

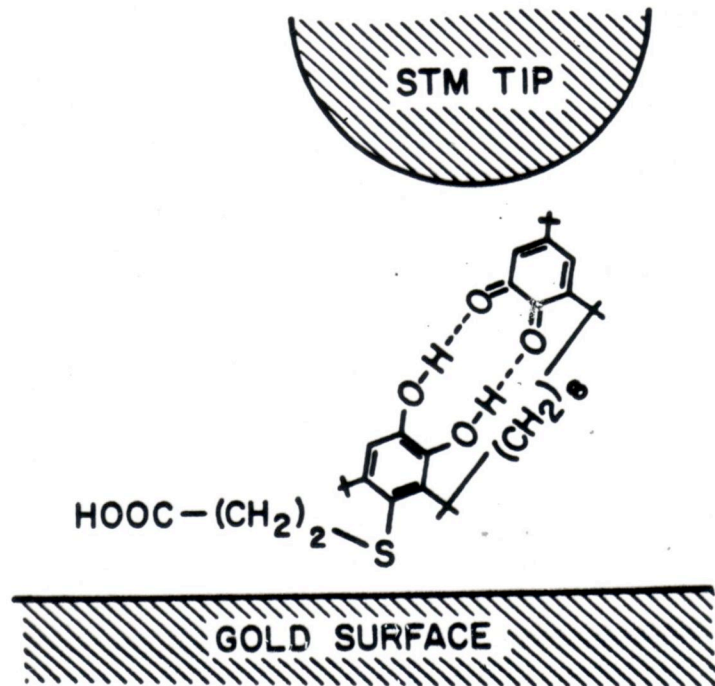


Calculating a tunneling current  
through a molecule  
&  
uni-molecular machines

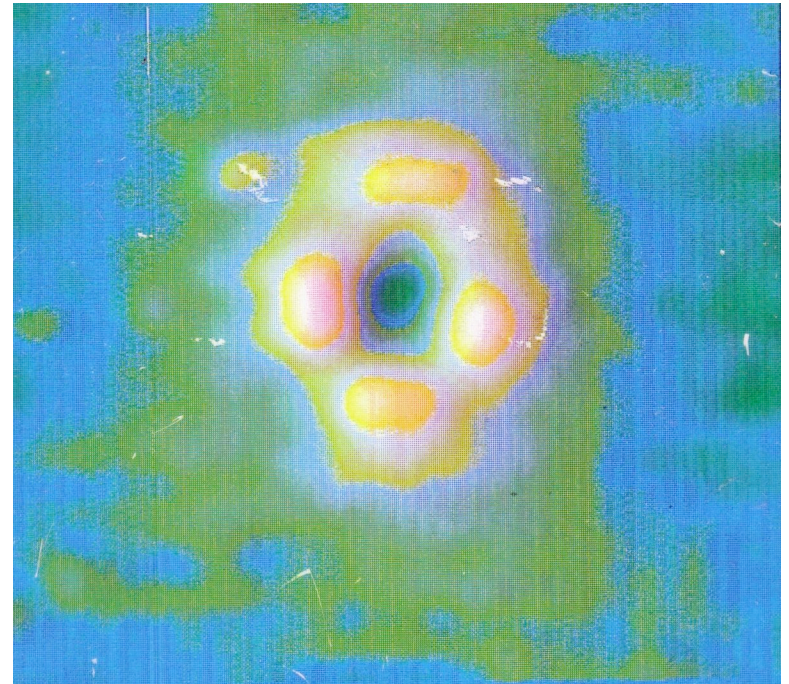
C. Joachim  
GNS CEMES/CNRS  
Toulouse, France

