Single molecule logic gates

Mohamed Hliwa

Hassan II University Casablanca-Morroco

AtMol International Workshop on Architecture and Design of Molecule Logic Gates and Atom Circuits

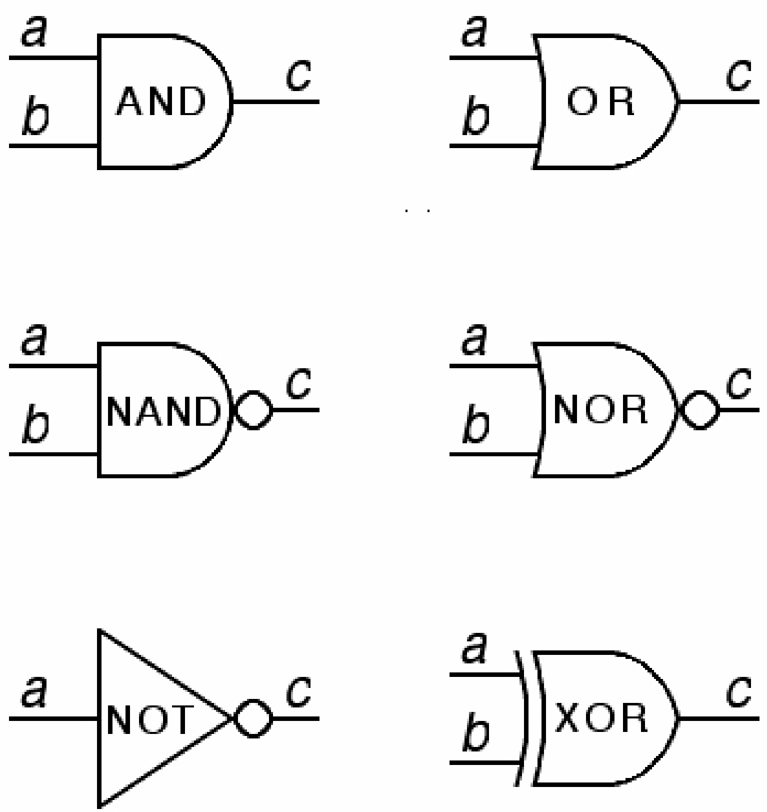
January 12-13 Barcelona-Spain

Outline

- Solid state diode based logic functions
- Examples of Molecule-Circuit
- Intramolecular node and mesh circuit laws
- N-electrode Elastic Scattering Quantum Chemistry technique
- Molecular conductance
- Diode based a single molecule logic gate : OR, AND
- Tunnel inelastic effect : an example of a current tranducer
- An XOR-molecule logic gate
- An OR-molecule logic gate whith no rectifier
- Balancing a Wheatstone Bridge

Diode based electronic circuits

Elementary logic functions



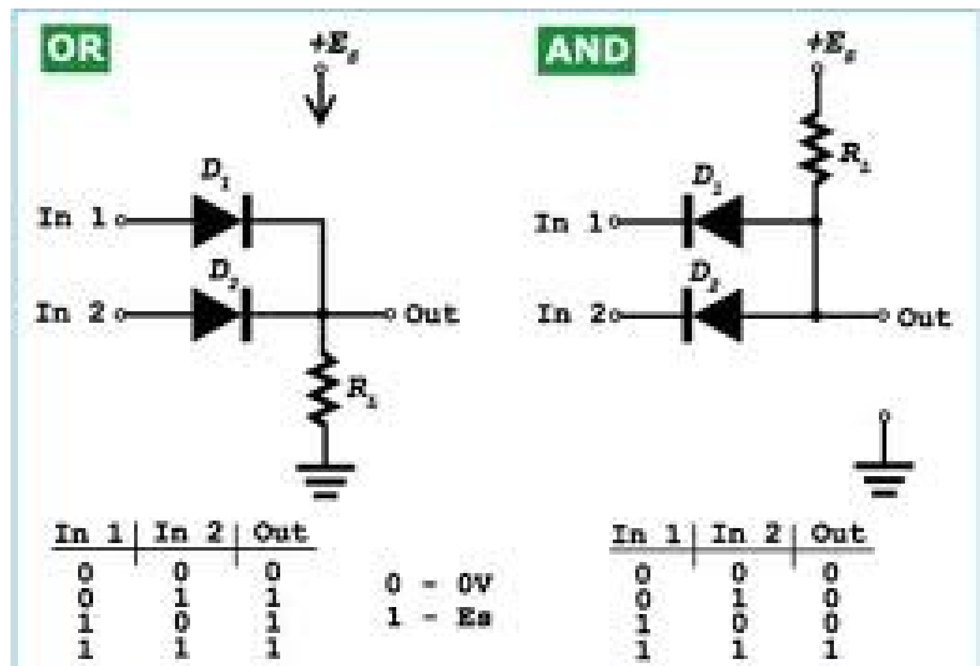
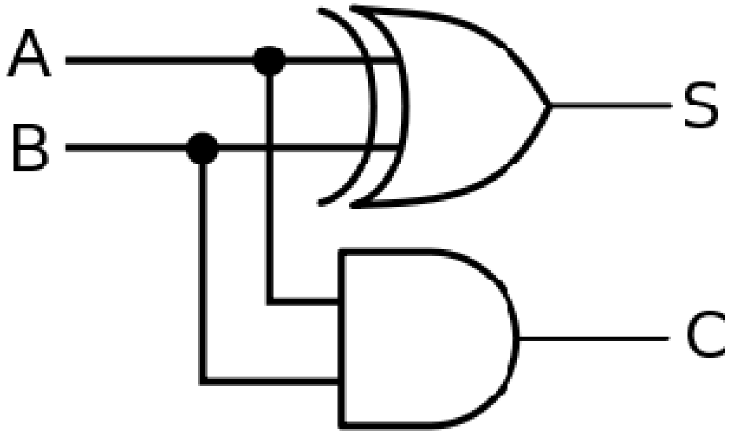


Fig. 2.1 p-n-junction diode's OR and AND gates.

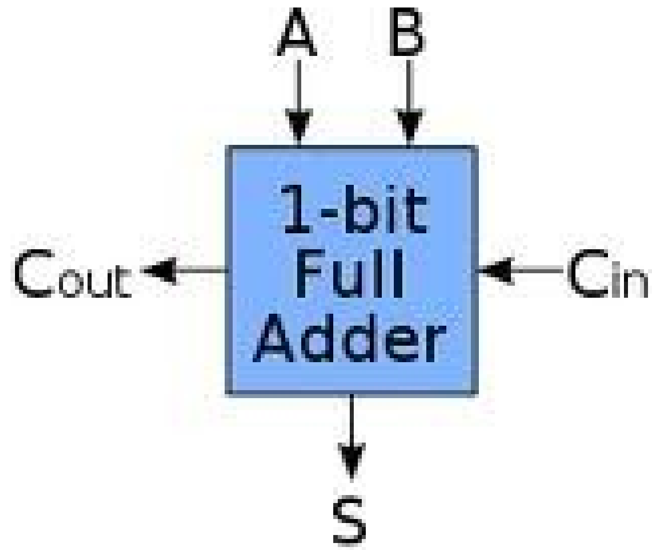
1-bit 2-input digital half adder

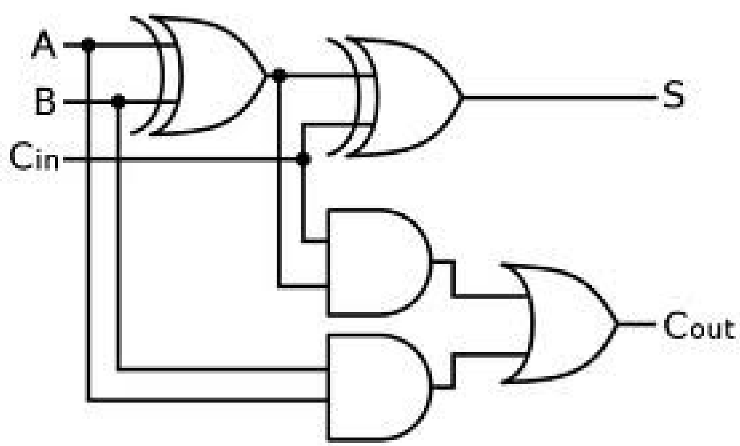


$$S = \overline{A}.B + A.\overline{B} = A \oplus B$$

$$C = A.B$$

A	B	C	S
0	0	0	0
0	1	0	1
1	0	0	1
1	1	1	0



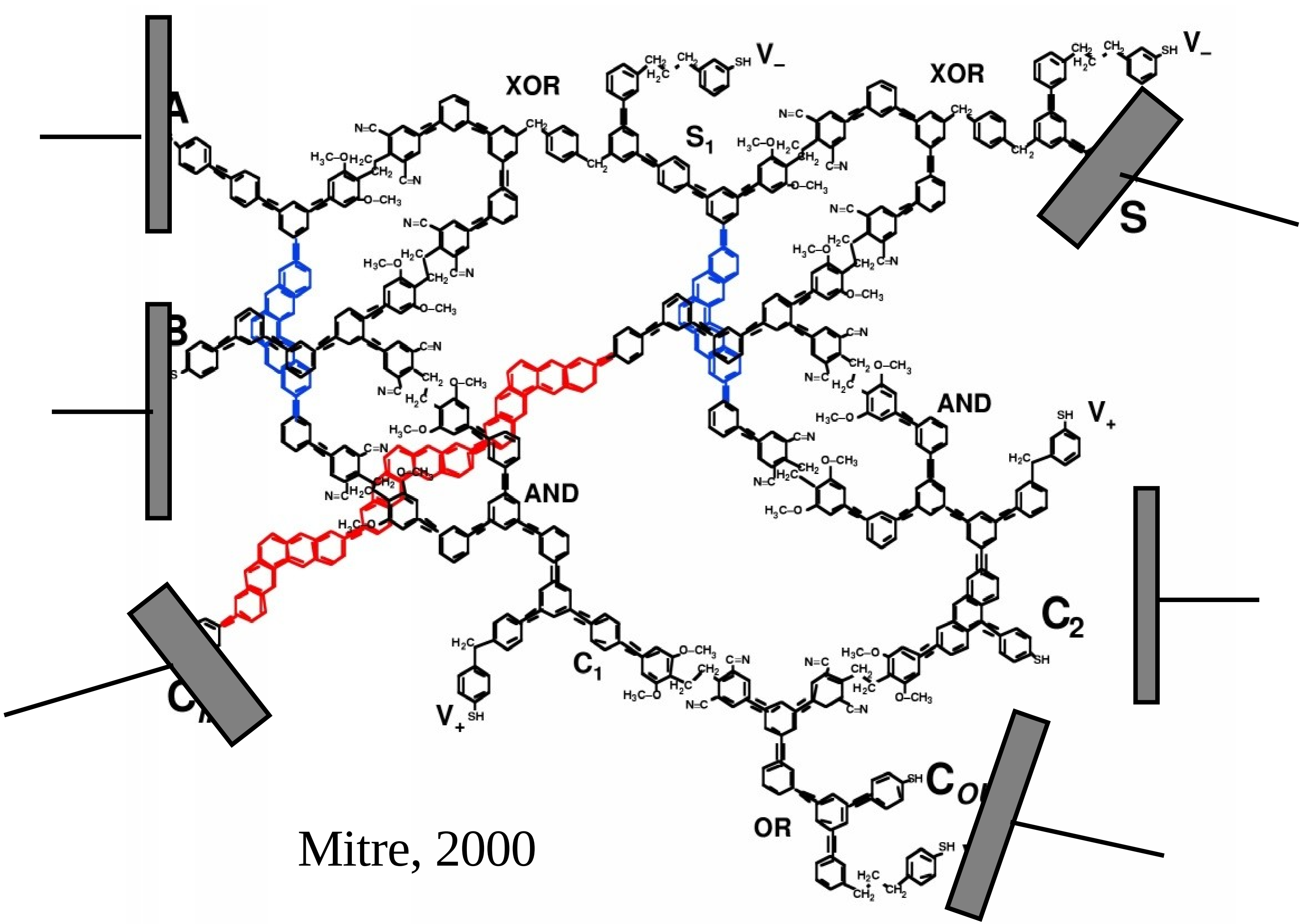


Input bit for number A	Input bit for number B	Carry bit input C_{IN}	Sum bit output S	Carry bit output C_{OUT}
0	0	0	0	0
0	0	1	1	0
0	1	0	1	0
0	1	1	0	1
1	0	0	1	0
1	0	1	0	1
1	1	0	0	1
1	1	1	1	1

Molecular Circuits

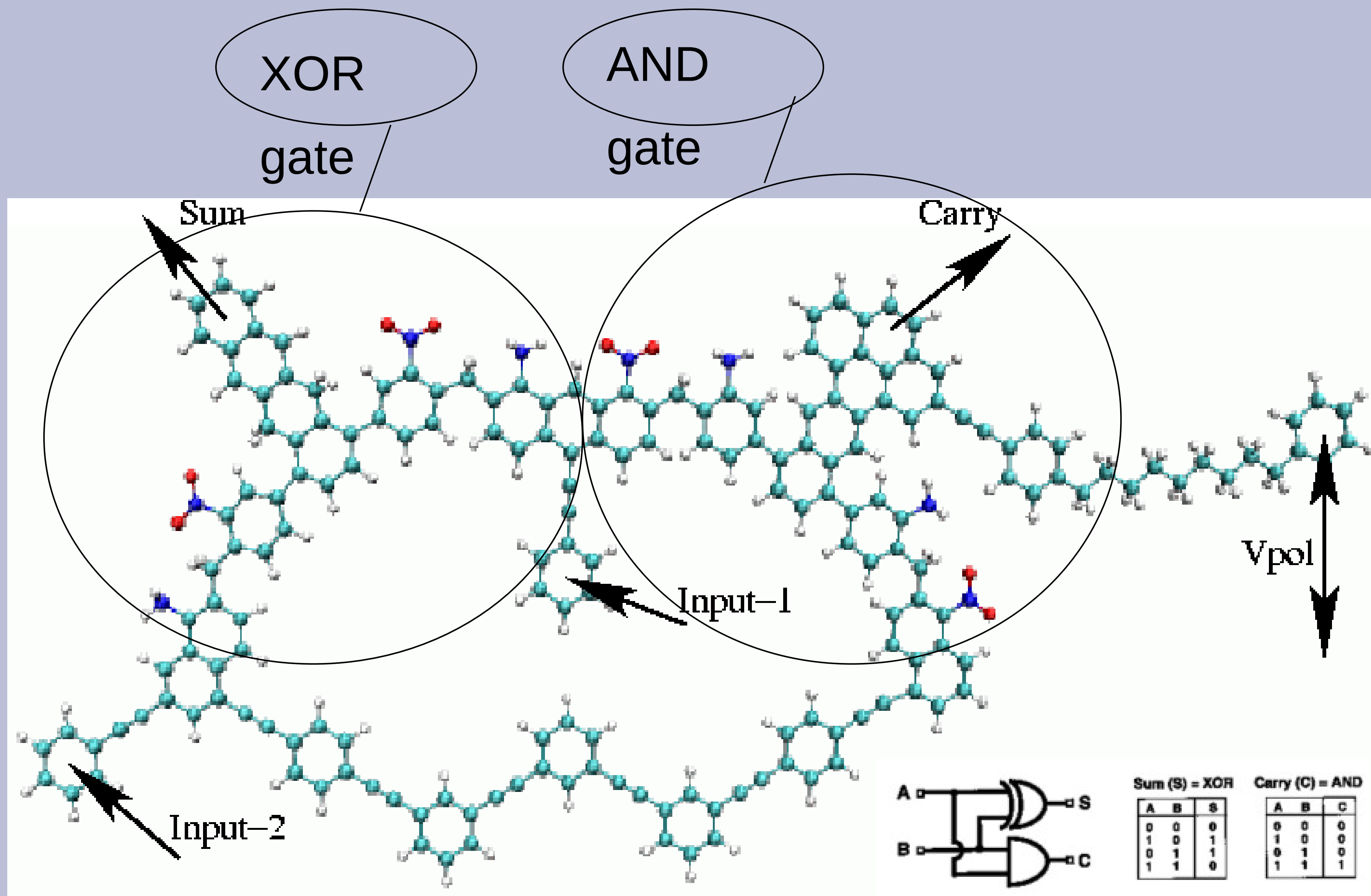
A molecular One bit full adder

J. C. Ellenbogen and J. C. Love, Proc. IEEE 88 (2000) 386



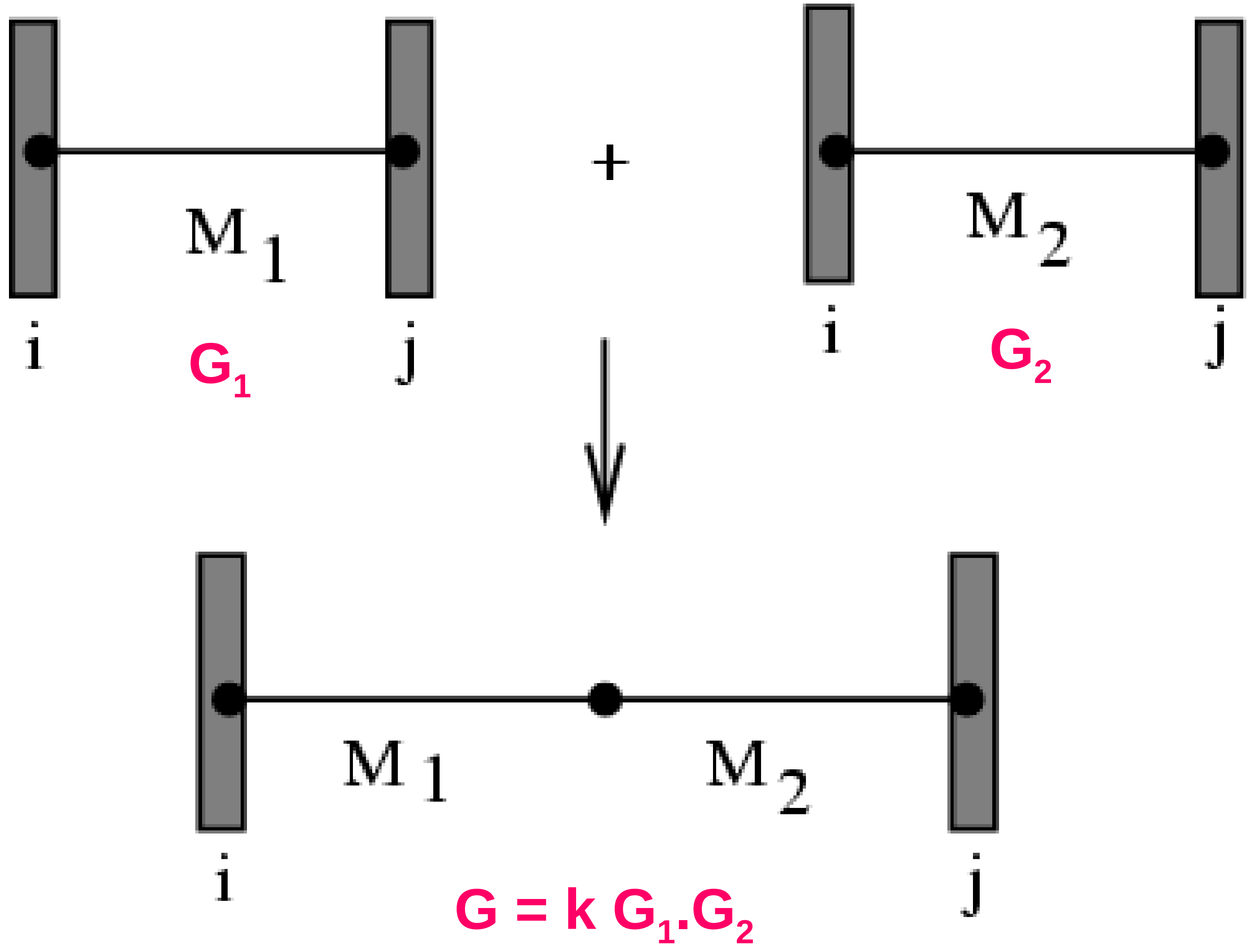
Mitre, 2000

Example of one bit a molecular half adder



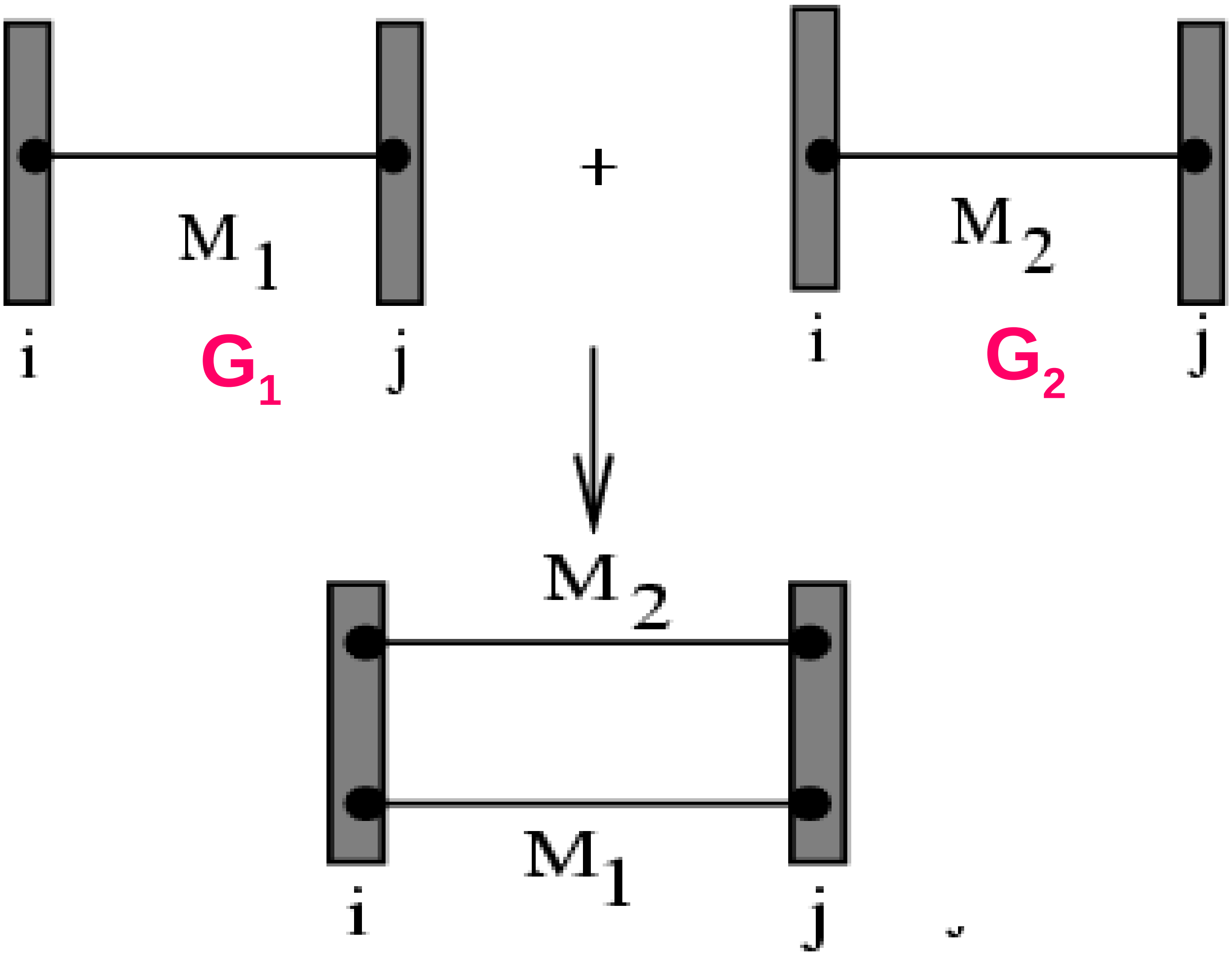
Intramolecular node and mesh circuit laws

Serial association of 2 molecular wires



M. Magoga and C. Joachim Phys. Rev. B 59 (1999) 16011

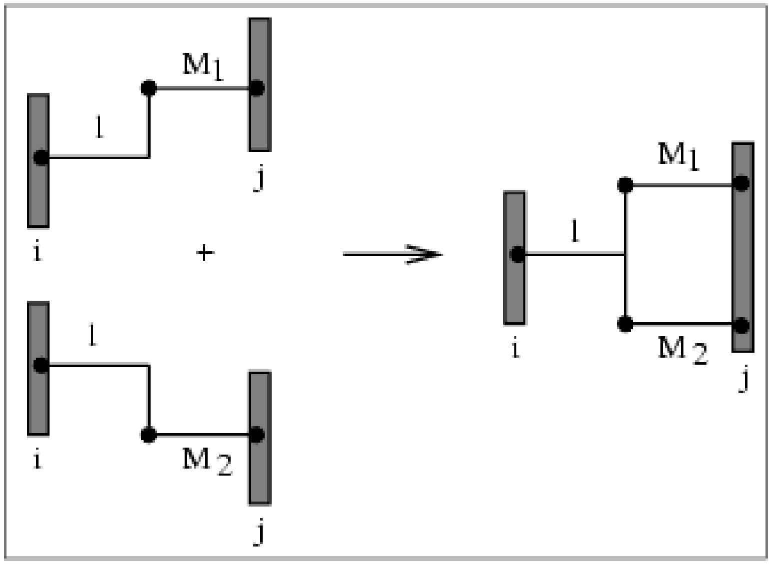
Paralel association of 2 molecular wires



$$G = G_1 + G_2$$

M. Magoga and C. Joachim Phys. Rev. B 59 (1999) 16011

Molecular wires association forming a single molecule With 1 intramolecular nodes

