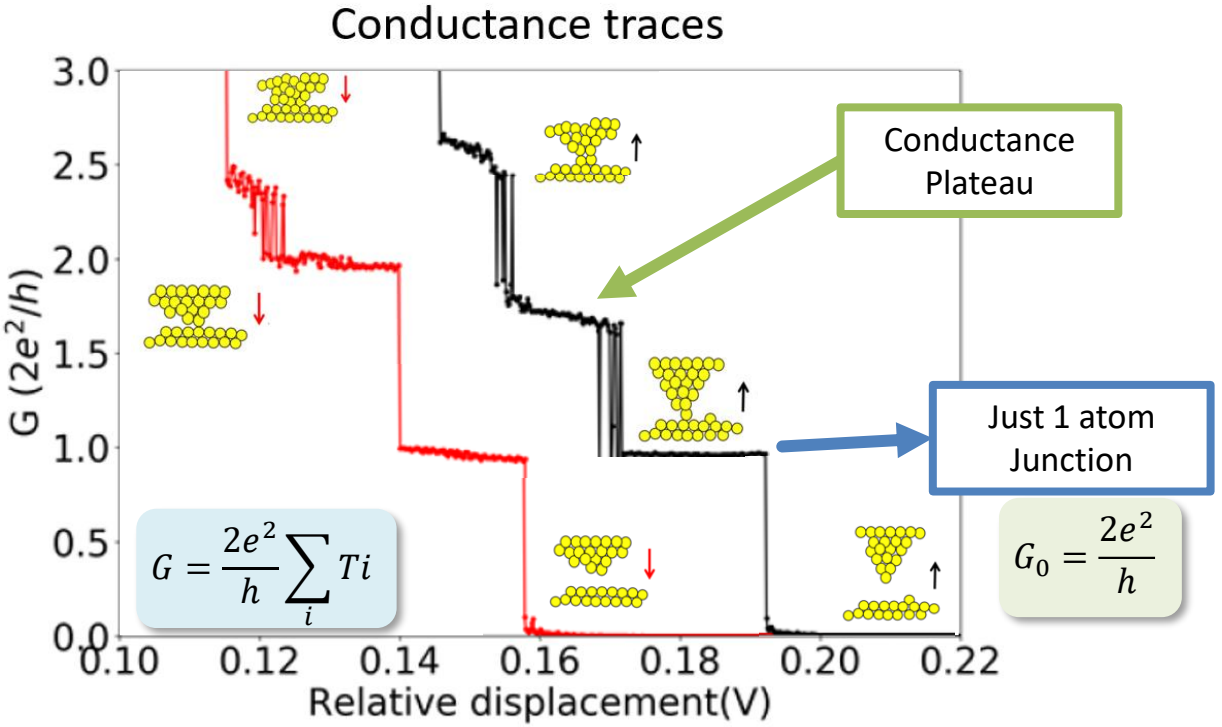
Electronic transport by Break Junctions Experiments





J. P. Cuenca *et al. arXiv* ***2025***





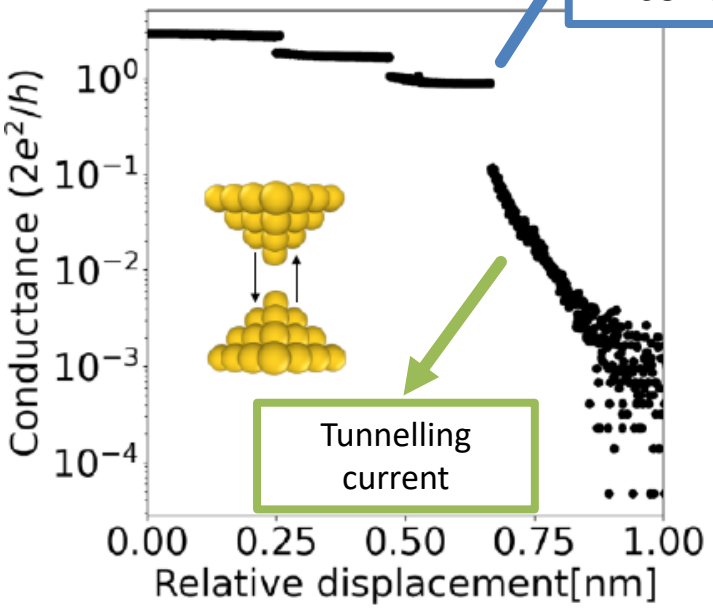
Y. Del Castillo Hernández. Master Thesis (UA) ***2020***

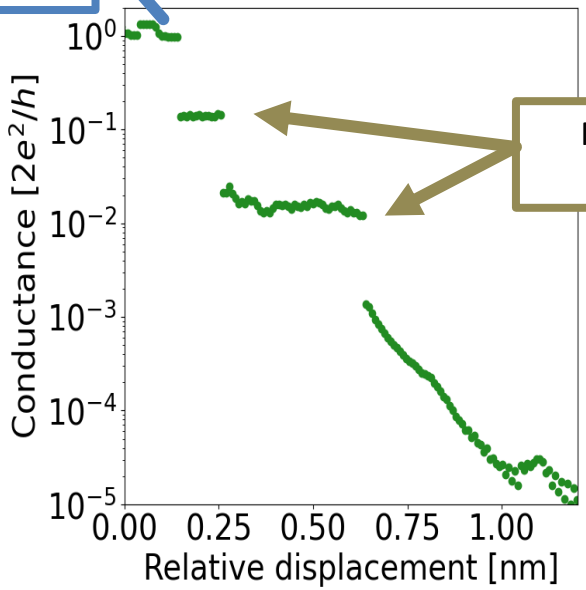
Electronic transport by Break Junctions Experiments

