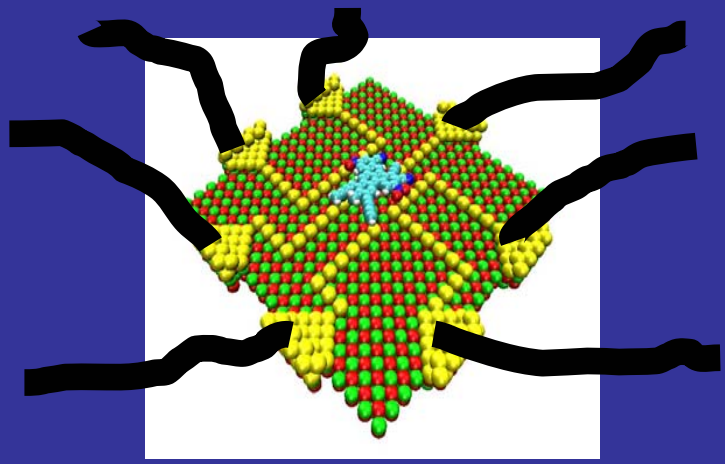
Pico-Inside

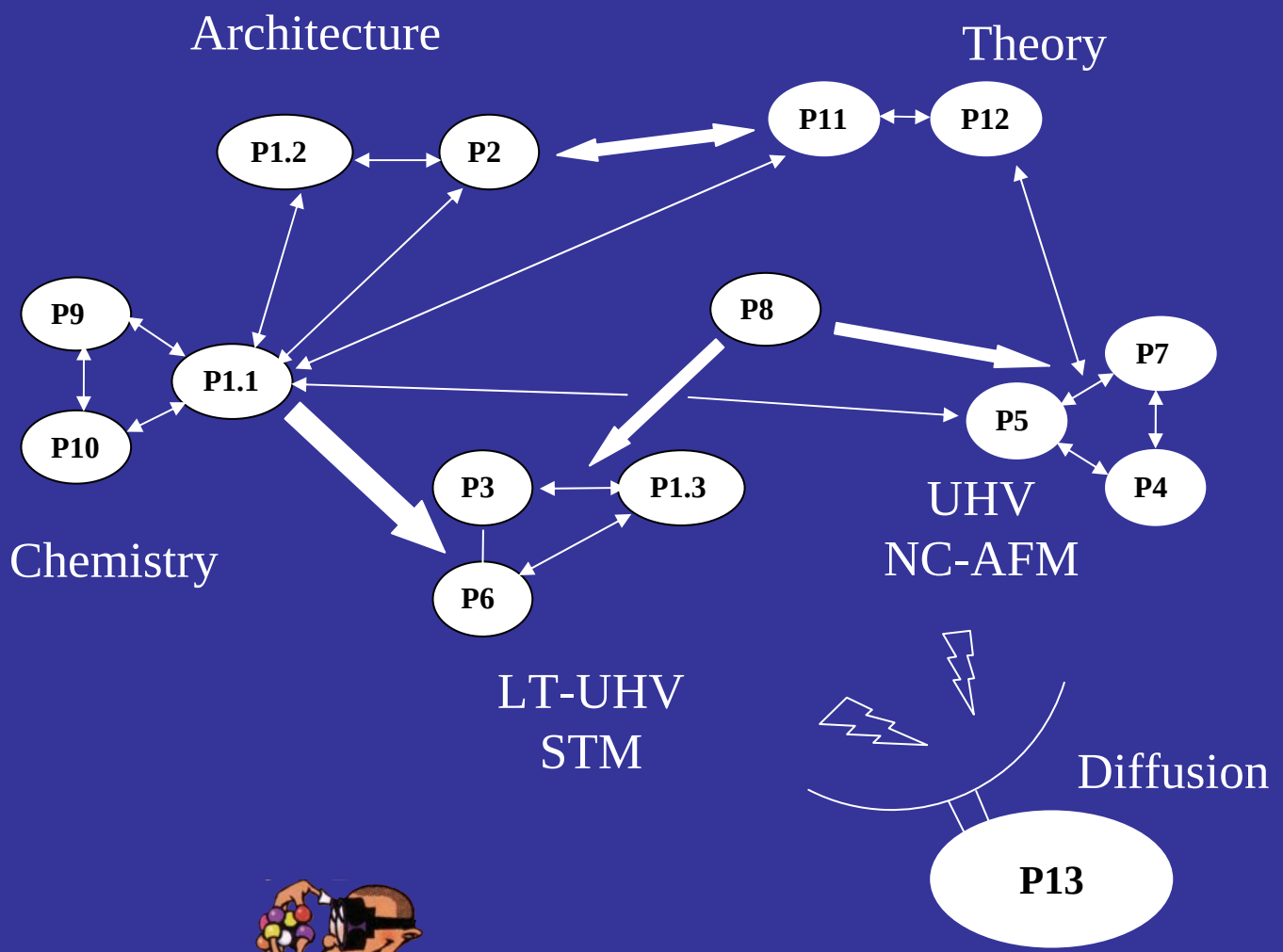
« Computing Inside a Single Molecule
using
Atomic Scale Technologies »

Can a single molecule compute by itself ?