2005 Feynman Prize Lecture

## Early day problems

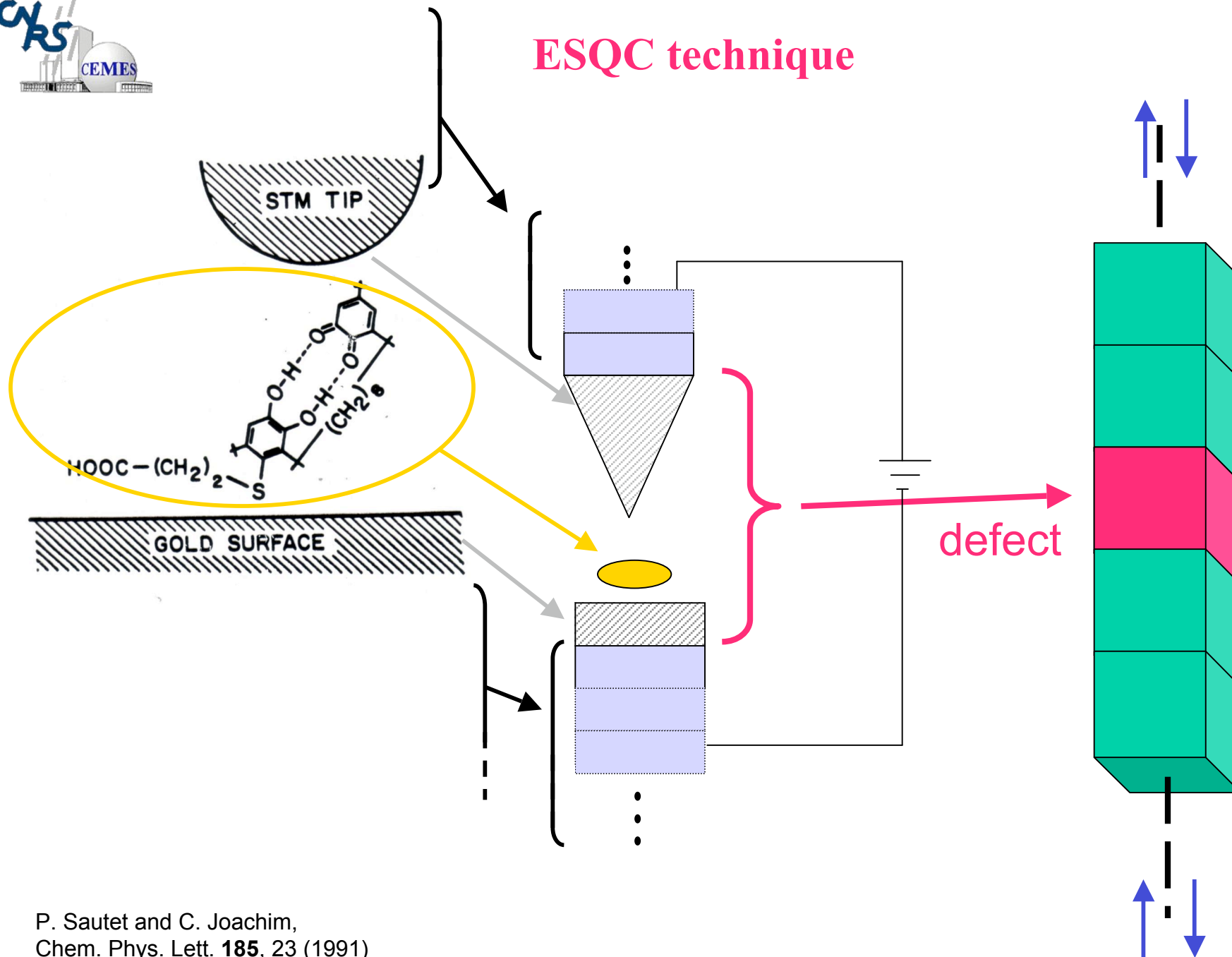


**1986-1988 :**  
**Switching with the STM**  
**with A. Aviram & M. Pomerantz**

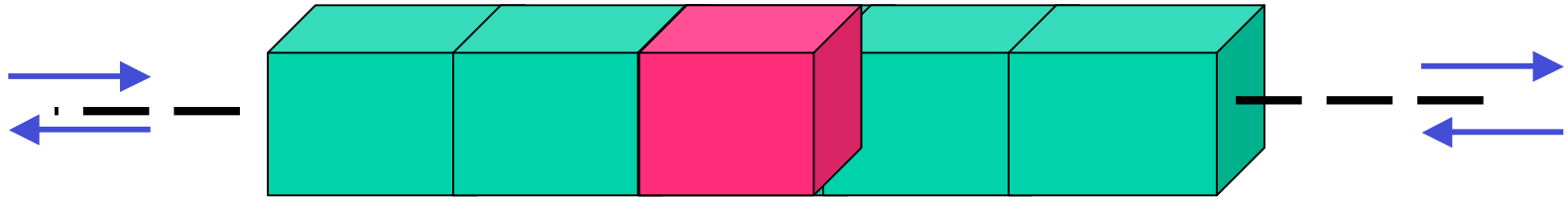


**1986-1987**  
**STM imaging of a Cu-Pc**  
**J.K. Gimzewski**

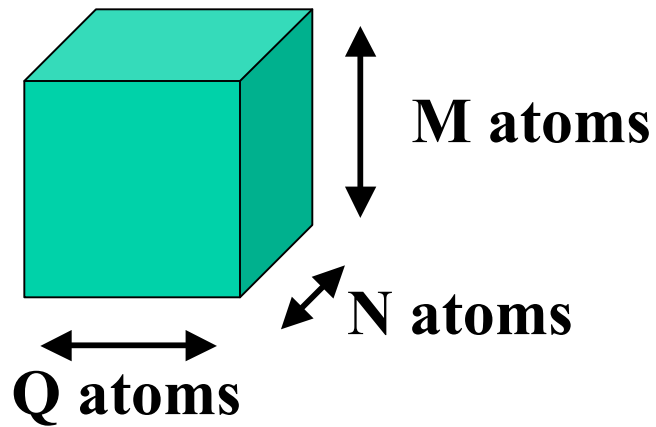
# ESQC technique



# Scattering matrix calculations



Electronic  
Hamiltonian

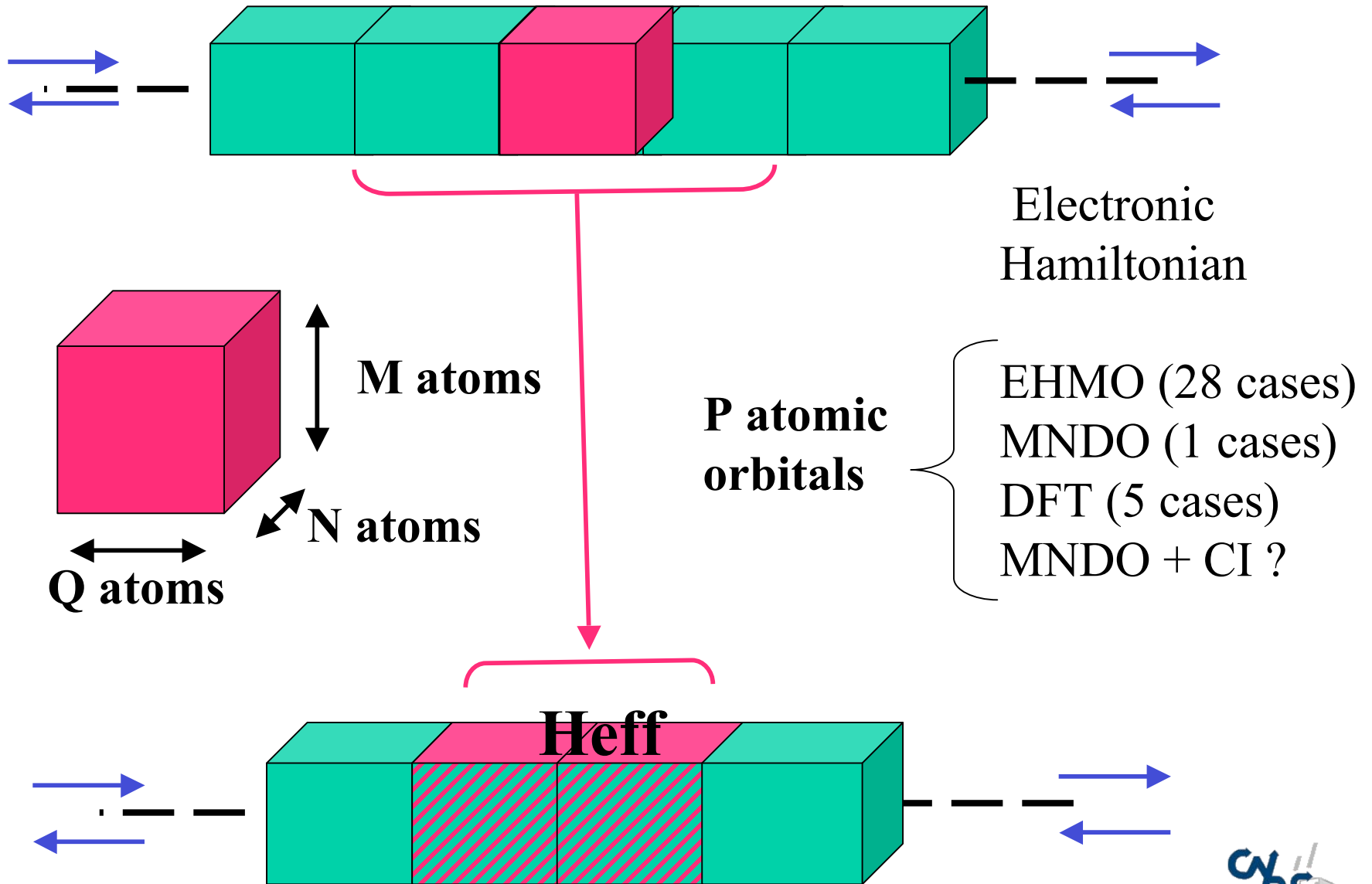


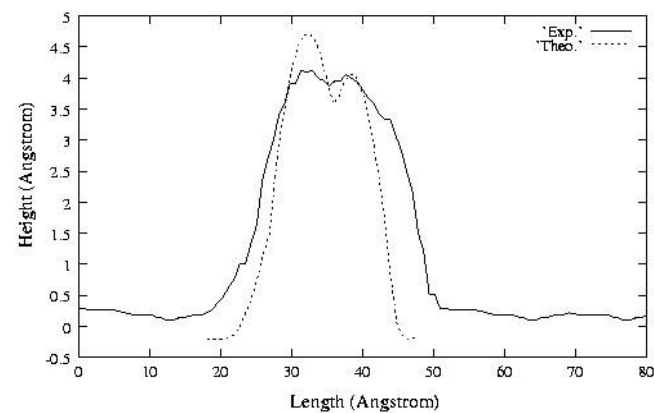
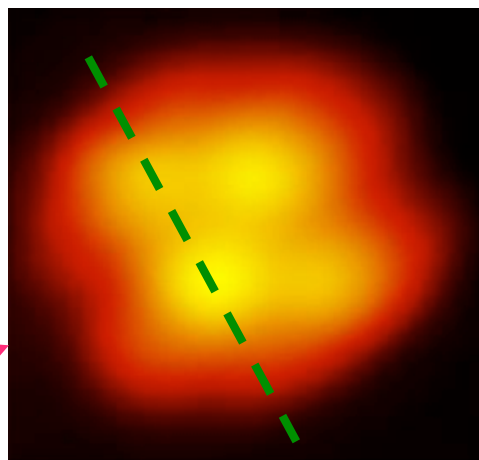
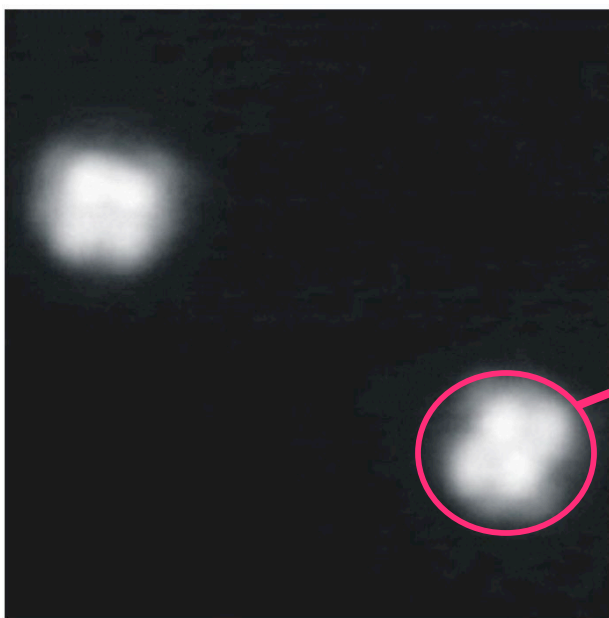
**P atomic  
orbitals**

EHMO  
MNDO  
DFT ?  
MNDO + CI ?

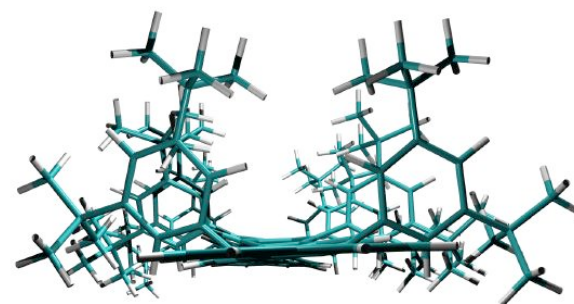
Metal or semi-conductor unit cell

# Scattering matrix calculations

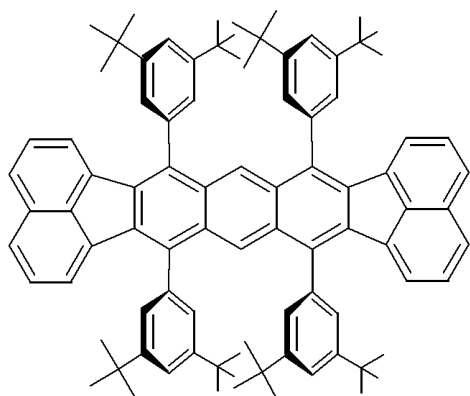




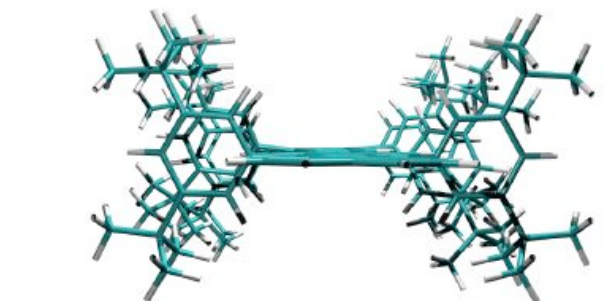
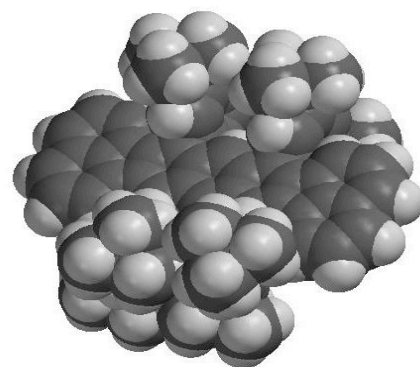
*Conformation refinement  
ESQC + MM2*



**Cu(100)**



M2

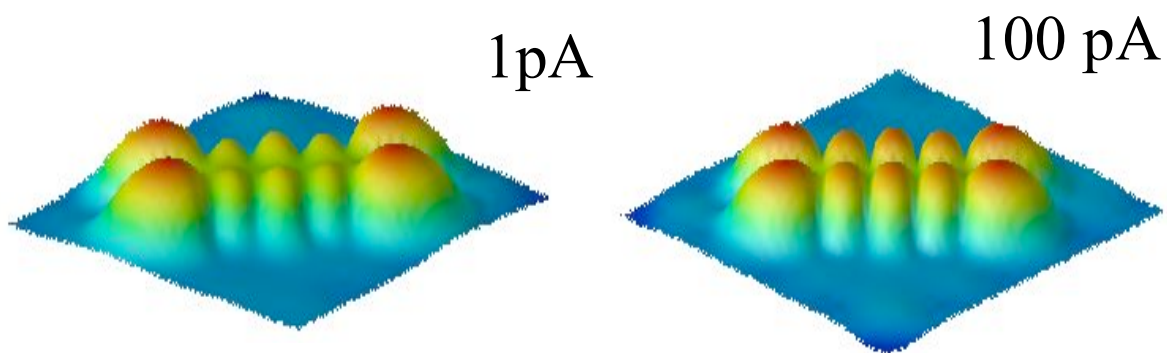
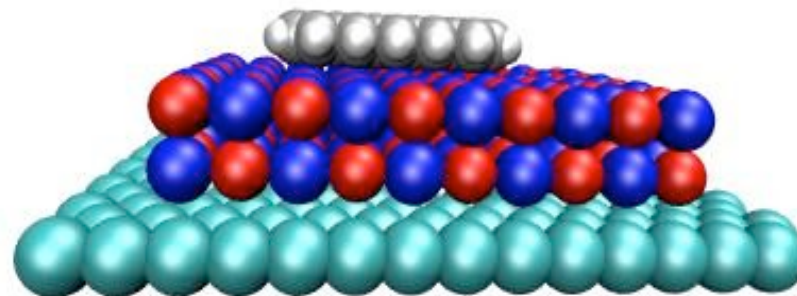


**Cu(100)**

# Pentacene on NaCl/Cu(111)



LT-UHV STM



ESQC calculated images

J. Repp and co-workers, Phys. Rev. Lett, 94, 026803 (2005)

ESQC

+ Molecular mechanics

STM manipulation signal

Design of uni-molecular machine

in Hybrid molecular electronics

Molecular wires, long range tunnel

Electronic contact resistance

Single molecule transistor

N-ESQC for Mono-molecular electronics

Intramolecular classical circuit

Quantum phase circuit

Quantum Hamiltonian logic gate

N-ESQC + Inelastic tunnel effect

Tunnel electron detector

Uni-molecular transducers





ESQC

+ **Molecular mechanics**

**STM manipulation signal**

**Design of uni-molecular machine**

in Hybrid molecular electronics

Molecular wires, long range tunnel

Electronic contact resistance

Single molecule transistor

N-ESQC for Mono-molecular electronics

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Quantum Hamiltonian logic gate