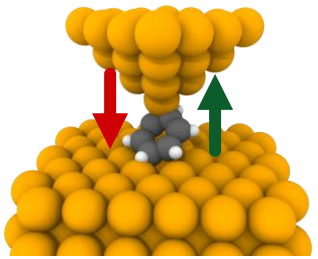
Pure Metallic atomic-sized contact

Just 1 atom contact

Single molecular Junctions





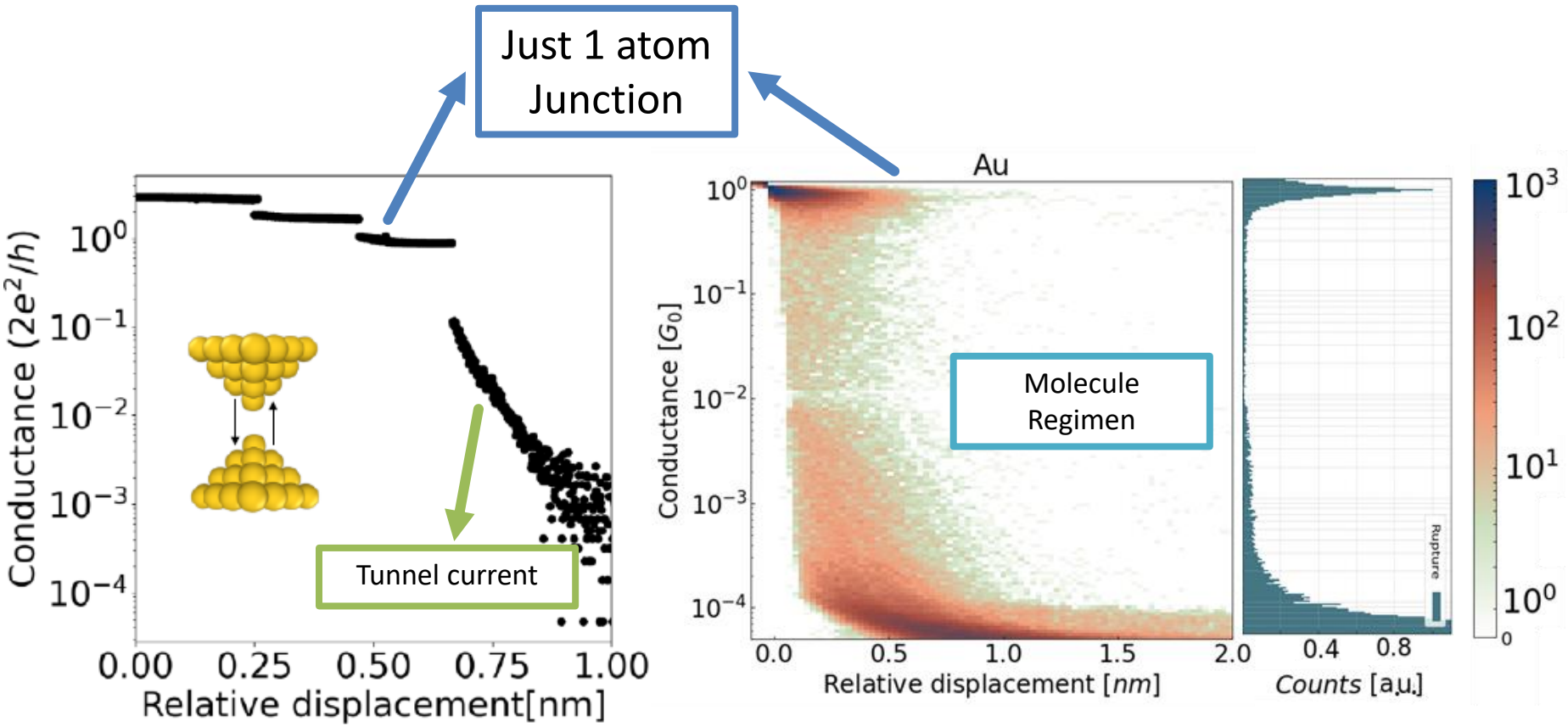


$$G = \frac{2e^2}{h}\sum_i Ti$$

Statistical analysis of electronic transport measurement by BJ approach

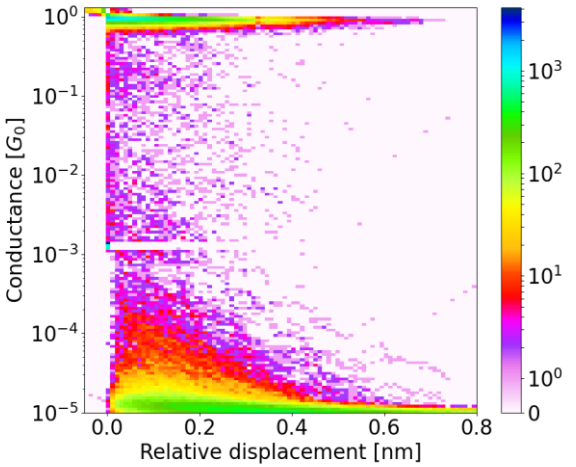
Gold as a benchmark

$$G = \frac{2e^2}{h}\sum_i Ti$$

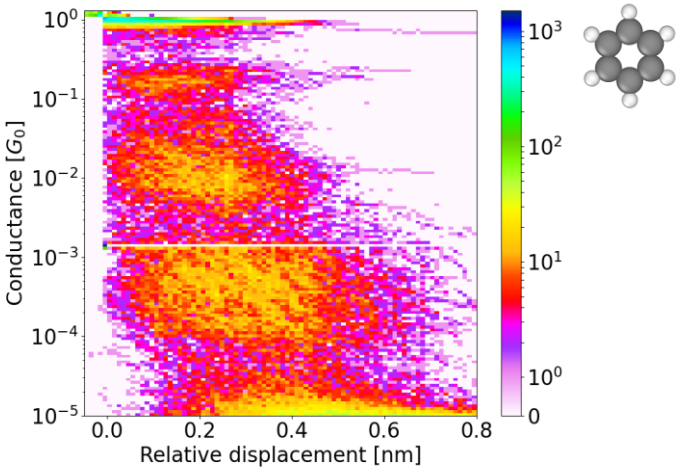


Electronic Transport Experiments

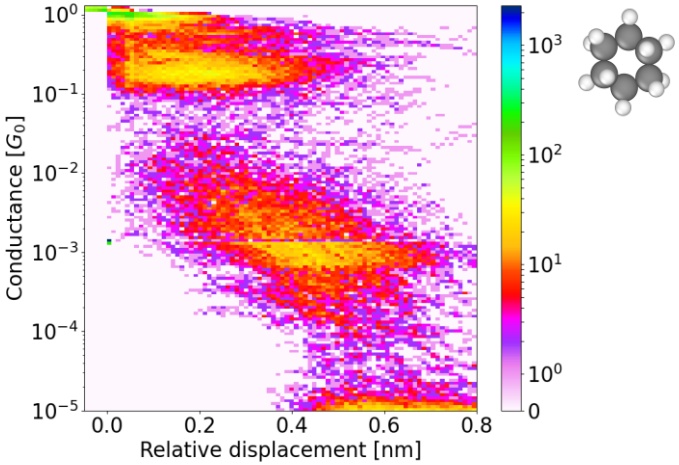
Gold



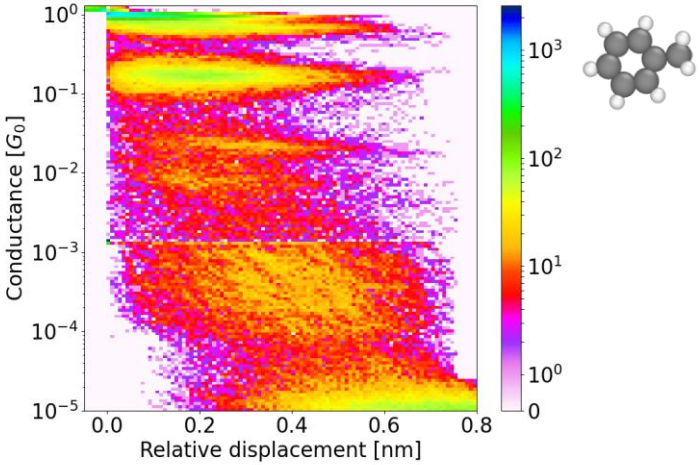
Benzene



Cyclohexane