Pico-Insiders

- P1.1: Toulouse
- P1.2: Paris
- P1.3: Orsay
- P2: Fujitsu
- P3: Berlin
- P4: Krakow
- P5: Osnabrück
- P6: Aarhus
- P7: Basel
- P8: Omicron
- P9: Prague
- P10: Tarragona
- P11: KCL
- P12:UCL
- P13: Madrid



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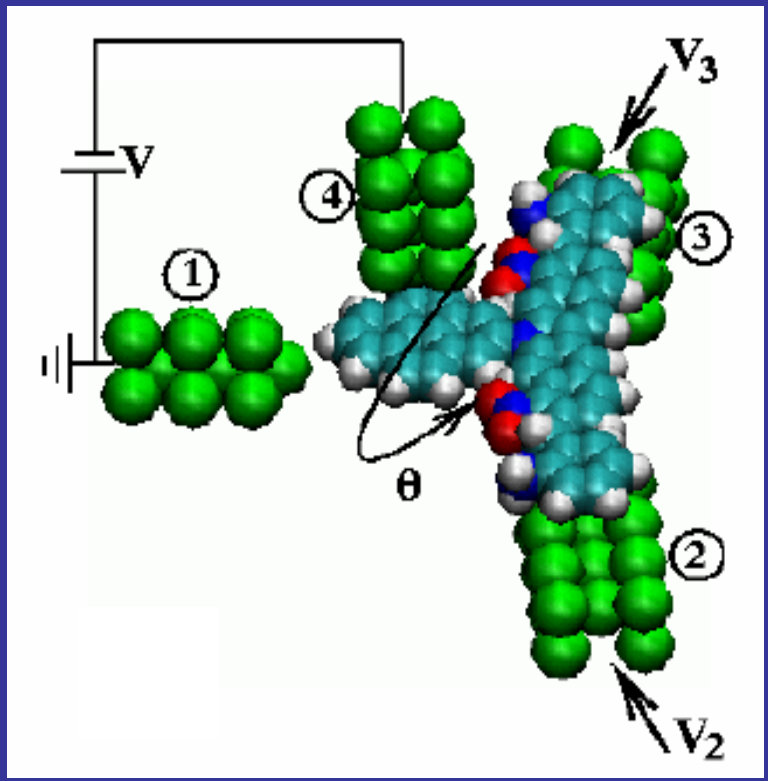
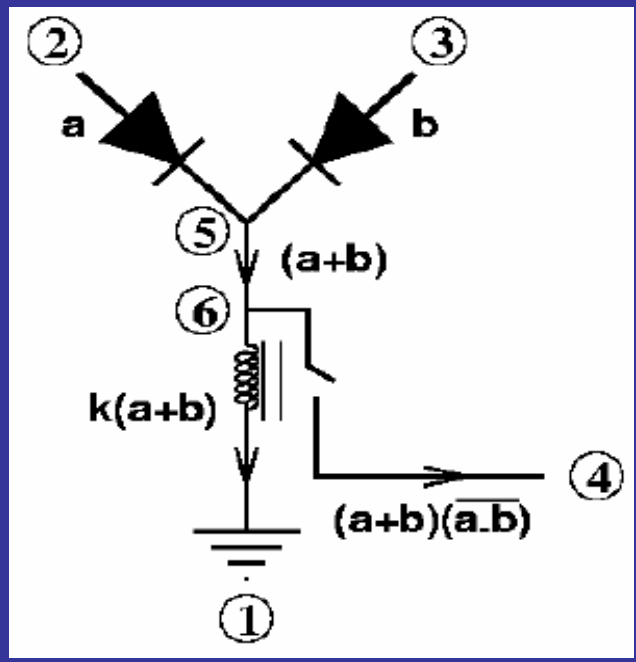
Unit 1
Intramolecular Architecture