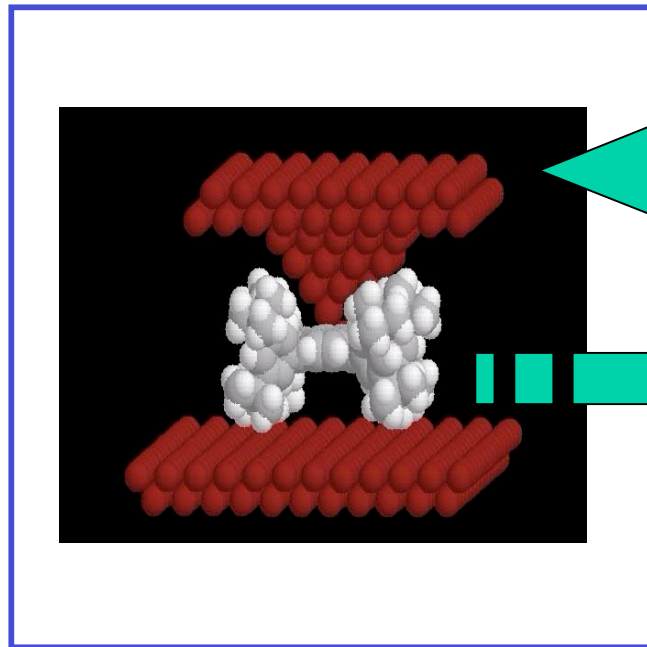
N-ESQC + Inelastic tunnel effect

Tunnel electron detector



# Calculation of STM Manipulation signal

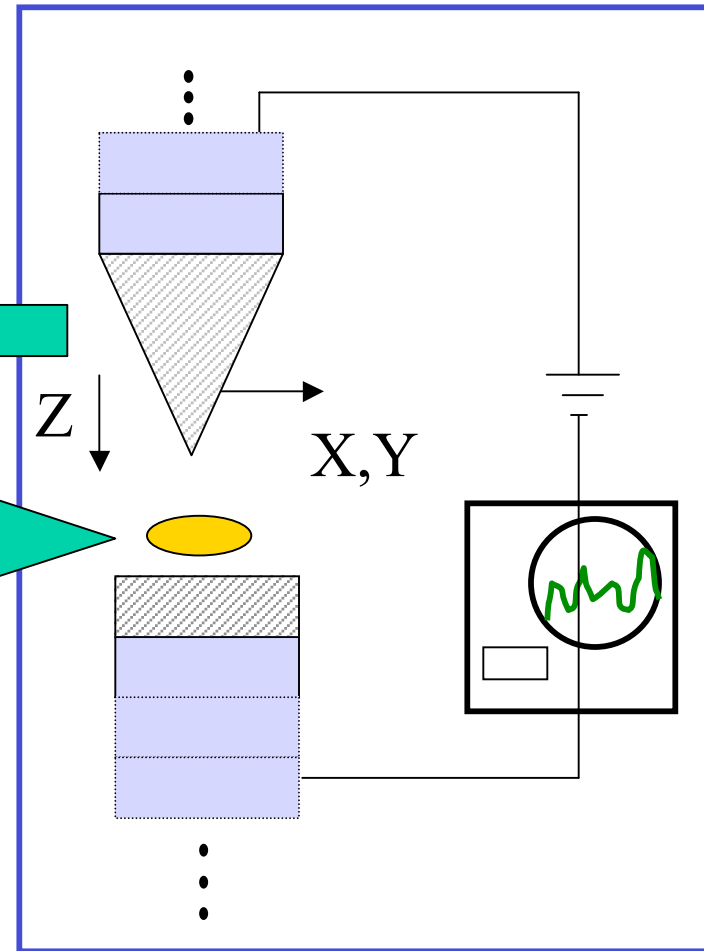
ASED +  
Molecular Mechanics MMX



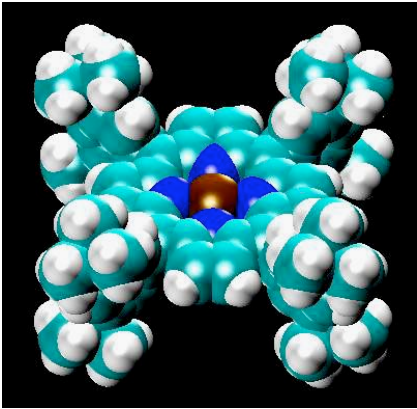
$X, Y, Z$

$(x_i, y_i, z_i)$

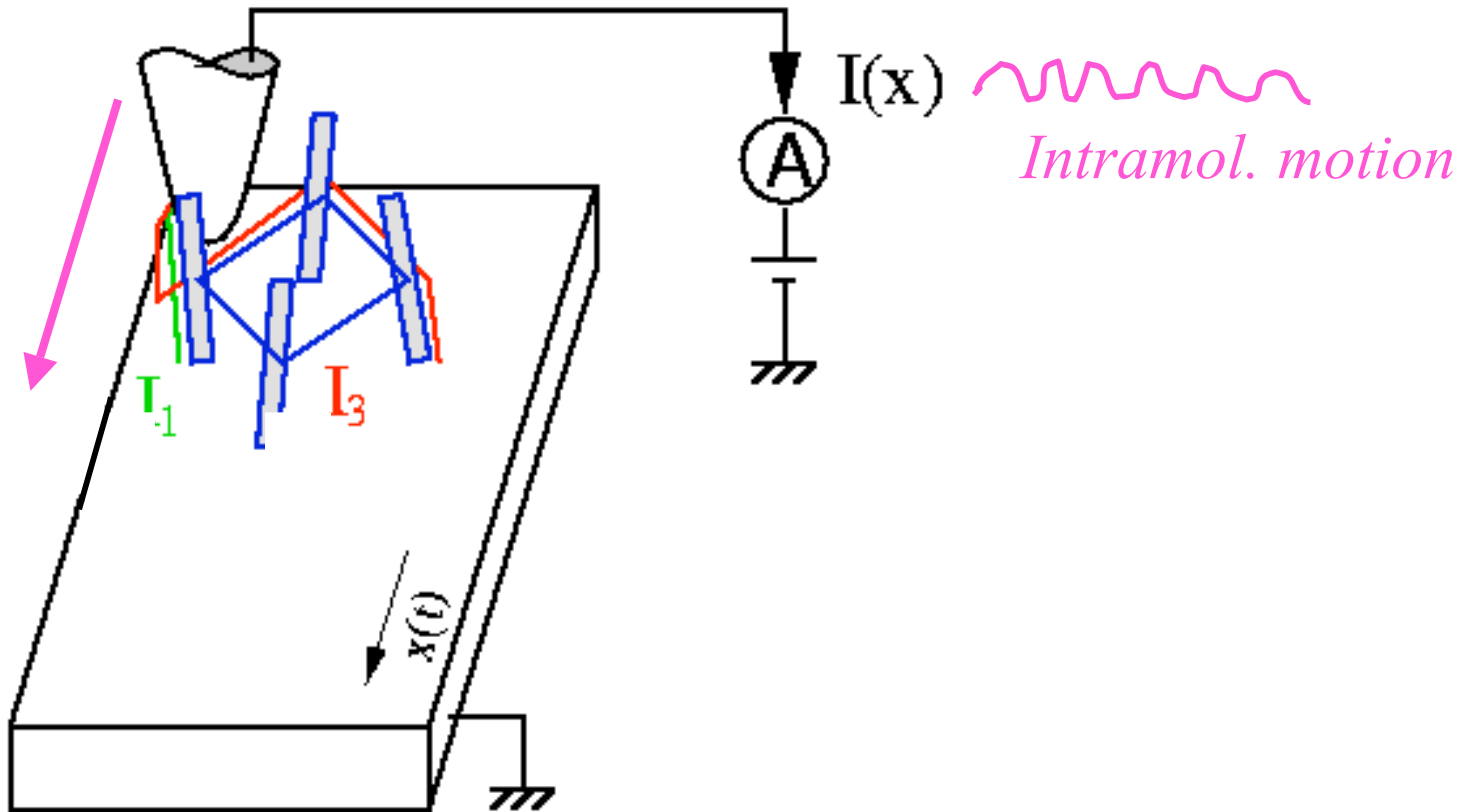
ESQC



T. Jung, J.K. Gimzewski and C. Joachim, Science (1996)



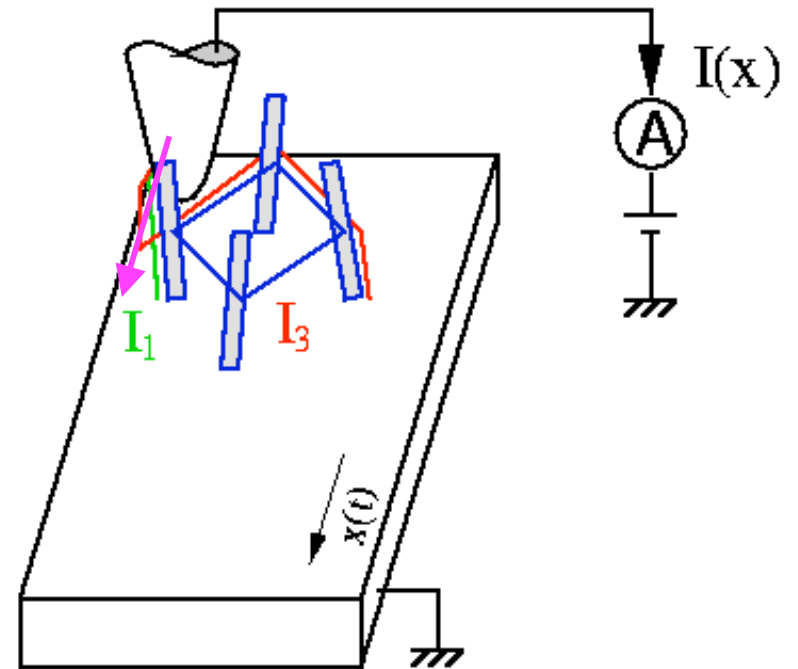
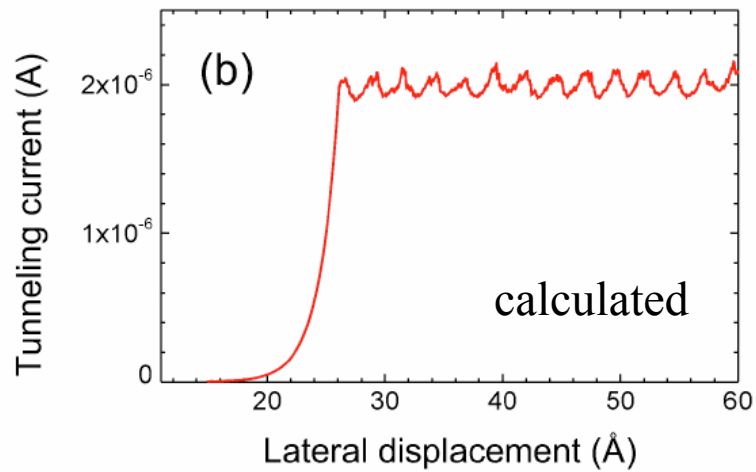
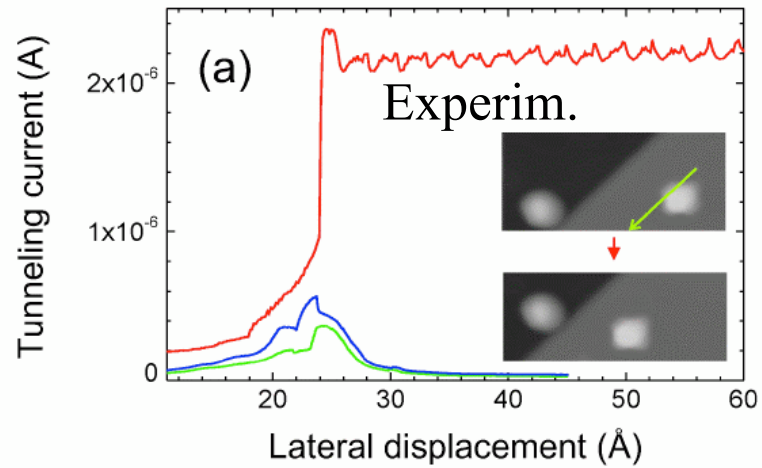
## STM constant Height manipulation



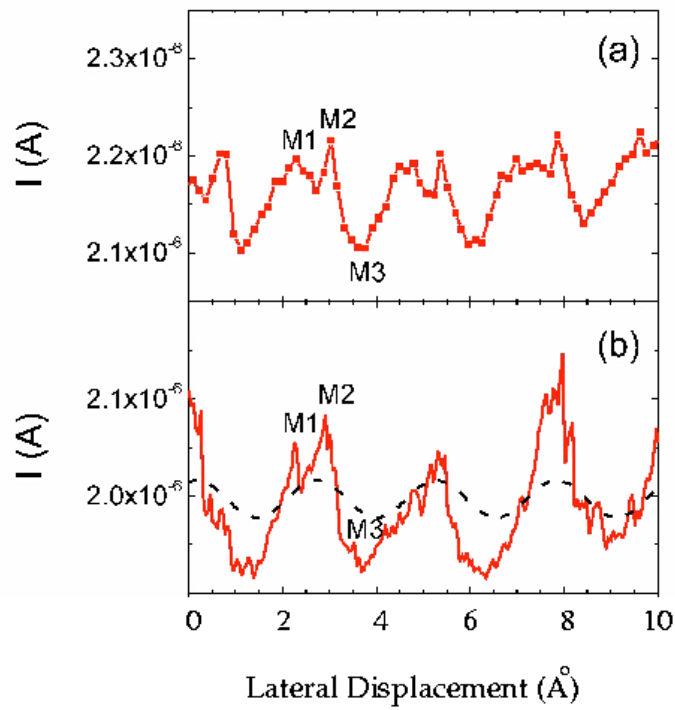
F. Moresco et col., PRL, 87,088302 (2001)



# Experimental and calculated signal

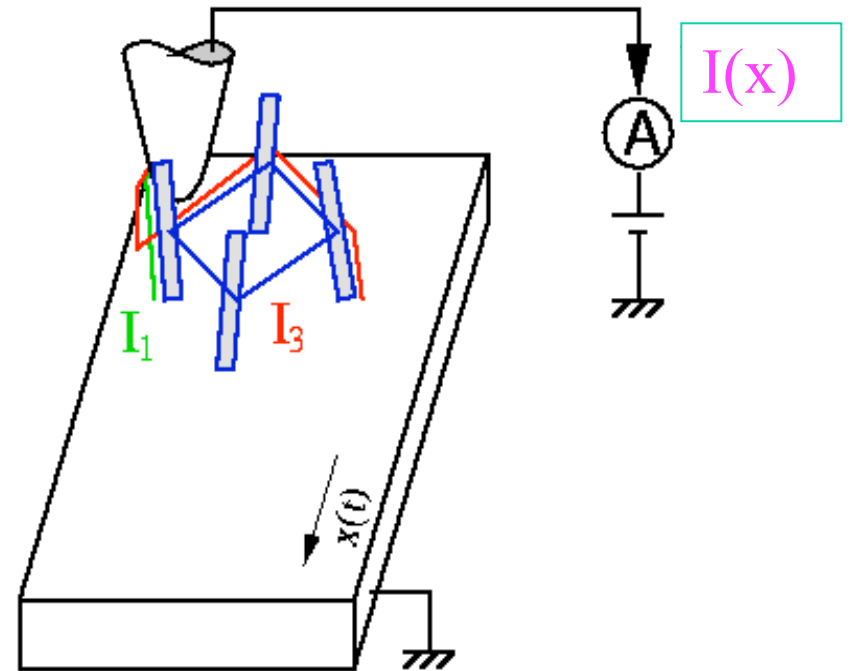


# Oscillation details in the STM manipulation signal

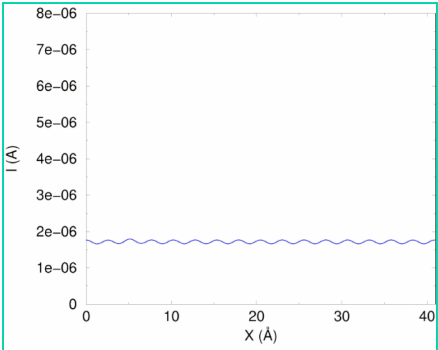
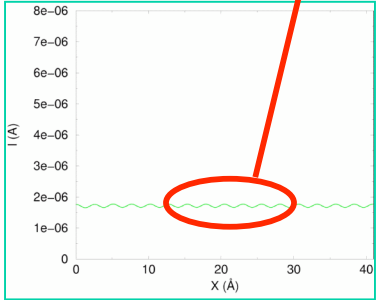
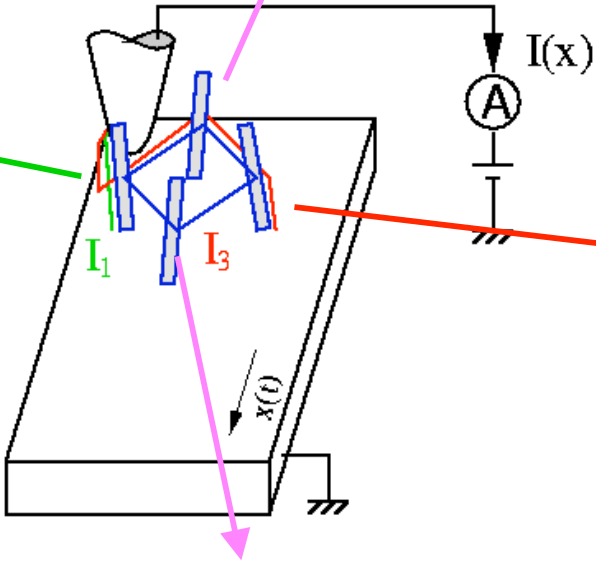
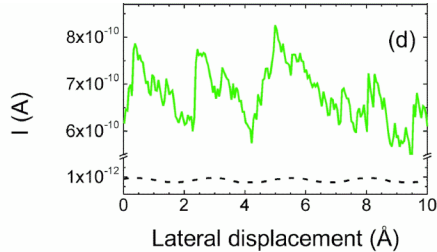
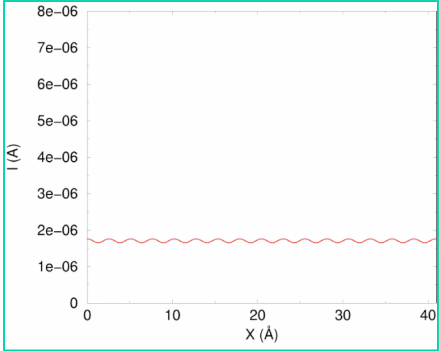
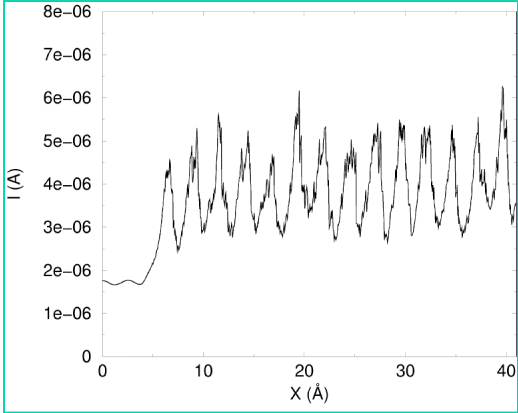


Exp.