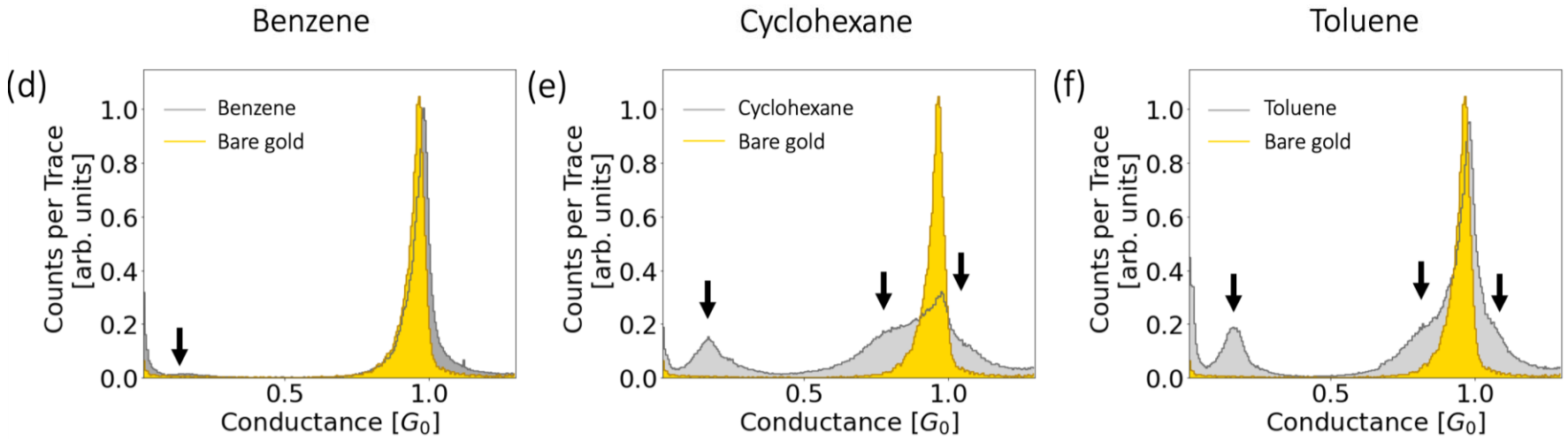
Toluene



T. de Ara *et al.* Materials Chemistry and Physics **291** (2022)

Electronic Transport Experiments

Linear Histogram

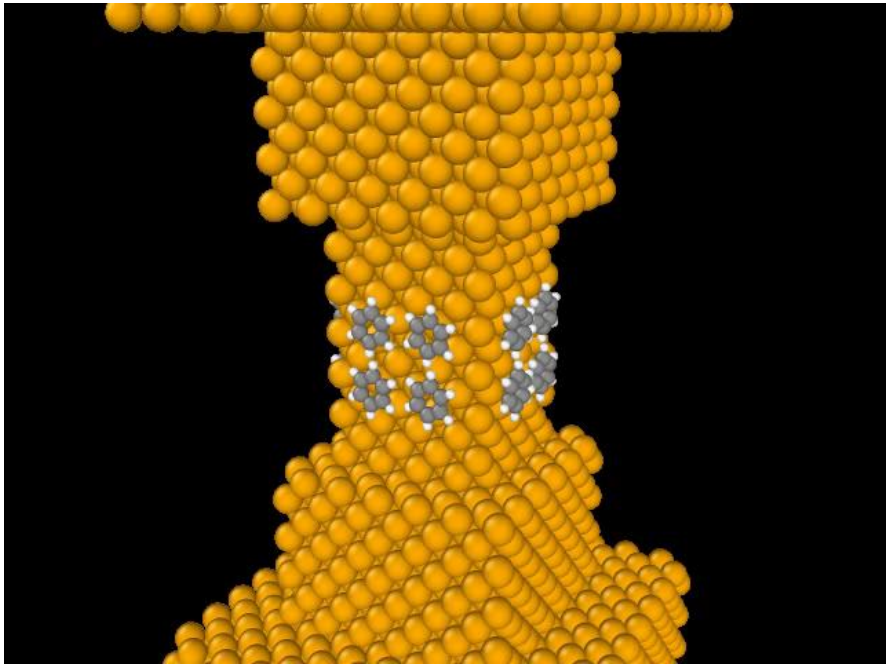


Broadened Peak at 1 G_0

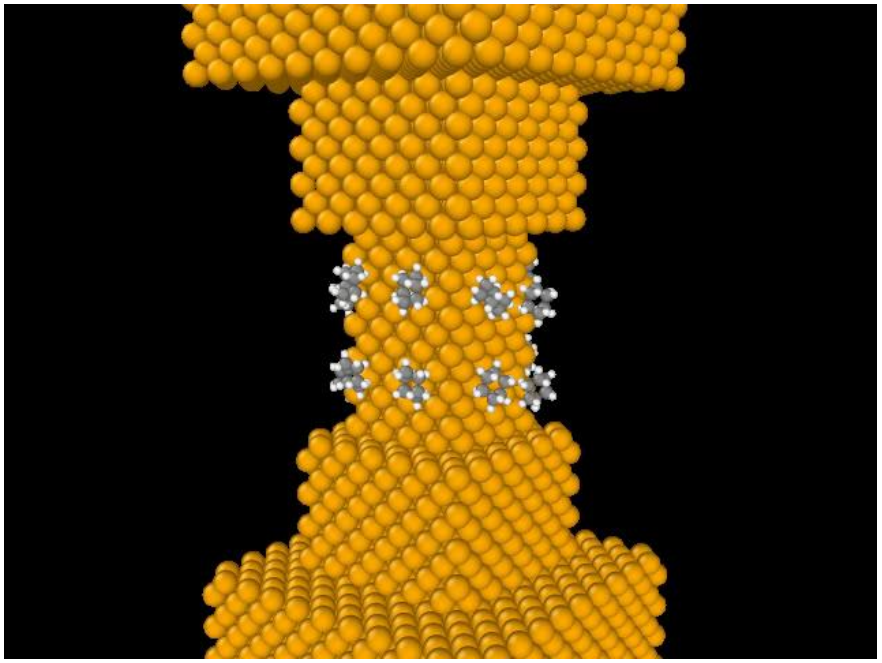
Molecular Dynamic Simulations

LAMMPS code with REAX FF potential at 300k

Benzene



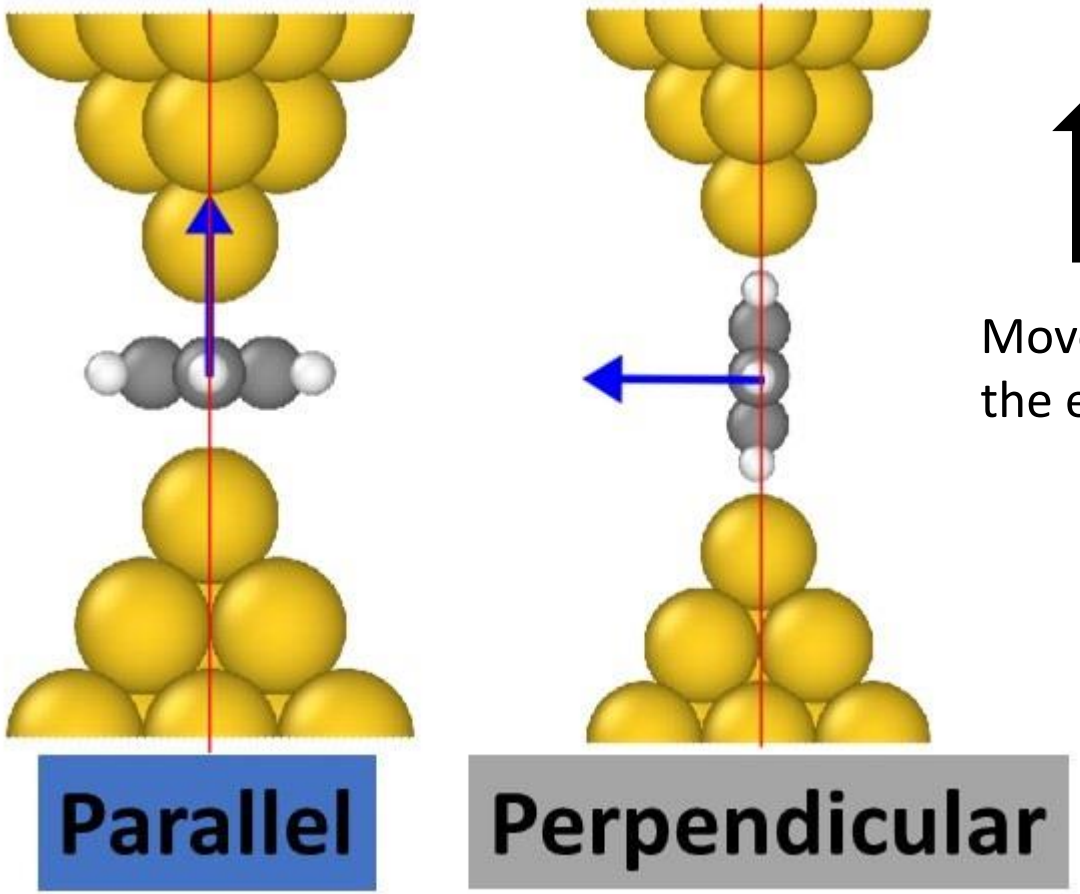
Cyclohexane



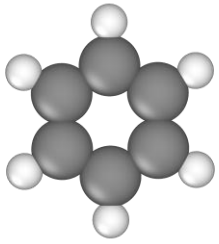
Electronic transport by DFT Calculations

We have computed the conductance using ANT.G code which based Gaussian.