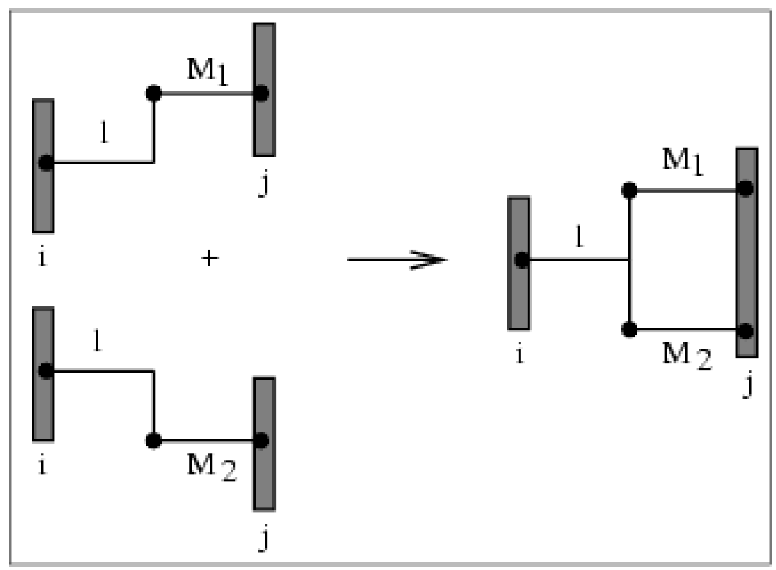


c

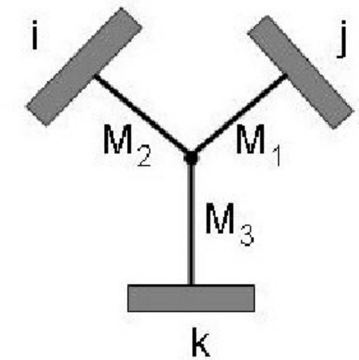
$$G = k\, g_l.(G_1+G_2)$$

Phys. Rev. B, 59, 16011 (1999)

Molecular wires association forming a single molecule
With 1 intramolecular nodes



c



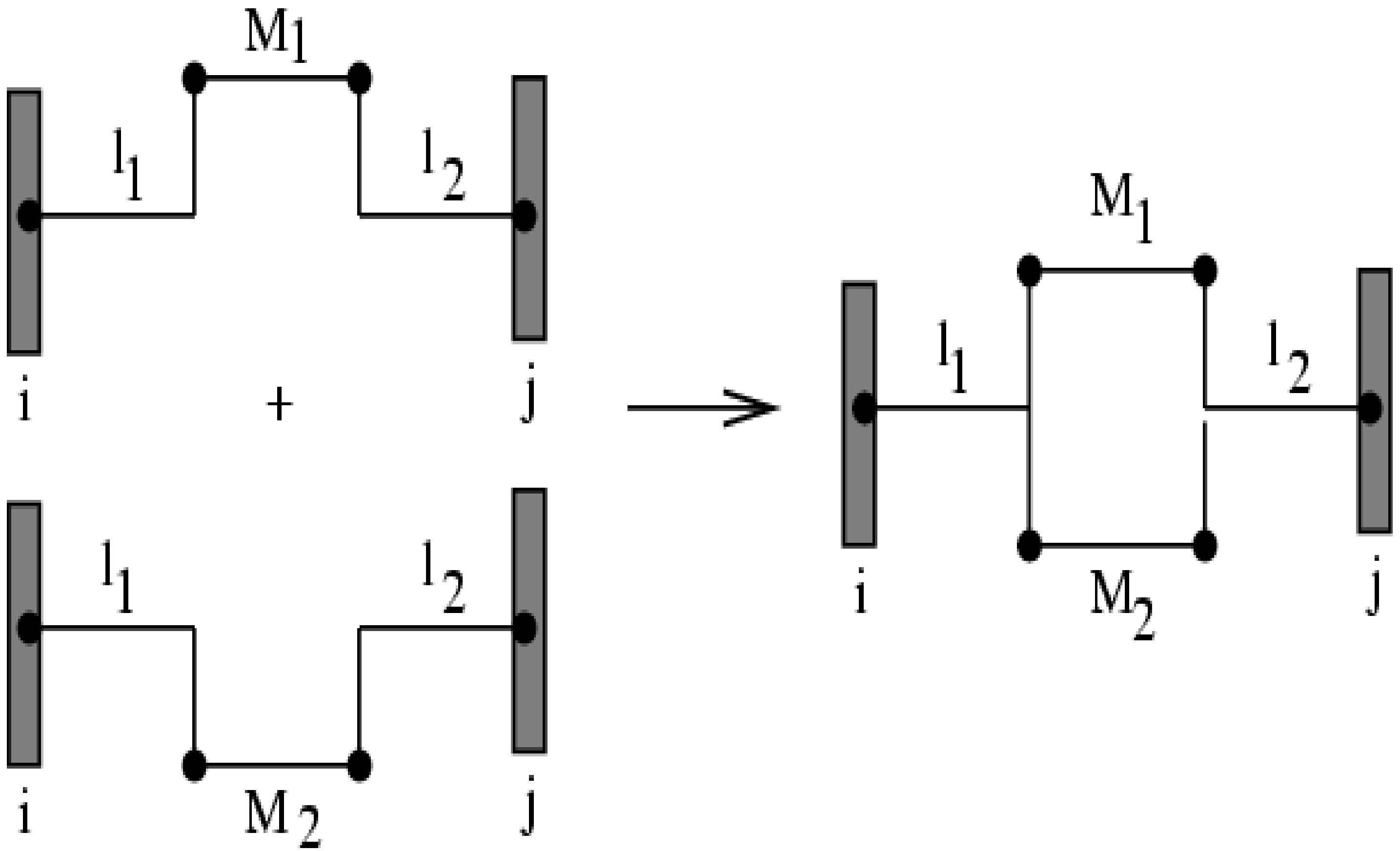
$$G = k\, g_l.(G_1+G_2)$$

Phys. Rev. B, 59, 16011 (1999)

Molecular wires association forming a single molecule
With 2 intramolecular nodes
(and 1 mesh)

G_1

G_2



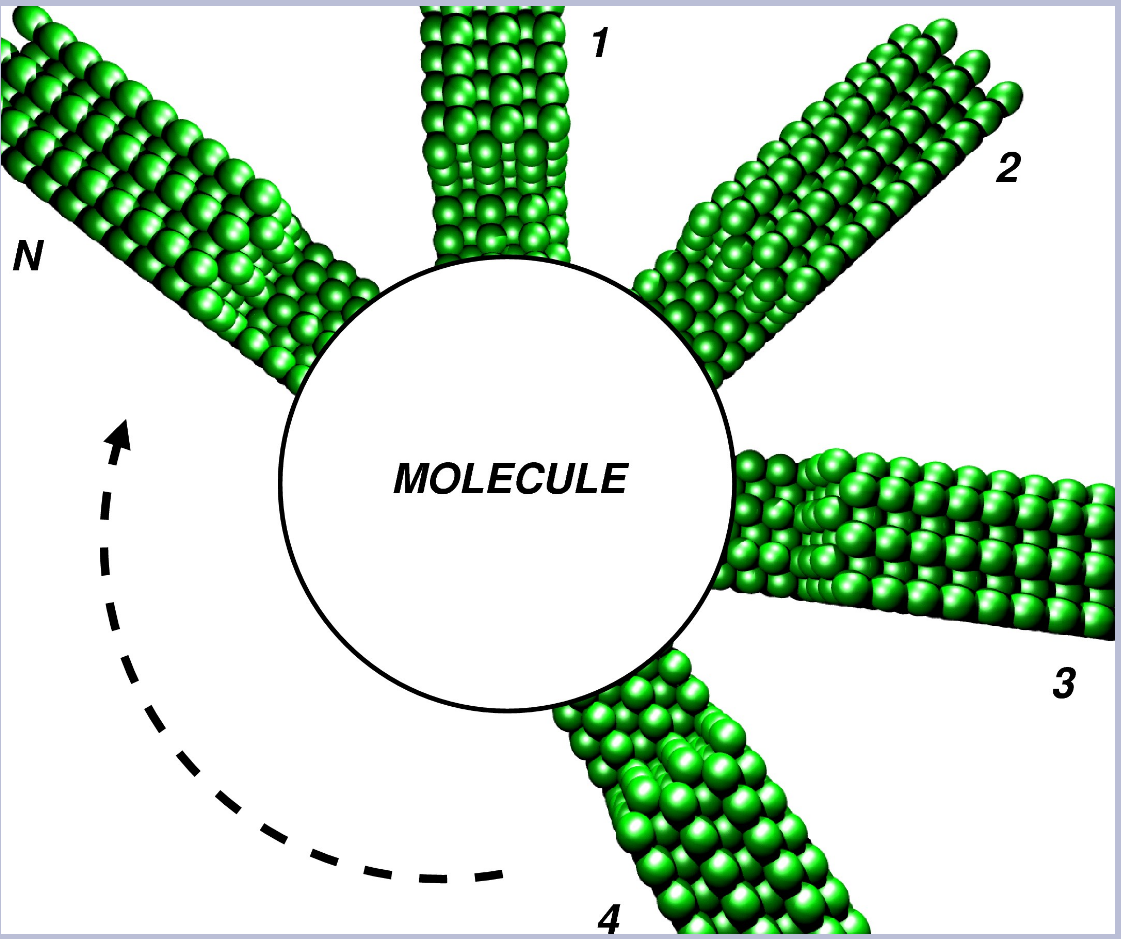
$$G = G_1 + G_2 + 2\,(G_1 \cdot G_2)^{1/2}$$

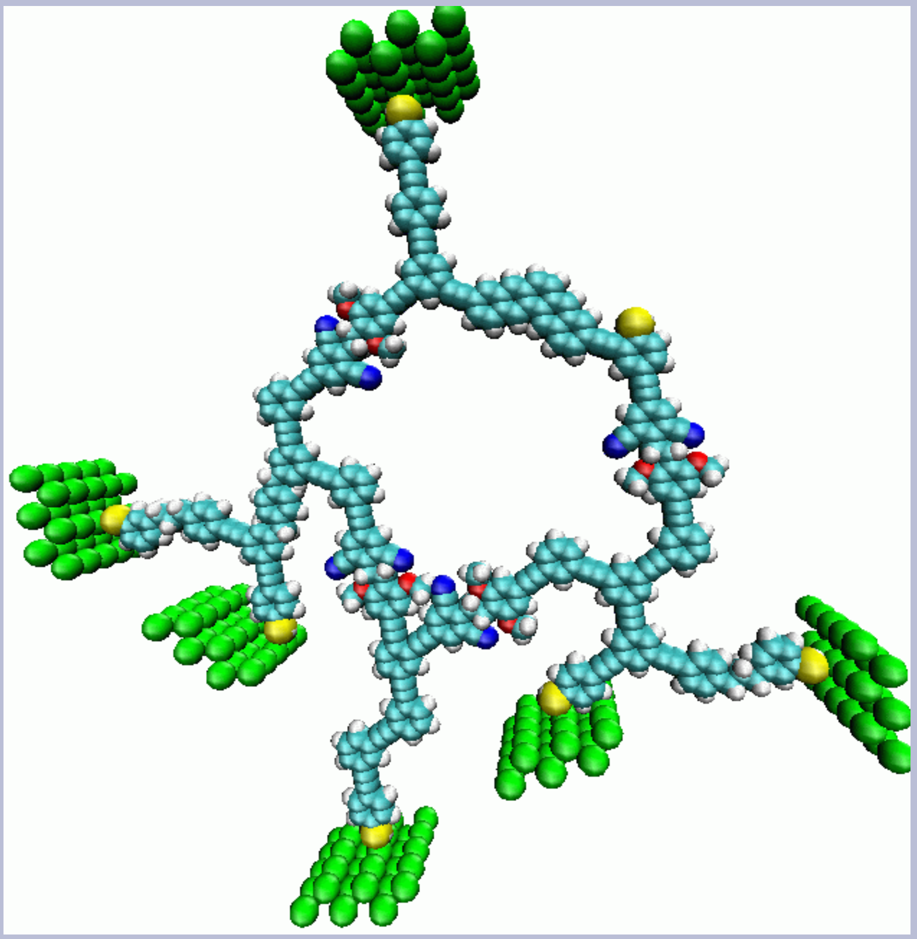
Phys. Rev. B, 59, 16011 (1999)

N-electrode Elastic Scattering Quantum Chemistry technique

(N-ESQC)

N-ESQC
Intramolecular electronic circuit simulator

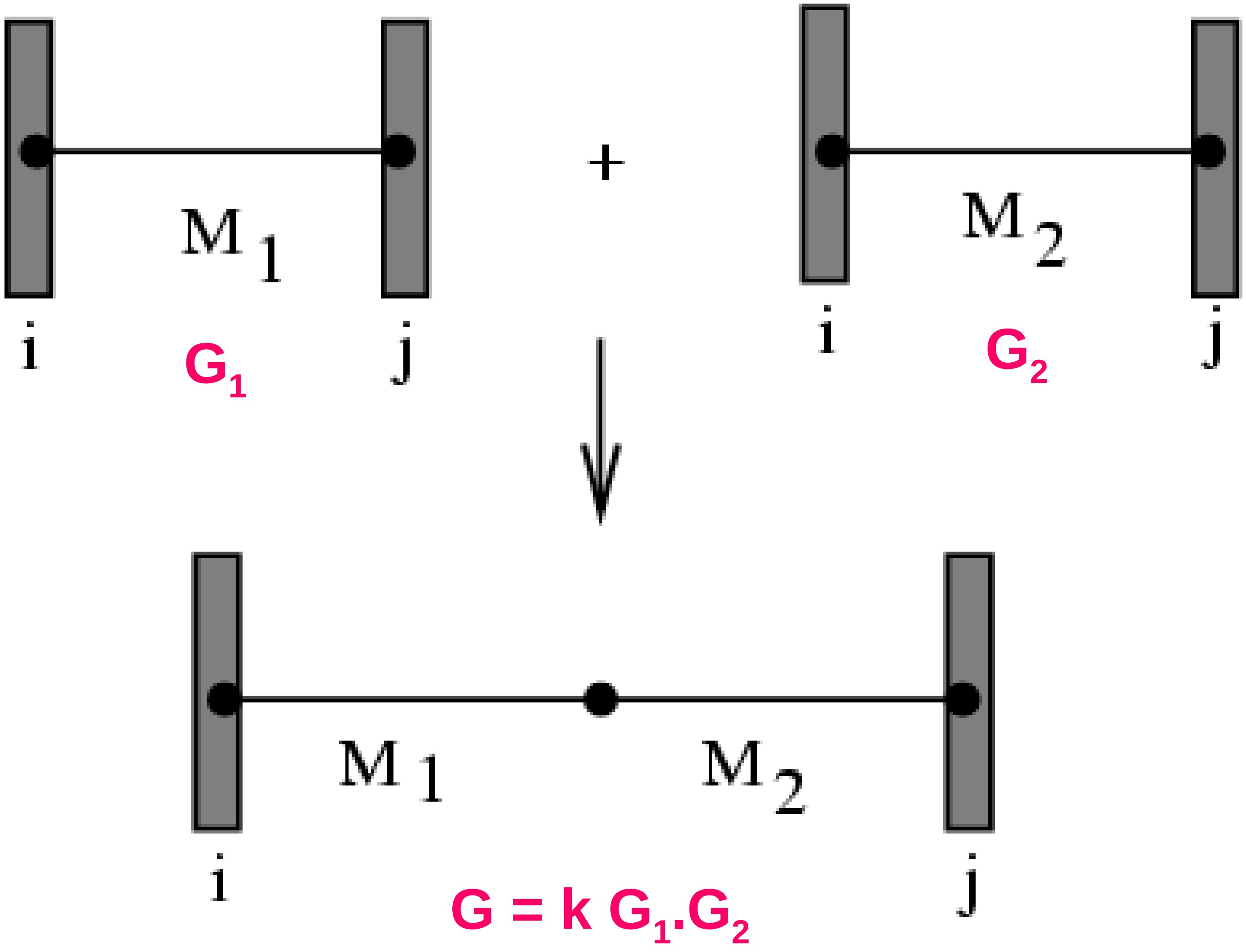




Chem. Phys. Lett. 367 (2002) 662

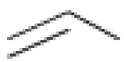
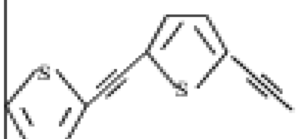
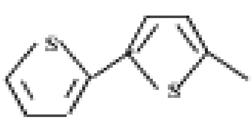
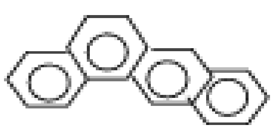
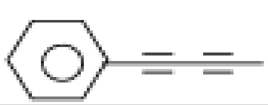
Molecular wires conductance

Serial association of 2 molecular wires



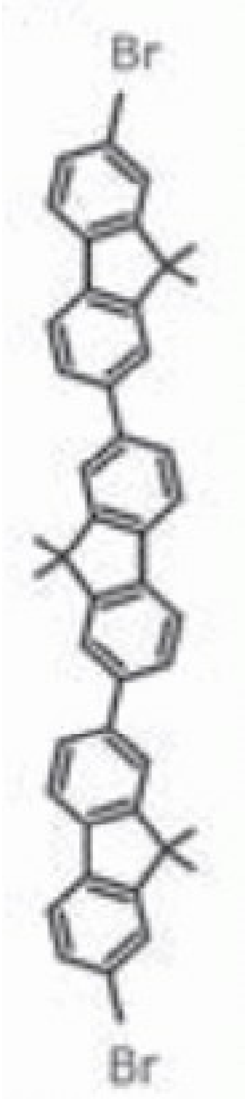
M. Magoga and C. Joachim Phys. Rev. B 59 (1999) 16011

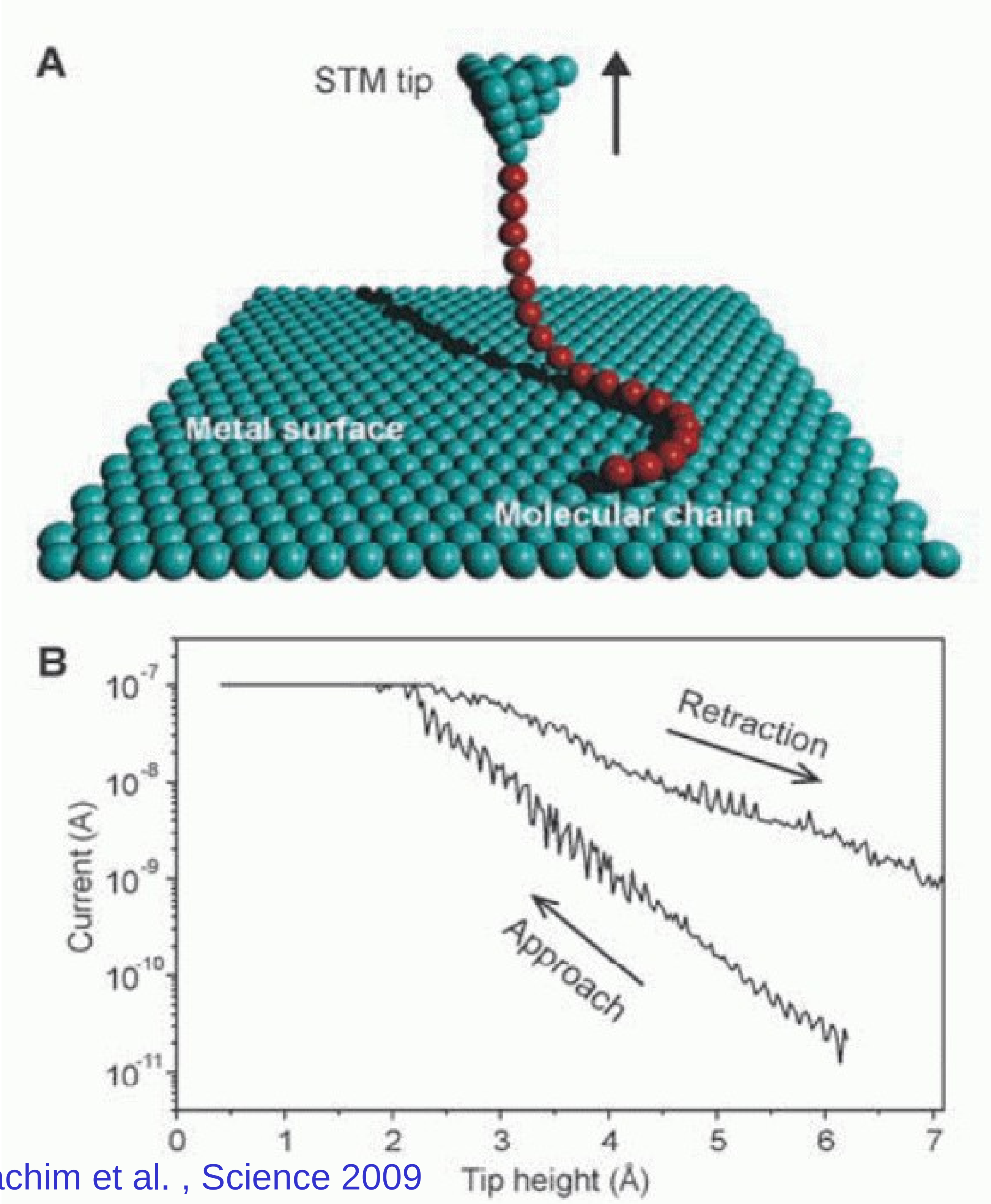
Organic molecular wires

Unite de fil molèculaire	γ ($Å^{-1}$)	$G_0(10^{-3})$	I(A)	E_g(eV)
Polyènes 	0.187	124	40×10^{-16}	1.11
Oligo(thiophène ethynylène) 	0.246	5.5	1.5×10^{-18}	1.22
Oligothiophène 	0.329	9.6	3.5×10^{-20}	1.53
Oligo(benzo Anthracène) 	0.395	41.3	7.8×10^{-23}	1.56
Oligo(phènyl–butadiyne) 	0.267	3.92	2×10^{-19}	1.75