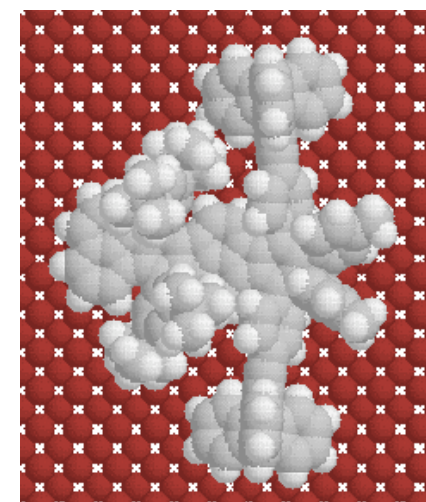
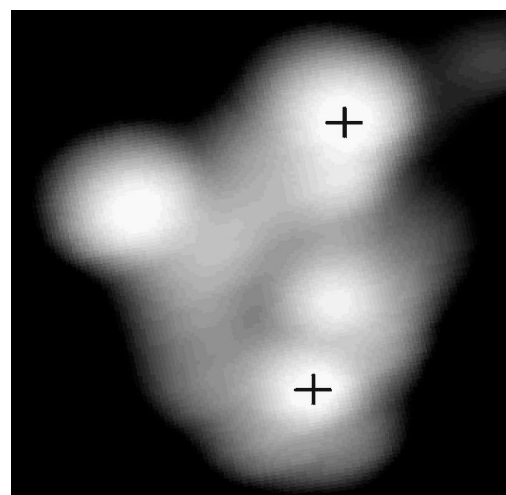
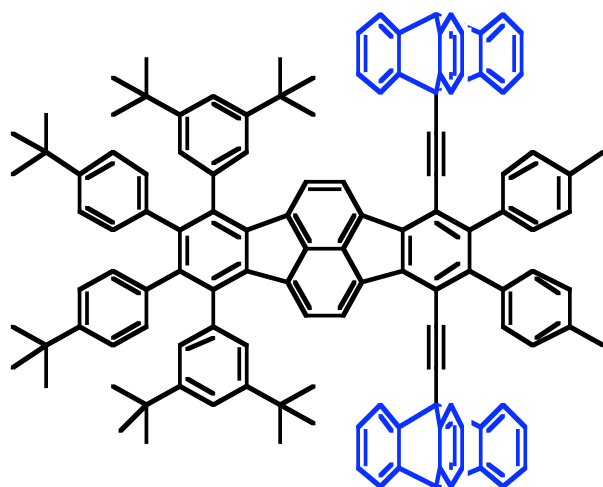
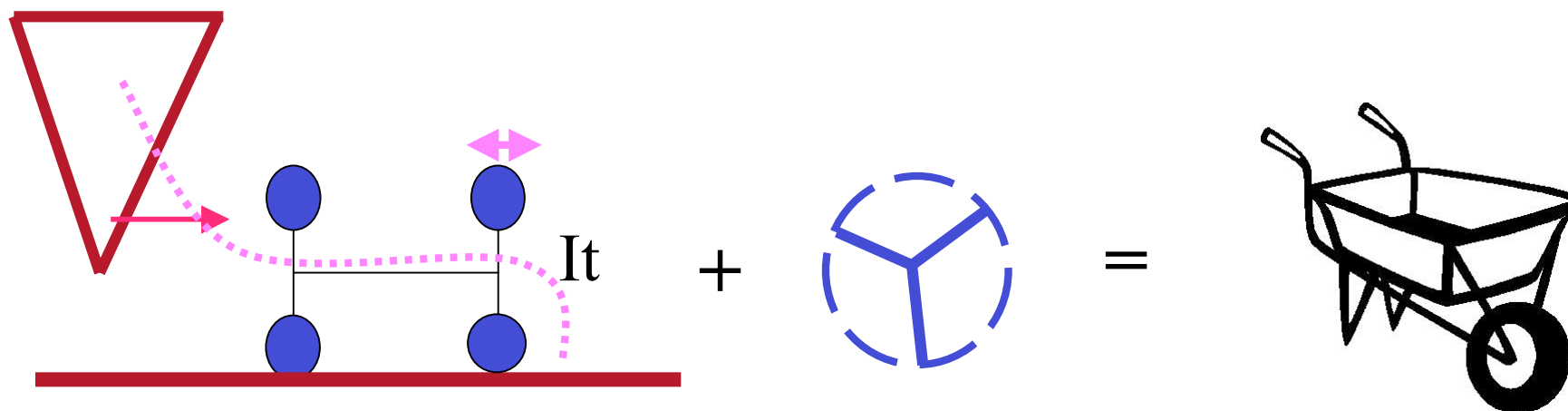
Calc.



# Leg per leg analysis



# An uni-molecular Barrow



Nanotechnology 2002, Tetra. Lett. 2003, Surf.Sc. Lett., 2005

ESQC

+ Molecular mechanics

STM manipulation signal

Design of uni-molecular machine

**in Hybrid molecular electronics**

**Molecular wires, long range tunnel**

**Electronic contact resistance**

**Single molecule transistor**

N-ESQC for Mono-molecular electronics

Intramolecular classical circuit

Phase circuit

Quantum Hamiltonian logic gate

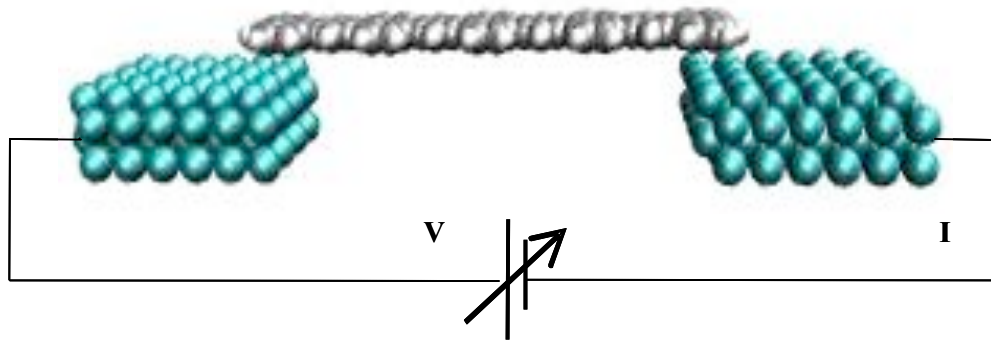
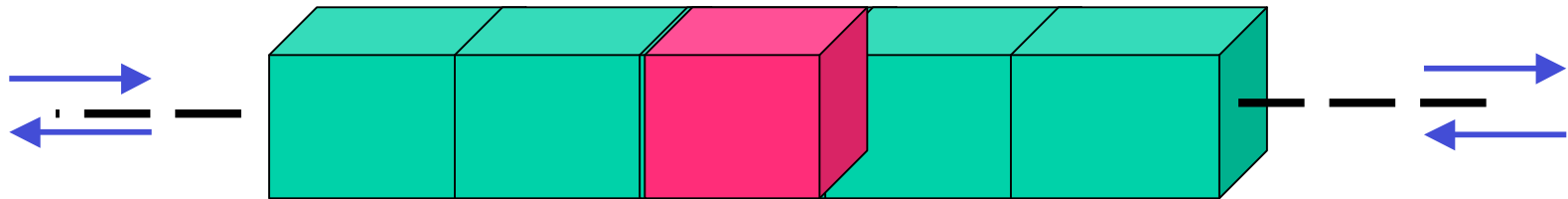
N-ESQC + Inelastic tunnel effect

Tunnel electron detector

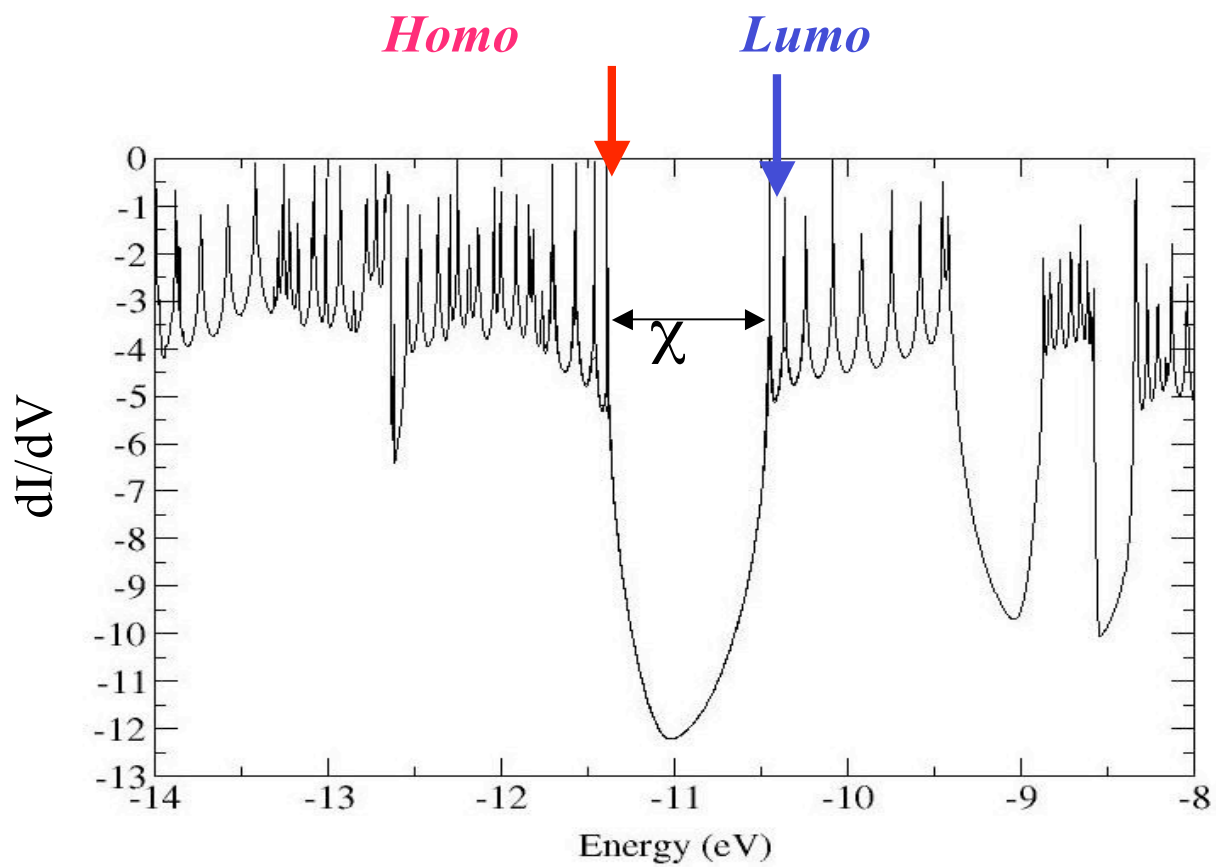
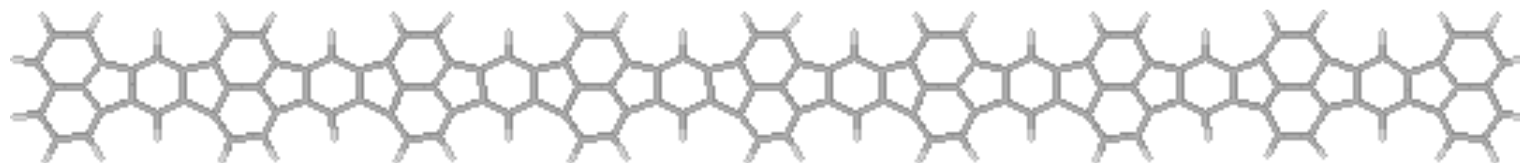




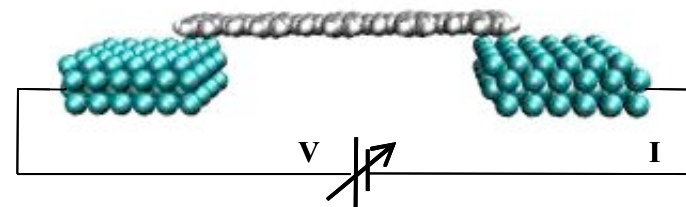
# Molecular wires, long range tunneling

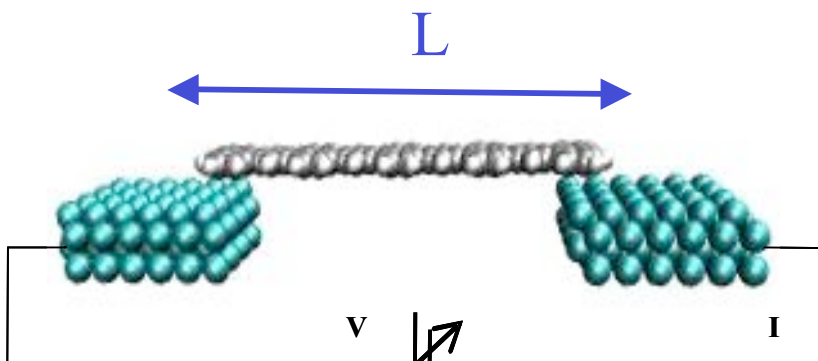


Scattering : 
$$I = \frac{e^2}{\pi \hbar} T(E_f) V$$



ESQC low voltage  $T(E)$  spectrum





$$G = G_0 \exp - 2\gamma_e L$$

$G_0$  ?