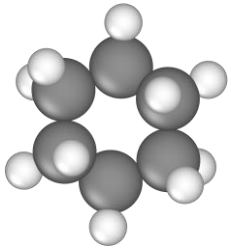
We have assumed these two structures



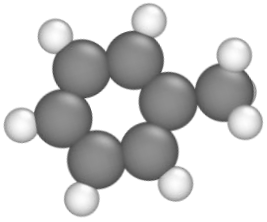
Break Junction exp + Mole. Dyna. + DFT



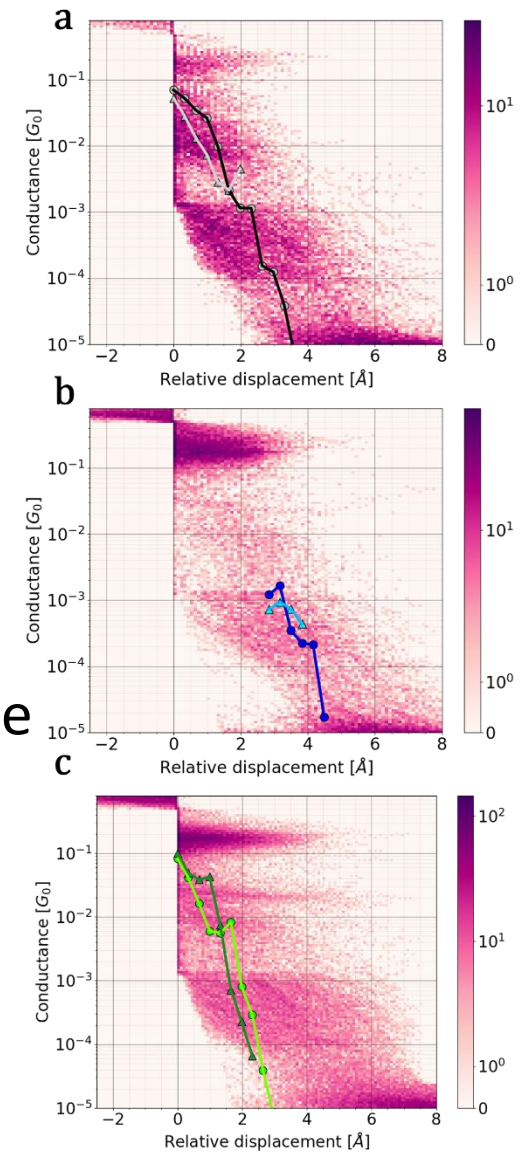
Benzene

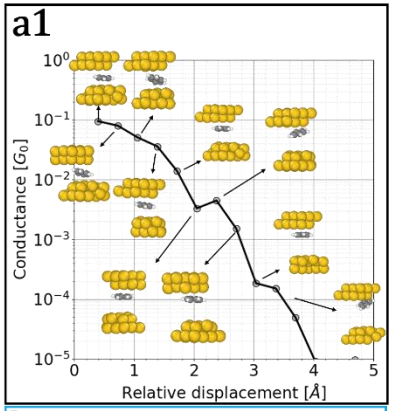


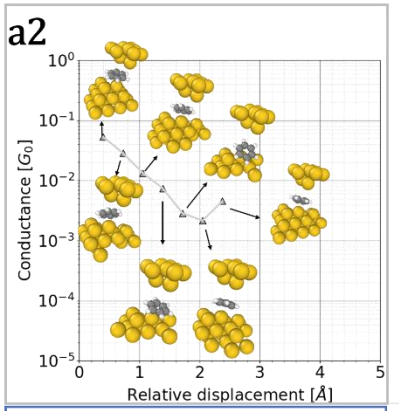
Cyclohexane

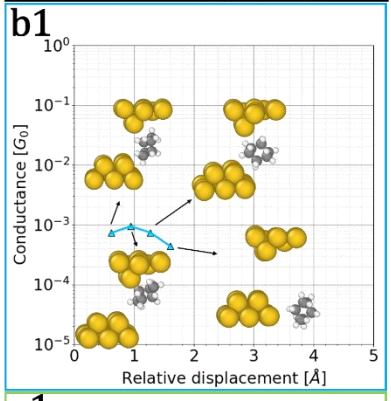


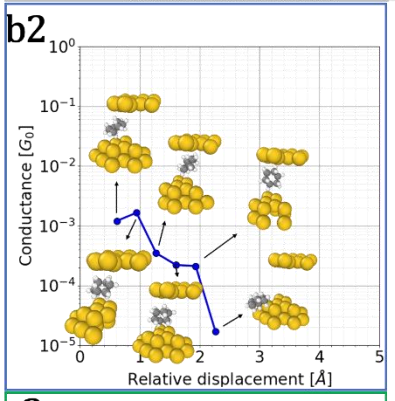
Toluene

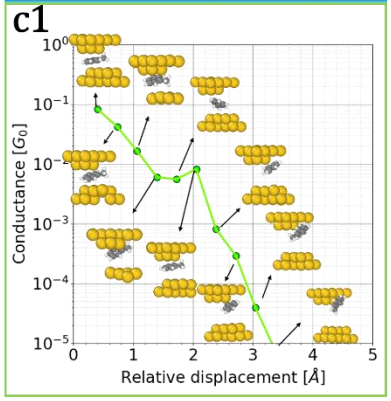


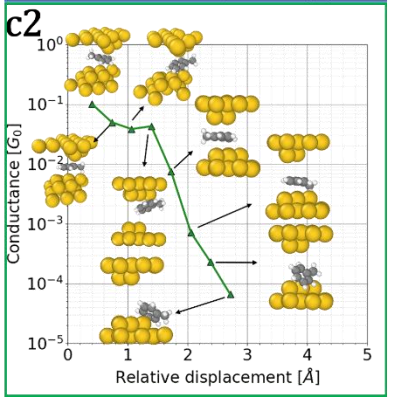




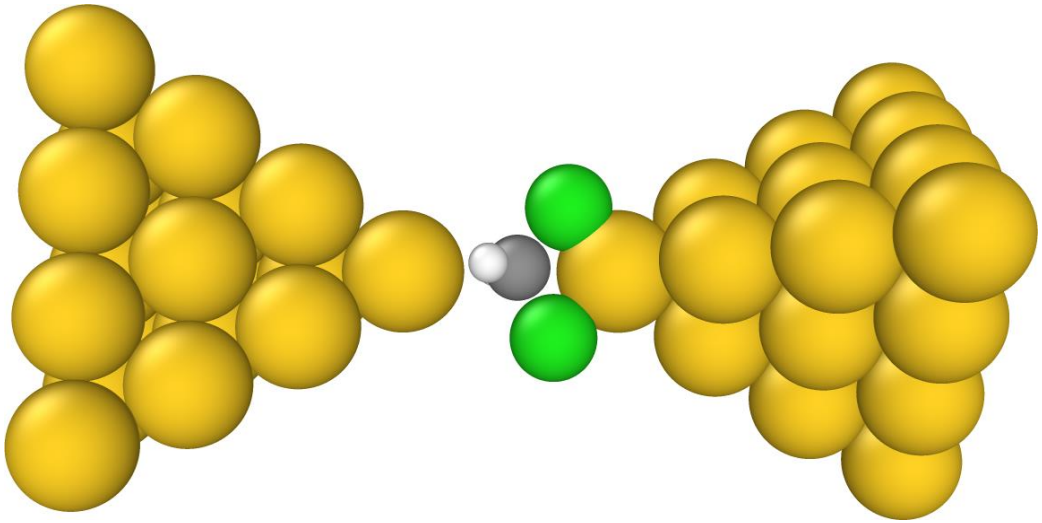


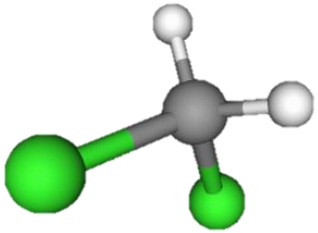






Halogenated Hydrocarbon Solvents Molecular Junctions



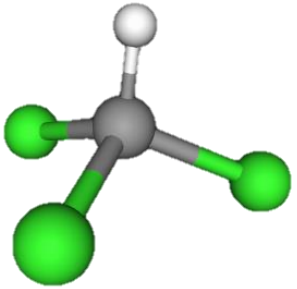


Dichloromethane

DCM

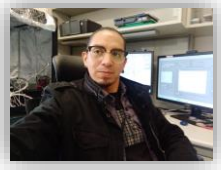
Patricia Ferrer

Juan Cuenca



Trichloromethane

TCM

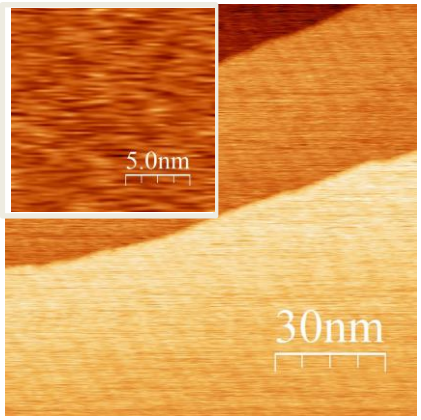


Jonathan Escorza

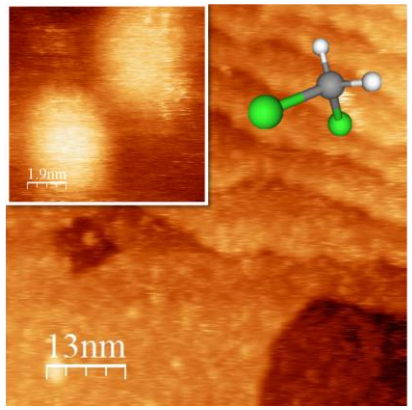
E. Guzmán

STM Images and STM-BJ in DCM and TCM

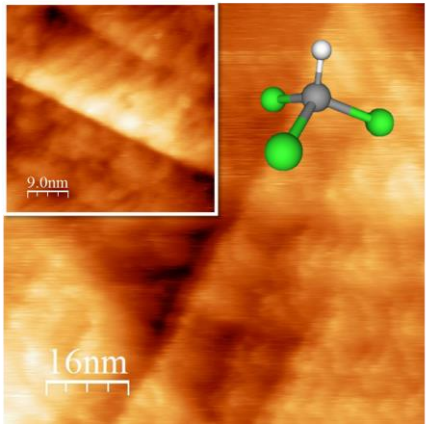
Au (111)

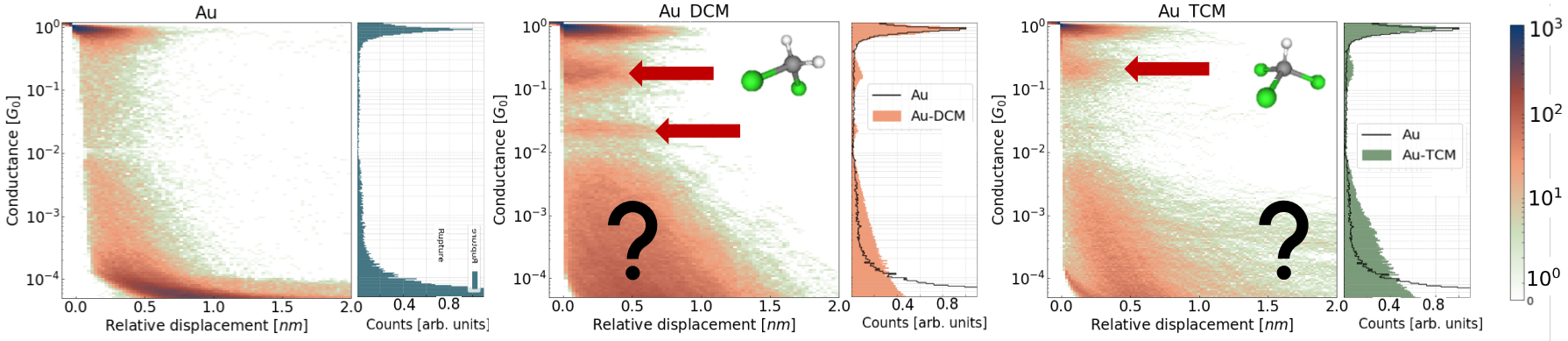


DCM



TCM

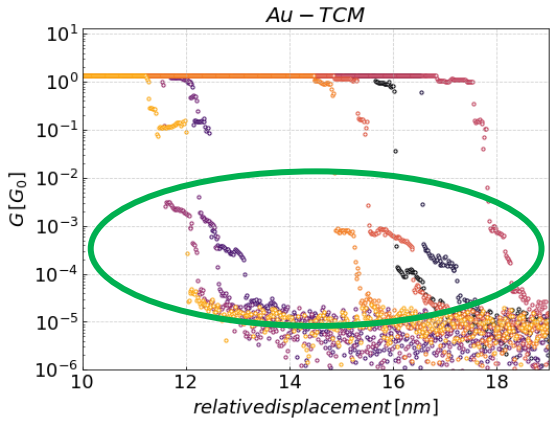


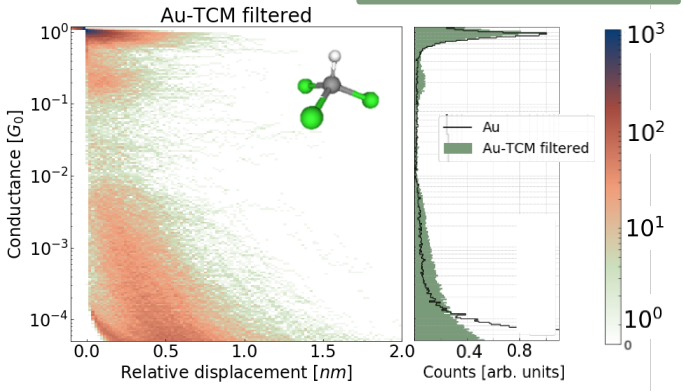


Au **DCM** **TCM**

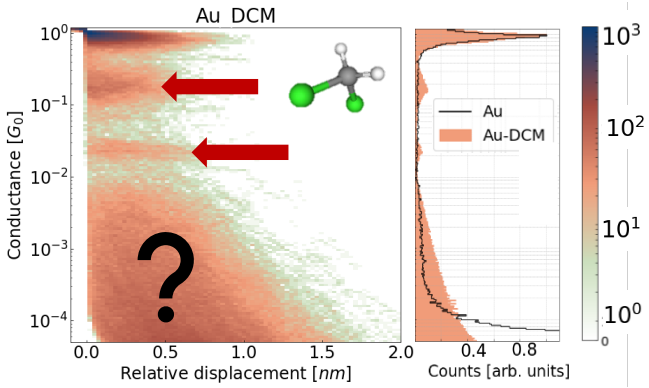
Histograms obtained by STM-BJ in DCM and TCM