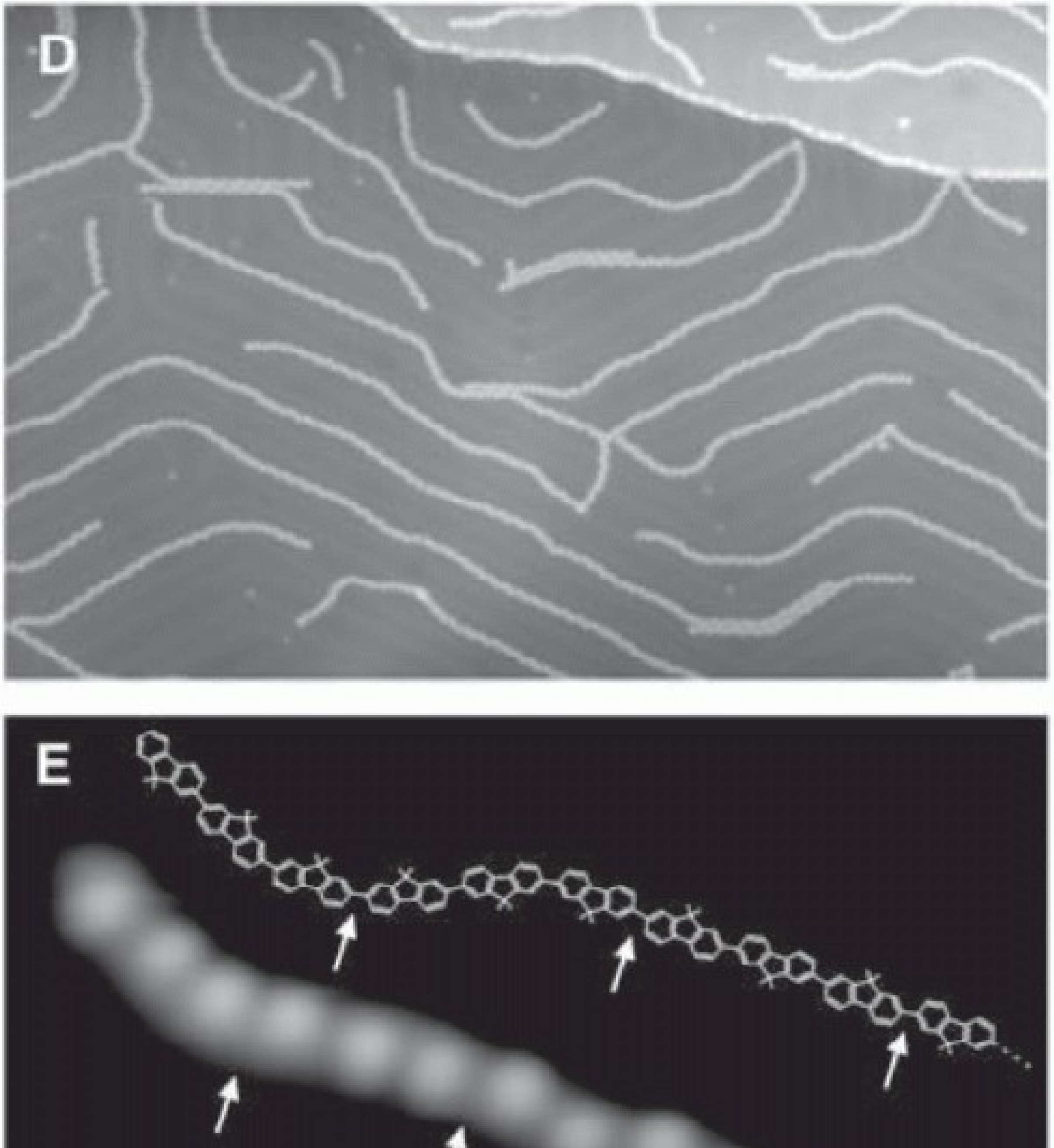
$$G=G_0\exp(-\gamma L)$$

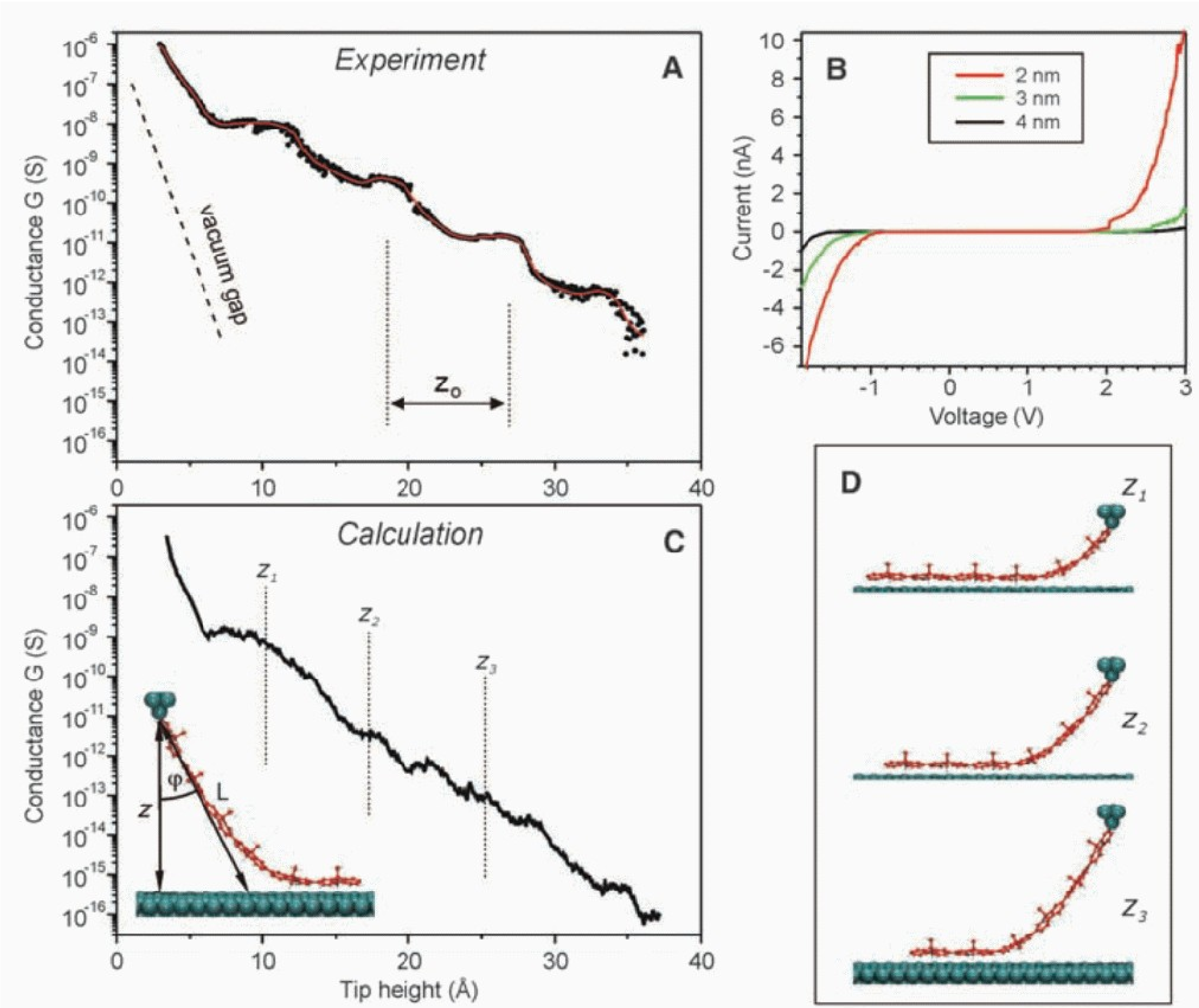
M. Magoga and C. Joachim; Phys. Rev. B (1999ç



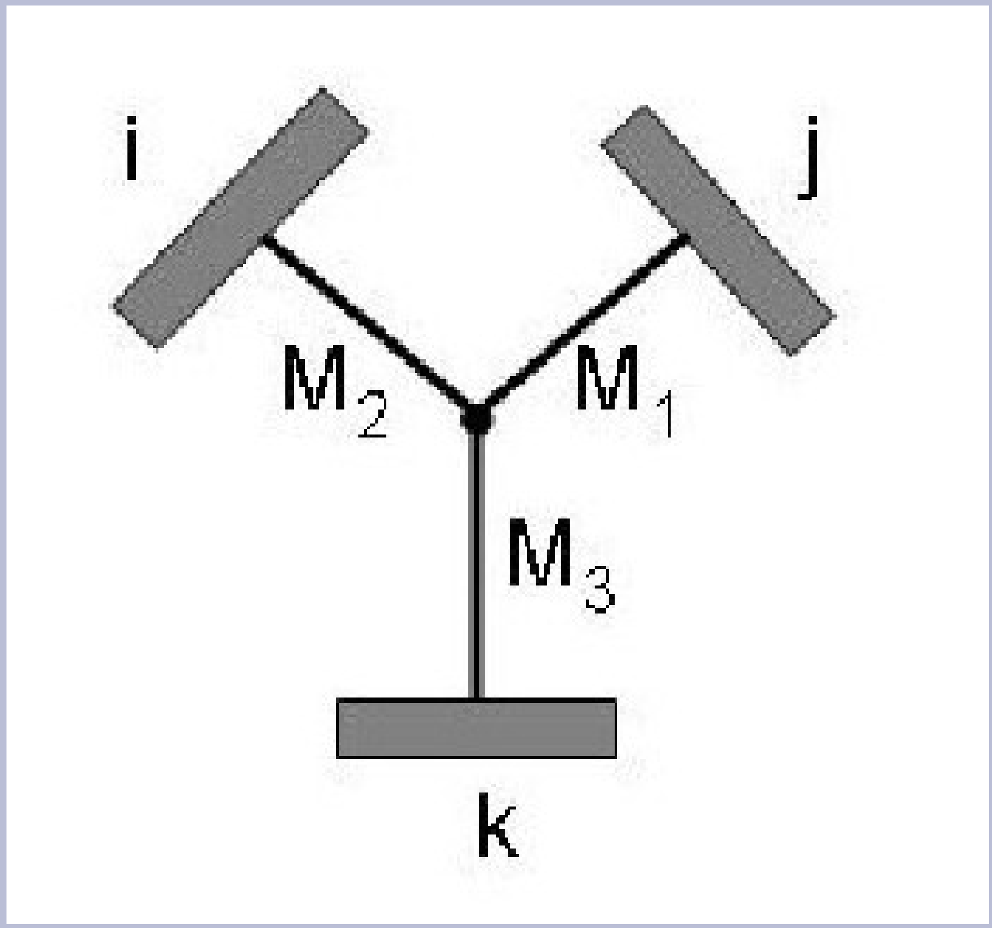


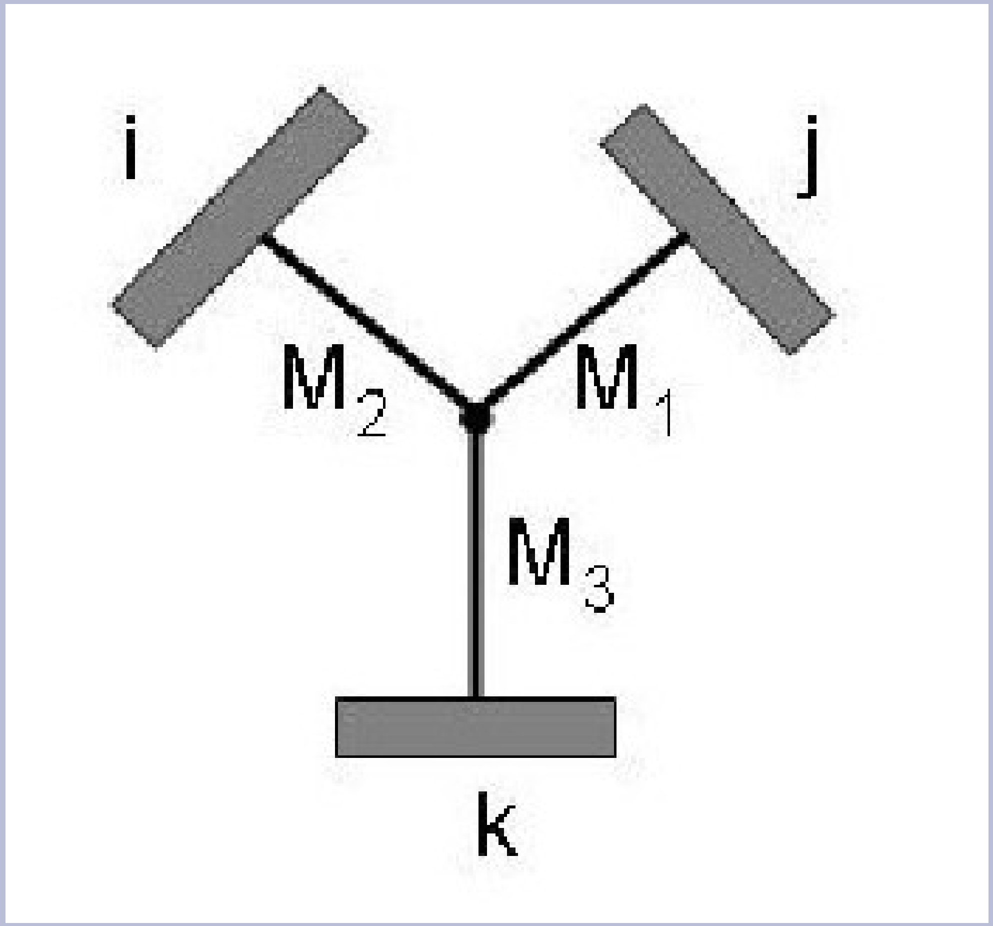
L. Grill, C. Joachim et al. , Science 2009

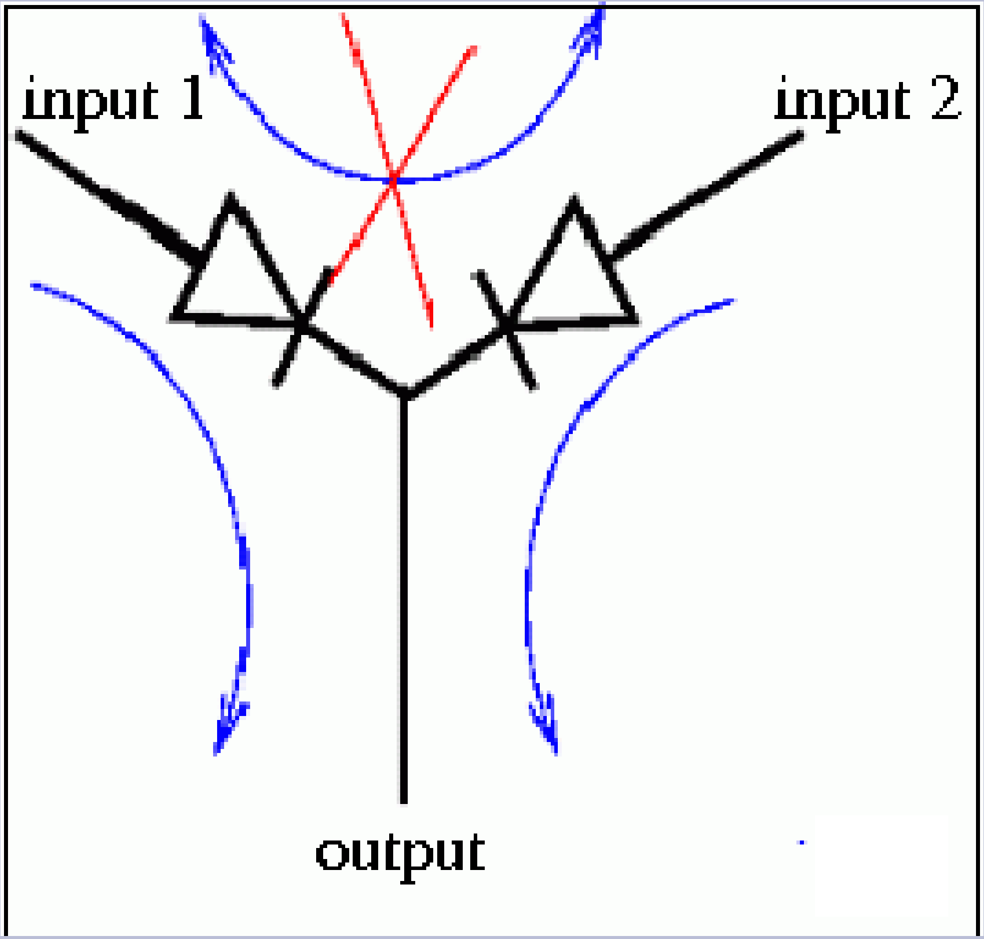

D
E



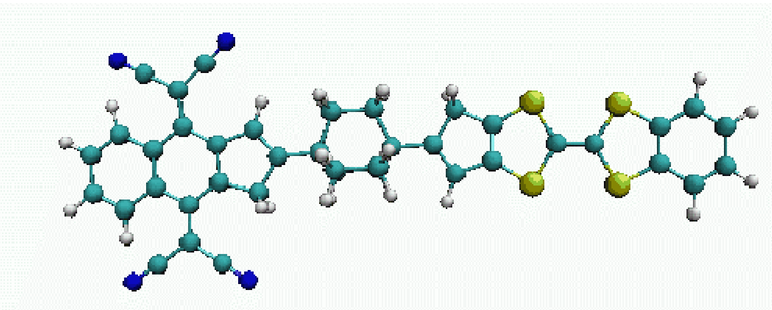
$$G=G_0\exp(-\gamma L)$$


i
j
M2
M1
M3
k


i
j
M2
M1
M3
k

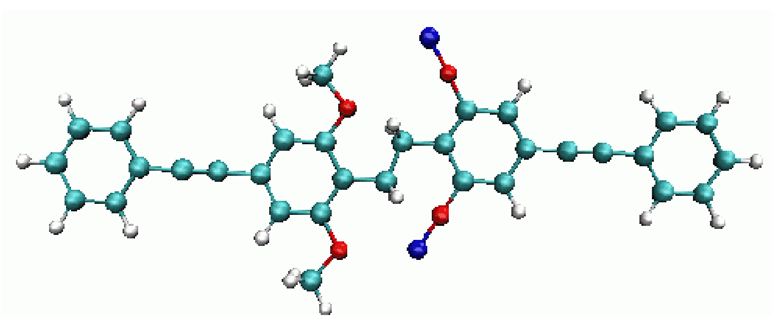

input 1
input 2
output

Diode based
single molecule logic gates



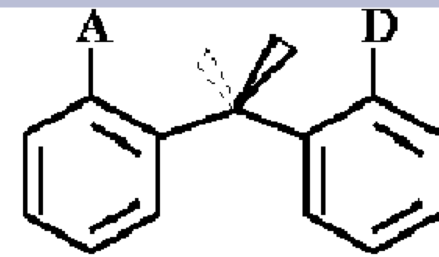
Aviram–Ratner diode

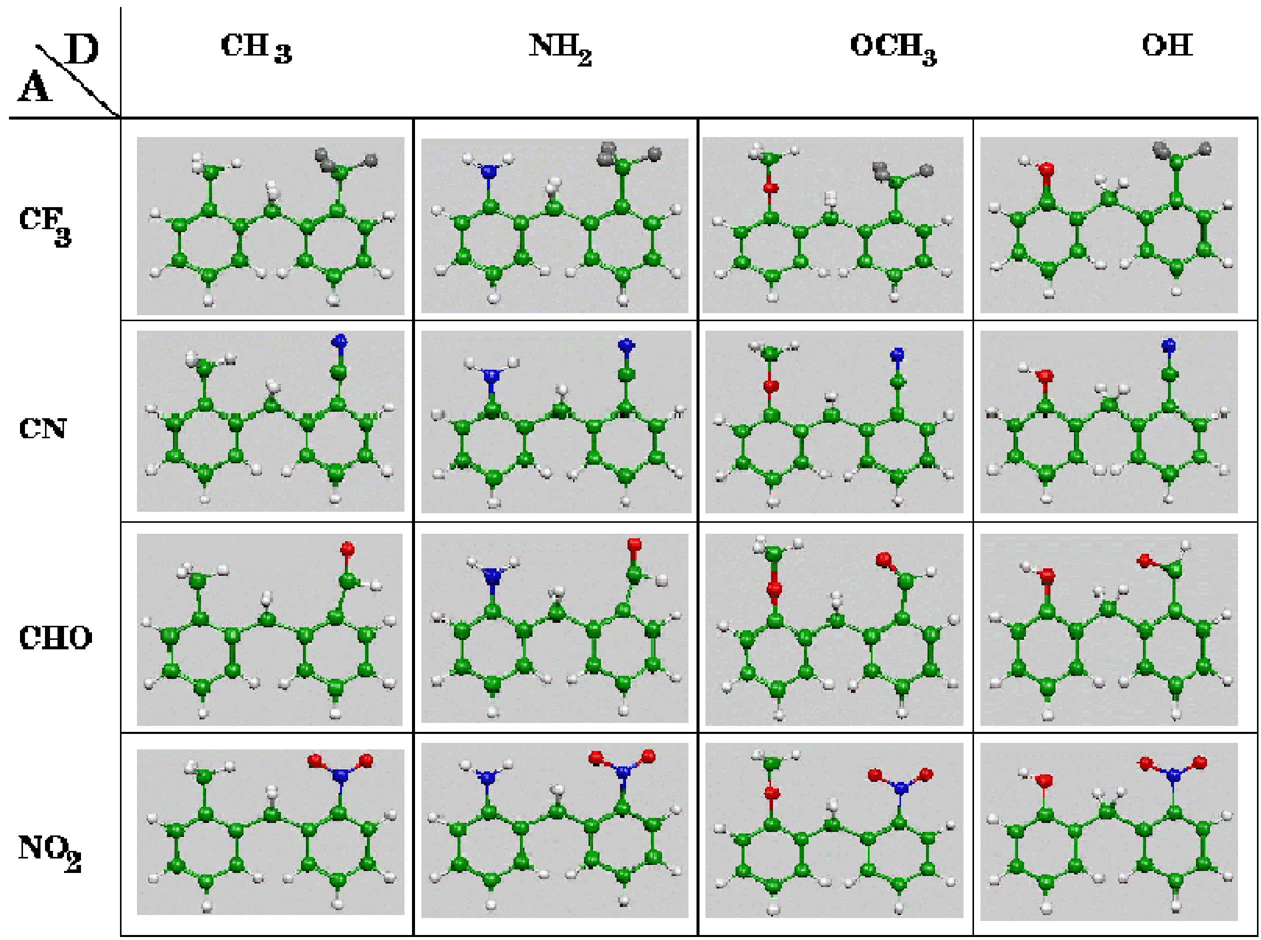
Chem. Phys. Lett. 29 (1974) 175



Ellenbogen–Mitre Corporation diode

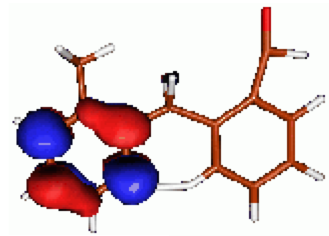
Proc. IEEE 88 (2000) 386



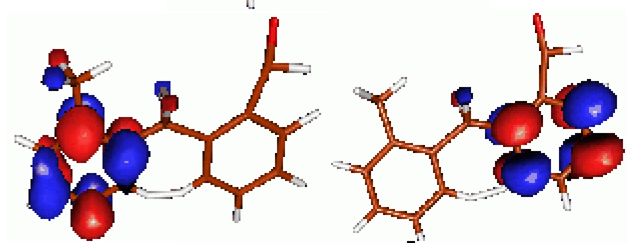


basical diodes

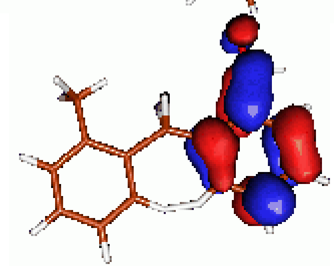
Diode : Frontier Molecular Orbitals



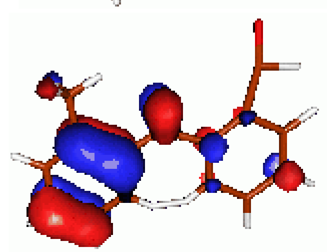
LUMO+2 : –8.39 eV



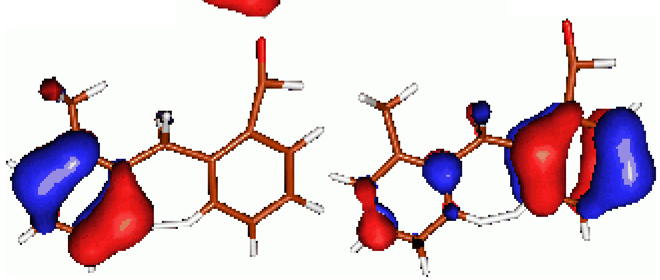
LUMOS+1 : –8.51 eV



LUMO : –10.12 eV



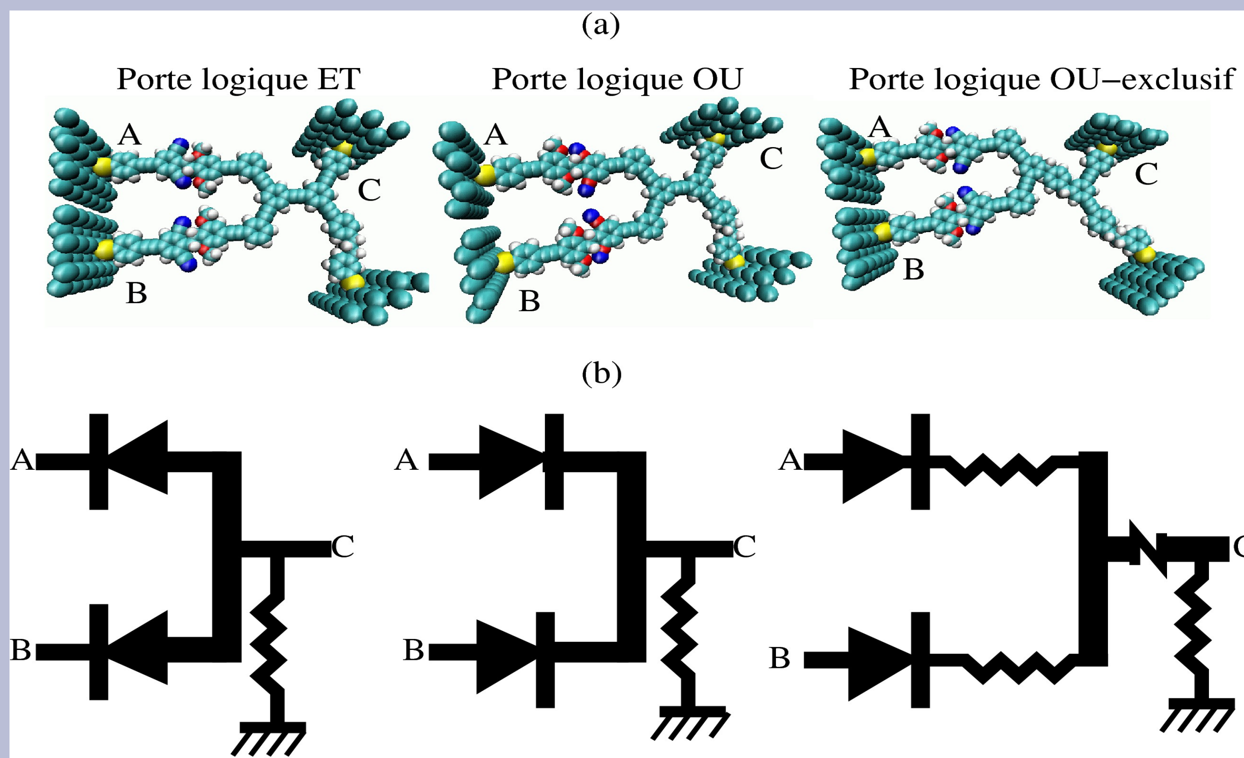
HOMO : –12.55 eV



HOMOS–1 : –12.90 e

Mono-molecular logic gate models

J. C. Ellenbogen and J. C. Love, Proc. IEEE 88 (2000) 386



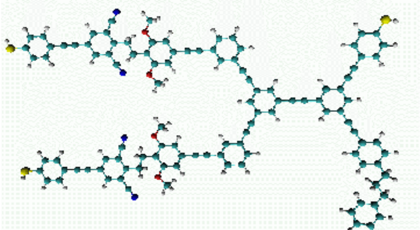
(c)