Option 1: An intramolecular semi-classical XOR gate





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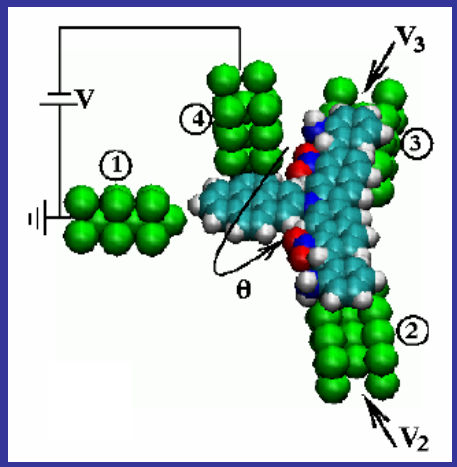
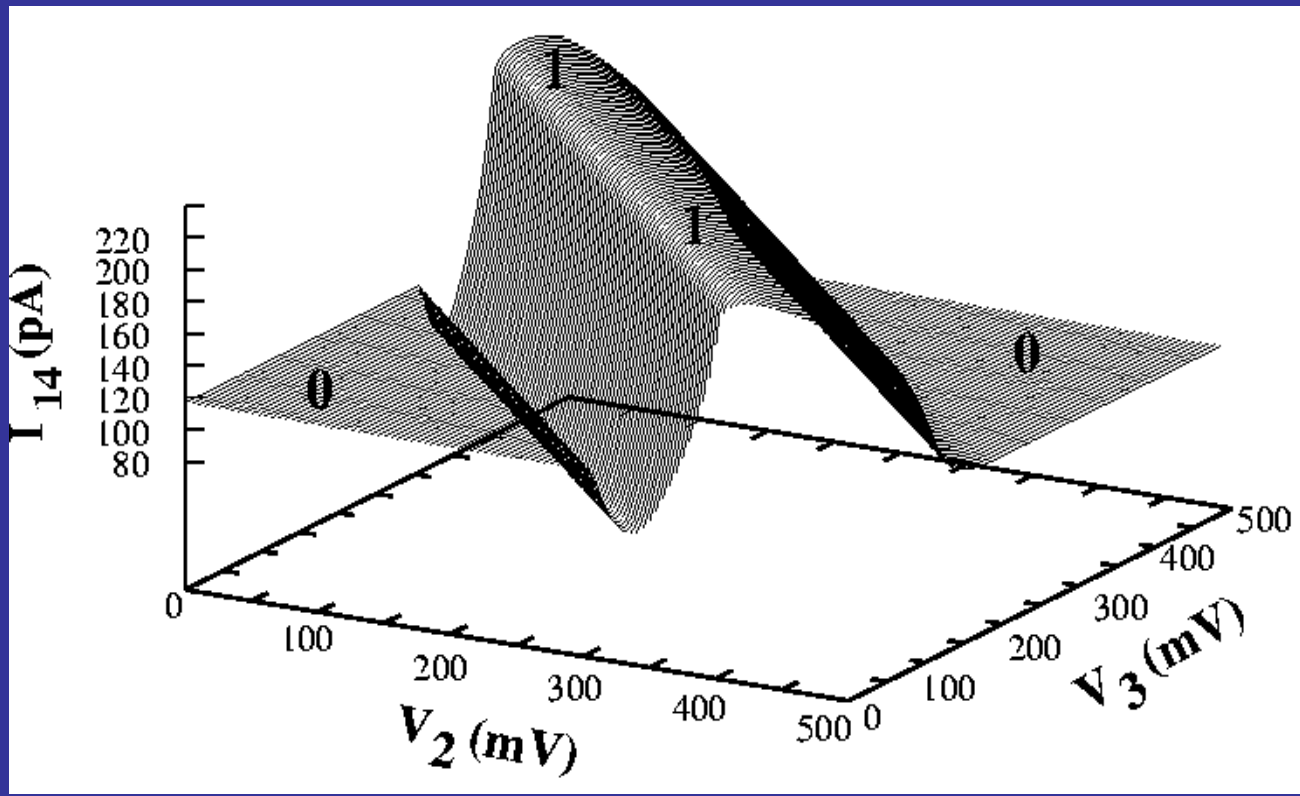
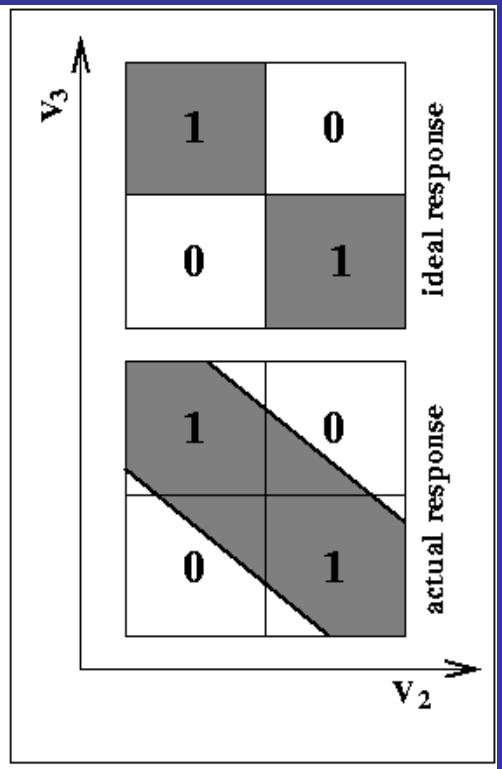
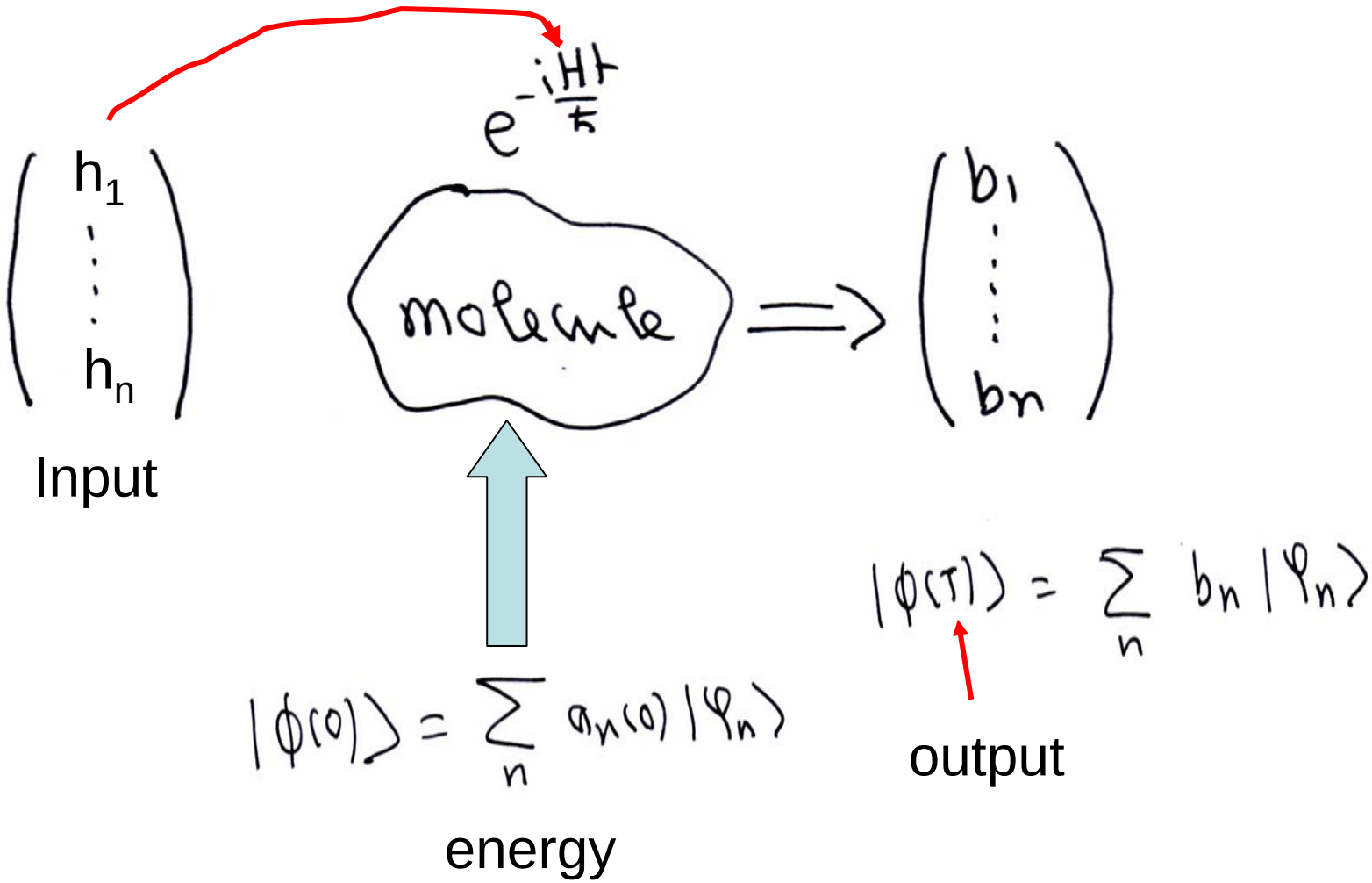
The XOR logic surface