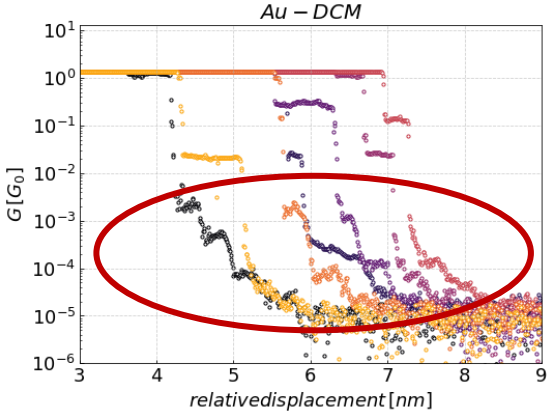
TCM Filtered

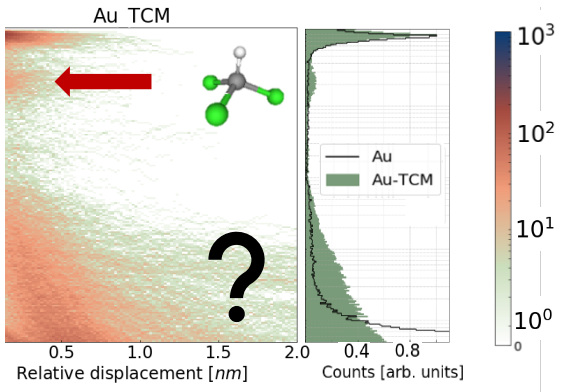




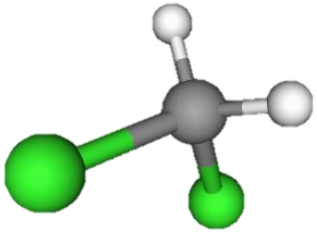
DCM



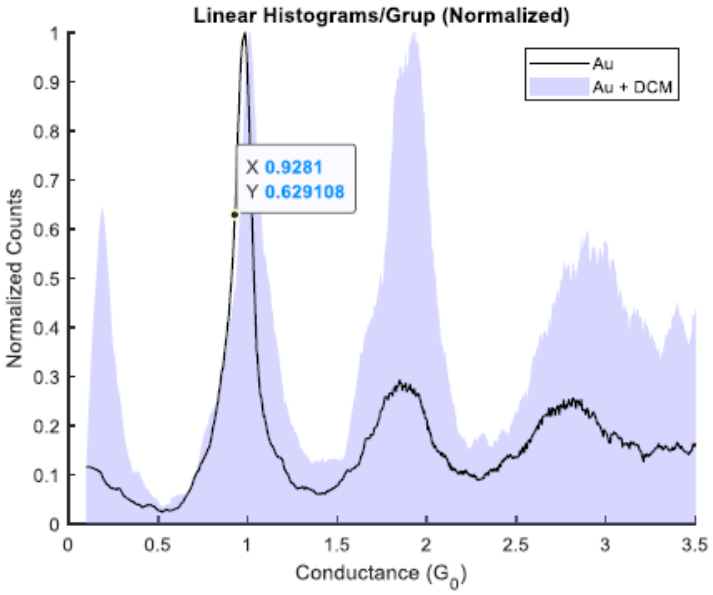


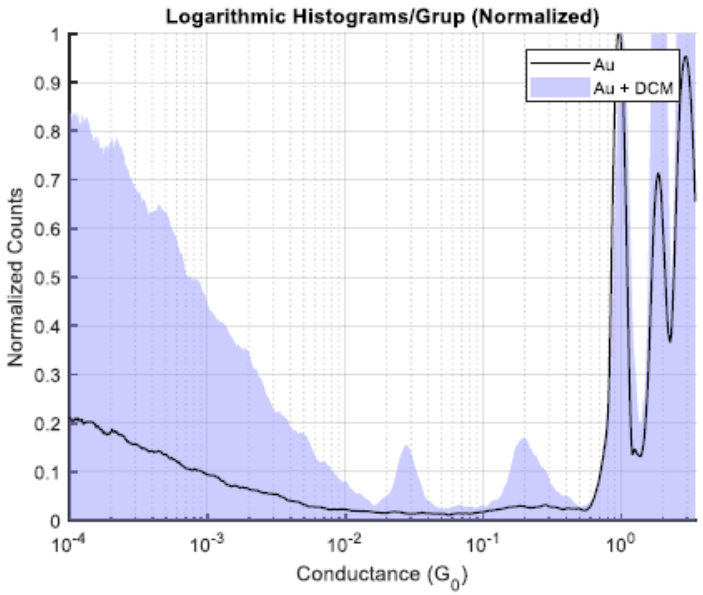


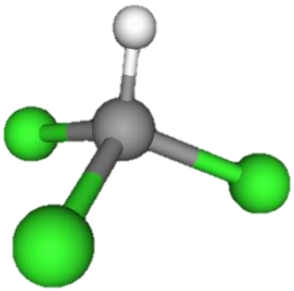
Histograms obtained by MCBJ in DCM and TCM



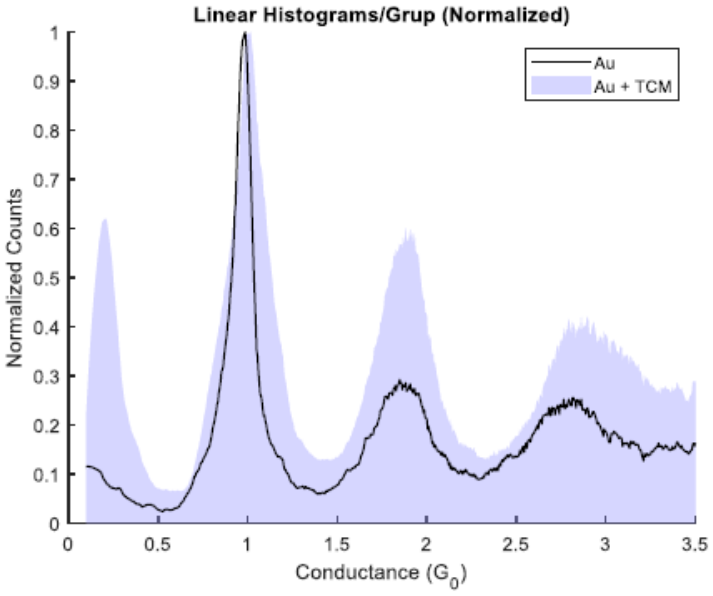
DCM

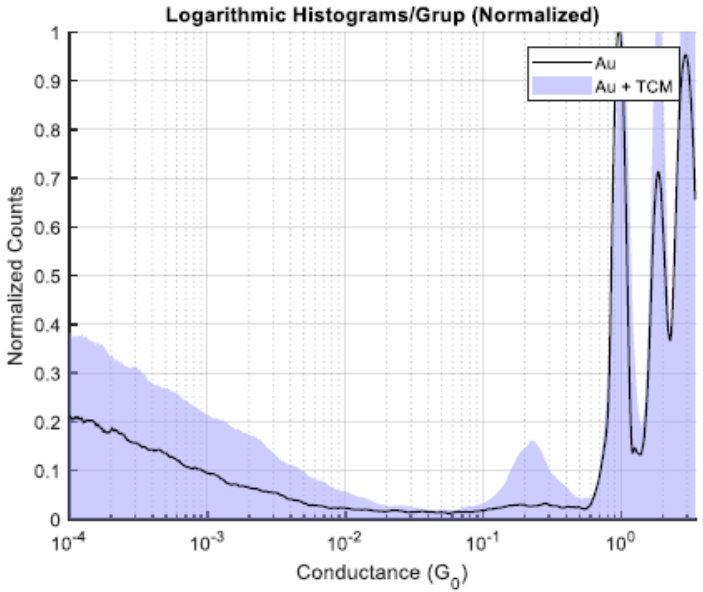




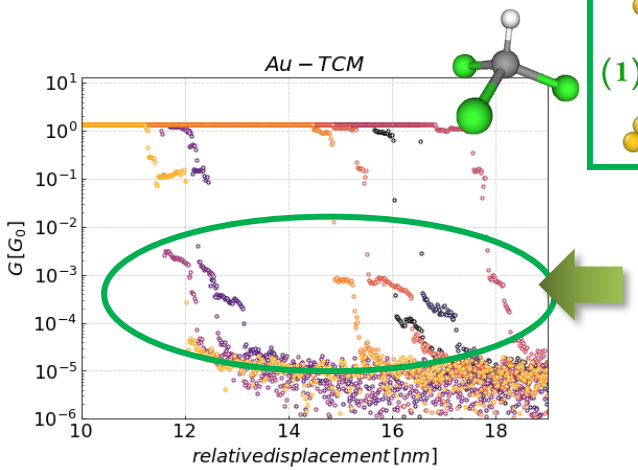


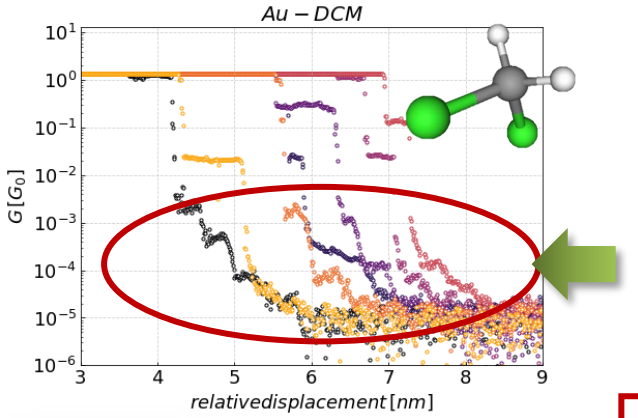
TCM

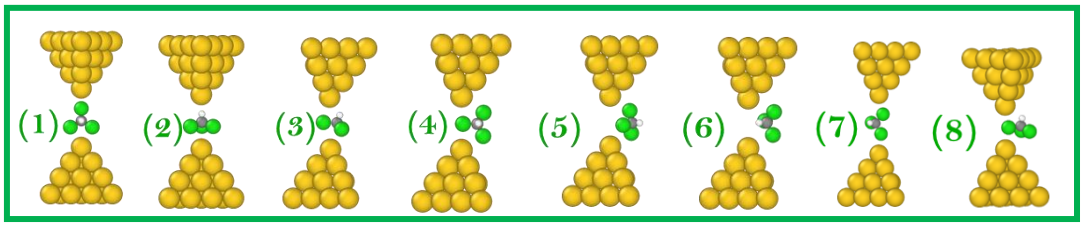


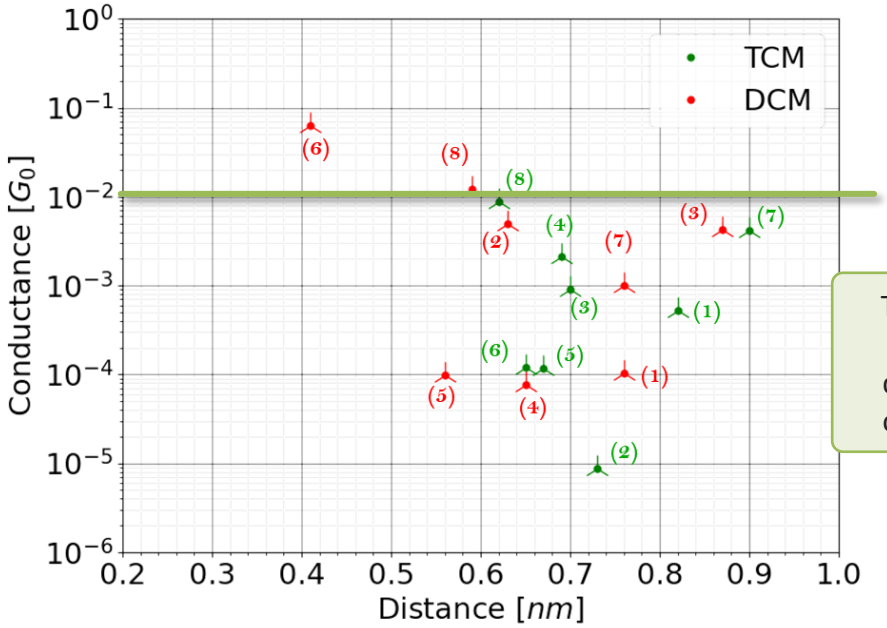


DCM AND TCM SOLVENTS

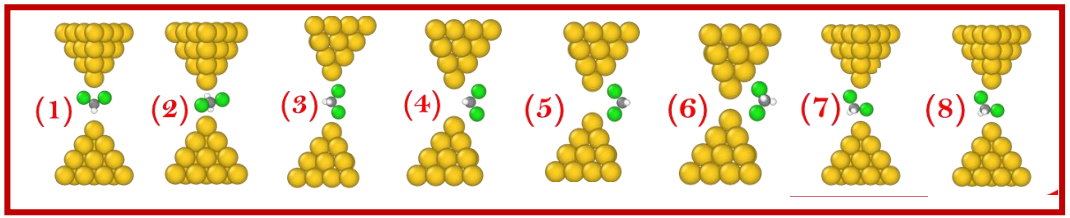


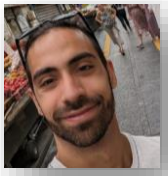






There is not a preferential configuration over the rest.