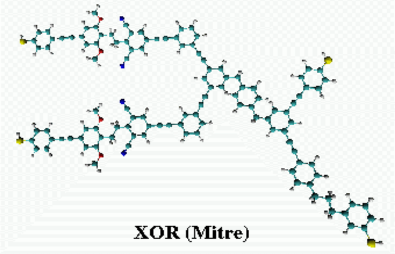
A	B	C
0	0	0
0	1	0
1	0	0
1	1	1

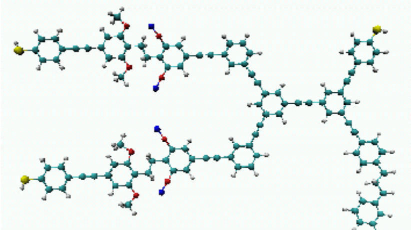
A	B	C
0	0	0
1	0	1
0	1	1
1	1	1

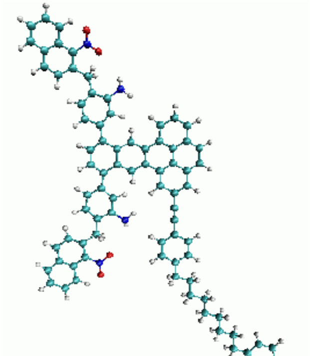
A	B	C
0	0	0
1	0	1
0	1	1
1	1	0

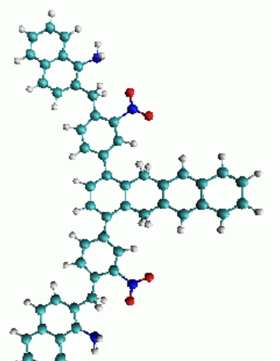
Examples of elementary logic gates

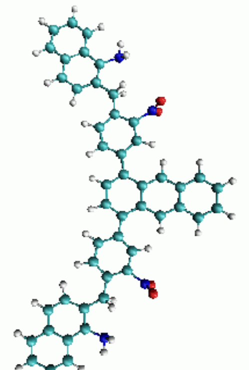

AND (Mitre)

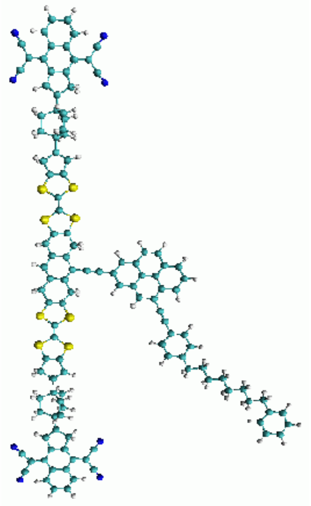

XOR (Mitre)

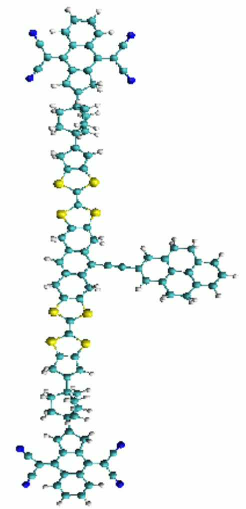

OR (Mitre)

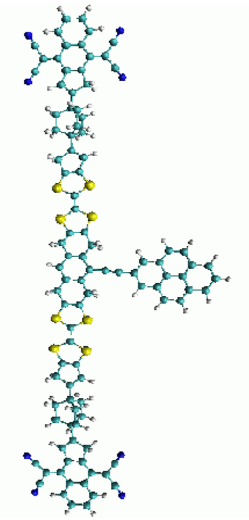

AND


XOR

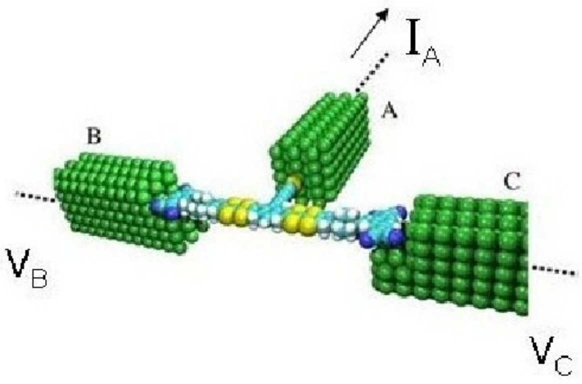

OR

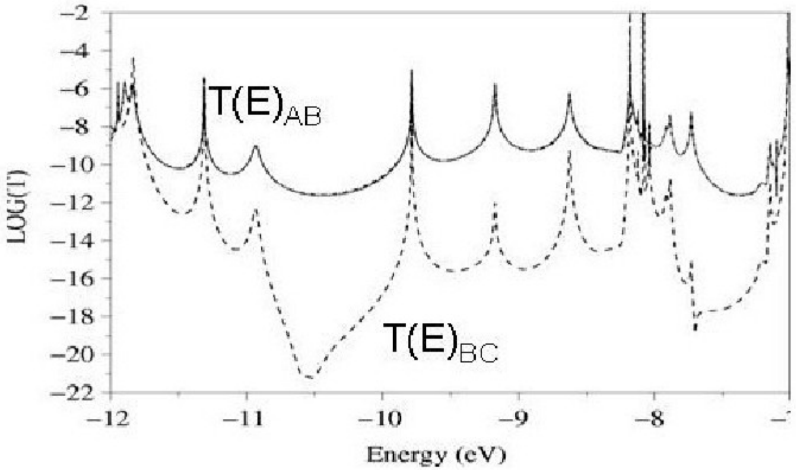

AND (Aviram)

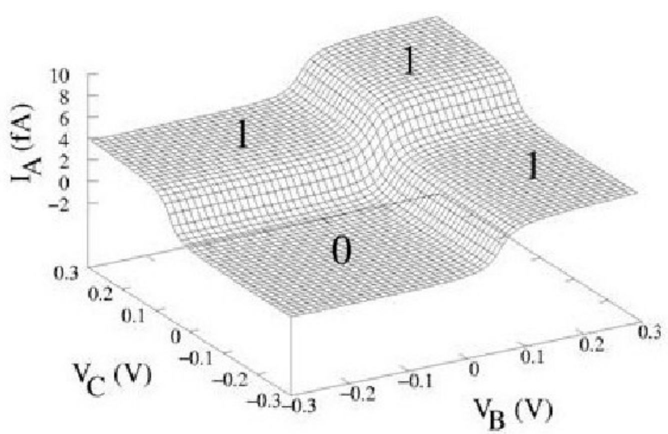

XOR (Aviram)


OR (Aviram)

An OR mono-molecular logic gate

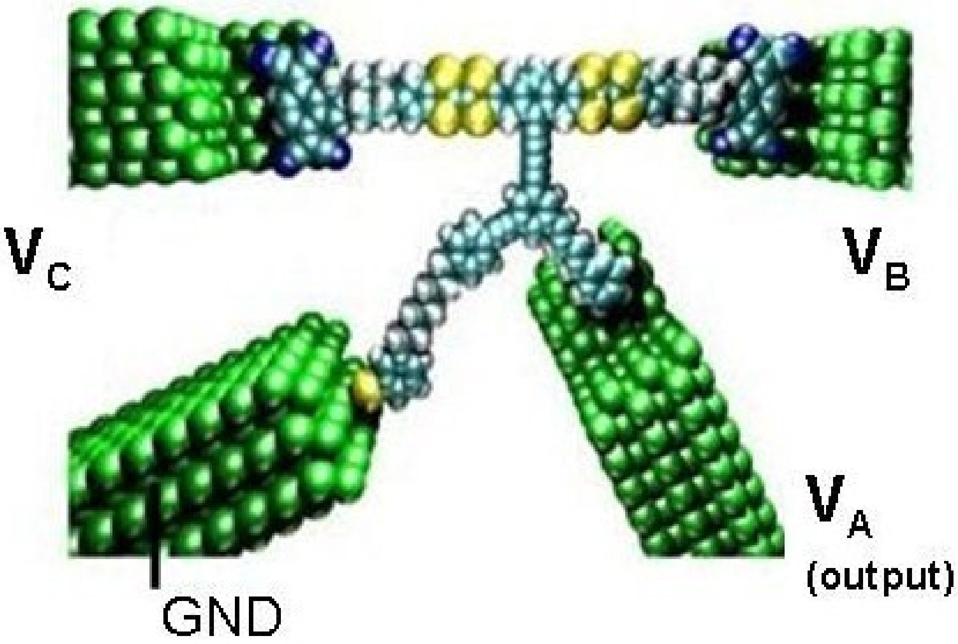


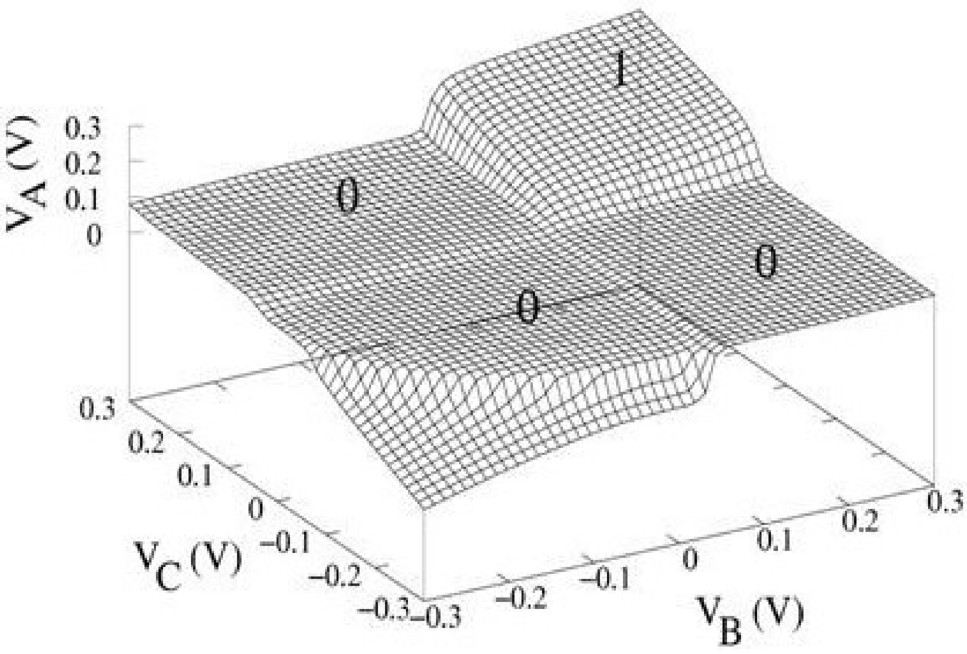




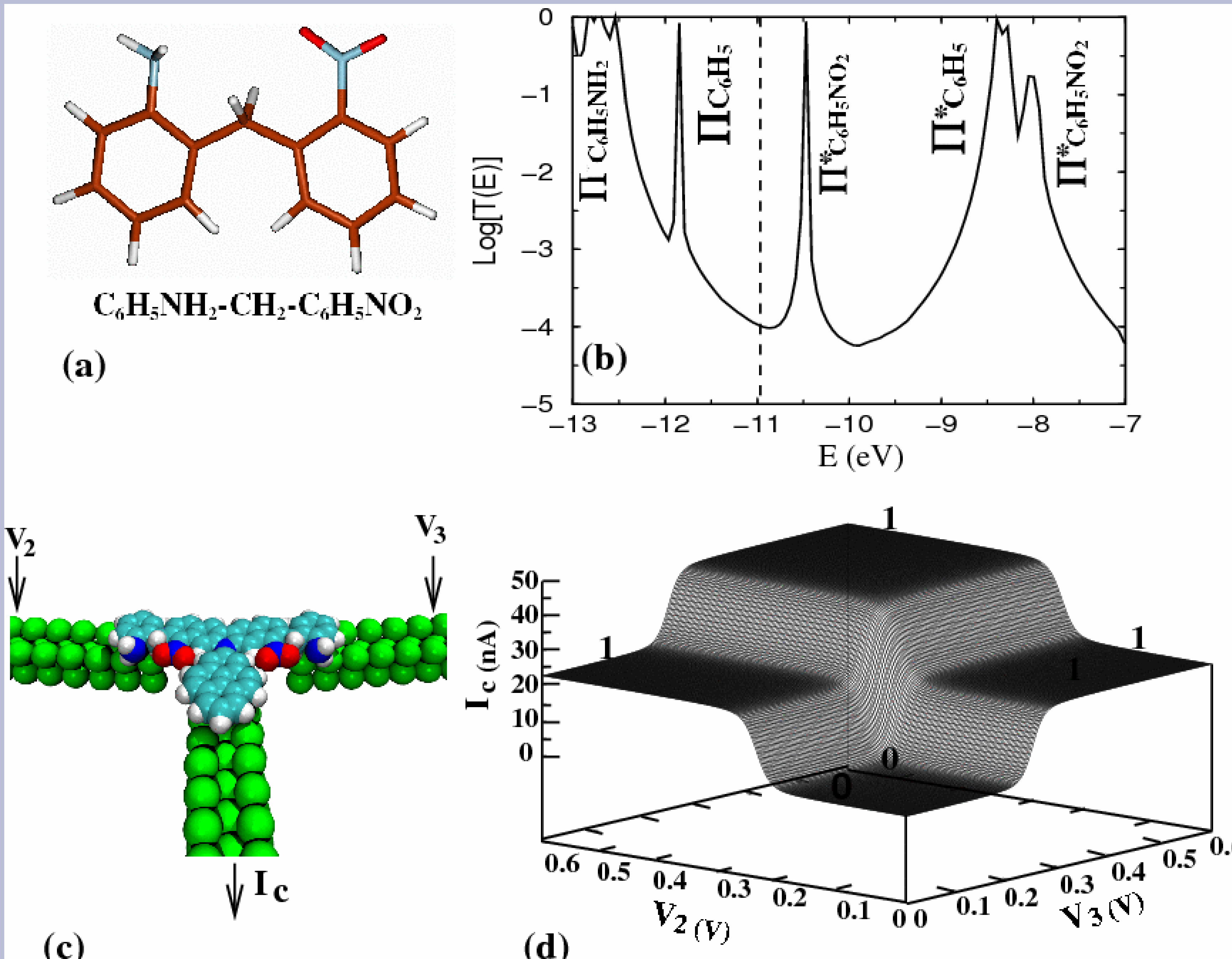
Chem. Phys. Lett. 367 (2002) 662

An AND mono-molecular logic gate





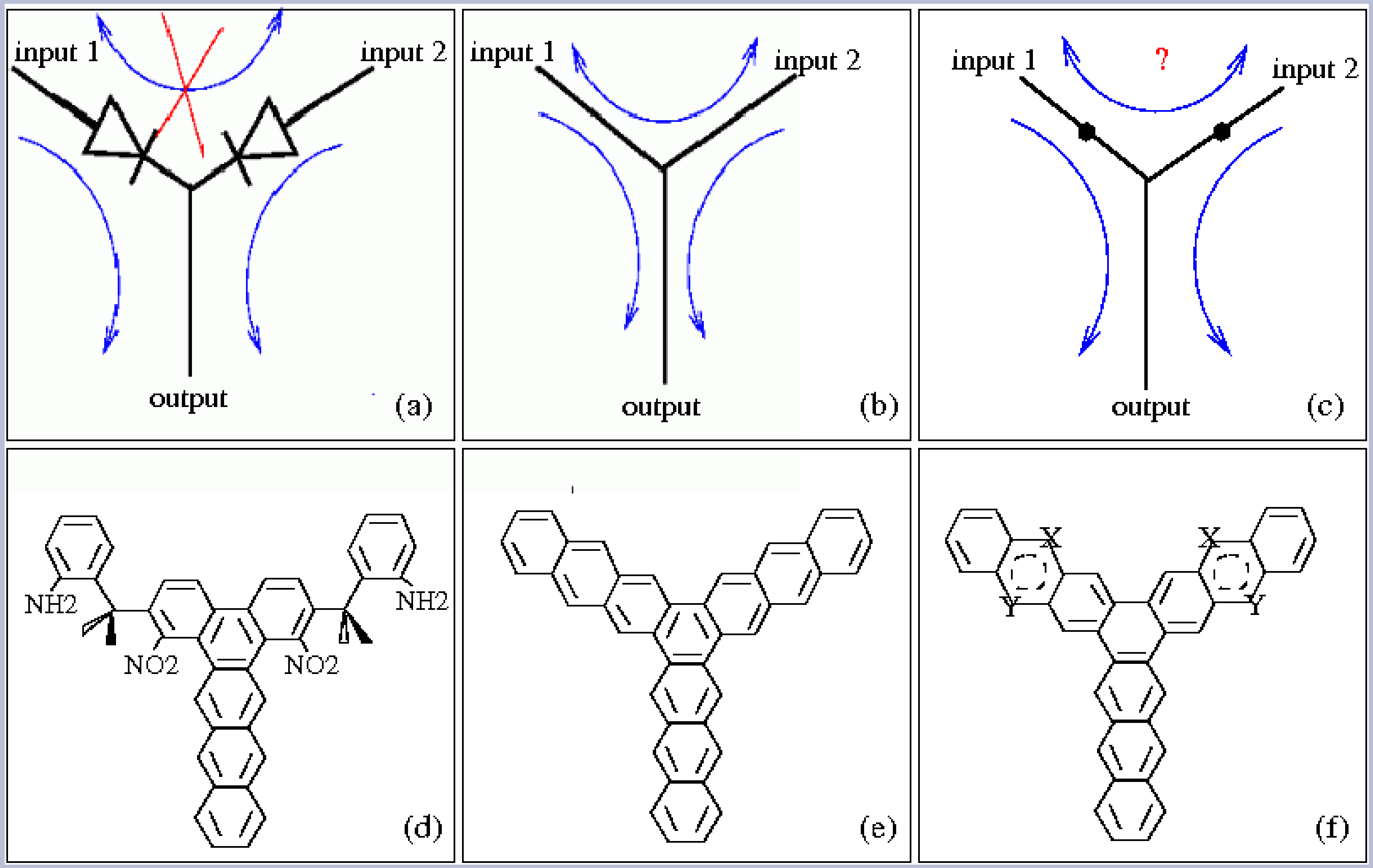
Chem. Phys. Lett. 367 (2002) 662



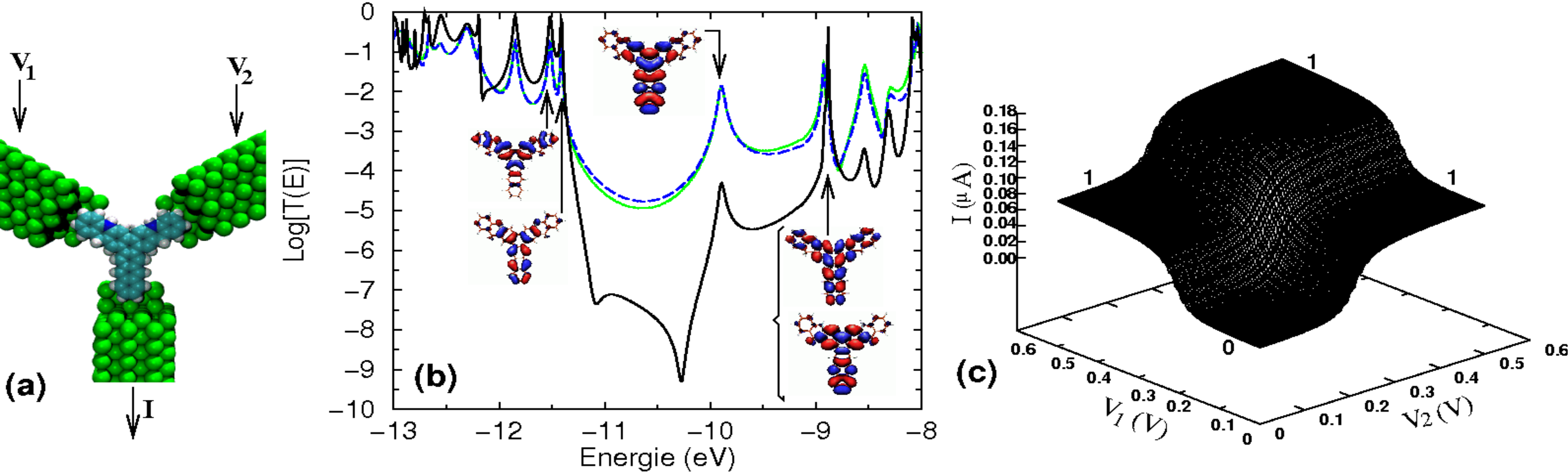
C6H5NH2-CH2-C6H5NO2
(a)
0
−1
−2
−3
−4
−5
Log[T(E)]
−13
−12
−11
−10
−9
−8
−7
E (eV)
Π C6H5NH2
Π C6H5
Π* C6H5NO2
Π* C6H5
Π* C6H5NO2
(b)
V2
V3
I c
(c)
50
40
30
20
10
0
I c (nA)
1
1
1
1
0
0
0.6
0.5
0.4
0.3
0.2
0.1
0
V2 (V)
0
0.1
0.2
0.3
0.4
0.5
0.6
V3 (V)
(d)