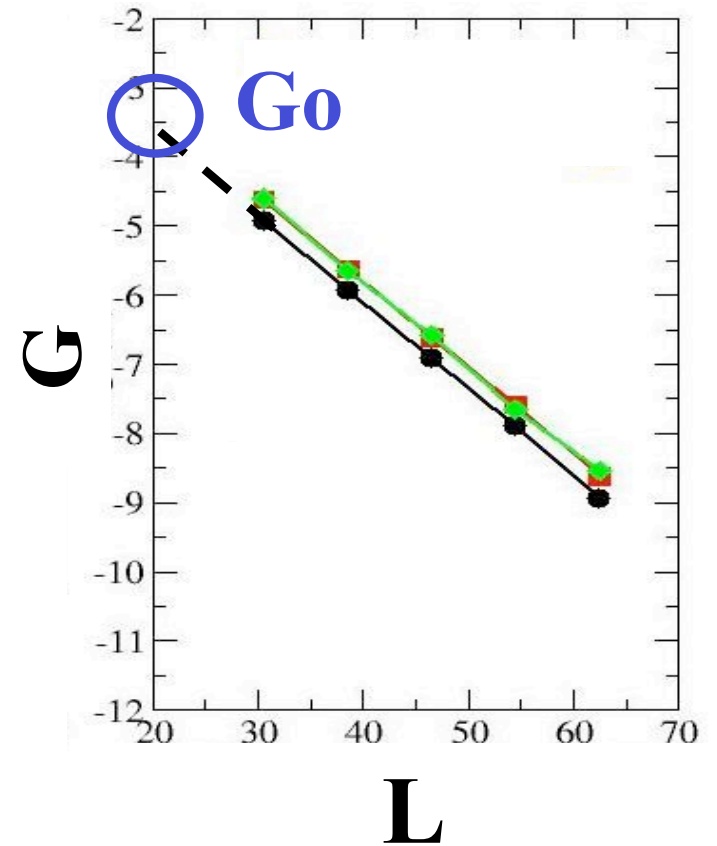
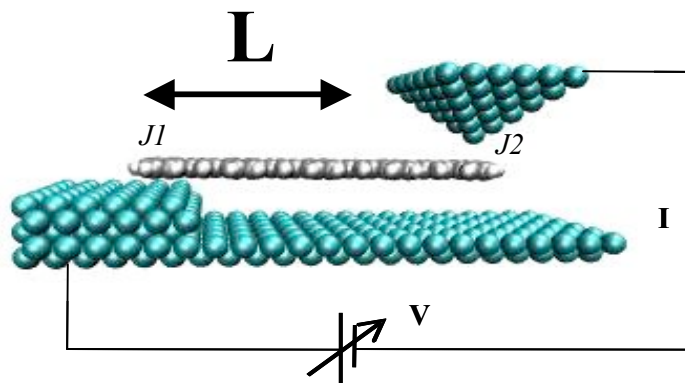
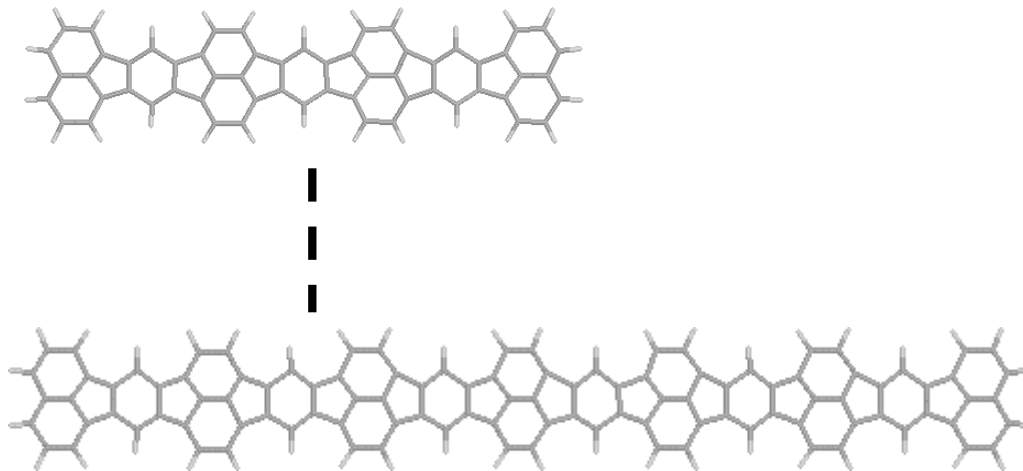
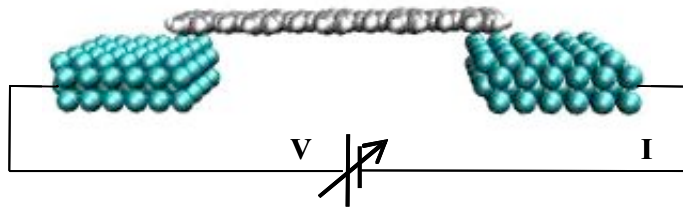
$$\gamma_e = \gamma_e(\chi, m^*) = \gamma_e(\chi, \rho)$$

$\chi$  = homo-lumo gap

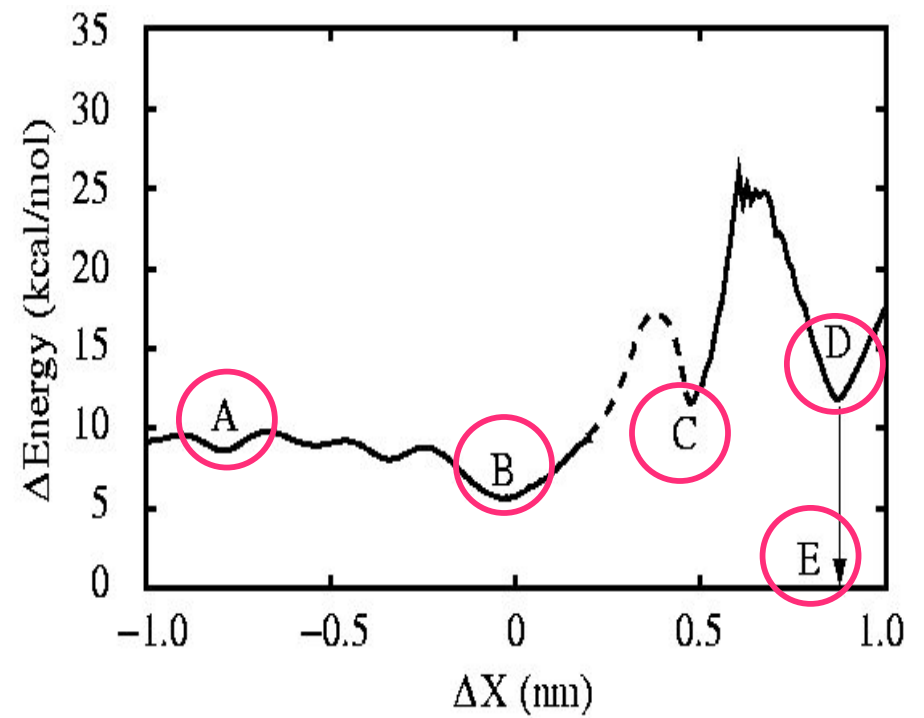
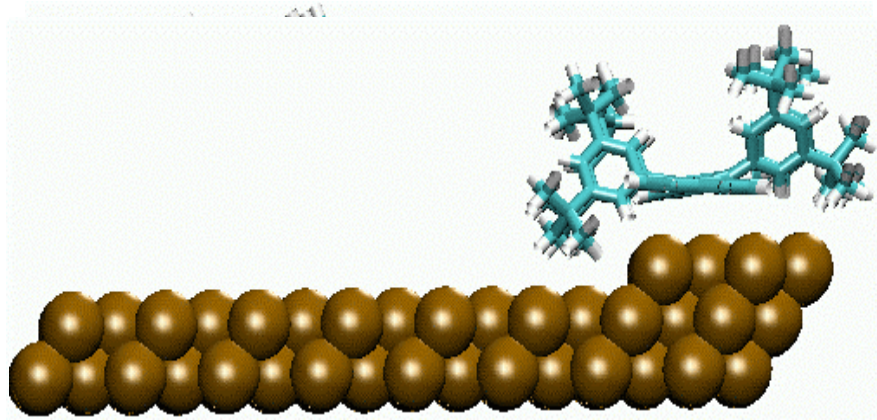
$m^*$  = effective masse of the tunneling electron

$\rho$  = the spectral repulsion factor

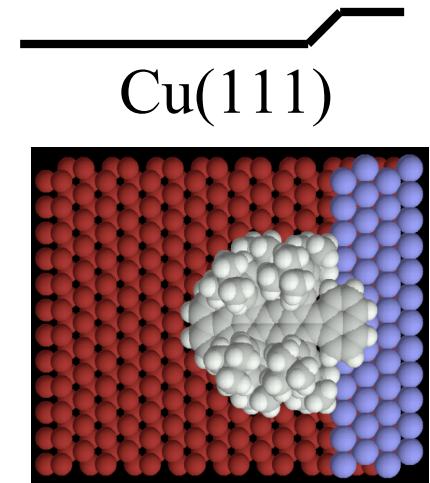
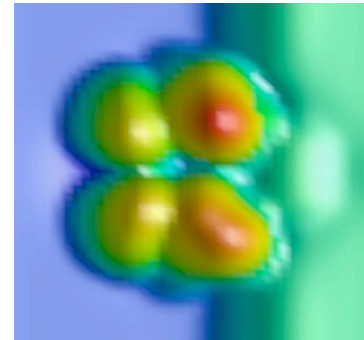
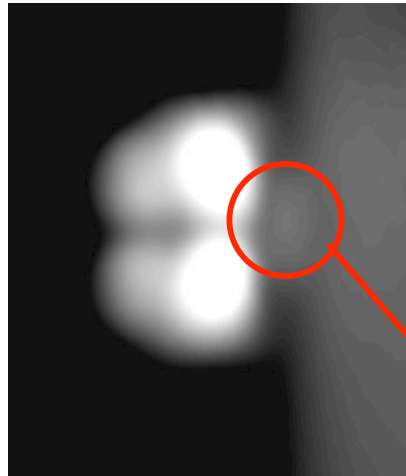
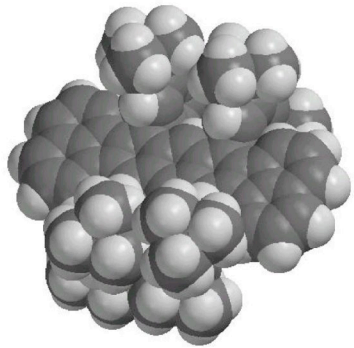
# How to get Go ?



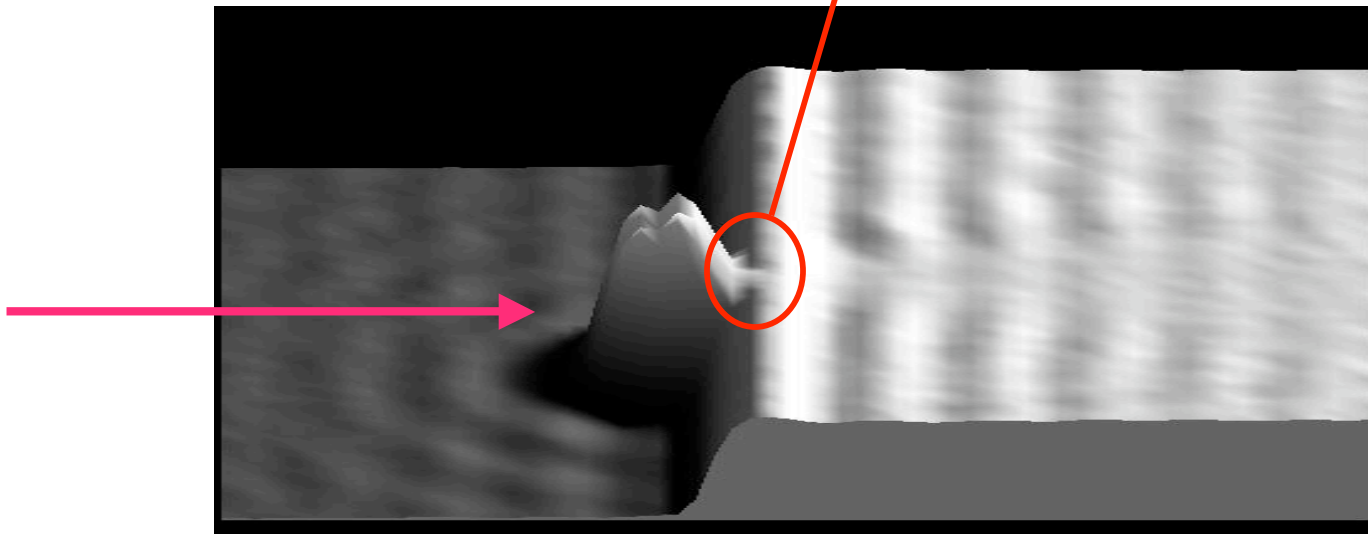
## Electronic contact mechanics



# Contacting $\perp$ to a step edge on Cu(111) ?



Contact bump



Conf. C

F. Moresco, C. Joachim, PRL, 91, 036601(2003)



ESQC

+ Molecular mechanics

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**N-ESQC for Mono-molecular electronics**