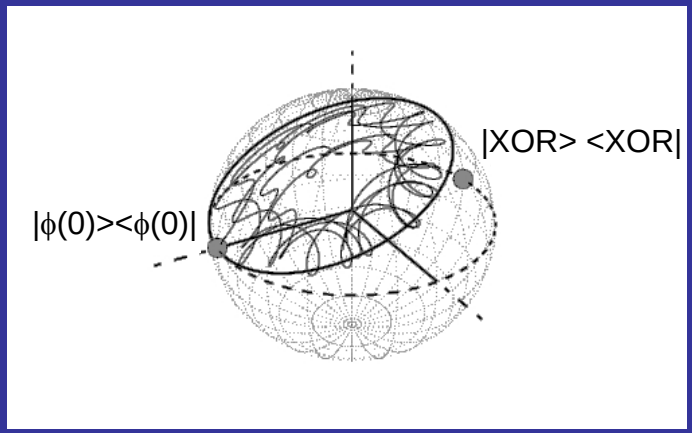




Option 2: Quantum Hamiltonian computing

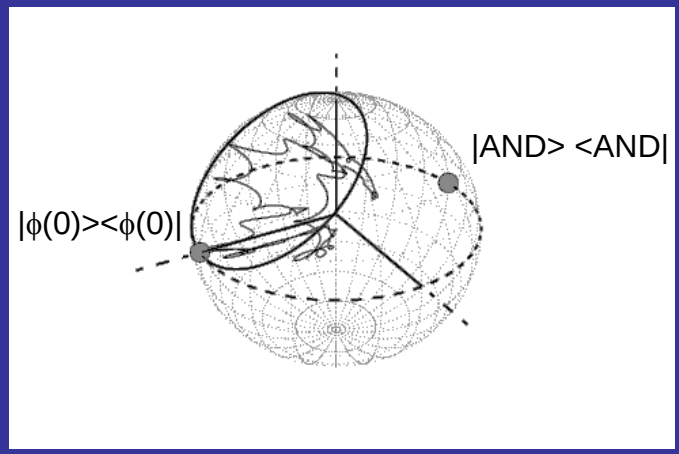


½ adder optimisation



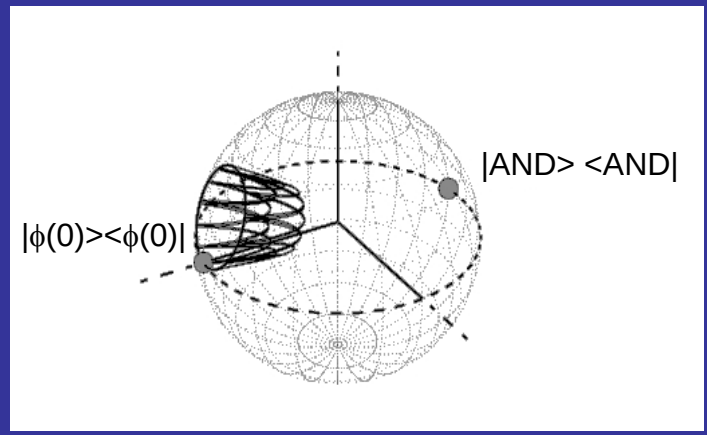
(0,1) input

3D Restricted Bloch sphere
Generated by |ϕ(0)> & |OUTPUT> states



(0,1) input

Pico-Inside



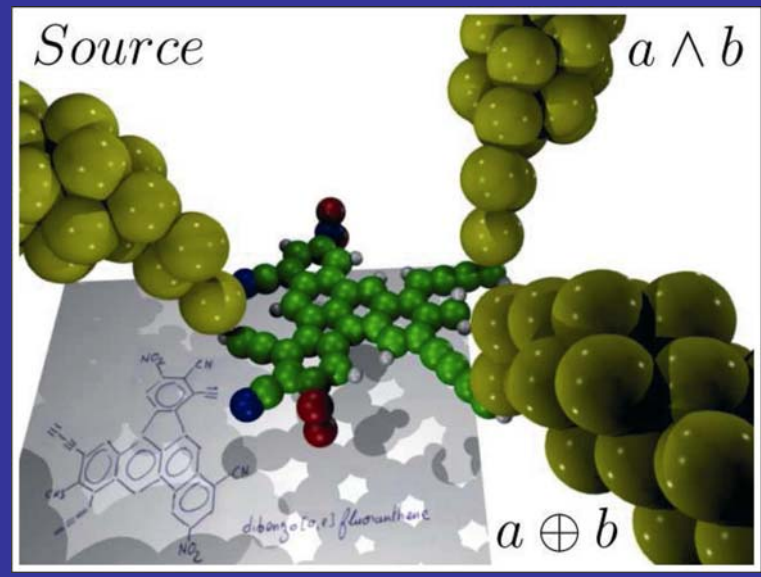
(1,1) input

N = 5 quantum states
hypersphere of dimension 24

Pico-Inside

Molecule ½ adder

input	R_{XOR}	R_{AND}
00	79.7 GΩ	516.0 GΩ