Anti-resonance peaks :
Use the interference effects

OR logic gate with no rectifier



OR-molecule logic gate
Involving interference effects

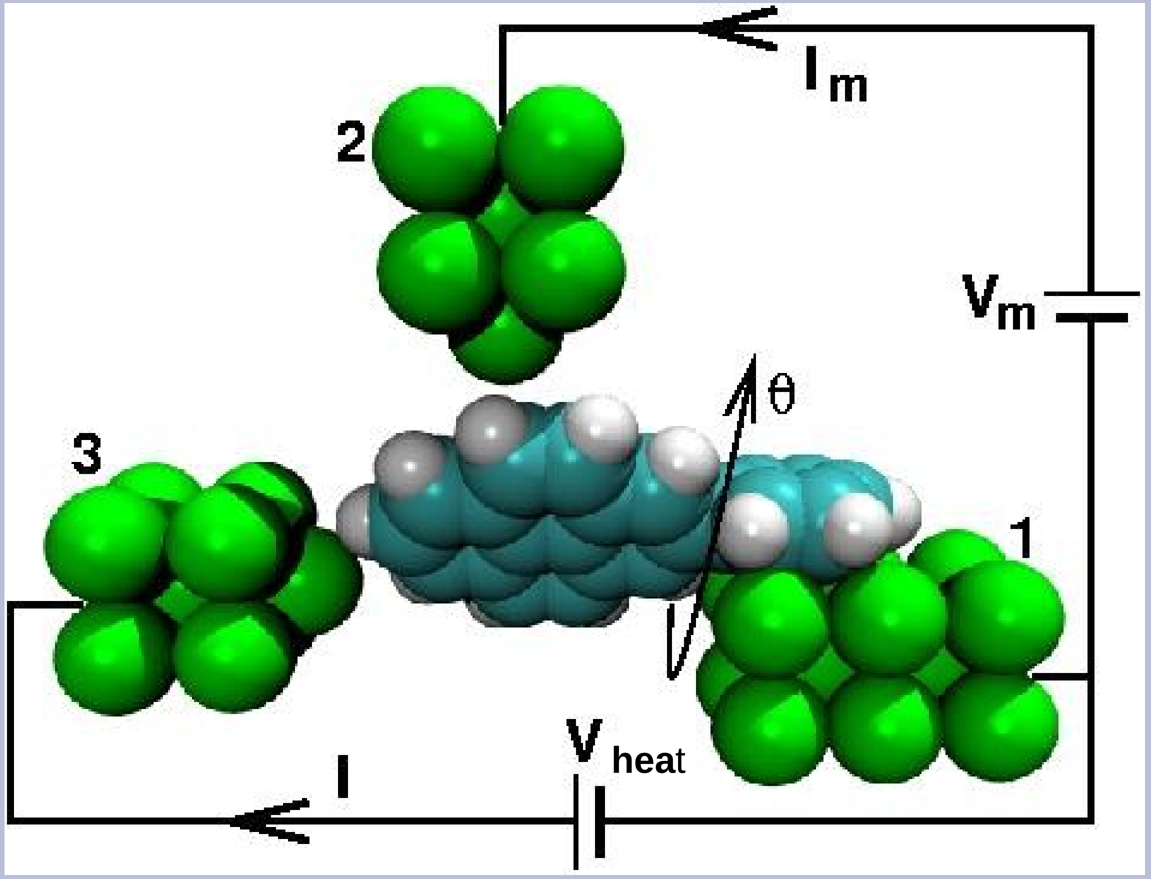


Chem. Phys. Lett. 470 (2009) 275

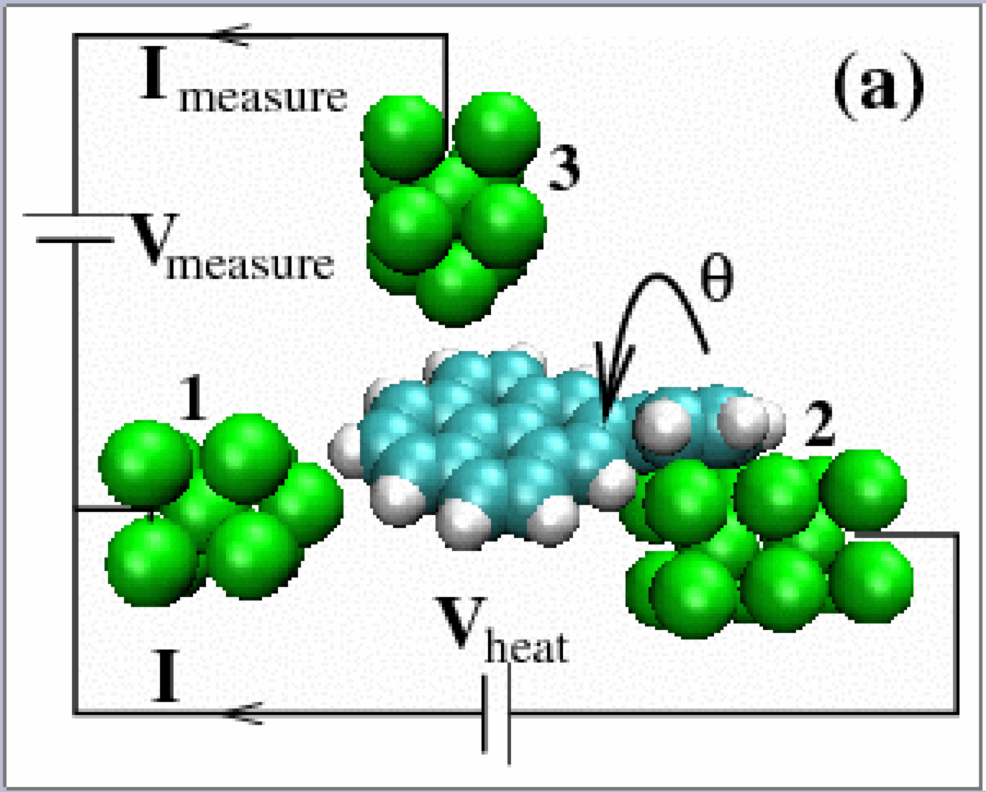
Tunnel inelastic effects

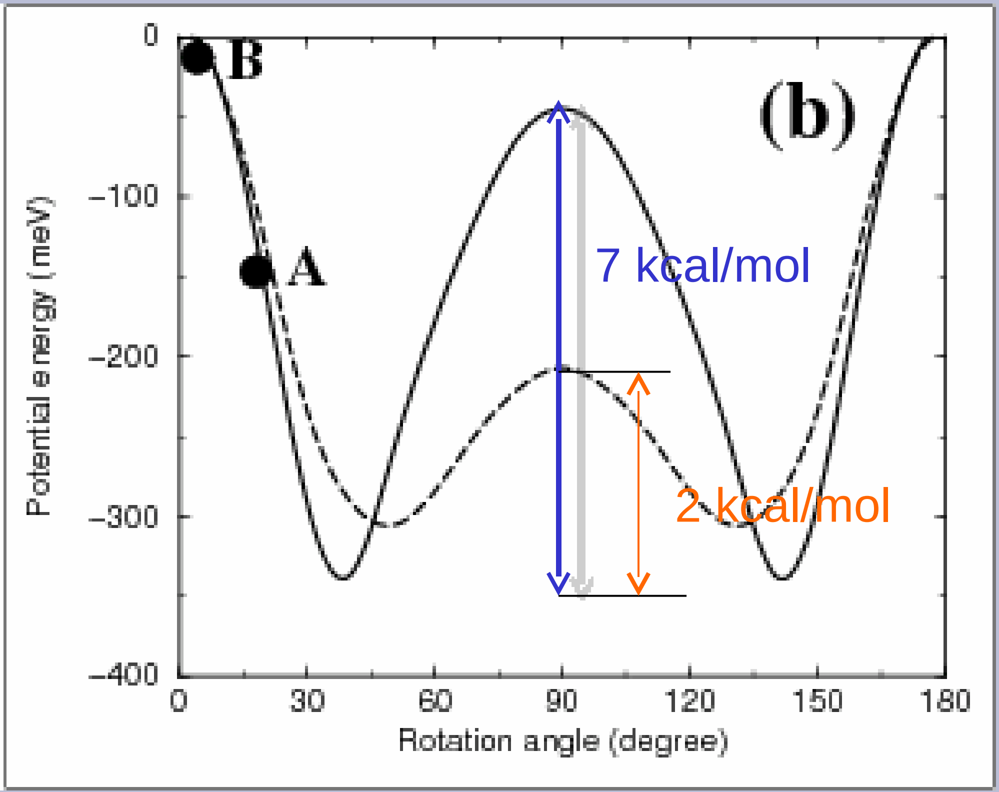
Current transduction effect

3-terminal transducer device



3-terminal transducer device



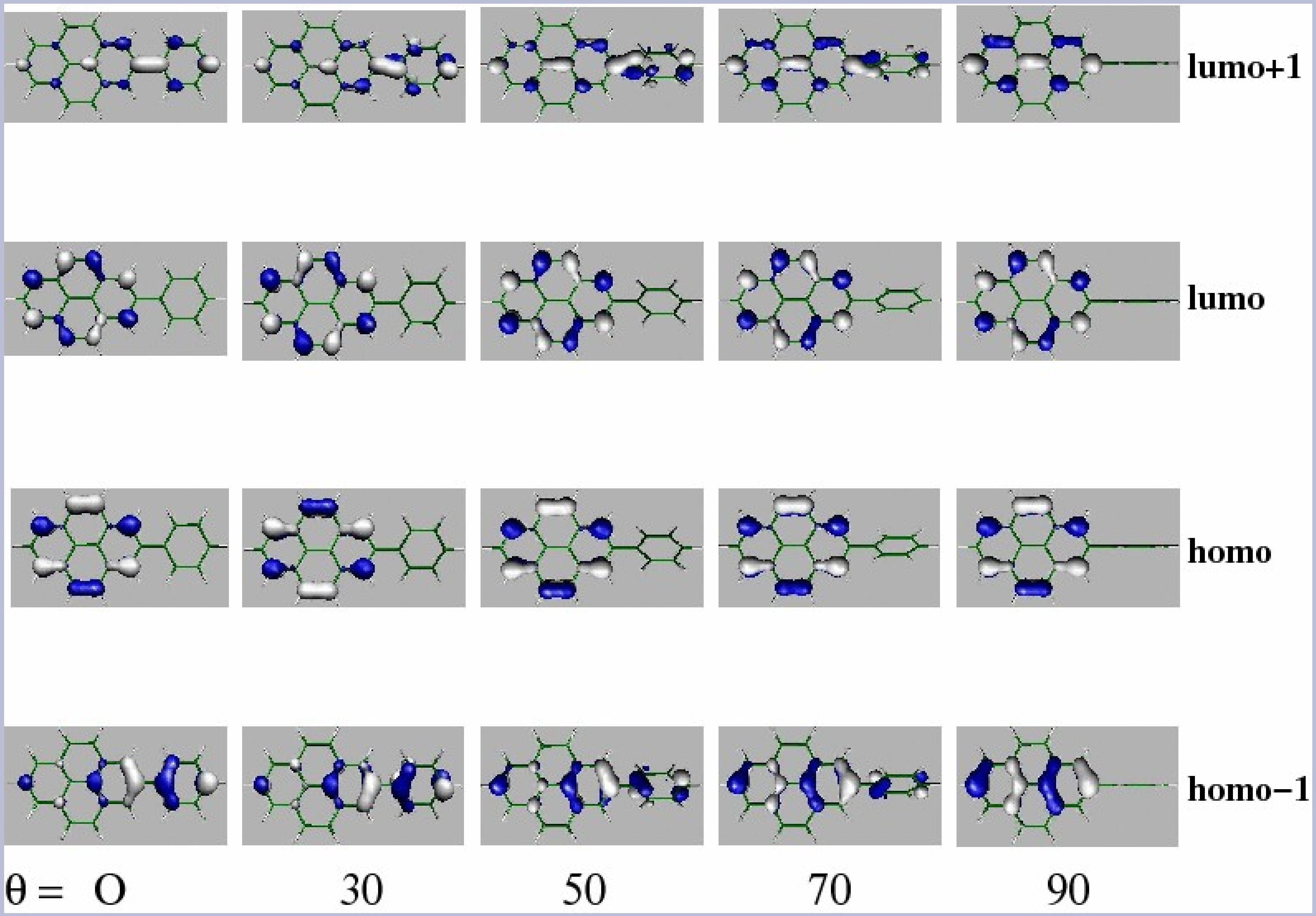


$K_{eq} = 4.61 \text{ N m}^{-1}$

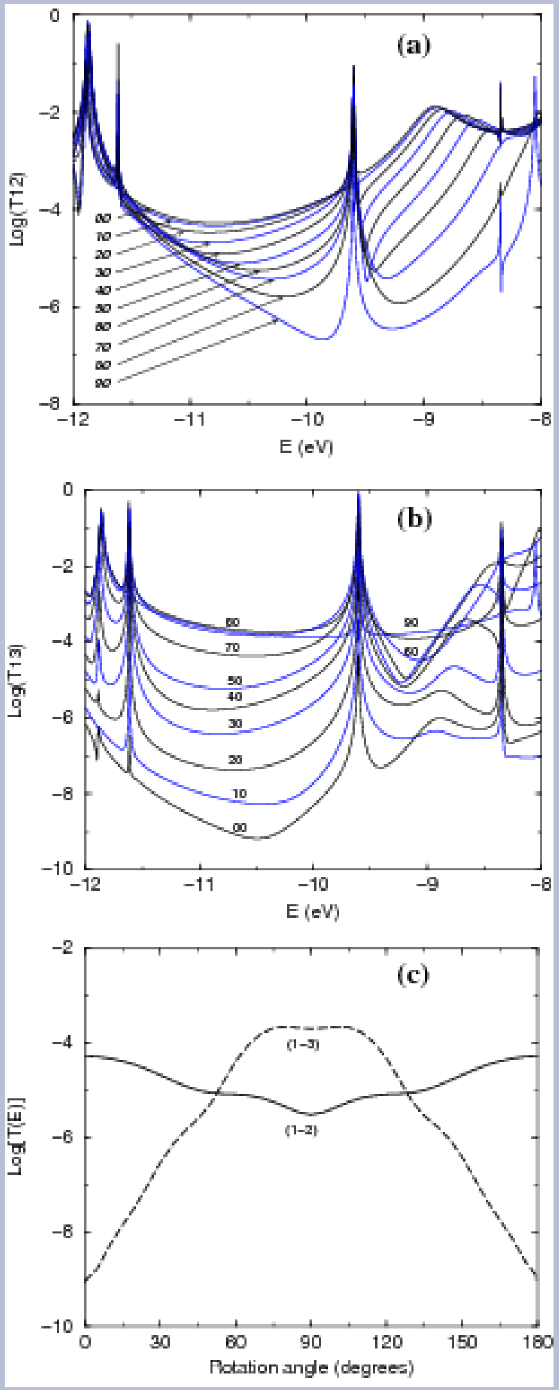
S. Ami, M. Hliwa, C. Joachim, Chem. Phys. Lett. 425 (2006) 356

Mono-molecular amperometer

FMO structures



Elastic tunnelling electron transmission spectra



Log{T(E,Θ)} at E =E_F = 10.8 eV

XOR logic gate : Inelastic force

$$J\frac{\partial^2\theta}{\partial t^2} = -\frac{\partial U(\theta)}{\partial\theta} + \eta J\frac{\partial\theta}{\partial t} + F_{in}(I,\theta)$$

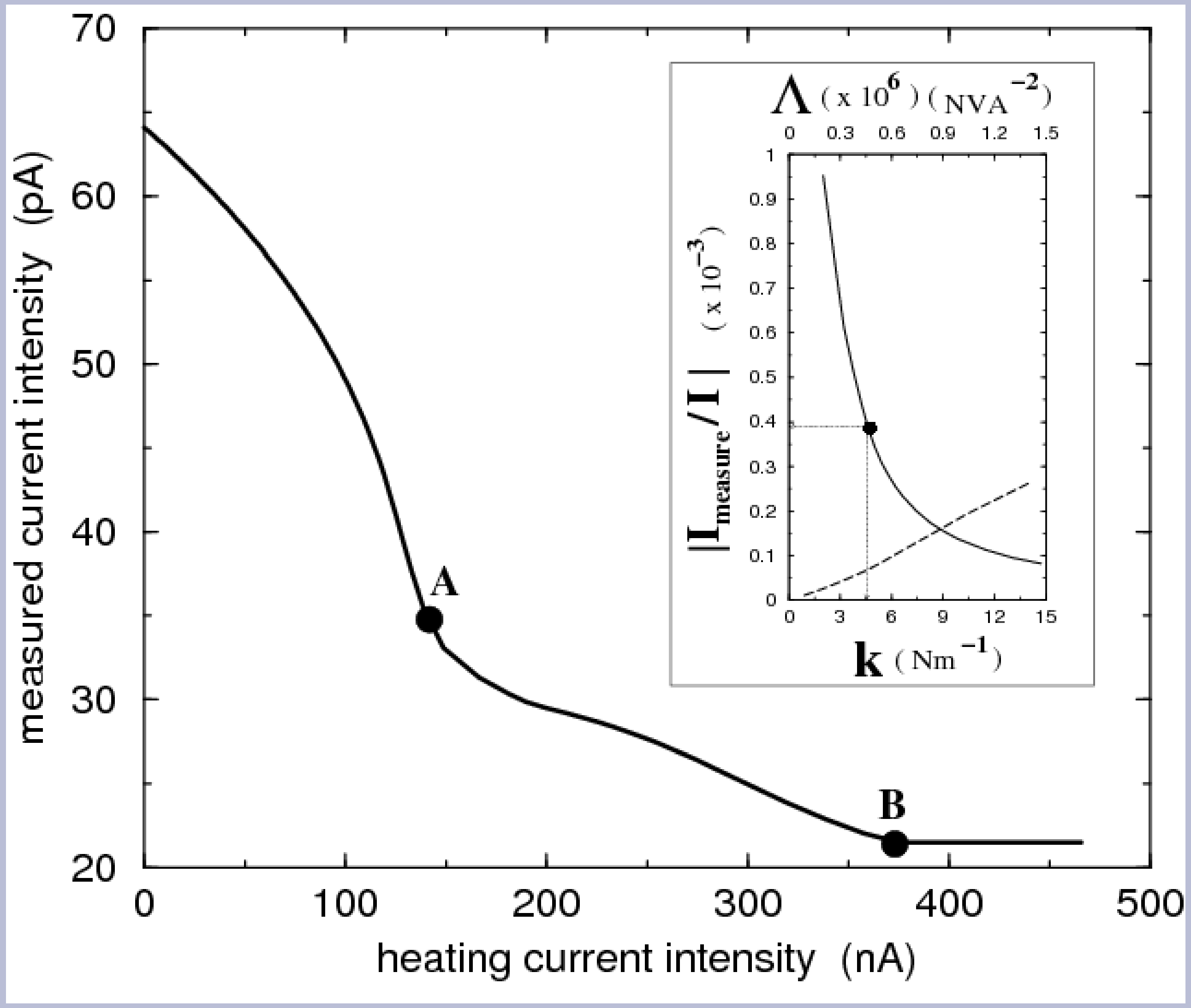
$$E_{in}(I,\theta) = 2\pi^2 g\gamma_{in}\lambda(\theta)\frac{\pi\hbar}{e^2 V_{heat}}\tau\frac{I^2}{e}$$

$$F_{in}(I,\theta) = \Lambda\frac{I}{V_{heat}}\frac{\partial I}{\partial\theta}$$

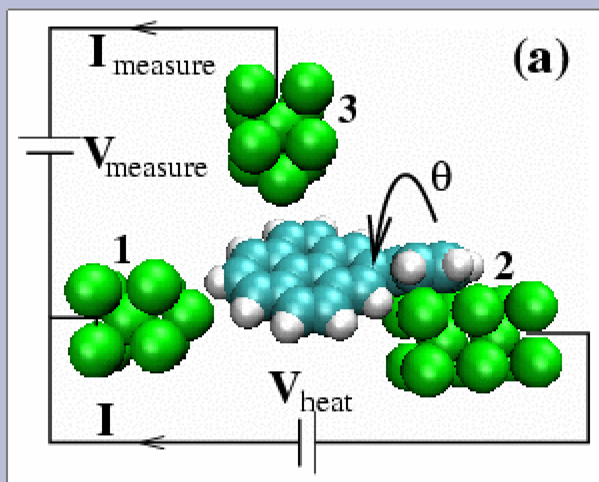
$$\Lambda = \frac{4\pi^2\lambda(\theta)}{e^2}\gamma_{in}\frac{\tau}{e}\pi\hbar$$

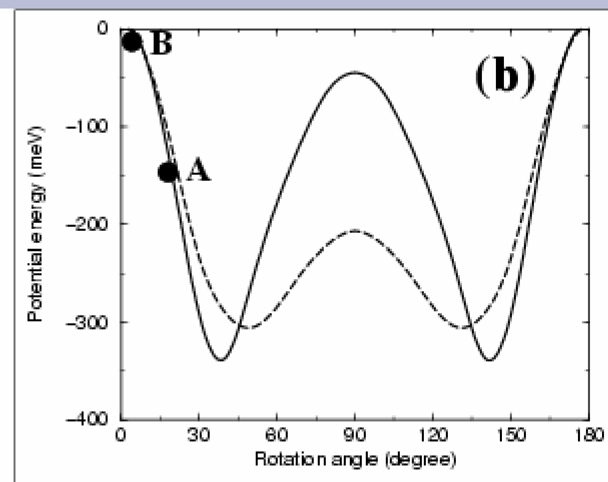
$$\lambda(\theta) = g\left\langle v_r\right|\hat{\theta}\left|v_s\right\rangle = g\sqrt{\frac{\hbar}{2J\omega}}$$