**Intramolecular classical circuit**

**Phase circuit**

**Quantum Hamiltonian logic gate**

N-ESQC + Inelastic tunnel effect

Tunnel electron detector



# Kirchhoff laws inside a molecule?

1845. ANNALEN No. 4.  
DER PHYSIK UND CHEMIE.  
BAND LXIV.

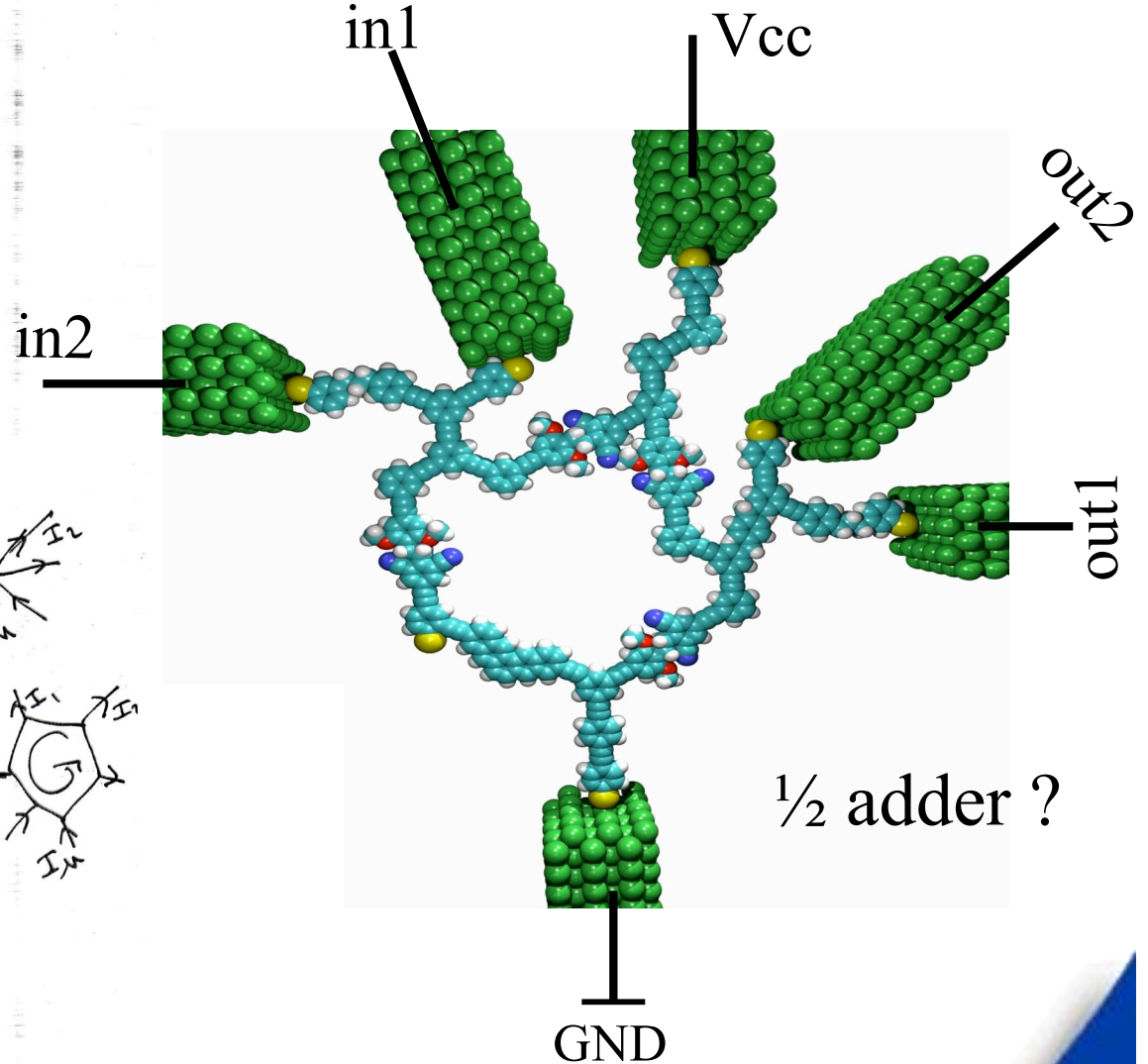
I. Ueber den Durchgang eines elektrischen Stromes durch eine Ebene, insbesondere durch eine kreisförmige; vom Studiosus Kirchhoff,  
Mitglied des physikalischen Seminars zu Königsberg.

Leitet man einen constanten galvanischen Strom durch eine Metallscheibe, so wird sich die Electricität in dieser auf eine bestimmte Weise vertheilen. Die Art der Vertheilung kann man nach den von Ohm aufgestellten Principien theoretisch ermitteln. Ich habe die dazu nöthige Rechnung unter der Voraussetzung, dafs der Zustand der Scheibe ein stationärer geworden sey, in dem Falle durchgeführt, dafs die Scheibe eine kreisförmige ist, und dafs die Electricität durch einen Draht in sie hinein, durch einen zweiten aus ihr heraustrete. Das Resultat wurde insbesondere einfach, wenn der Ein- und der Austrittspunkt in der Peripherie der Scheibe liegen, in diesem Falle habe ich dasselbe durch  $\nabla$  geprüft und, wie es mir scheint, eine Bestätigung gefunden. Ich will meine Betrachtungen an  $1, 2, \dots, \mu$  in einem Punkte zu schreiben.

1) wenn die Drähte  $1, 2, \dots, \mu$  in einem Punkte zusammenstoßen,  $I_1 + I_2 + \dots + I_\mu = 0$ , wo  $I_1, I_2, \dots$  die Intensitäten der Ströme bezeichnen, die jene Drähte durchfließen, alle nach dem Berührungspunkte zu als positiv gerechnet;

2) wenn die Drähte  $1, 2, \dots, \nu$  eine geschlossene Figur bilden,  $I_1 \cdot \omega_1 + I_2 \cdot \omega_2 + \dots + I_\nu \cdot \omega_\nu = 0$ , = der Summe aller elektromotorischen Kräfte, die sich auf dem Wege:  $1, 2, \dots, \nu$  befinden; wo  $\omega_1, \omega_2, \dots$  die

Poggendorff's Annal. Bd LXIV. 33



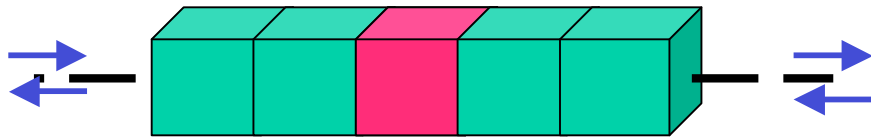
1/2 adder ?



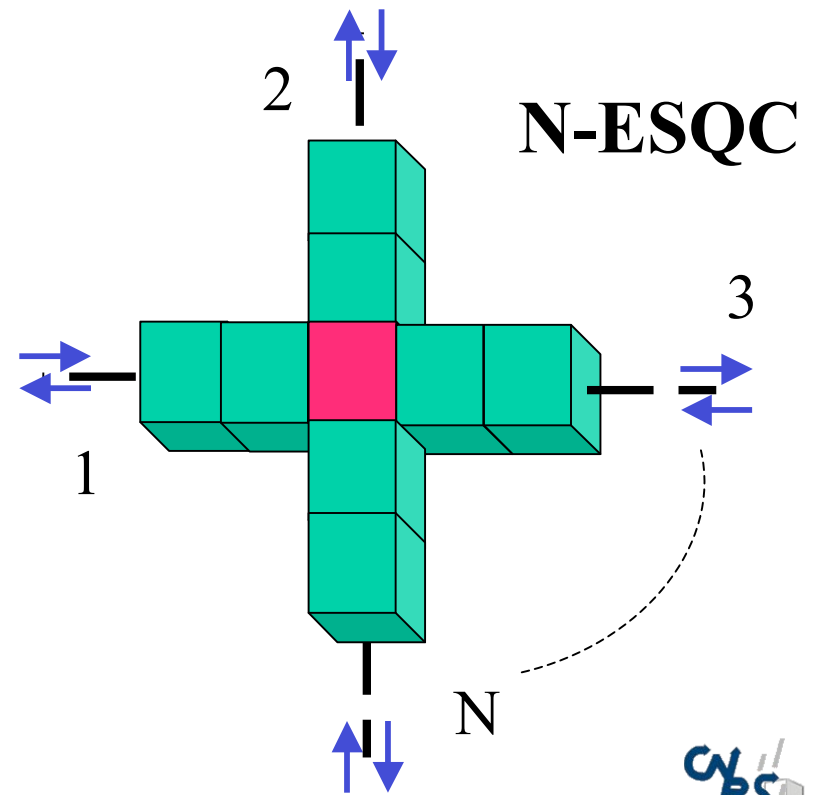
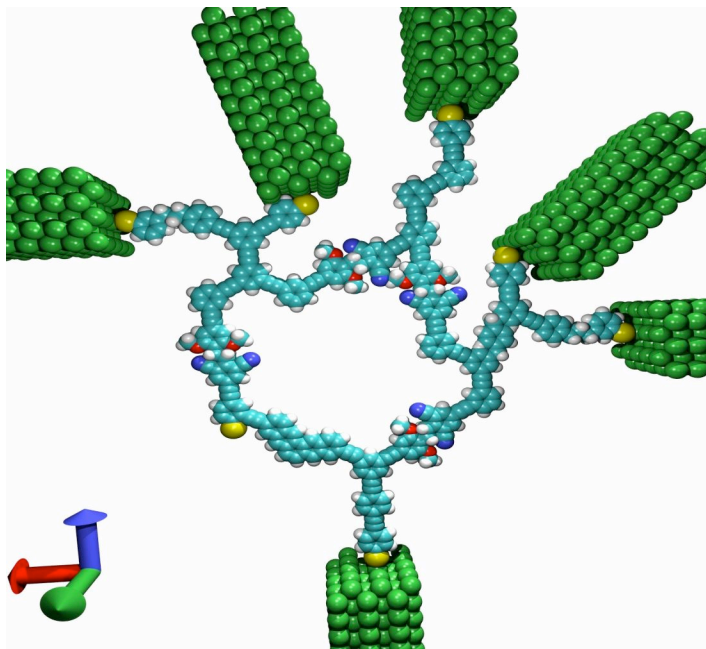
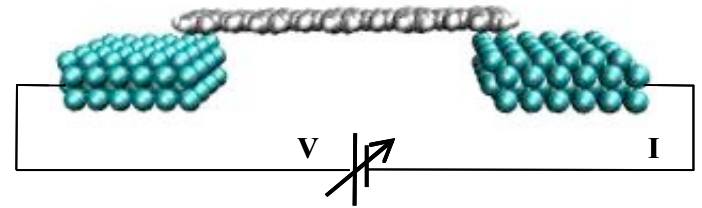
N-ESQC method, Chem. Phys. Lett (2003)