01	4.79 GΩ	3.46 GΩ
10	1.86 GΩ	1.13 GΩ
11	147.0 GΩ	6.22 MΩ



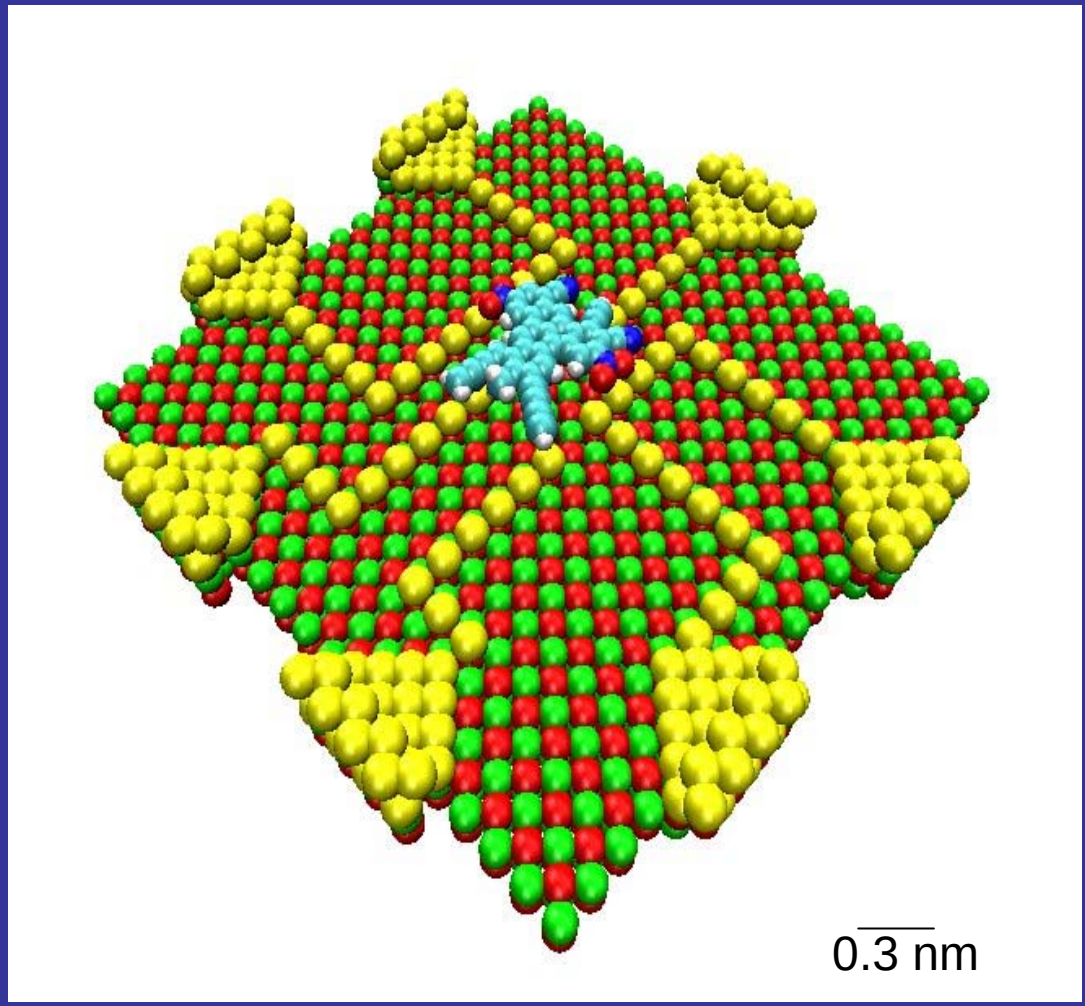
196 Molecular orbitals

5 are « computing »

Molecule OR, AND, NOR, XOR, CNOT have been optimized

Nanolett. Submit.

Surface implantation?



NaCl
KBr
Mica

Si02

Nanostencil

Insulator

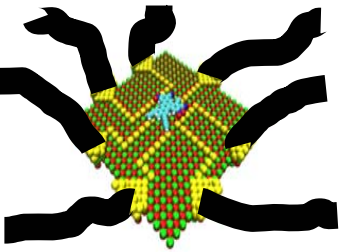
Au/KBr

Metal
Mesa?

KBr pits

Surf. Prep.

Surf. Sci.



5 nm

Atom & molecular manipulation

Semi-conductor

Metal
Mesa?

Surf.
« Passivation »

Surf. Sci.