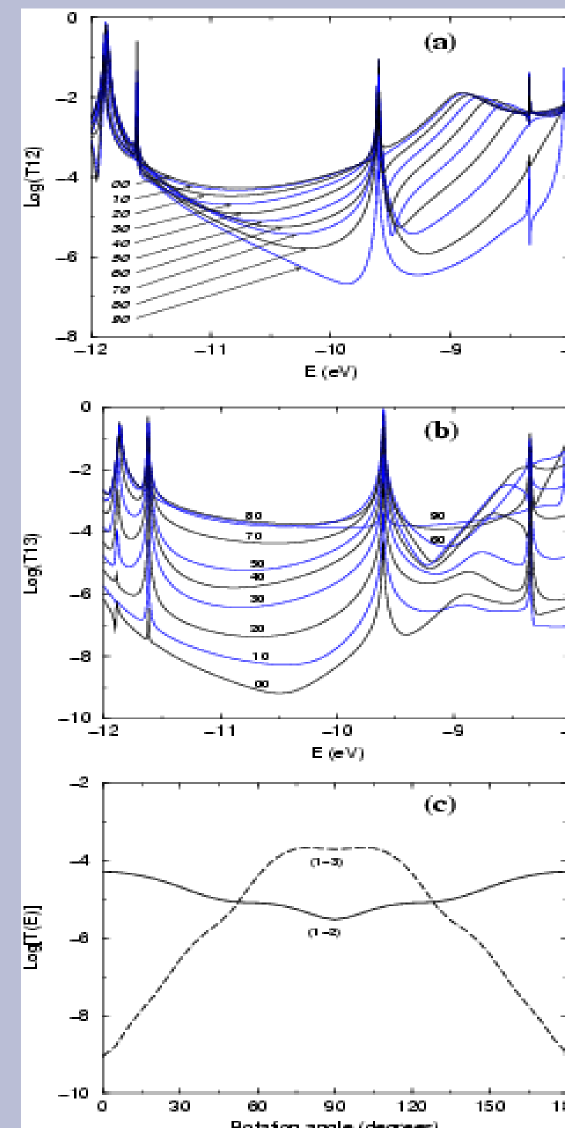
Current transduction effect

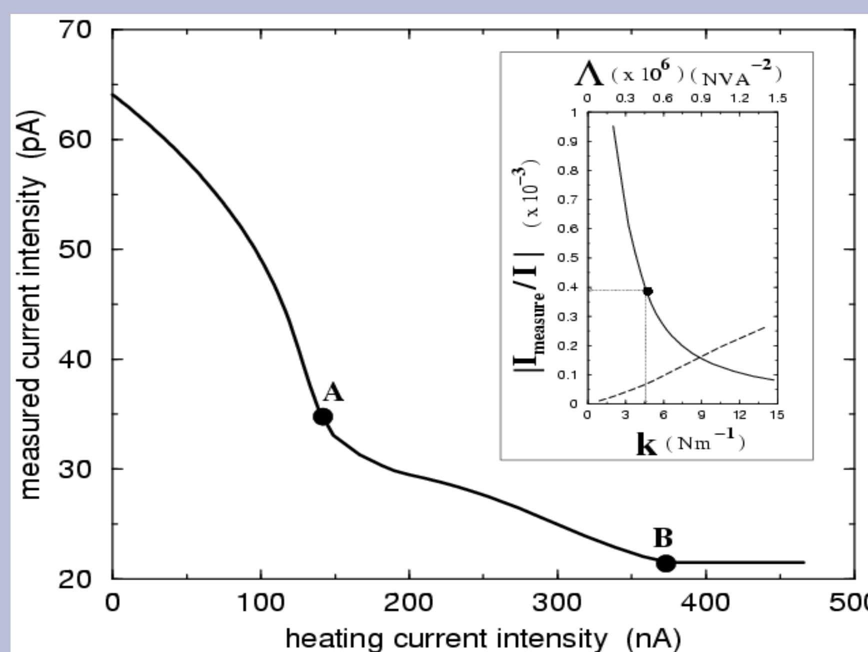


Mono-molecular amperometer





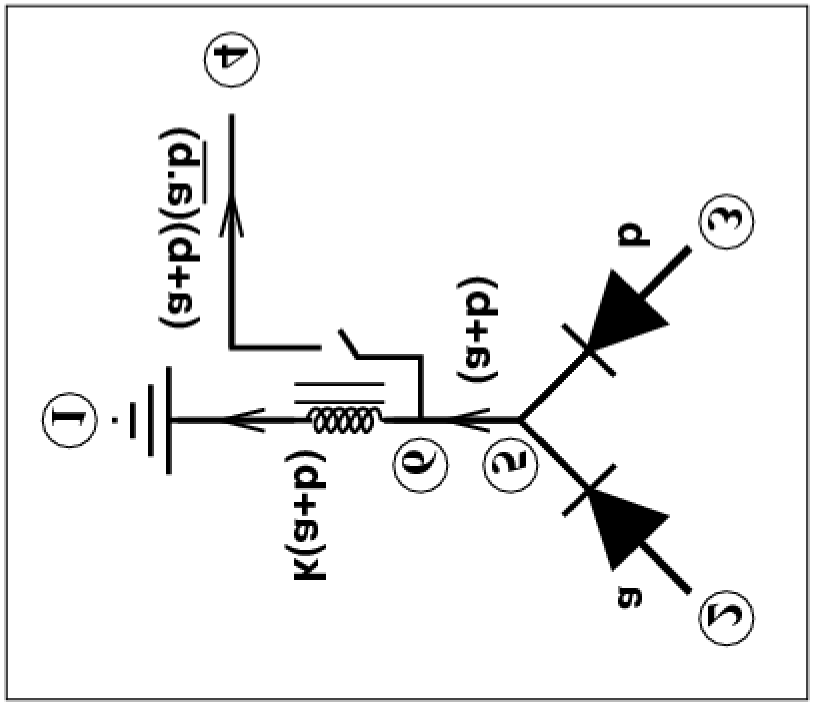


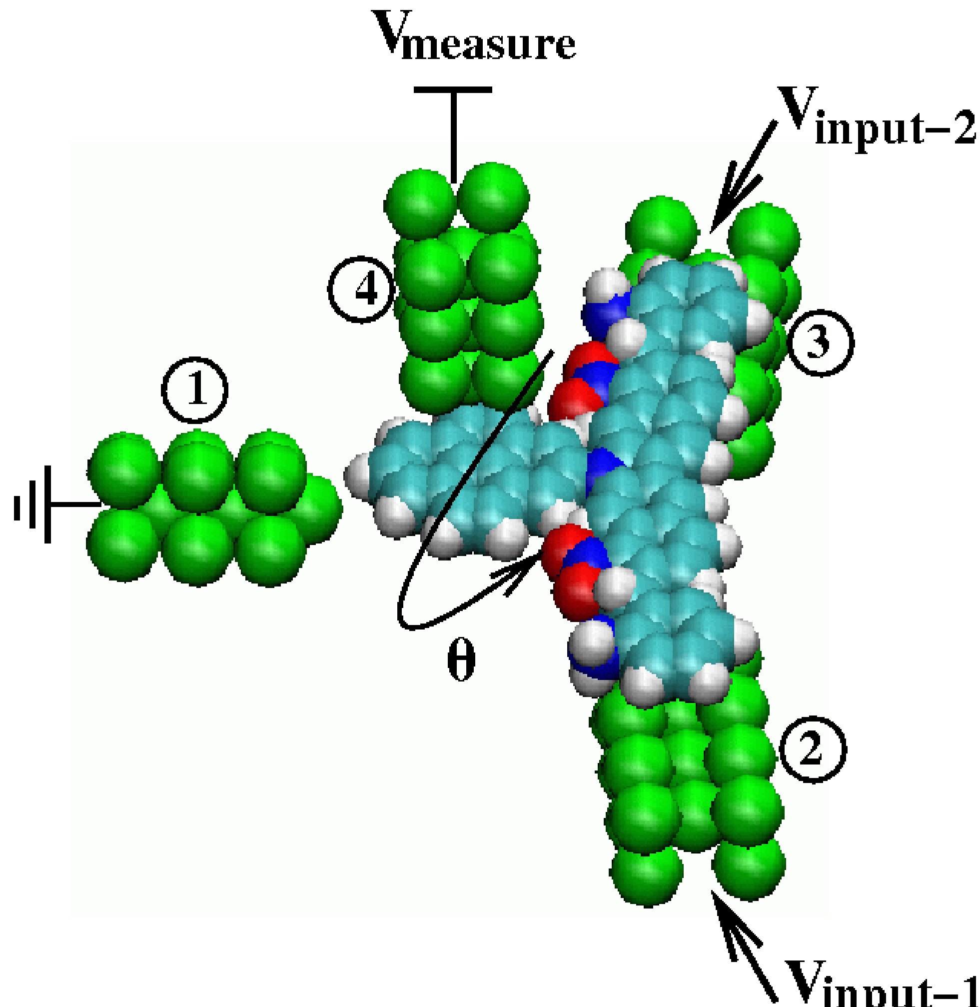


S. Ami, M. Hliwa, C. Joachim

Chem. Phys. Lett. 425 (2006) 356

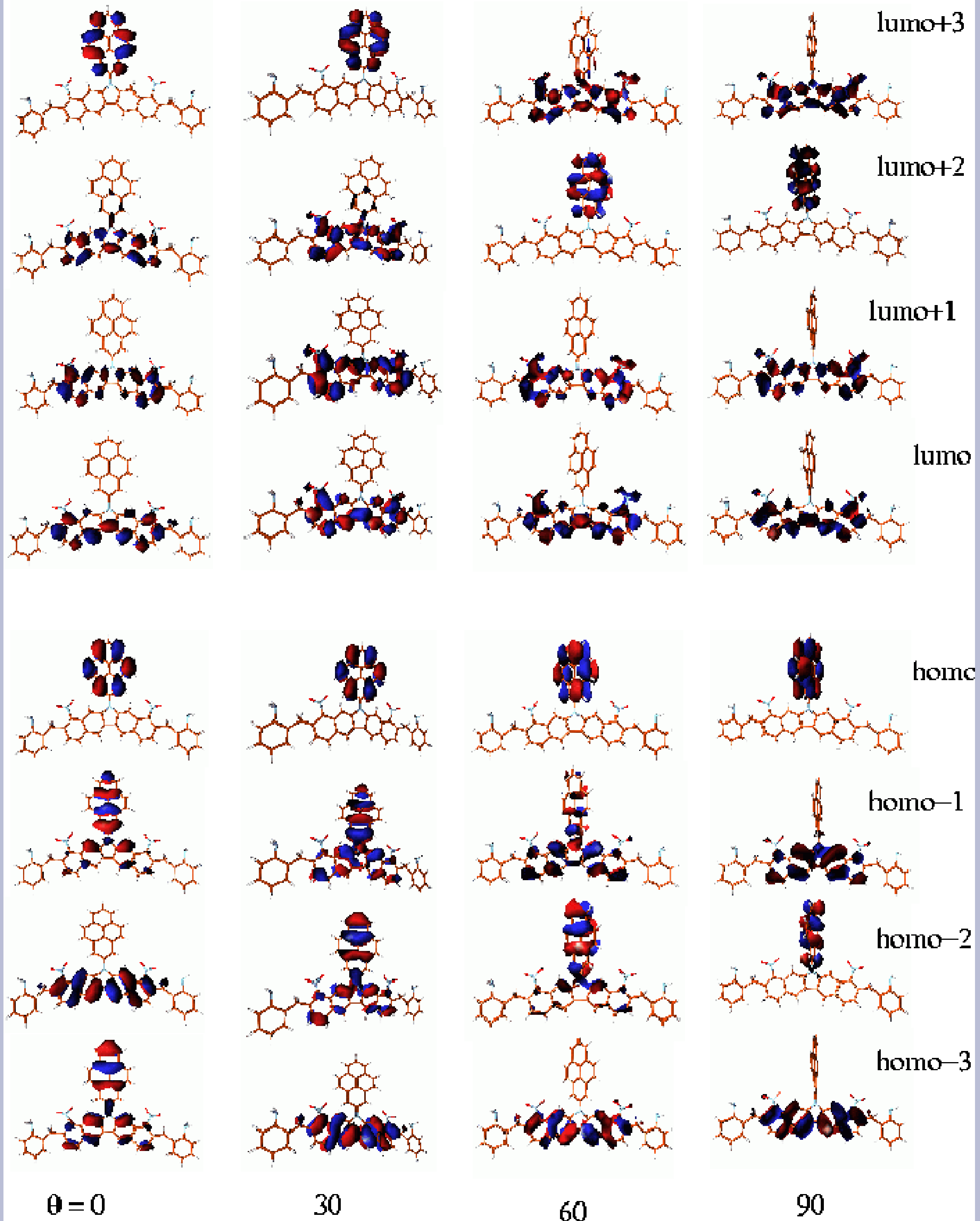
A mono-molecular XOR logic gate



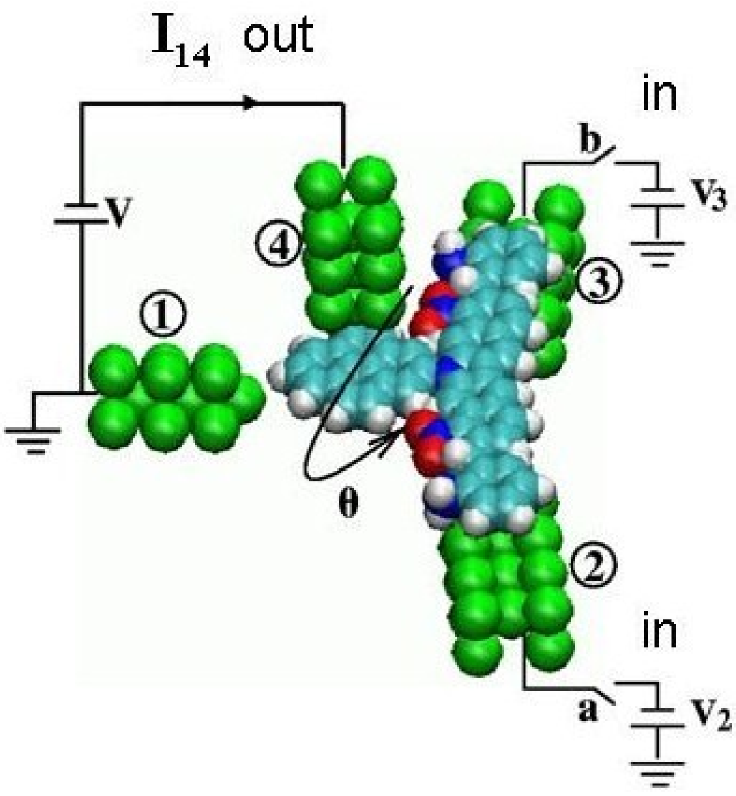


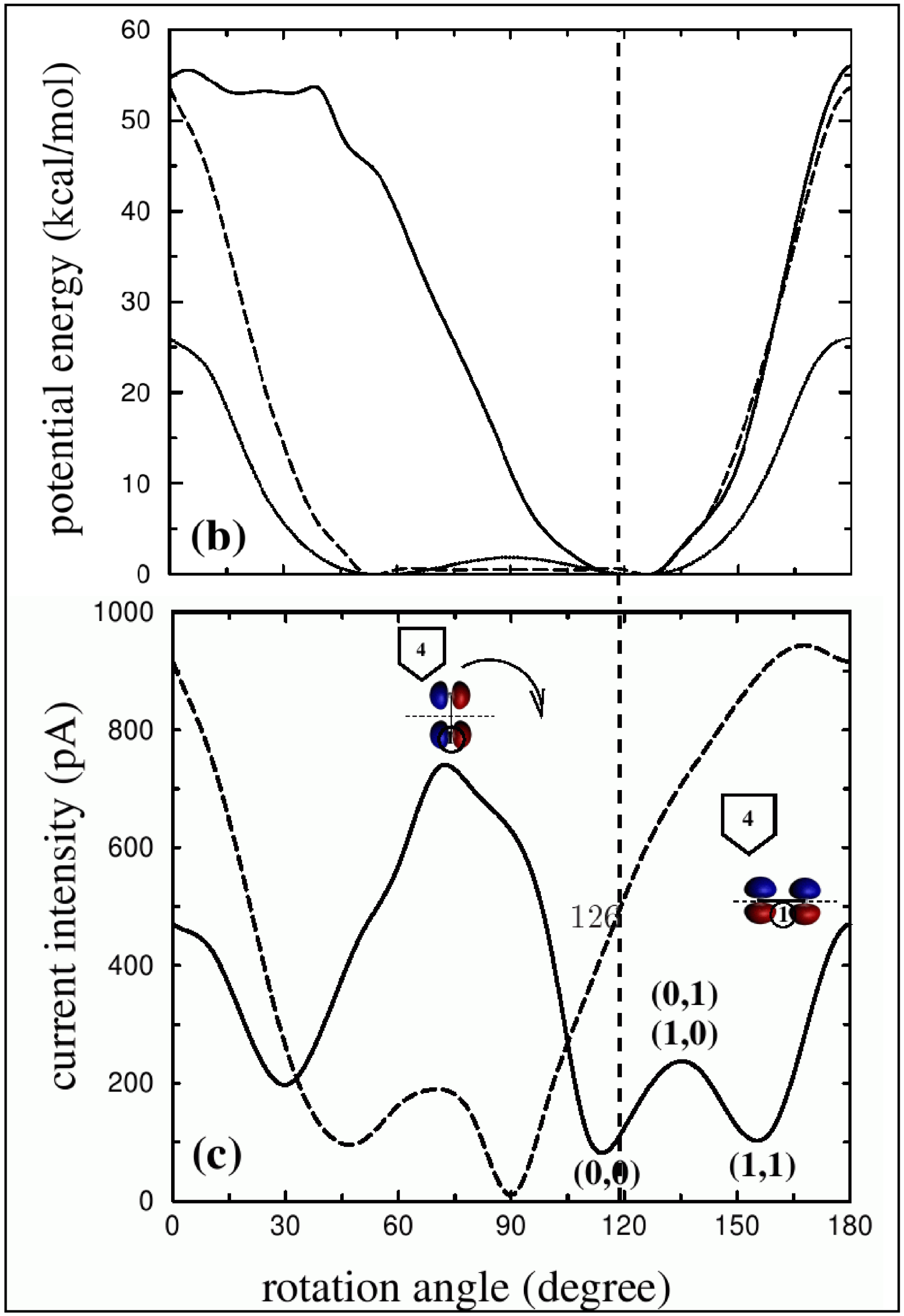
N. Jlidat, M. Hliwa and C. Joachim ; Chem. Phys. Lett. 451 (2008) 270.

FMO structures

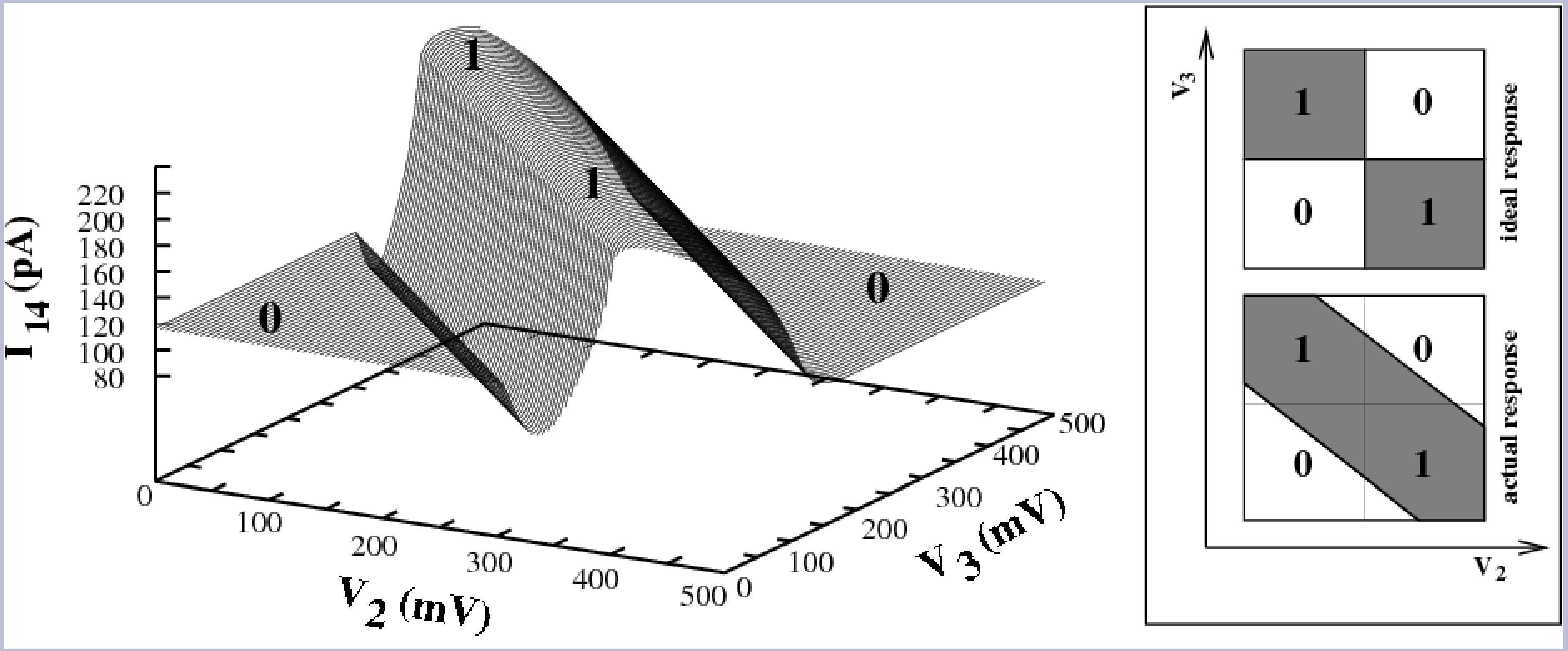


Mechanical and electrical characteristics





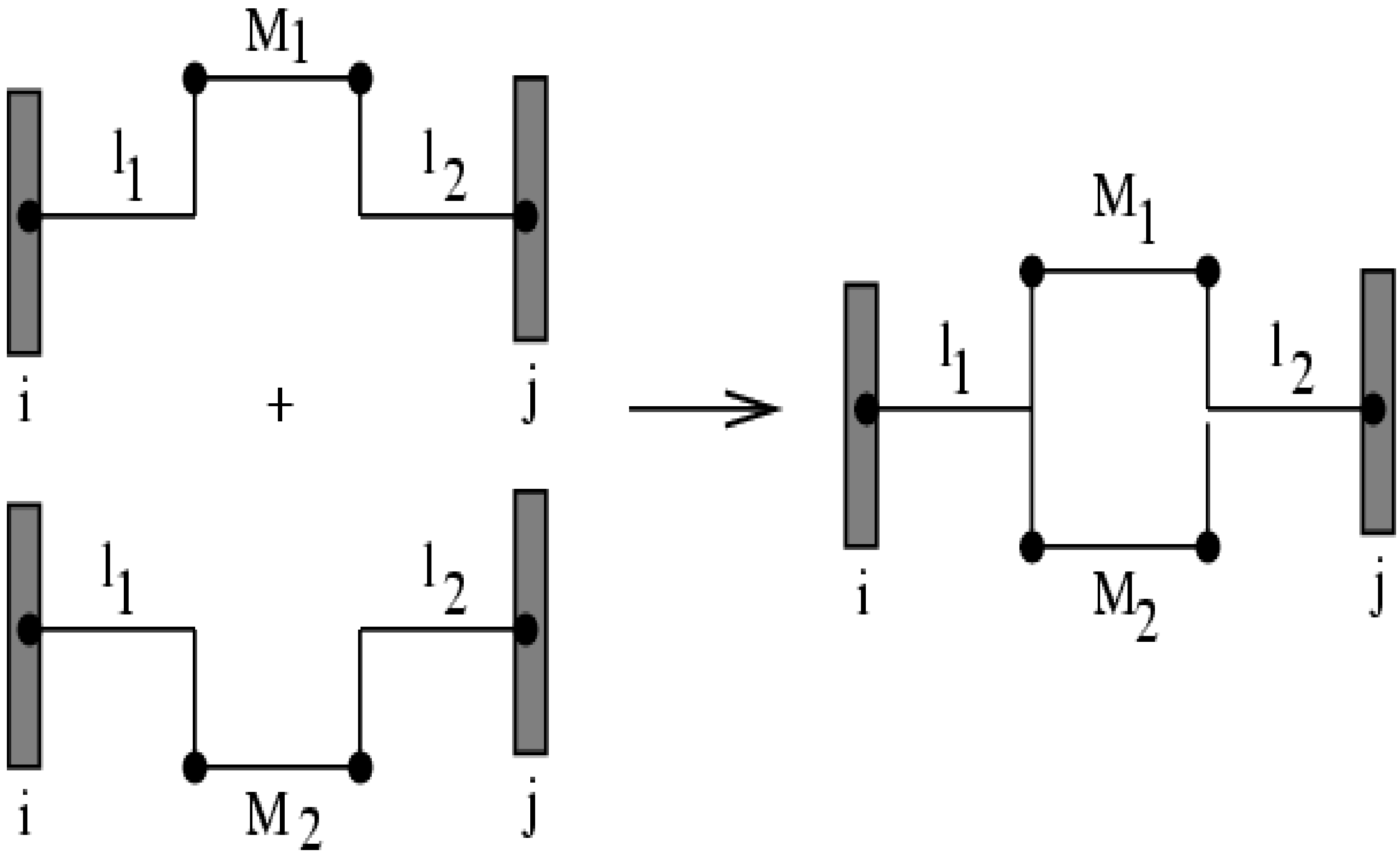
XOR-Molecule logic surface



Molecular wires association forming a single molecule
With 2 intramolecular nodes
(and 1 mesh)

G_1

G_2

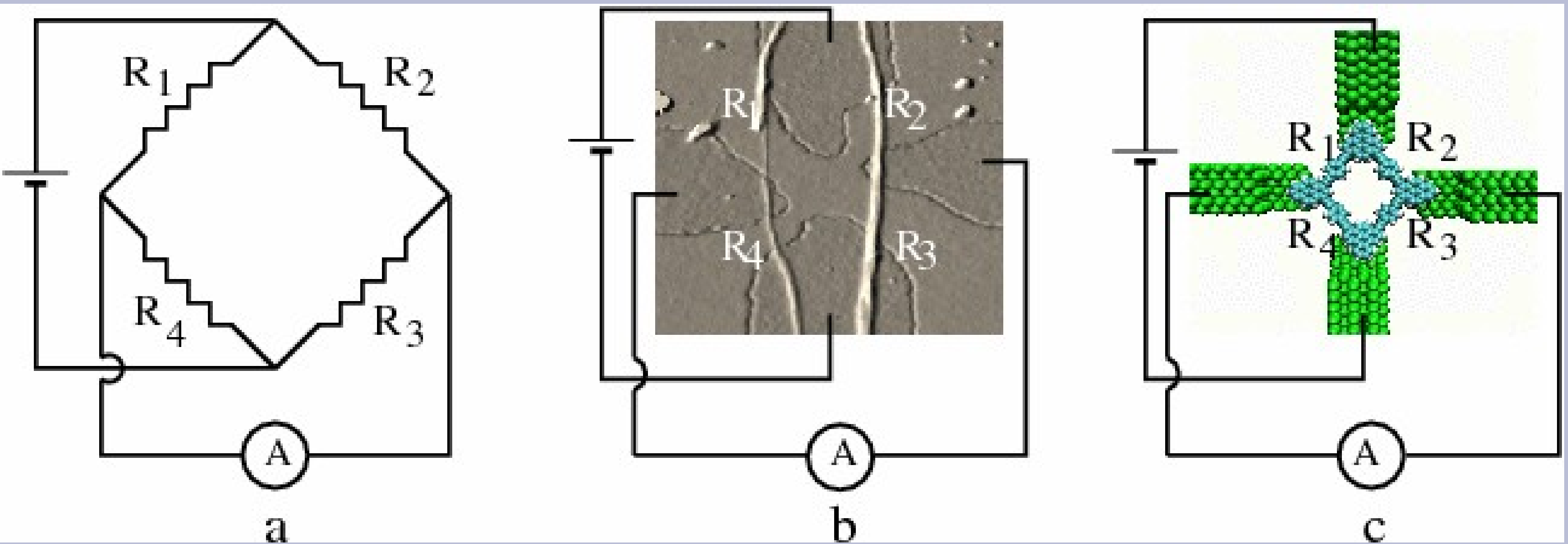


$$G = G_1 + G_2 + 2\,(G_1 \,.\, G_2)^{1/2}$$

Phys. Rev. B, 59, 16011 (1999)

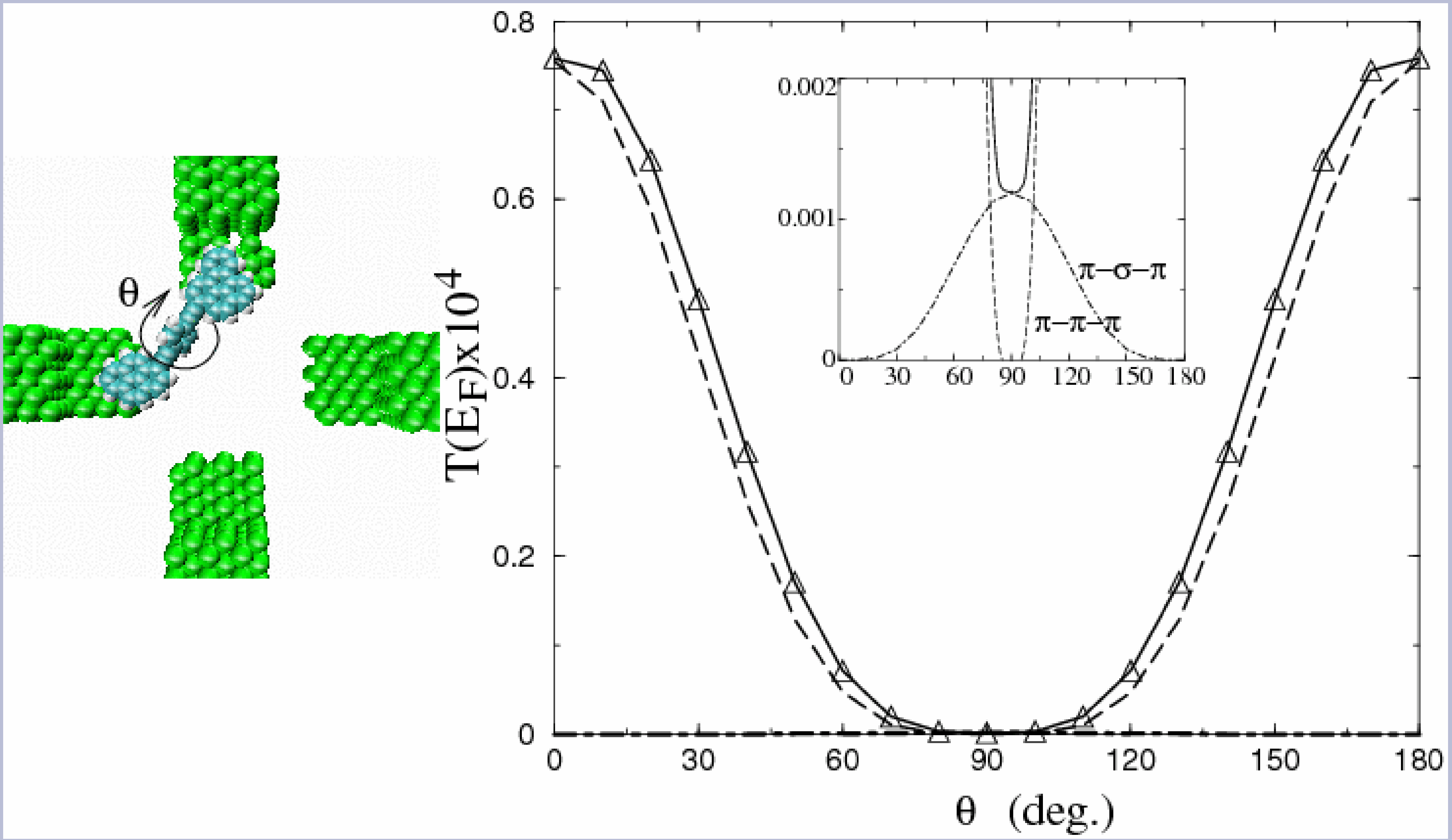
Balancing a Wheatstone bridge

Four-branch Wheatstone bridge



(b) T. Ondarçuhu et al., Rev. Sci. Instrum 71 (2000) 2087
(c) S. Ami, M. Hliwa anc C. Joachim, Nanotechnology 14 (2002) 283