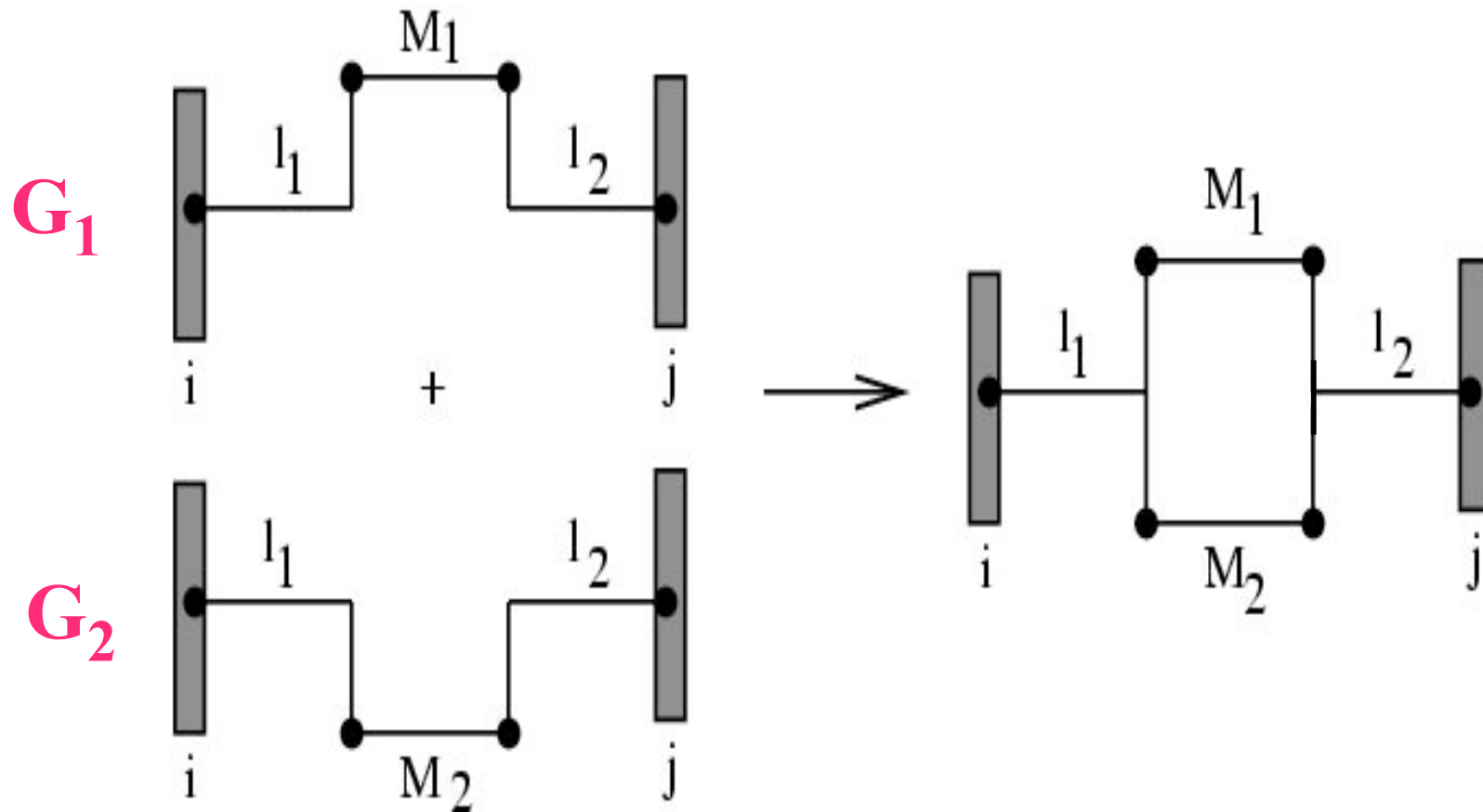






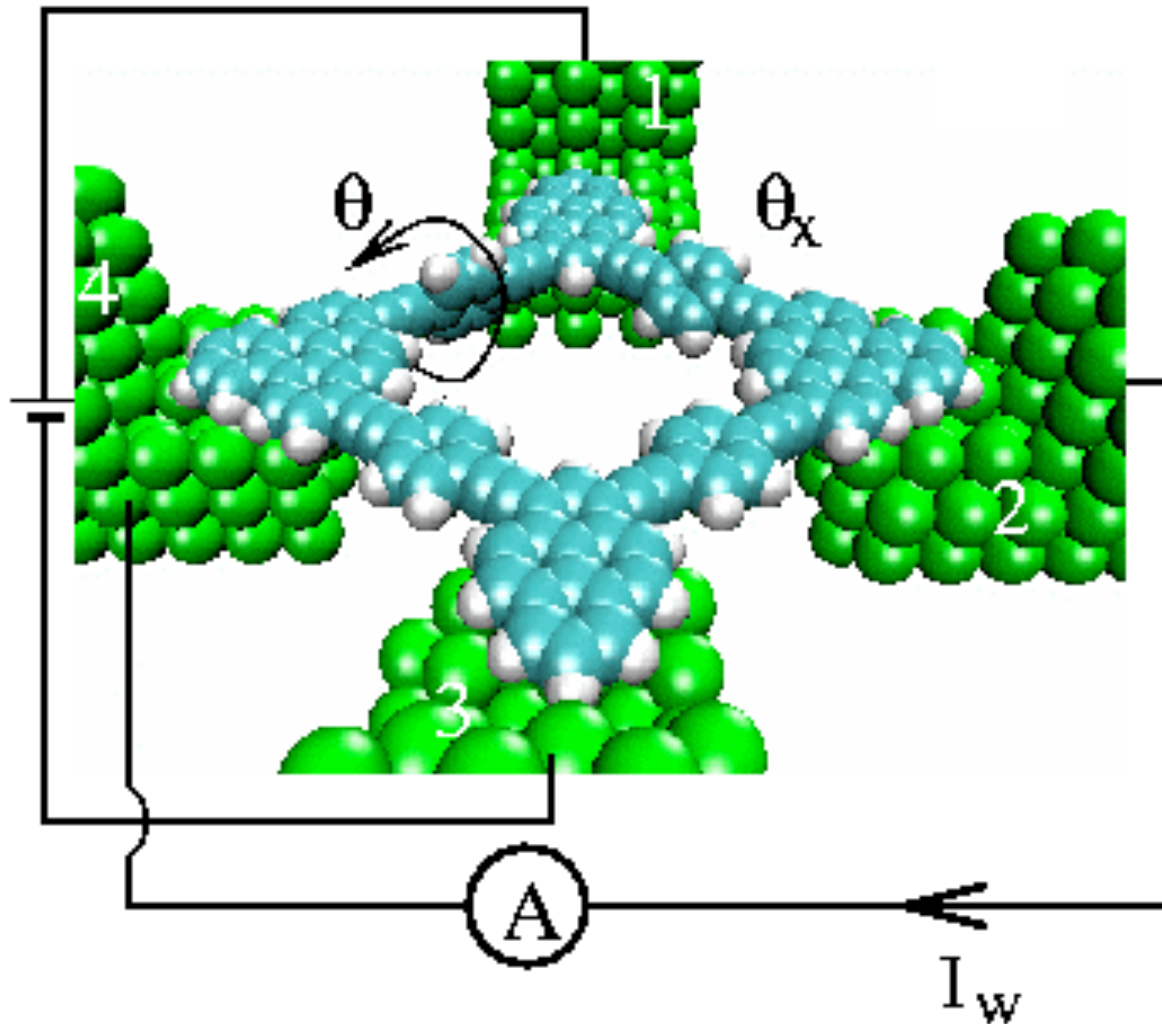
**ESQC**





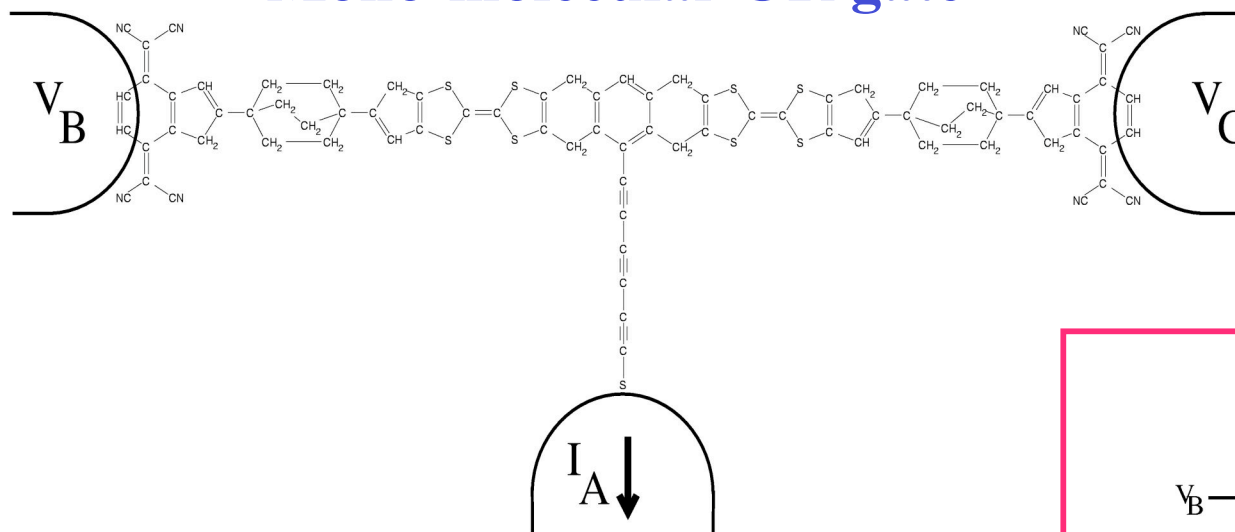
$$G = G_1 + G_2 + 2 (G_1 \cdot G_2)^{1/2}$$

# Equilibrer un pont de Wheatstone?

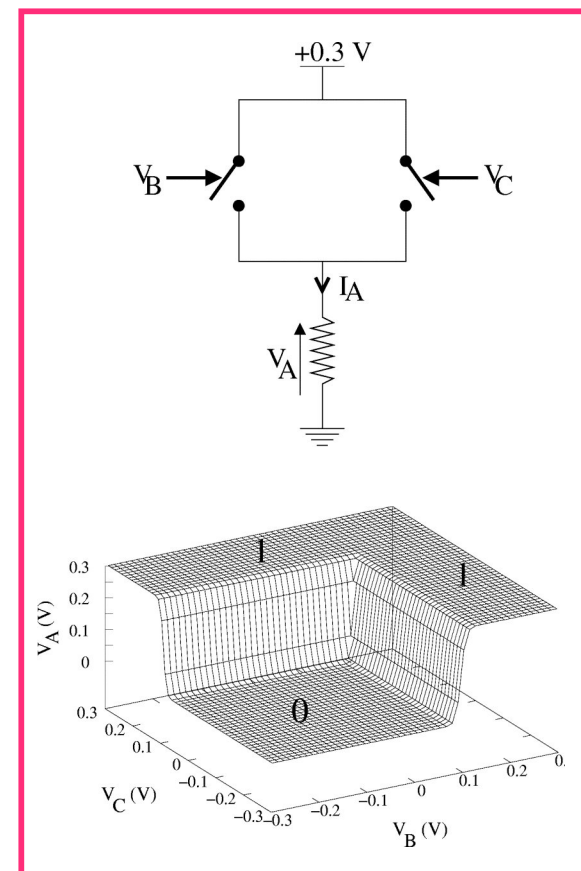
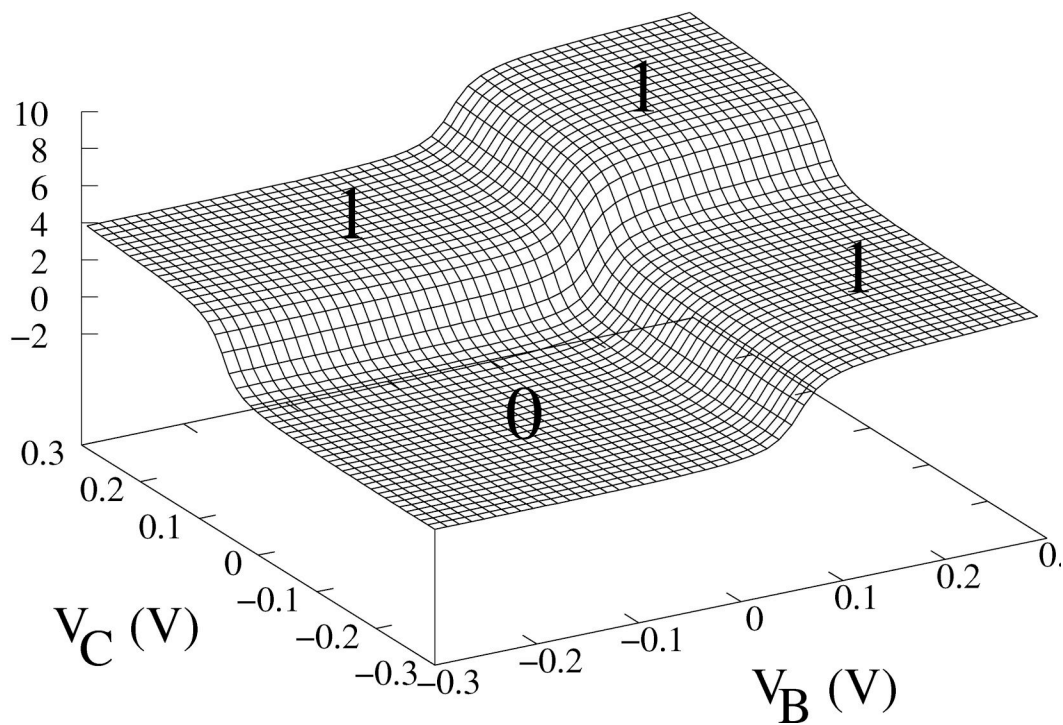


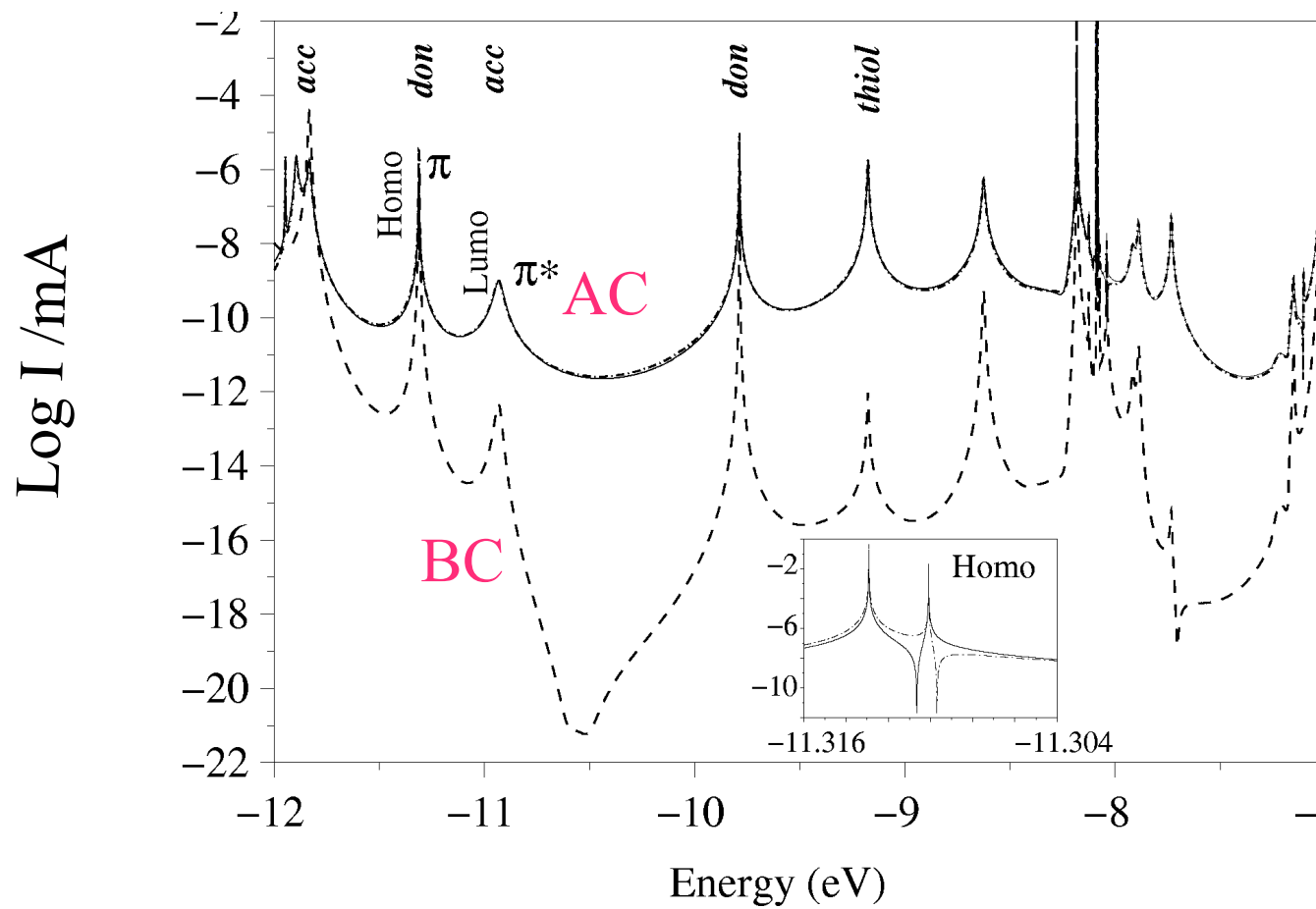
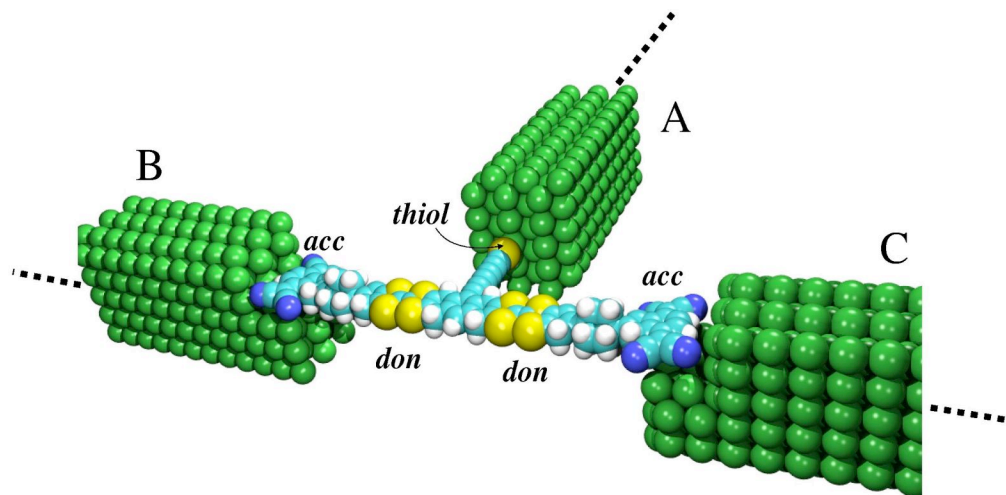
Nanotechnology, Feb. 2003