4 Probes

MoS2

Au/MoS2

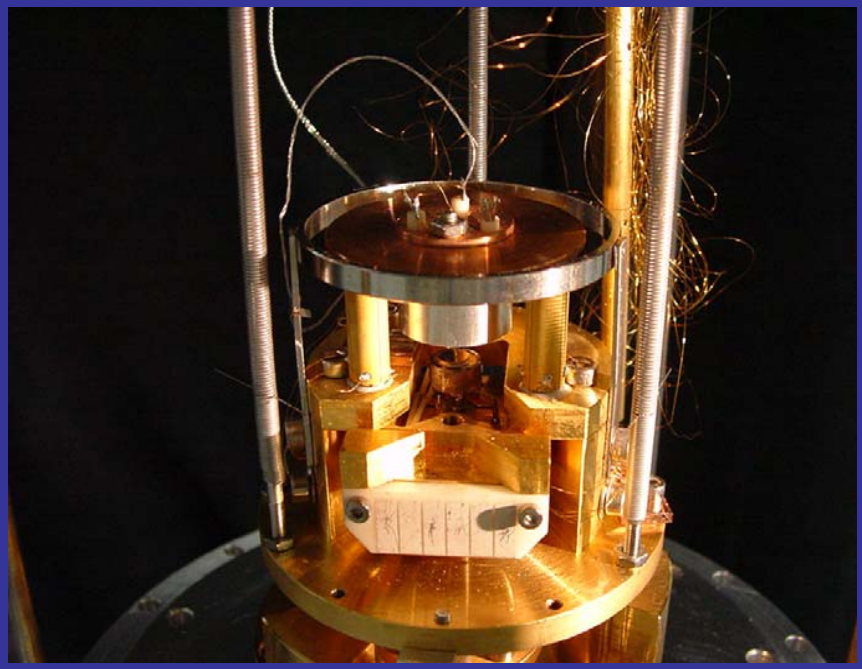
NaCl/Cu(111)
Si(100)X
MoS2

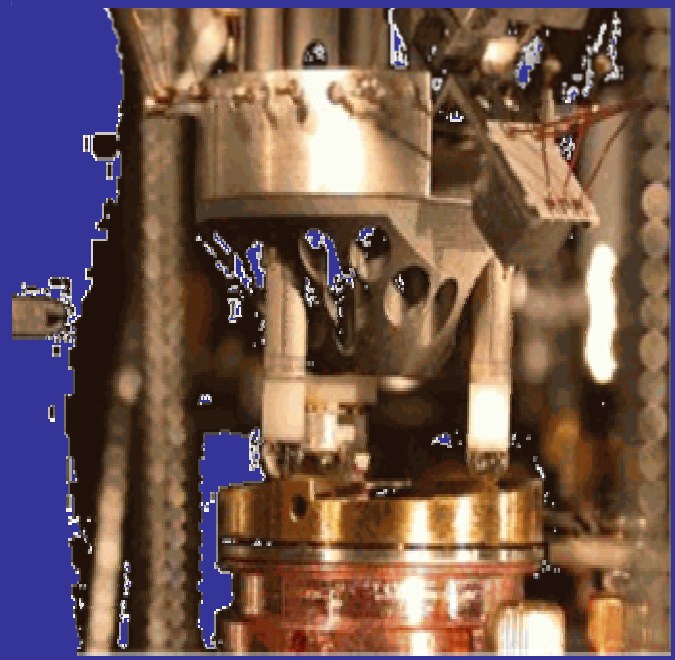
InSb
Si(100)X
MoS2
SiC

Surf. Leak. Current

Pico-Inside

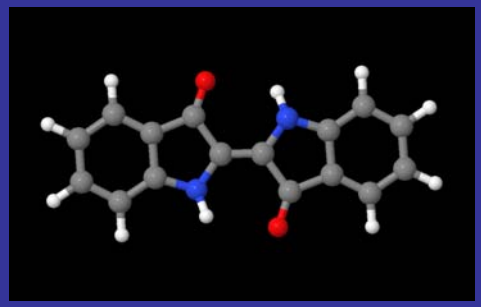
Unit 2
Single molecule(s) on surface
LT-UHV-STM & LT-NC-UHV-AFM





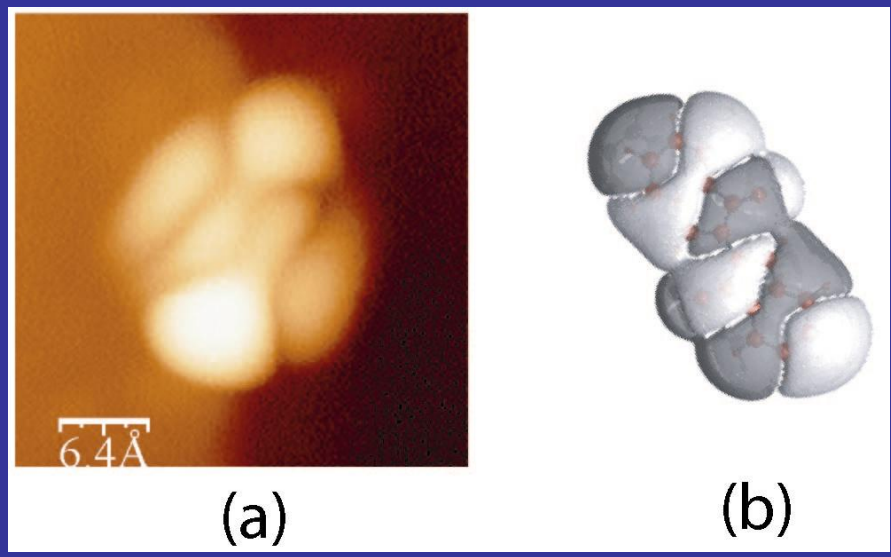
Single molecules on NaCl/Cu(111): Indigo