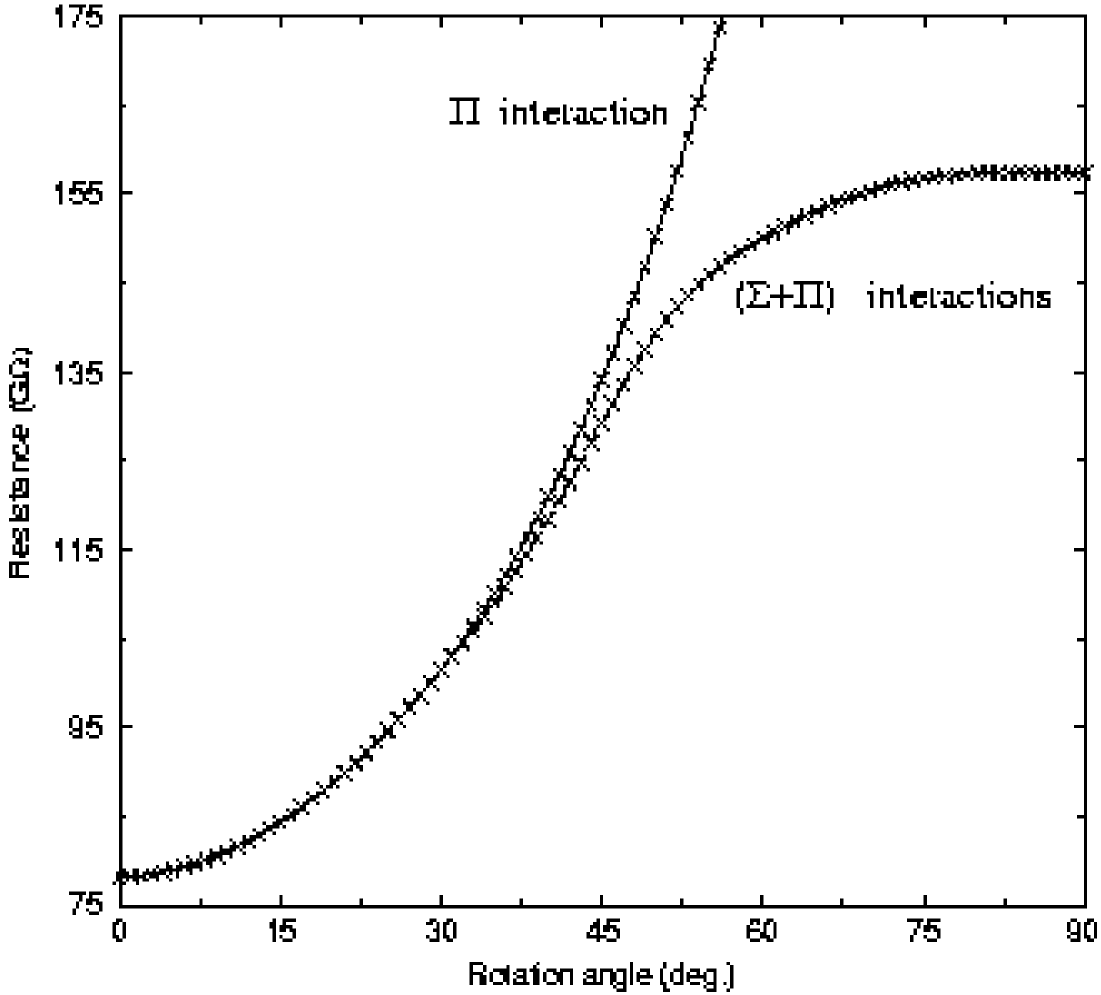
One branch Transmission coefficient variation



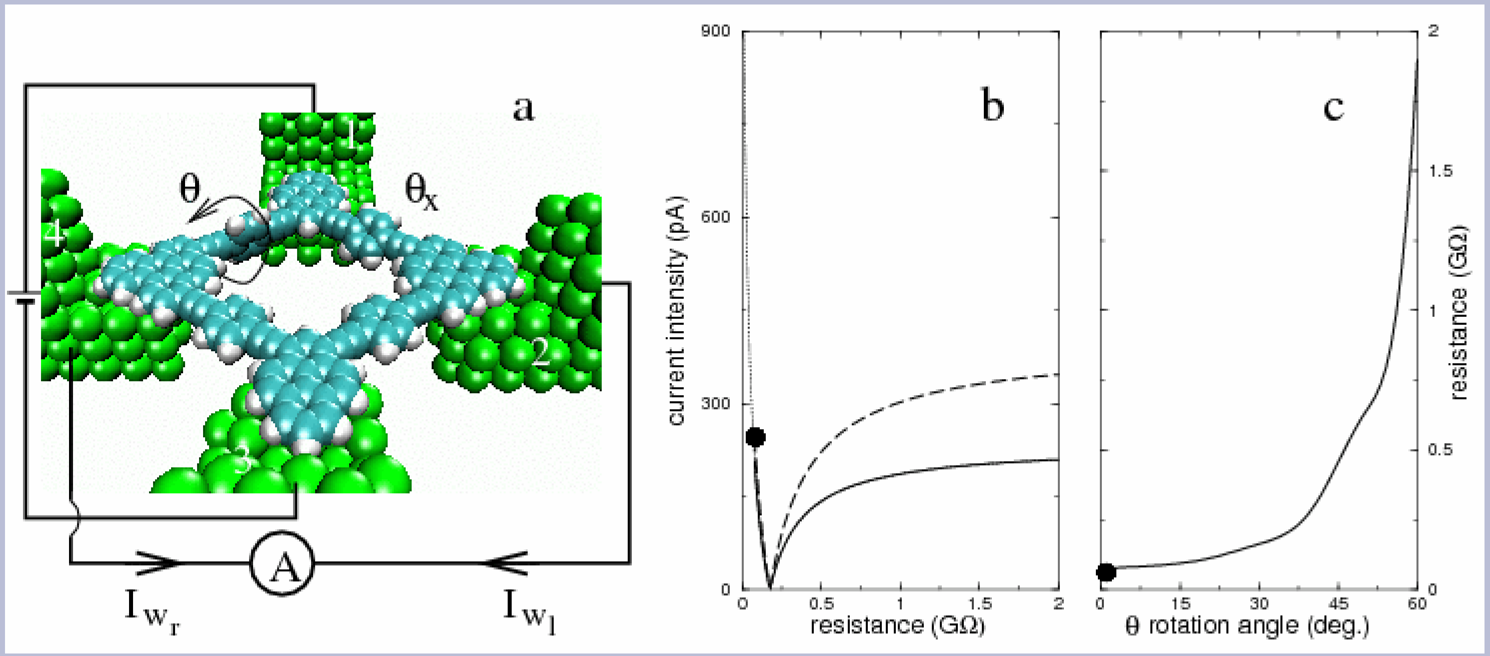
$T_{12} = T_{\pi\pi} \cos^4(\Theta) + T_{\sigma\pi} \sin^4(\Theta)$

, Nanotechnology 14 (2002) 283

One branch Resistance variation



Nanotechnology 14 (2002) 283



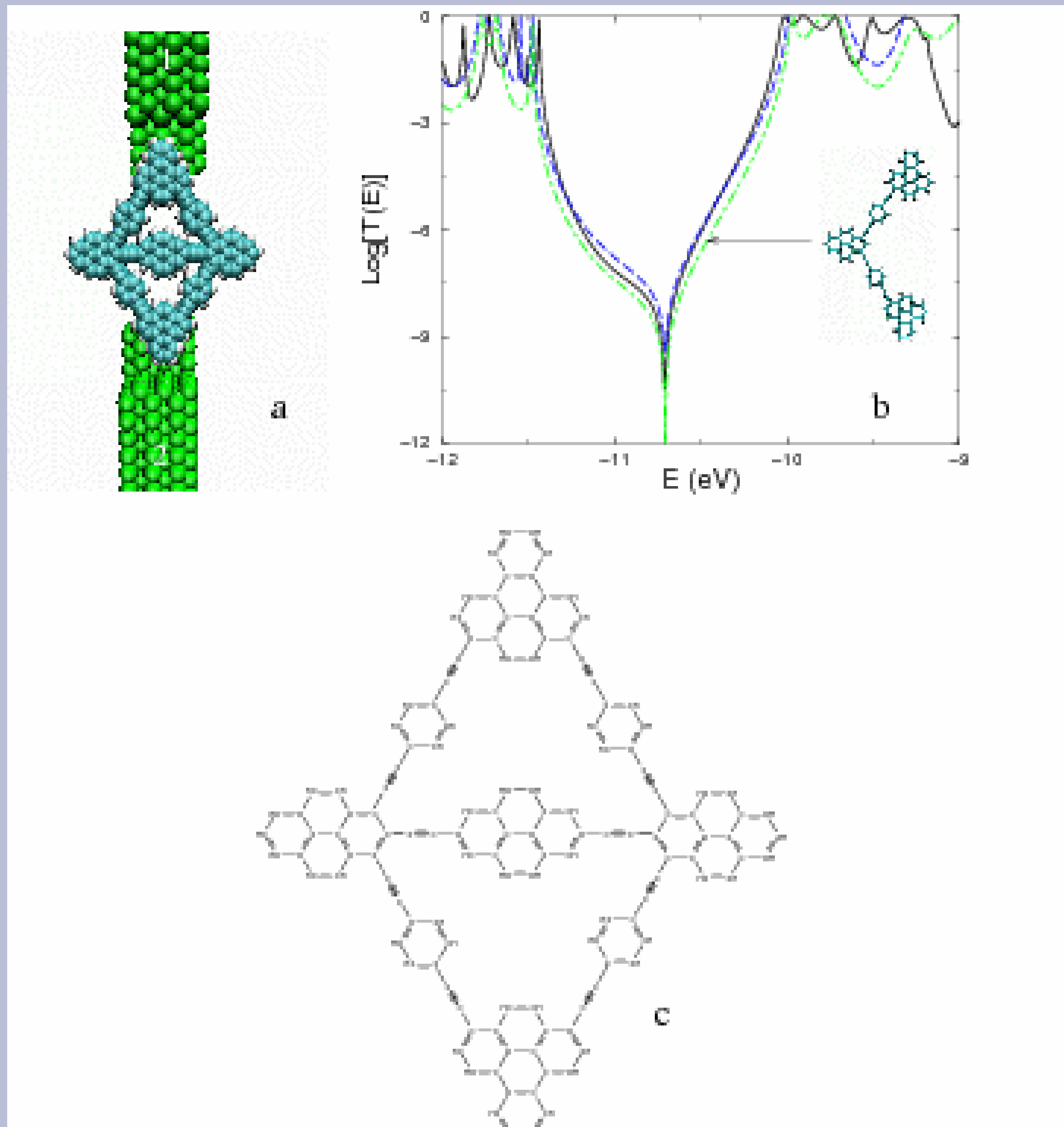
Θ_X = 30 deg., R_X = 175MΩ

R23 = R34 = 78MΩ (minimum value for Θ= 0)

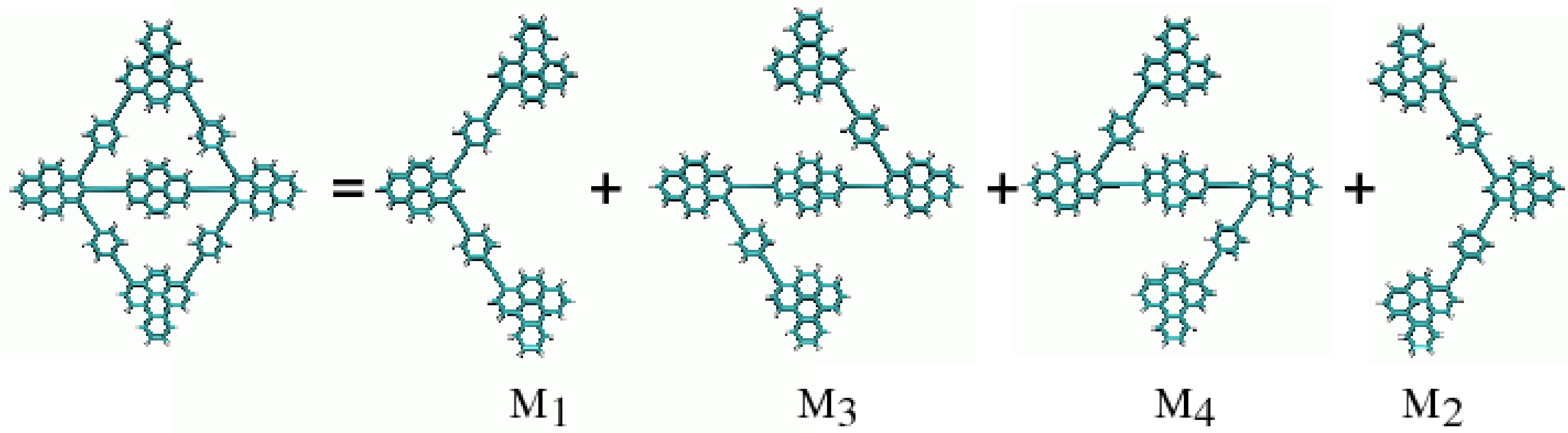
Classical standard Wheatstone bridge mesh and node laws (Kirshhoff) → $R_\Theta R_{23} = R_X R_{34}$

Quantum intramolecular circuit rules → $R_\Theta + R_{23} = R_X + R_{34}$

5-branch Wheatstone bridge



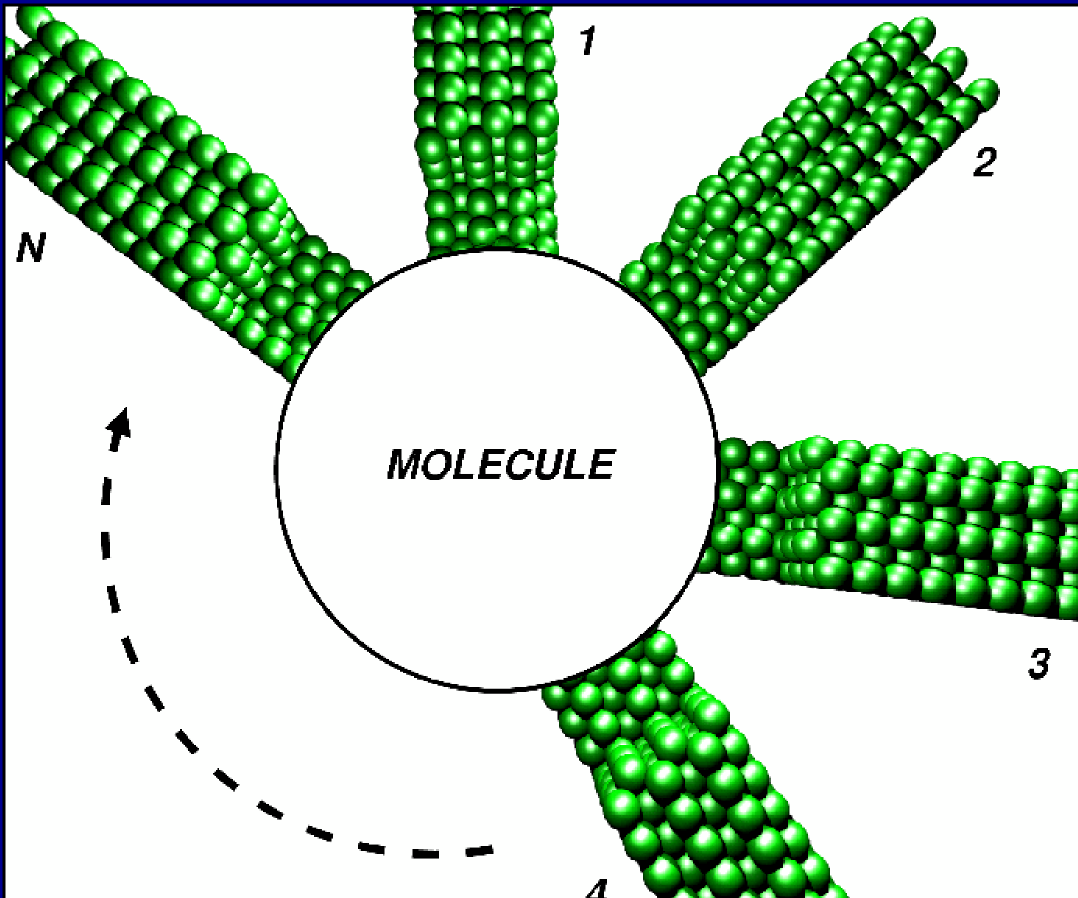
Specific superposition rules for 5-branch Wheatstone bridge

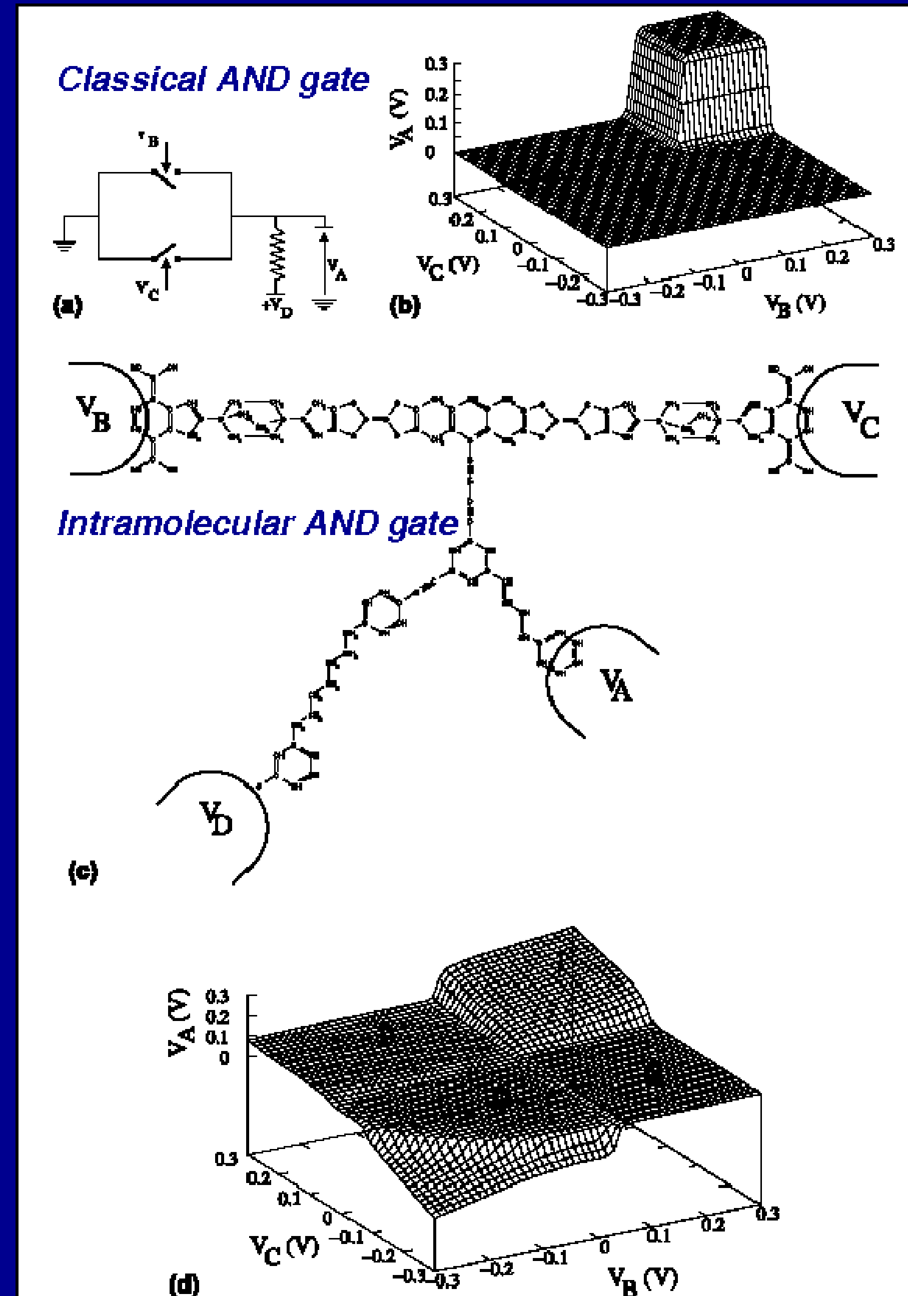


$$G = 4G_1 + 4G_3 + 8(G_1 x G_3)^{1/2} \quad ; \text{with } G_1 = G_2 \text{ and } G_3 = G_4$$

Summary

Intramolecular circuit simulator
N–electrode Elastic Scattering Quantum Chemistry (N–ESQC)

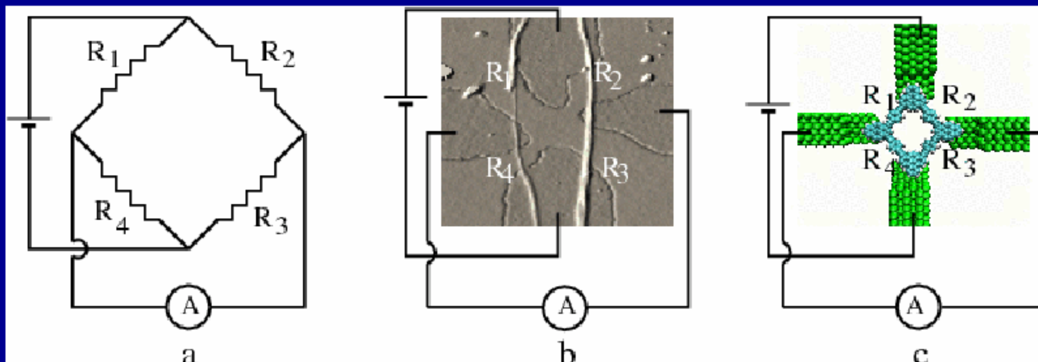




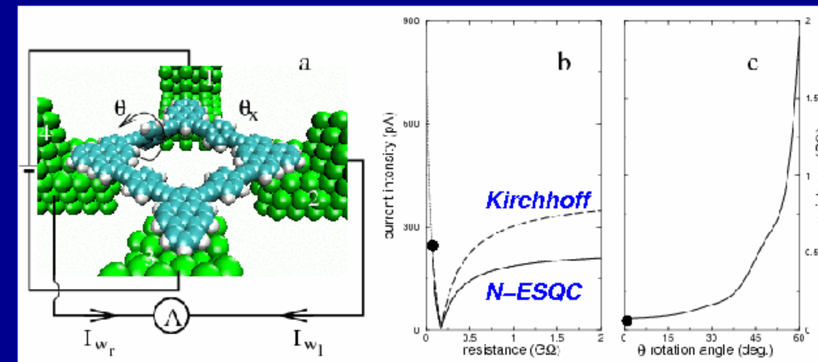
based on elastic scattering quantum chemistry technique, an intramolecular circuit simulator is presented for the design of electronic logic functions integrated in a single molecule interconnected to the N electrodes.
The scattering circuit is made of central molecule interacting with N electrodes
The full circuit is calculated tacking into account the EHMO valence orbitals of the central molecule and the band structure of the electrodes in interaction with the molecule.
Using molecular rectifier groups, an AND–molecule is designed, its current – voltage characteristic and its logic response are calculated. The AND gate works only in an output voltage mode.