# Mono-molecular OR gate

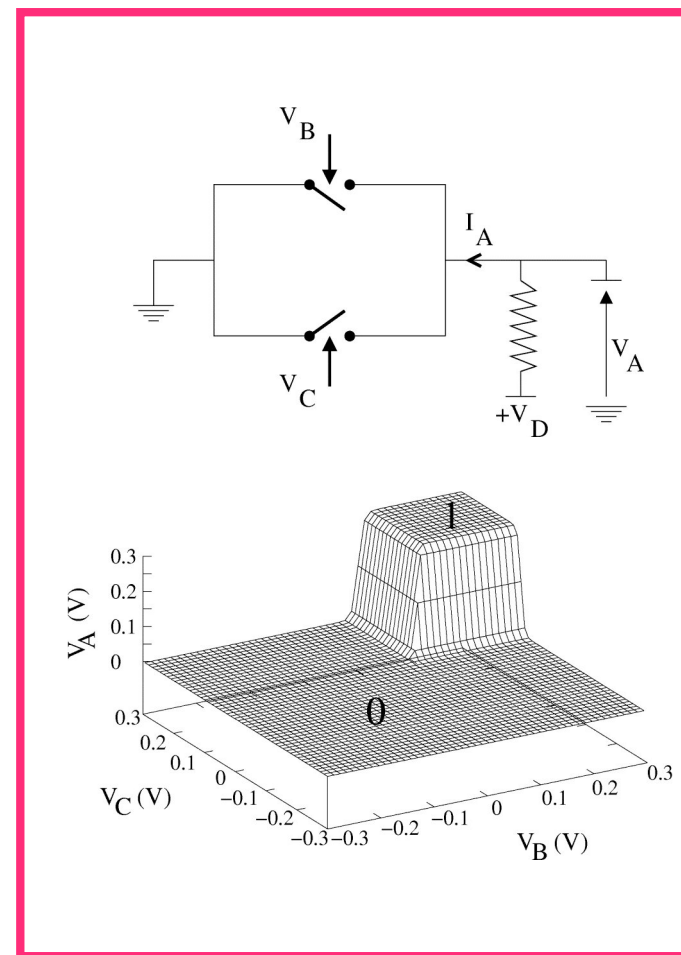
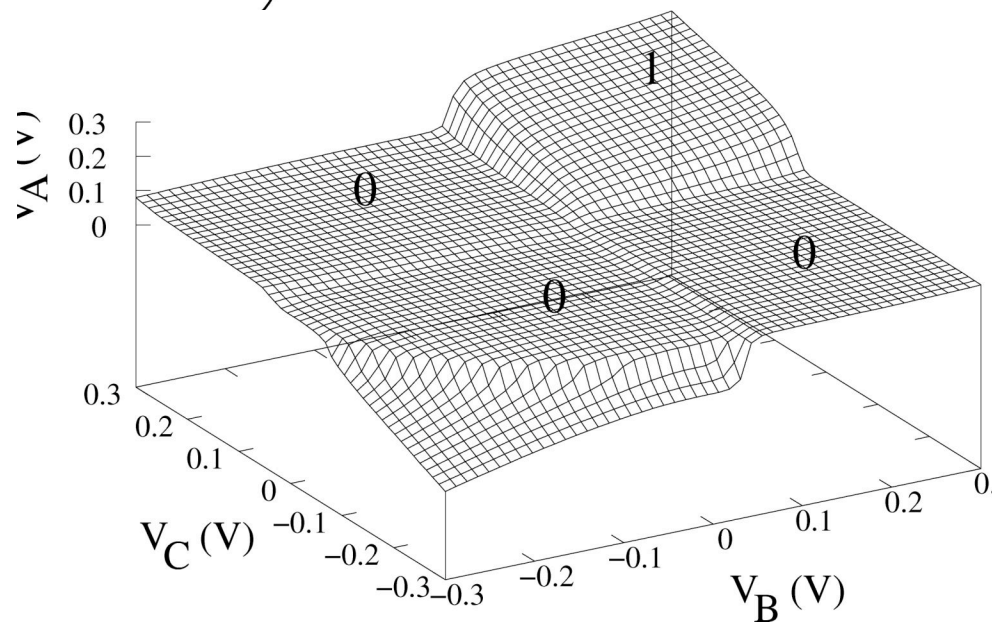
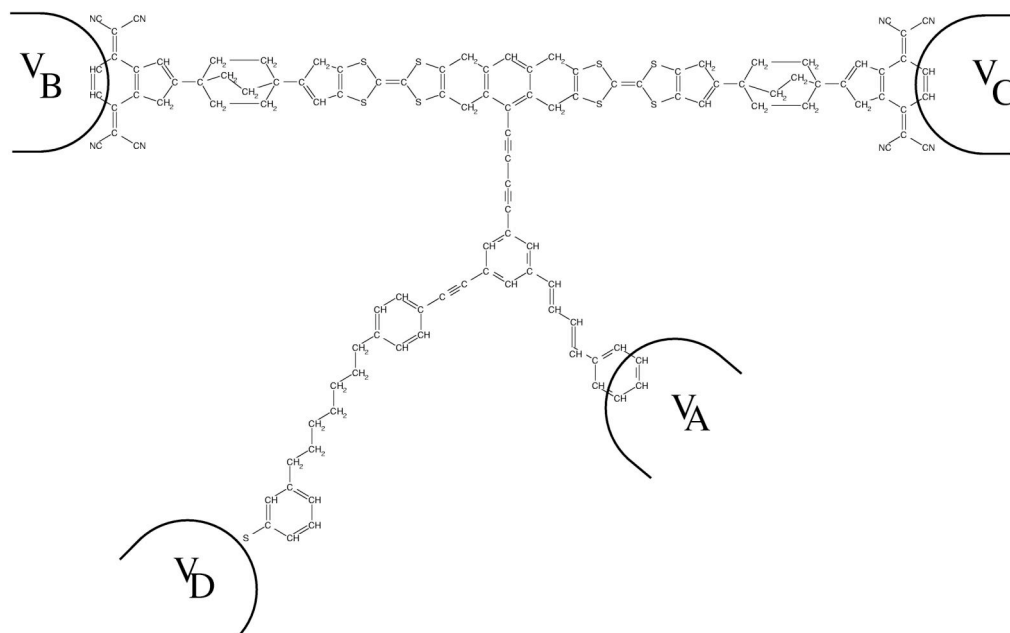


$I$  (fA)

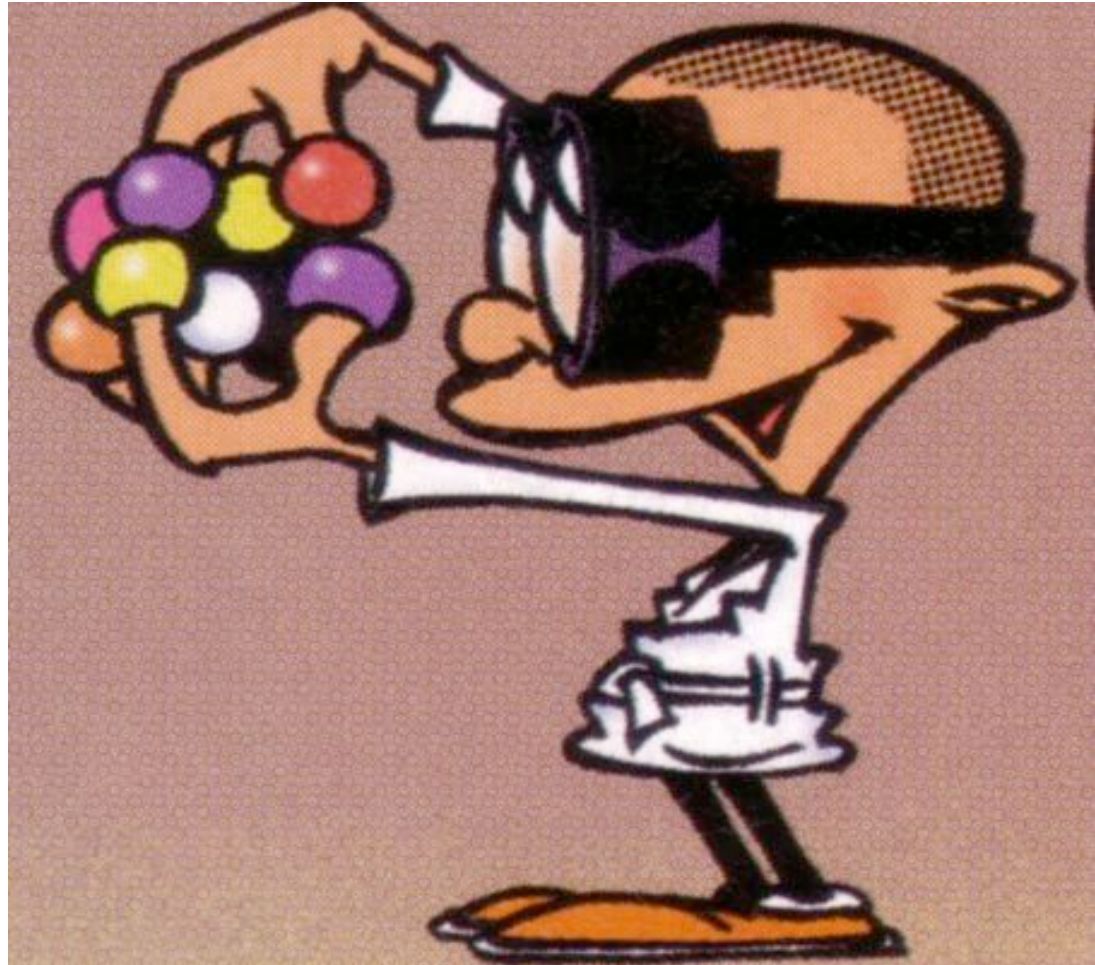
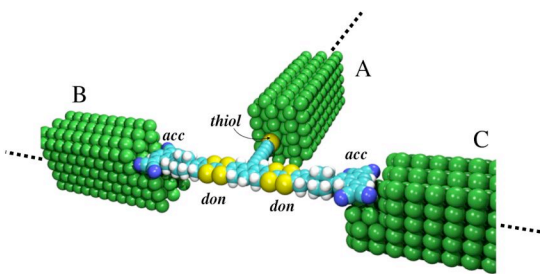
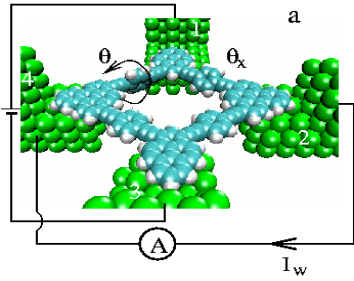
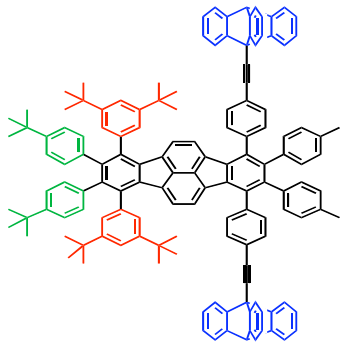




# Mono-molecular AND gate

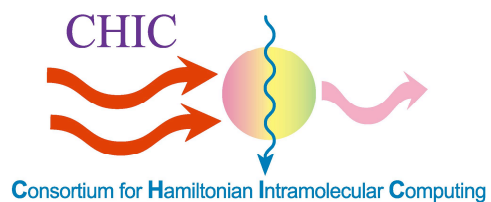


S. Ami, M. Hliwa and C. Joachim,  
Chem. Phys. Lett. , 367, 662 ( 2003)





theGNS



Pico-Inside