Indigo molecule



$C_{16}H_{10}N_2O_2$

STM image Calculation



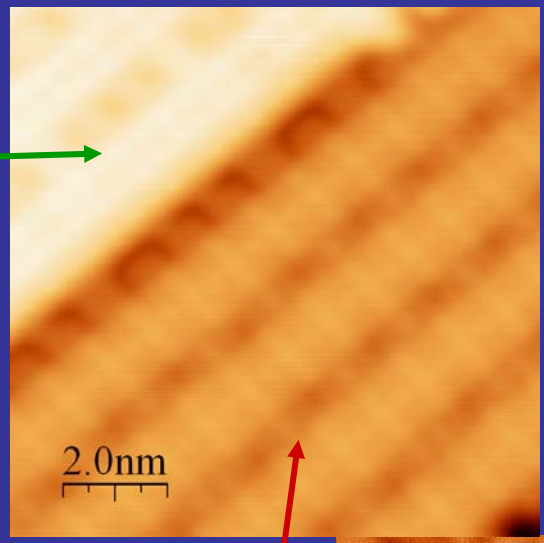
(a) STM image of a molecule on a step edge at V= +1.5V,
(b) LUMO of the free molecule.

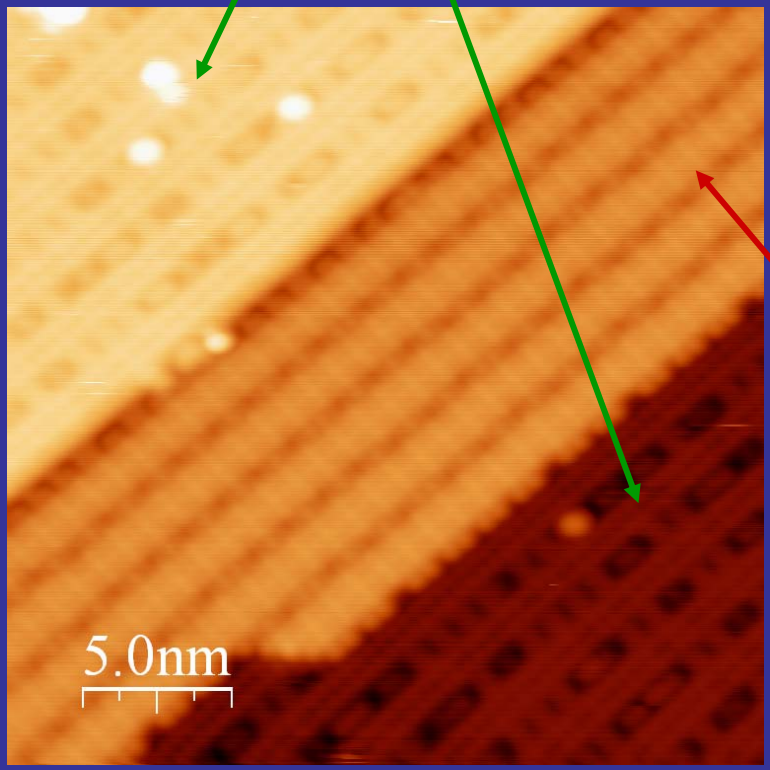
- *Orbitals are resolved*
  Good agreement with calculations at the extremities of the molecule, but less in the centre

Pico-Inside

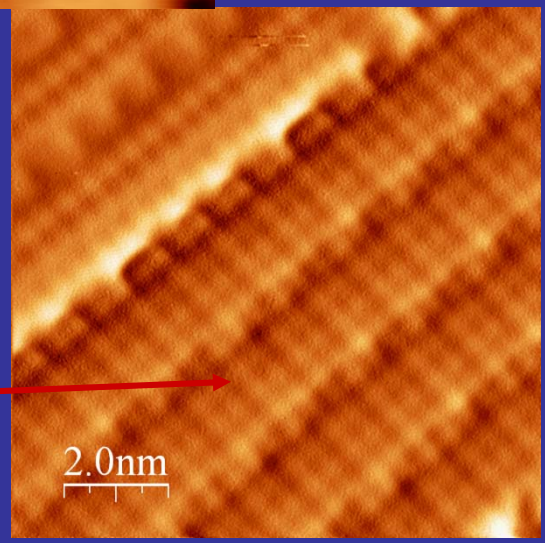
Ultra-thin KBr islands on InSb(001)