Balancing a nano-scale Wheatstone bridge

Wheatstone bridges at 3 different scales

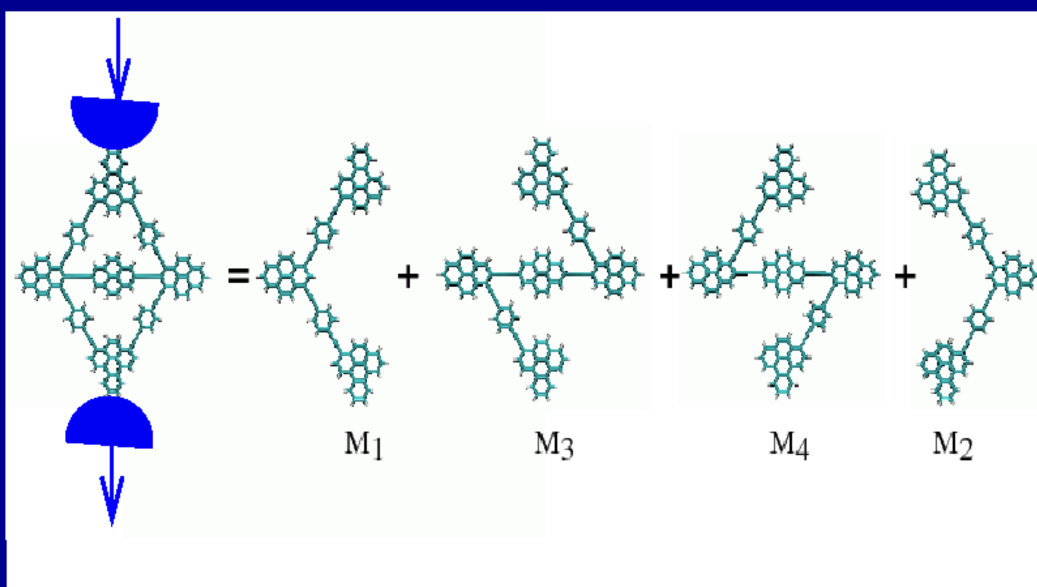


Variation of the balancing tunneling current

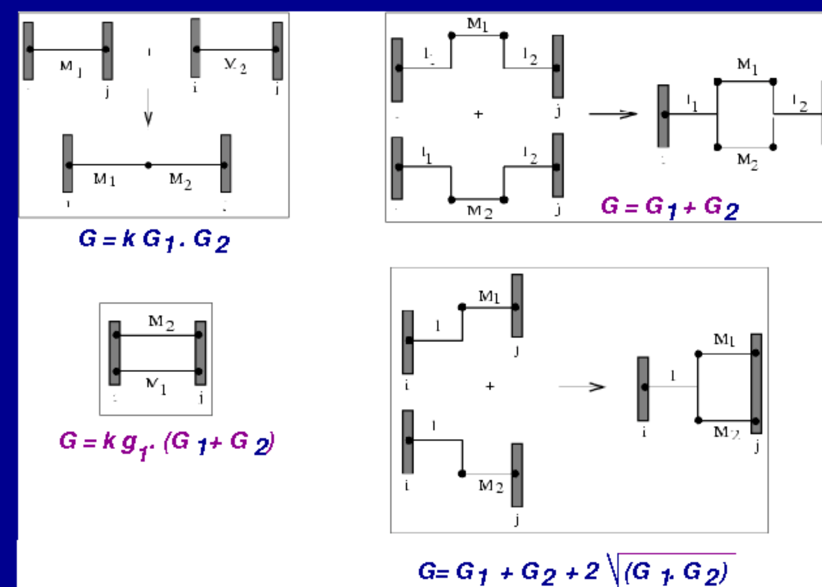


Specific rules for the 5–branche Wheatstone bridge

$G = 4G_1 + 4G_3 + 8\sqrt{G_1 . G_3}$; $G_1 = G_2$ and $G_3 = G_4$

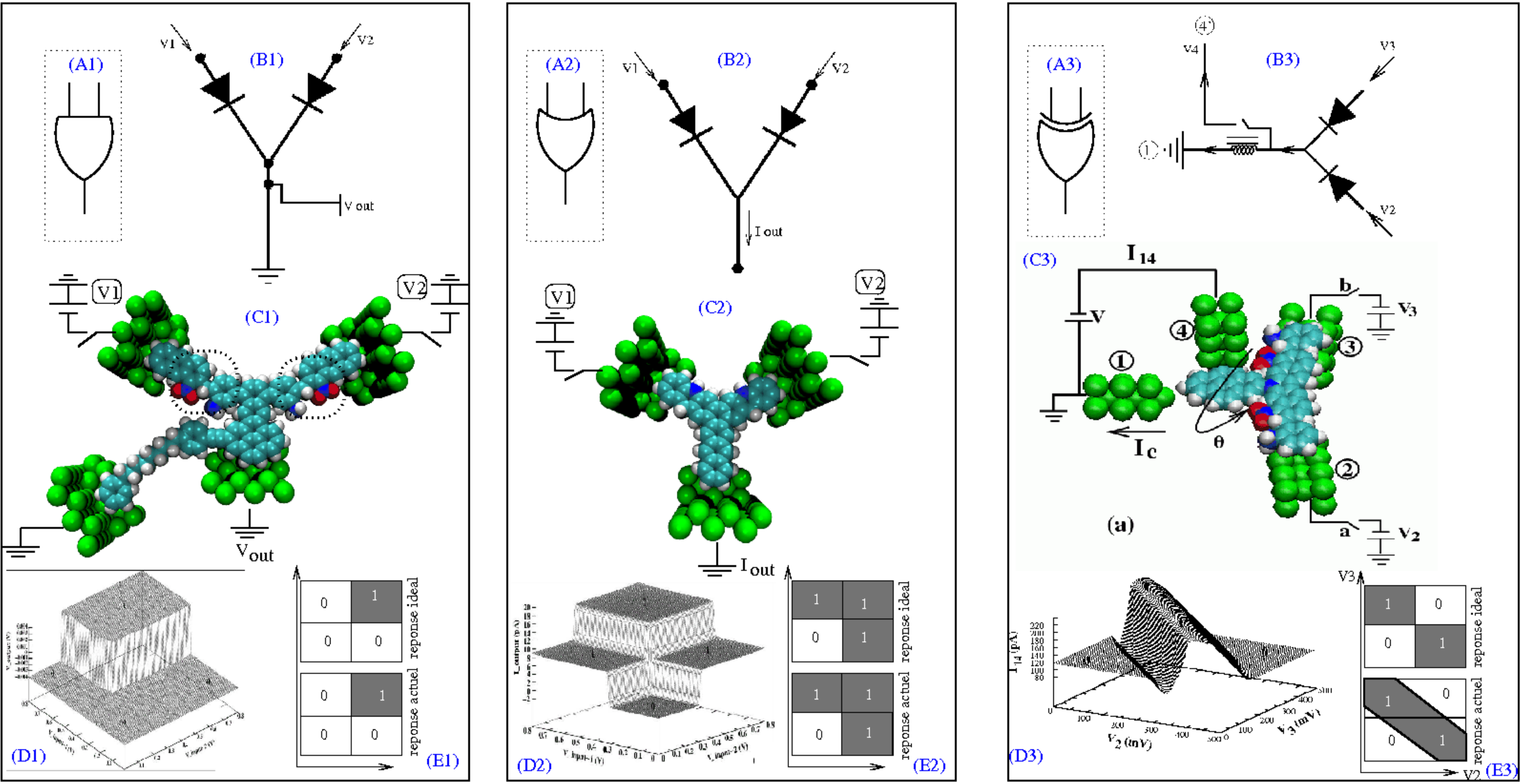


Intramolecular tunneling circuit superposition rules



Using the EHMO–NESQC technique , the scattering electronic properties of mono–molecular Wheatstone bridges are studed. Simple intramolecular circuit rules are given for the design of an intramolecular electronic circuit integrated in a single molecule. The balancing condition of the 4–electrode monomolecular Wheatstone bridge is provided. The value of the tuning resistance is the same applying the new circuit rules and the standard Kirchhoff node and mesh laws.

Monomolecular Logic gates



(a) N. Jlidat, M. Hliwa and C. Joachim ; Chem. Phys. Lett. 451 (2008) 270.
(b) **N. Jlidat, M. Hliwa and C. Joachim** ; Chem. Phys. Lett. (2008).

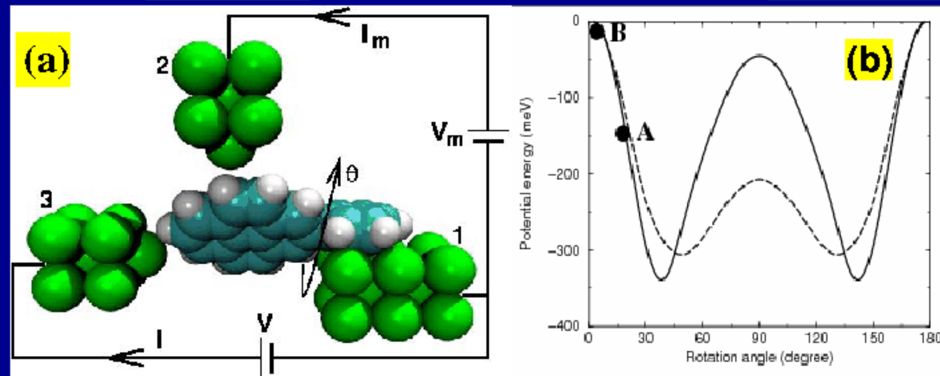
A 3-terminal single molecule nano-scale amperometer

The setup

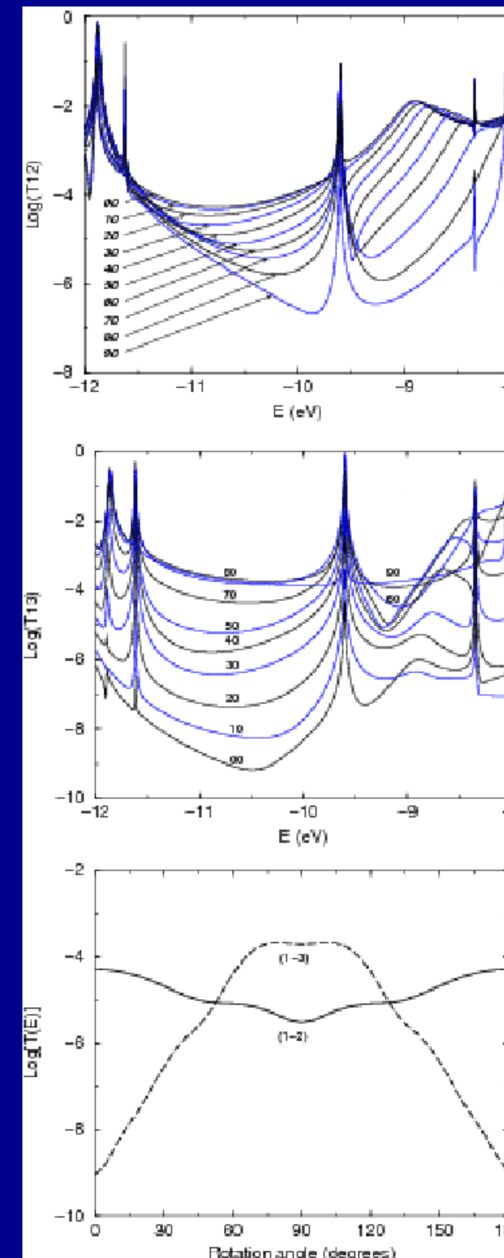
This 3-terminal single molecule tranducer is able to measure tunnel current intensities. The conformation of pyrene-phenyl molecule is changed under an intramolecular inelastic current effect. This conformation change is detected by a third lateral electrode ineracting also with the molecule. The full multi-channel electronic scattering matrix of the device is calculated taking into account the chimisorption of the molecule at one end and the details mechanics of the conformation change of this molecule. A semi-classical model is used to describe the intramolecular trans-duction effect between the electrons transferred through the molecule and its conformation change. It results a linear tranduction curve between the input and the detection currents of the device for a range of tunnel current of interest fo mono-molecular electronics.

(a) Desription of the used setup to heat the pyrene-phenyl molecule under the voltage V and to detect the molecule response via Im were Theta is the rotation angle between the phenyl and pyrenyl planes.

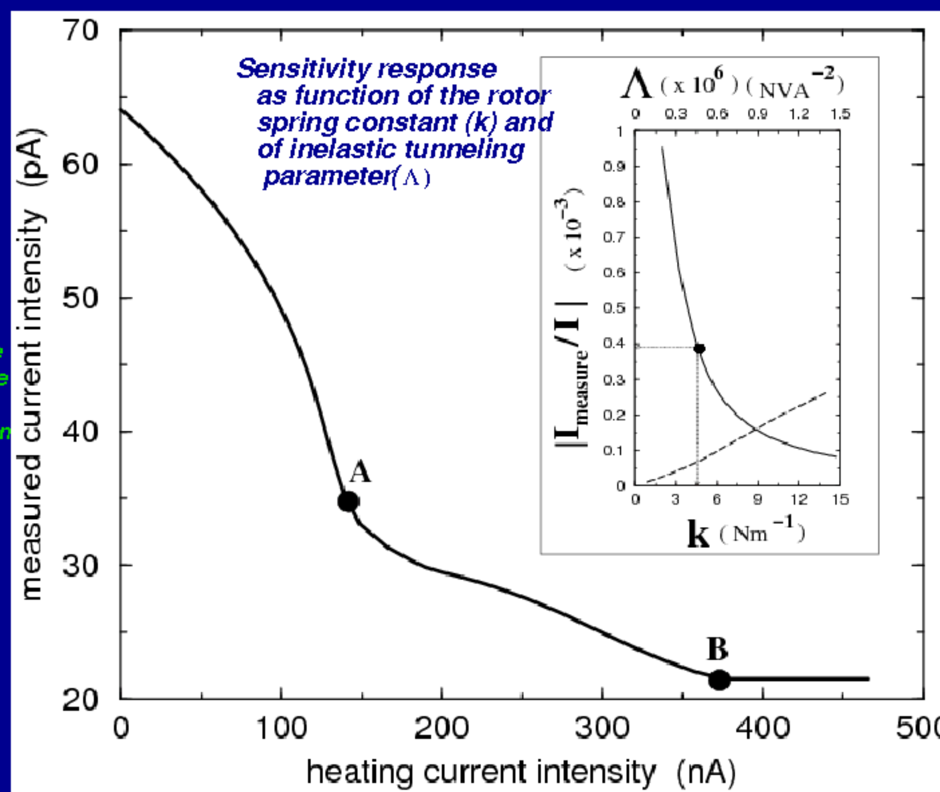
(b) Potential energy curves U(theta) for and for the molecule (dashed line)



Elastic tunneling electron transmission spectra

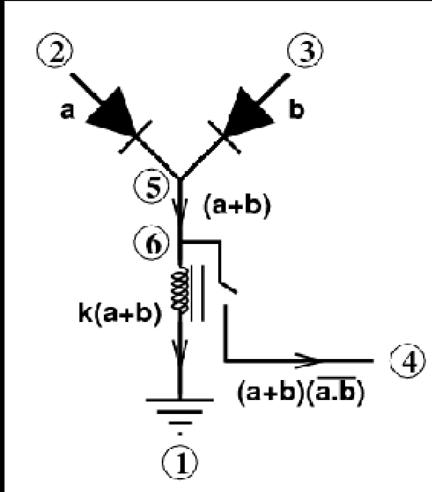


Transduction curve



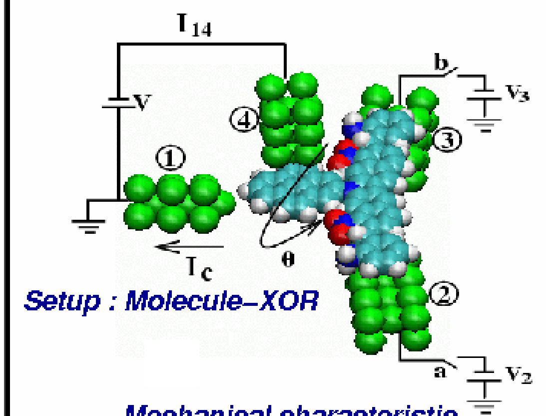
A semi-classical XOR logic gate integrated in a single molecule

XOR gate transcripted in an electrical circuit

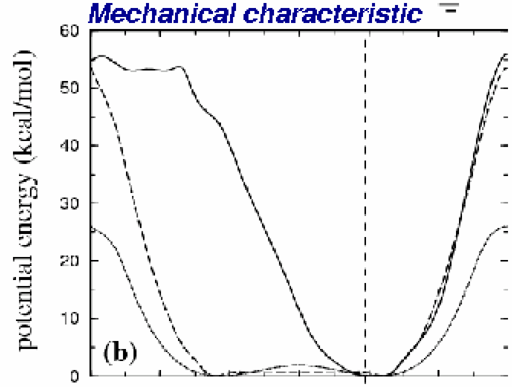


Improving the design of molecular rectifiers, a molecule is presented performing the digital XOR function where the output circuit is independent of the inputs. An intermolecular inelastic effect was optimised to get the non-linear effect for an XOR to work. This demonstrates how an intraolecular circuit can be designed where energy is provided along the molecule independently of the inputs. The electronic characteristics of this molecule-XOR were calculated using the N-ESQC technique for N=4 interconnects at a semi-empirical level of description. Inside a single molecule, pilling up classical functions implemented each by a specific chemical group (2 rectifiers and a rotor for the XOR) is limited in the final molecule by the spectral mixing of the molecular orbitals of each function.

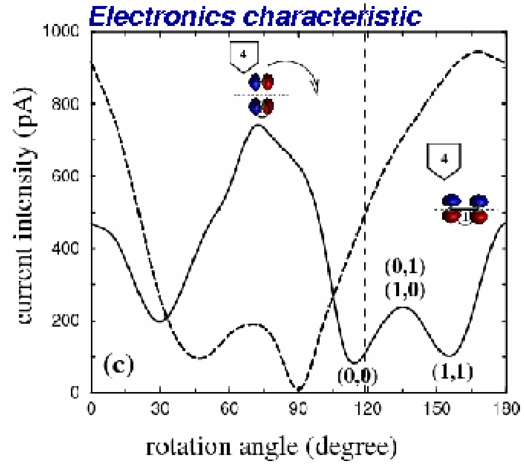
Design and principle of an molecule-XOR gate



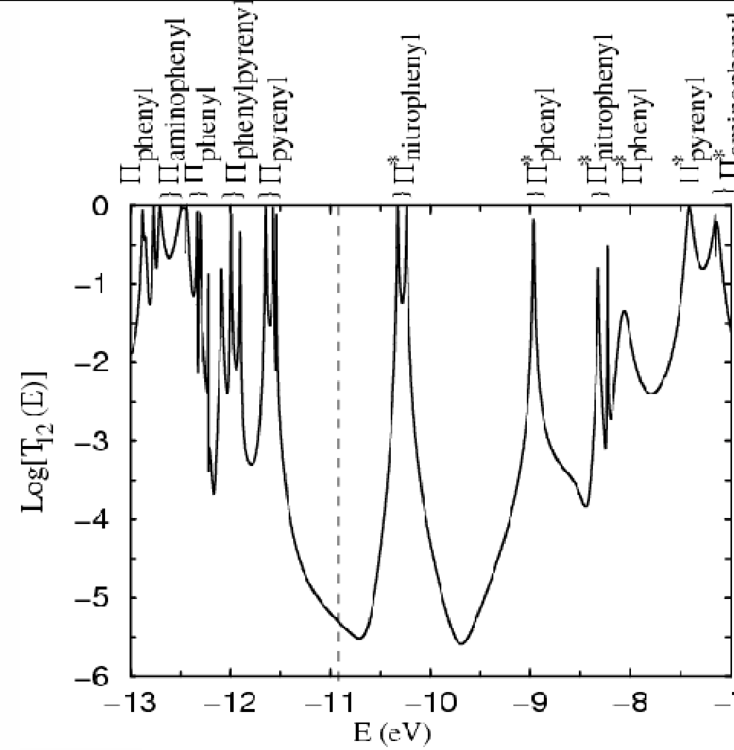
Mechanical characteristic



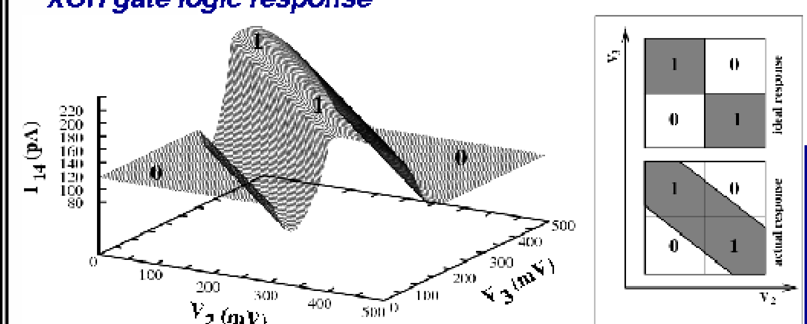
Electronics characteristic



Input-Output tunnel electron transmission coefficient and logic surface



XOR gate logic response

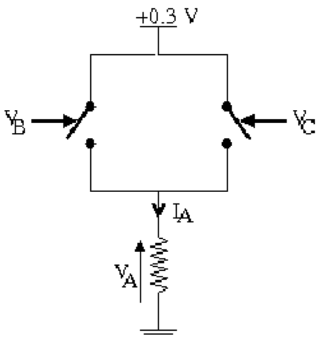


Mono-molecular OR logic gate

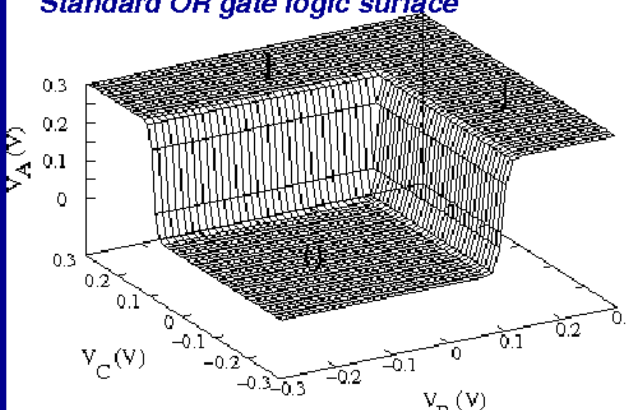
Classical OR gate

Molecule-OR gate

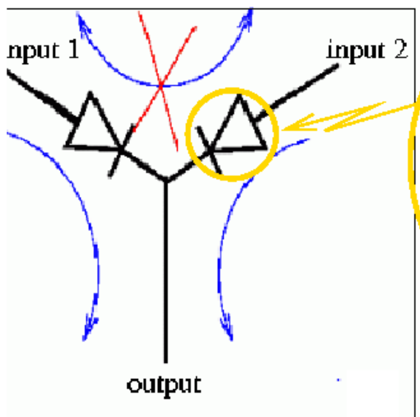
Electric OR gate circuit

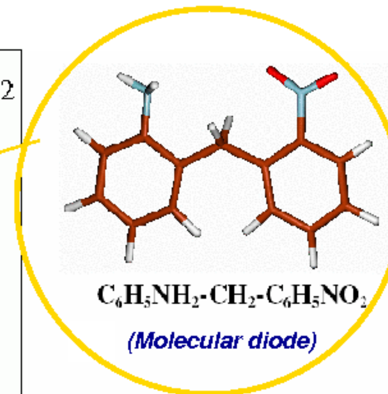


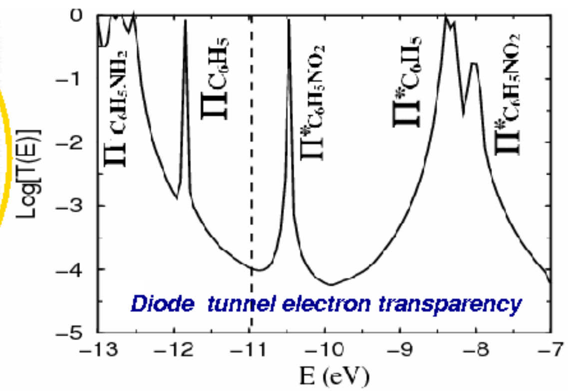
Standard OR gate logic surface



Diode based OR gate

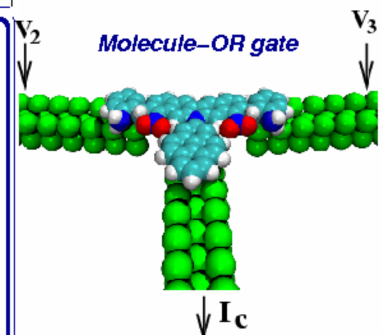




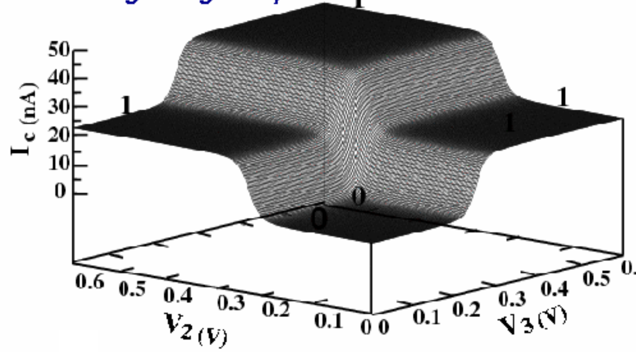


Diode based molecule–
OR logic gate is designed.
Tahe law of te superposition
of the tunneling current
inside the molecule works
perfectly as compared to
the ideal OR logic surface.
But from inside the molecule,
there is no means to equalize
the "1" resulting from one
input set at 0.3 V. This well
have to be performed outside
the molecule–OR

Molecule–OR gate



OR gate logic response



Aknowledgments

- **NanoSciences Group** (GNS-CEMES-CNRS-Toulouse)

www.cemes.fr

- Christian Joachim
- Nicolas Renaud
- Stephane Ami
- Nozha Jlidat
- Mike Magoga

Thanks for your attention