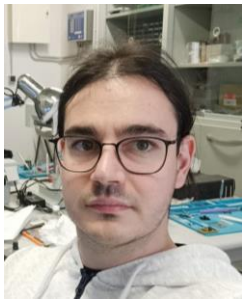


ANDRÉS MARTINEZ

DFT PRELIMINARY CALCULATIONS

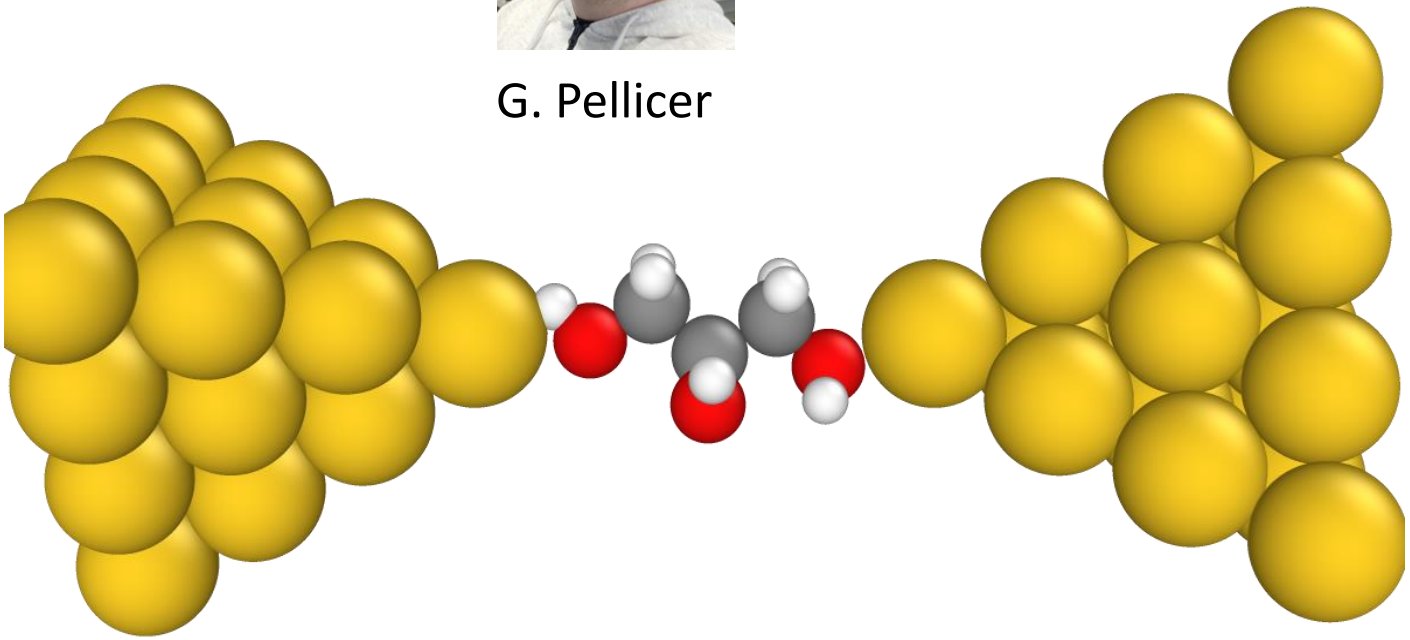
Molecular Junctions Glycerol

Quantum Transport in Single Molecule Junctions of Glycerol: Extending the conductance range Using Logarithmic Amplifiers



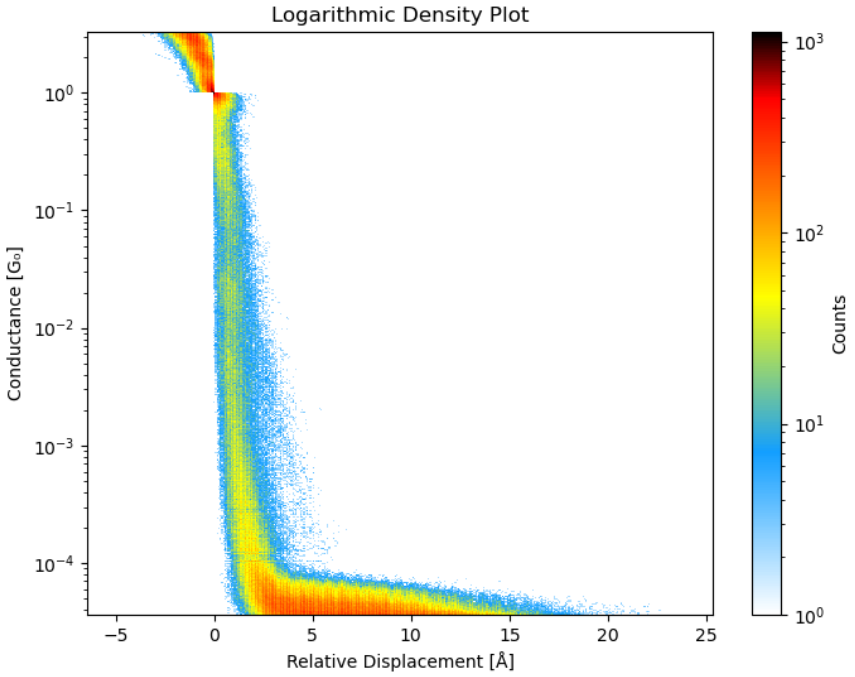
G. Pellicer

Thursday @ 19:30

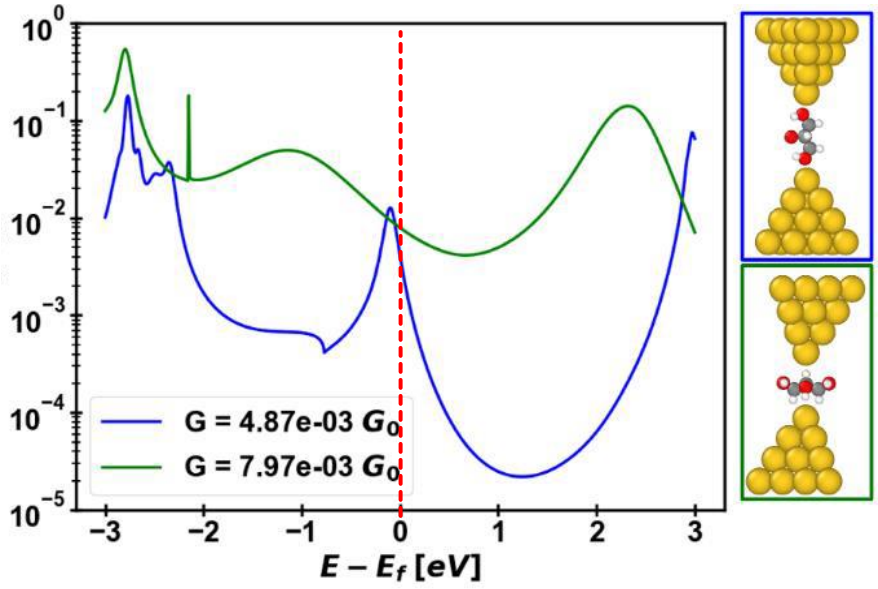


Molecular Junctions Glycerol

BJ - Experiments



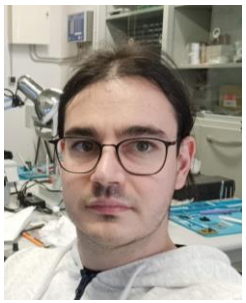
DFT-NEGF



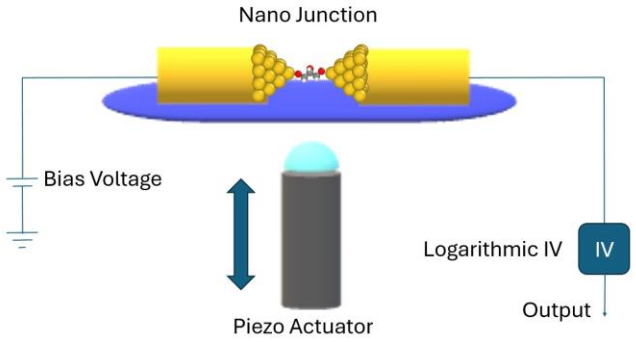
Identifying Clean and Contaminated Gold Atomic-sized Contacts at Room Conditions

- Can we use a clustering machine learning algorithm to identify clean and contaminated gold atomic-sized contacts at room conditions?

  Yes, we can. In our case we have used DBSCAN method

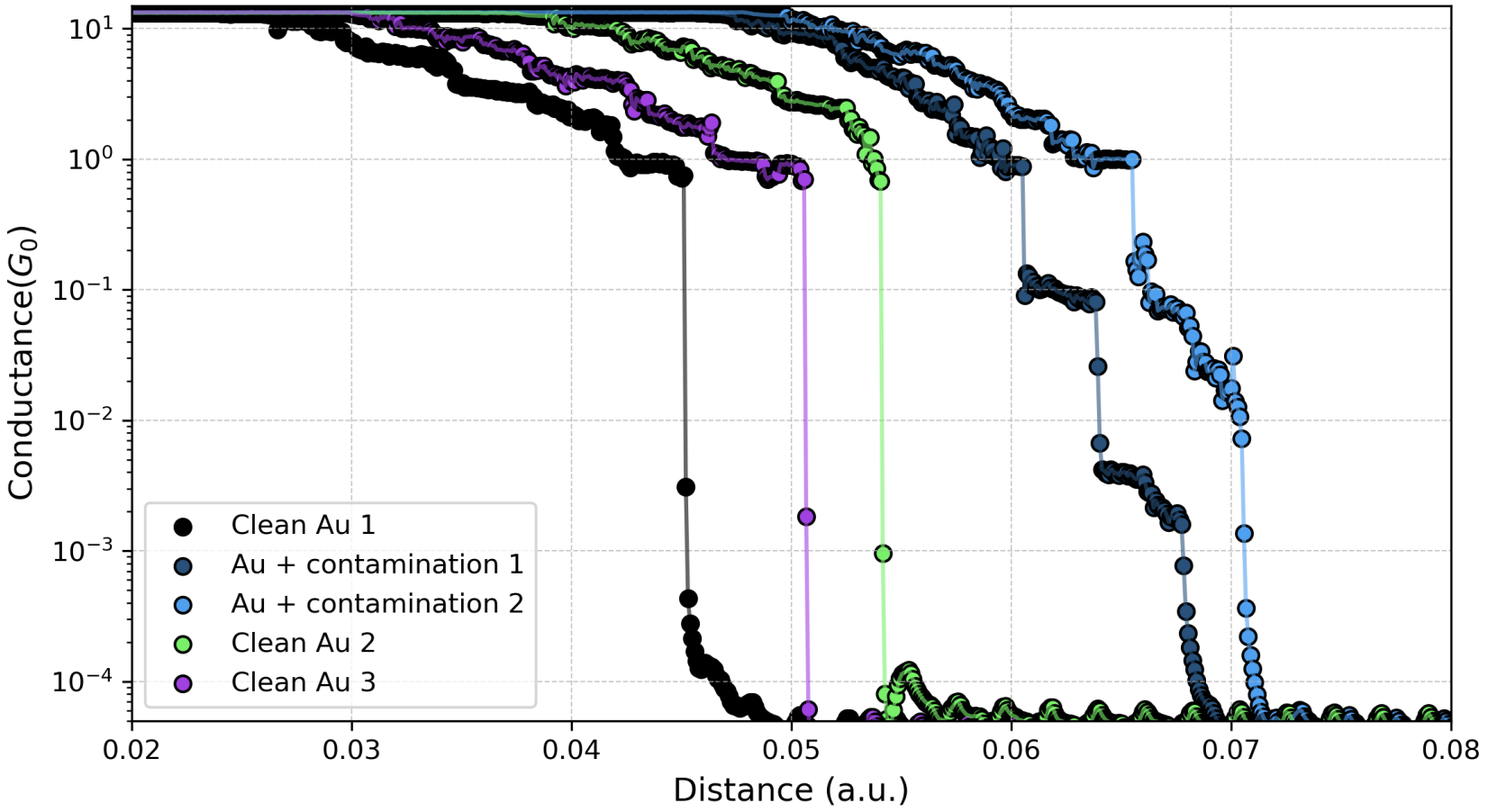


G. Pellicer



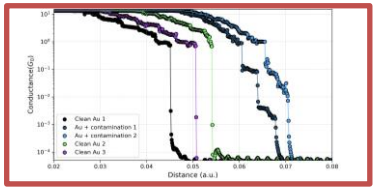
Identifying Clean and Contaminated Gold Atomic-sized Contacts at Room Conditions

We have obtained 8000 curves of this stile



Identifying Clean and Contaminated Gold Atomic-sized Contacts at Room Conditions

Input



Eps

Min samples

DBSCAN ALGORITHM

Output

Number of cluster (in our case 2)

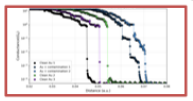
Number of outliers (minimum)

Min samples and Eps are numbers unknown in advance

D. Cabosart et al. APL, 114, **2019 (K-mean algorith)**

Identifying Clean and Contaminated Gold Atomic-sized Contacts at Room Conditions

Input



Eps

Min samples

DBSCAN ALGORITHM

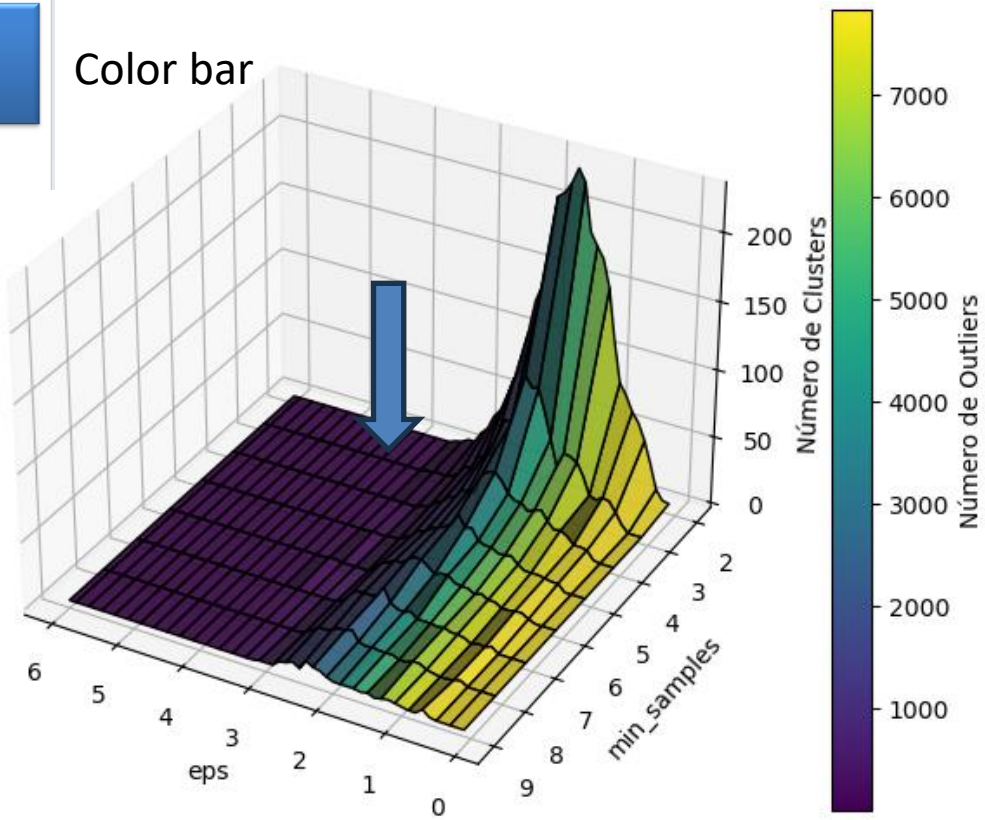
Output

Number of cluster (in our case 2)

Number of outliers (minimum)

Z-axis

Color bar

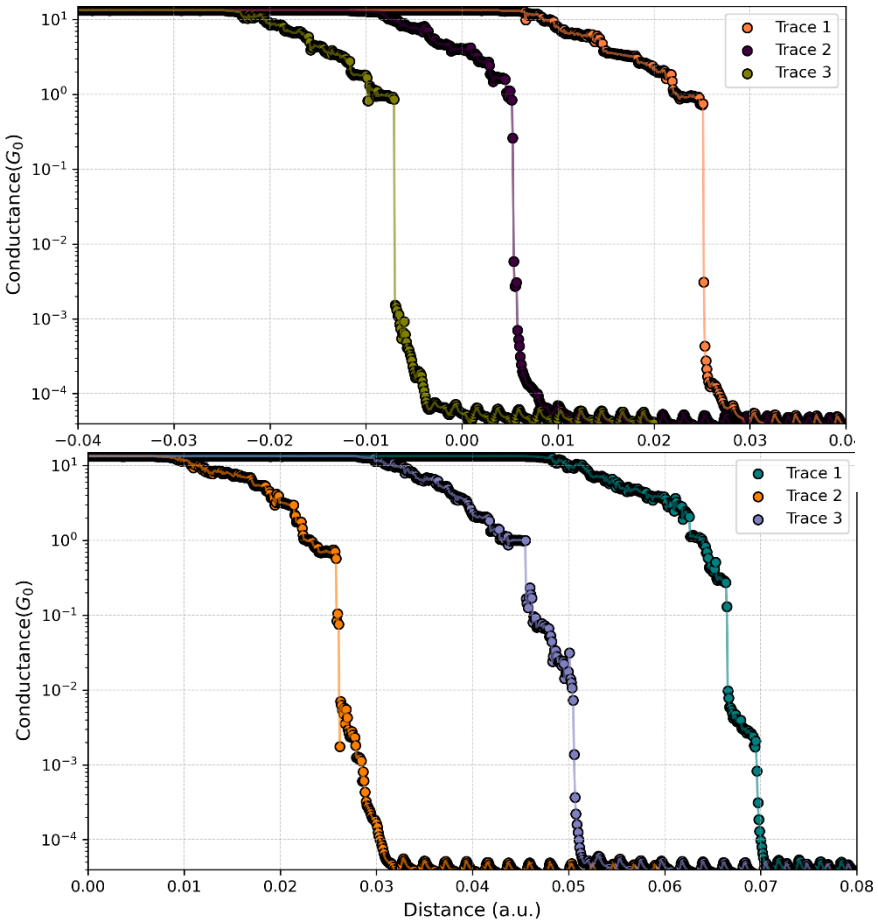


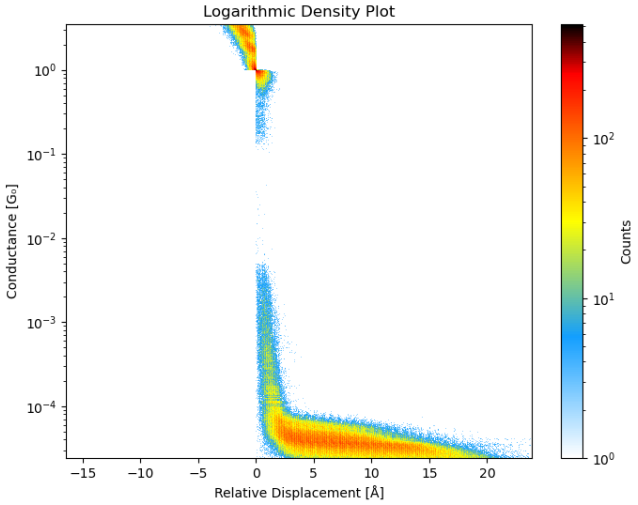
Identifying Clean and Contaminated Gold Atomic-sized Contacts at Room Conditions

DBSCAN Algorithm

Clean

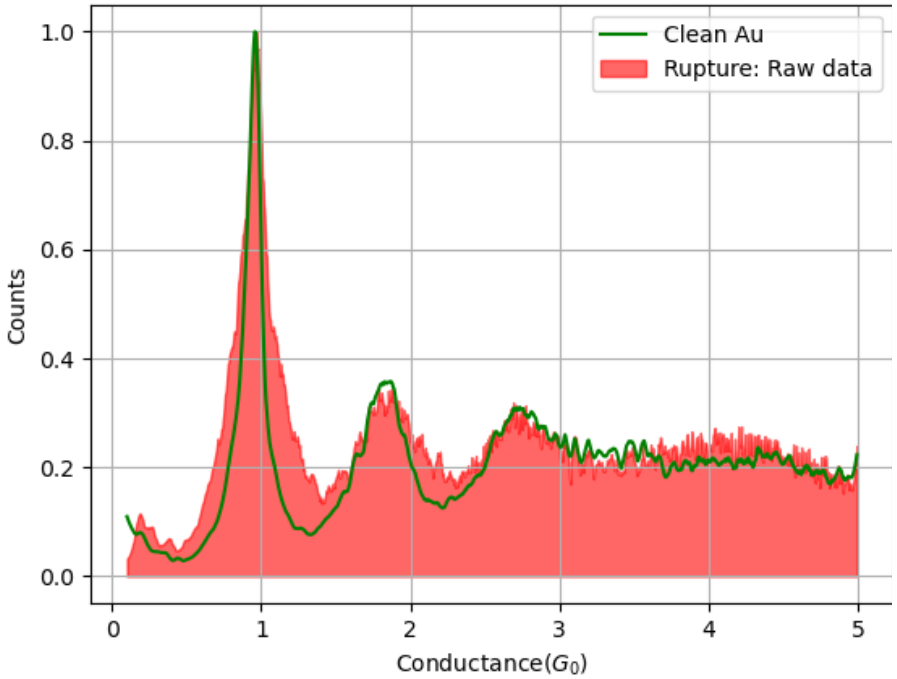
Environmental contaminations



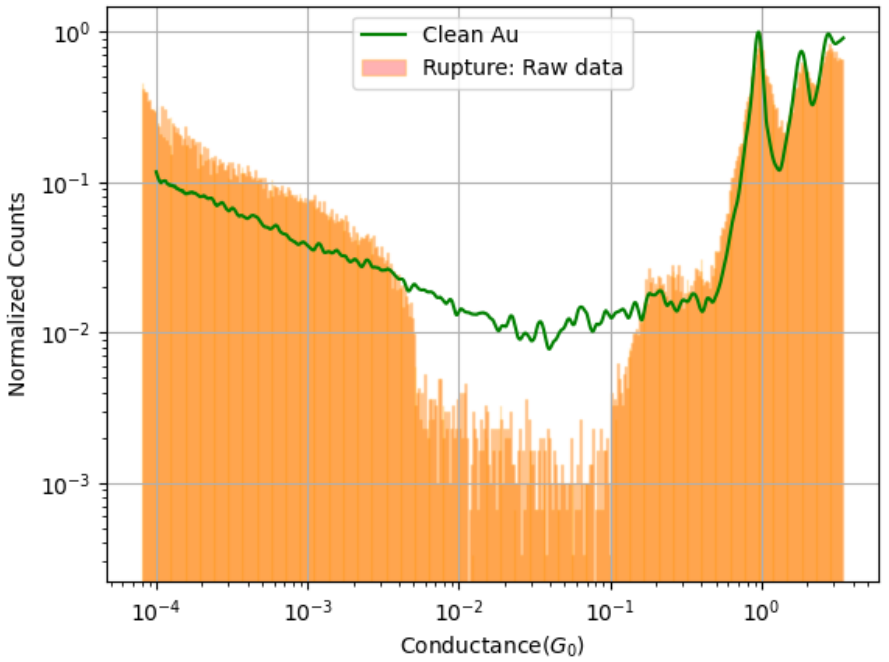


Identifying Clean and Contaminated Gold Atomic-sized Contacts at Room Conditions

Linear Histogram

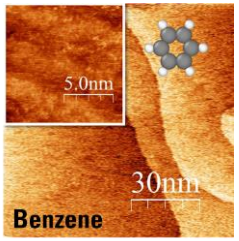


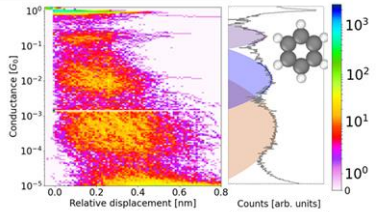
Logarithmic Histogram



Conclusions

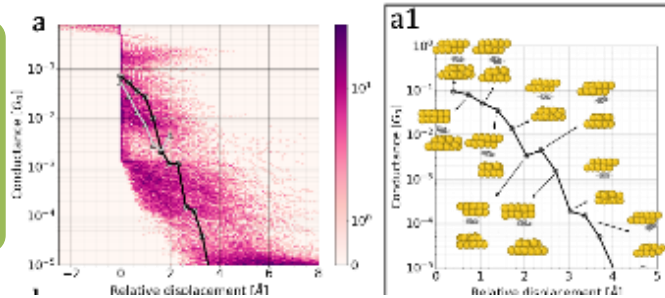
Organic solvents are not fully evaporated

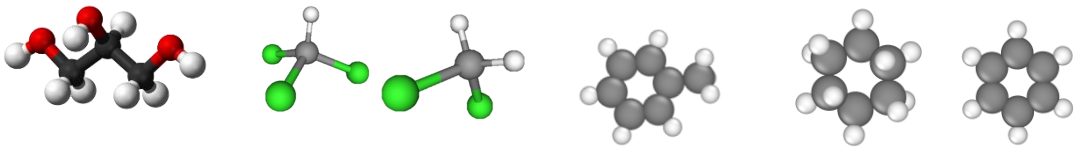


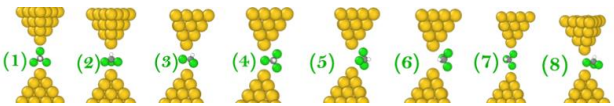


Solvents play a role in molecular electronics

We have characterized the conductance “fingerprint” of the typical solvents with different polarities

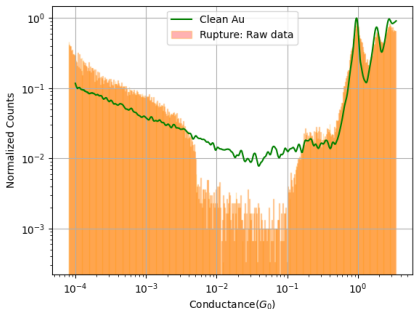






We can relate the trace of conductance with molecular orientation in the electrodes

DBSCAN Clustering help us to classify pure metallic traces form contaminated



Summary in one sentence

Sabatier’s Principle.

It states that the interactions between the catalyst and the reactants should be "just right"; that is, neither too strong nor too weak

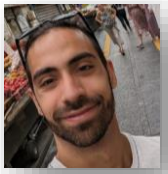
Sabater’s Principle.

Electronic transport is key to understanding atomic and molecular structures.

Researchers involved

Dr. Tamara de Ara

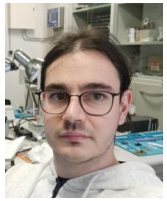
Patricia Ferrer



Andrés Martinez

Juan Cuenca

E. Guzmán



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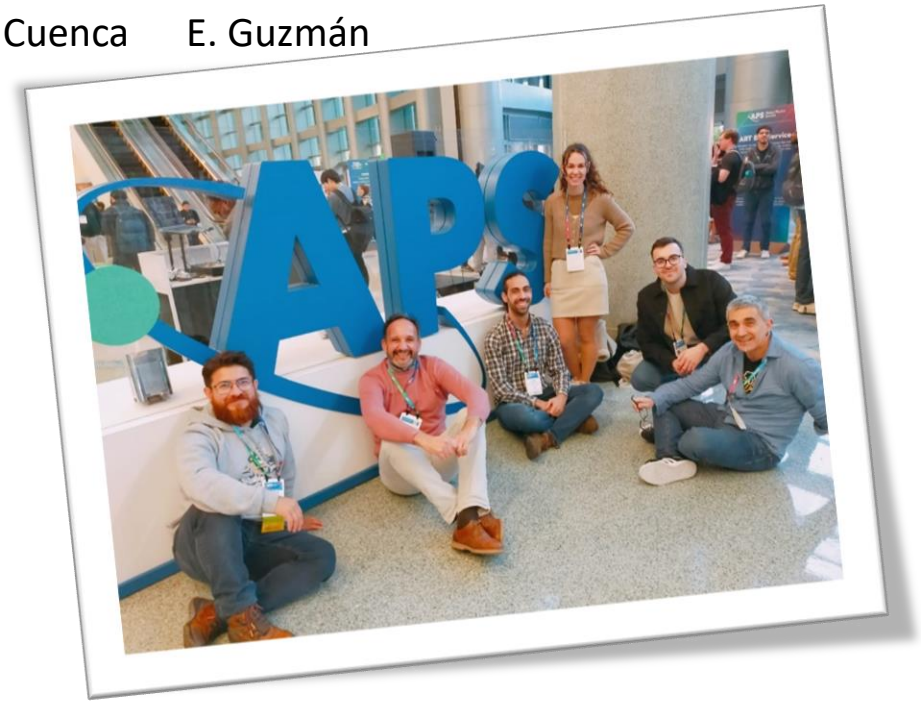
Jonathan Escorza

M. Navarro

Dr. Carlos Sabater

Prof. Carlos Untiedt



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Questions?