New low temperature phase of InSb(001) surface





1 ML KBr

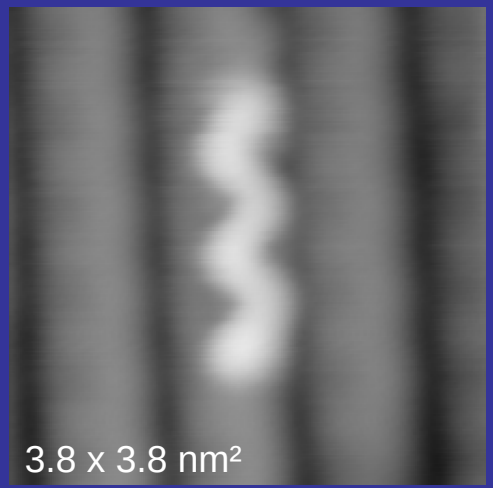


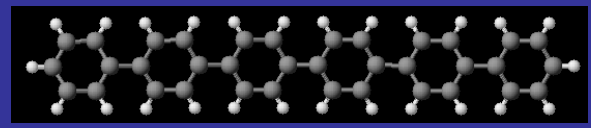
Images taken at 77 K

Adsorption of hexaphenyl on CaF_2 striped phase

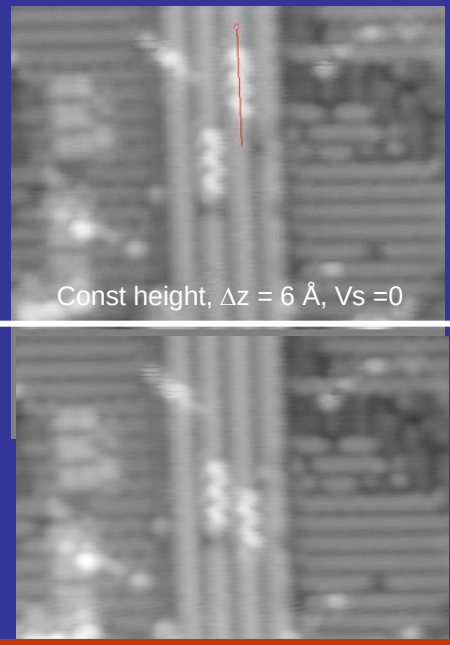
Pico-Inside

Vs = -2.5 V , 60 pA

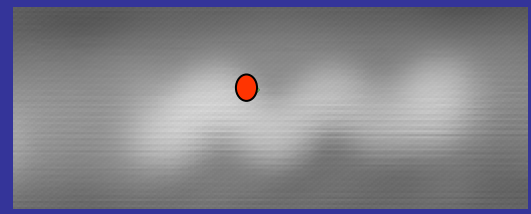




Tip manipulation



Voltage pulses

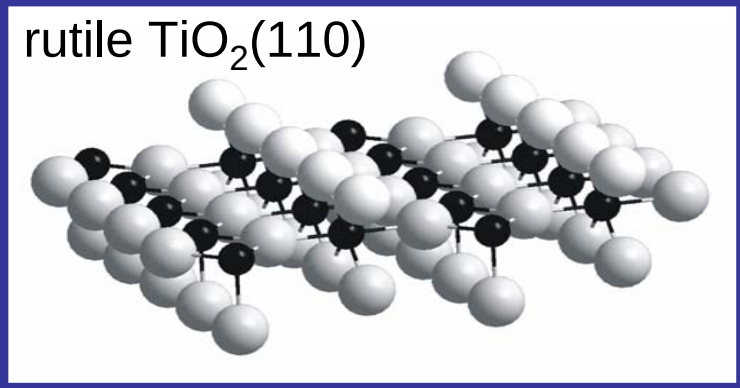


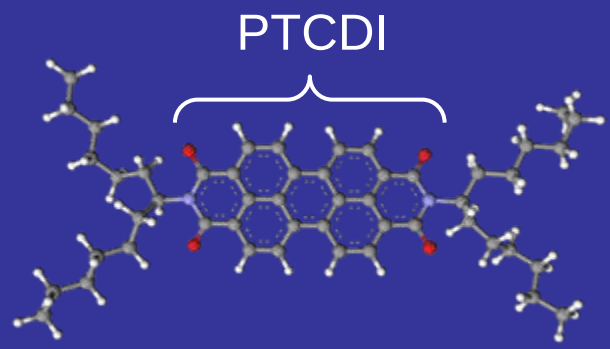
Vs = -3.5 Volts, 1 nA, 4 sec.

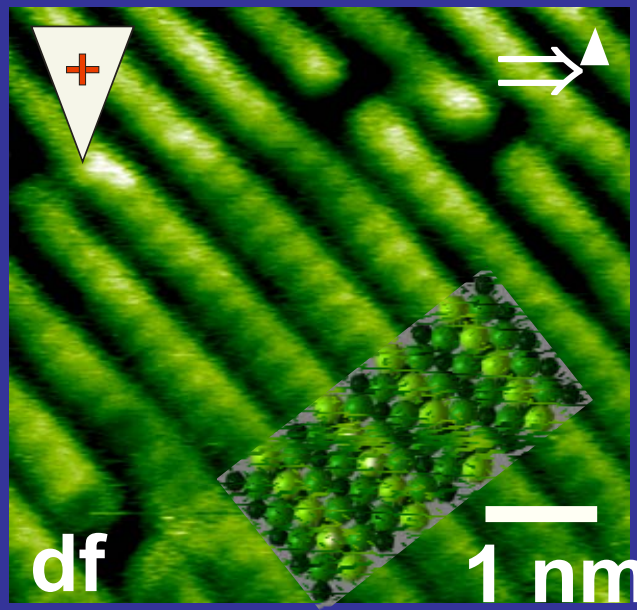
⇨Single hexaphenyl molecules can be aligned and positioned along insulating CaF_2 stripes on Si(100)

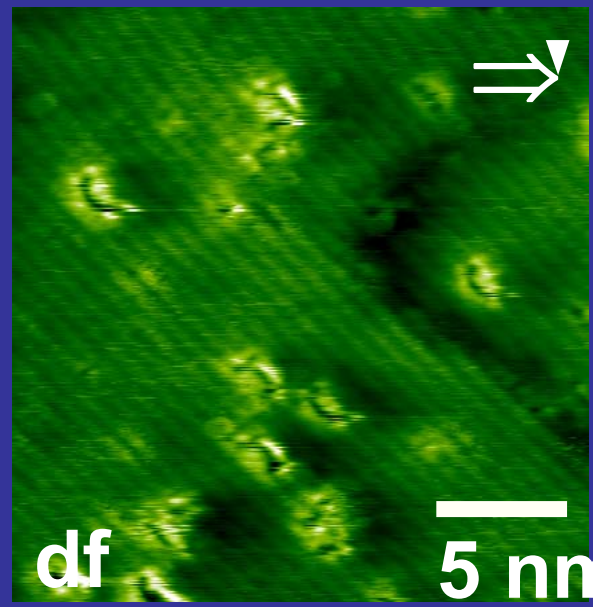
0.2 L Hexaphenyl adsorbed at 5K

NC-AFM the perylene derivative on rutile TiO_2(110)



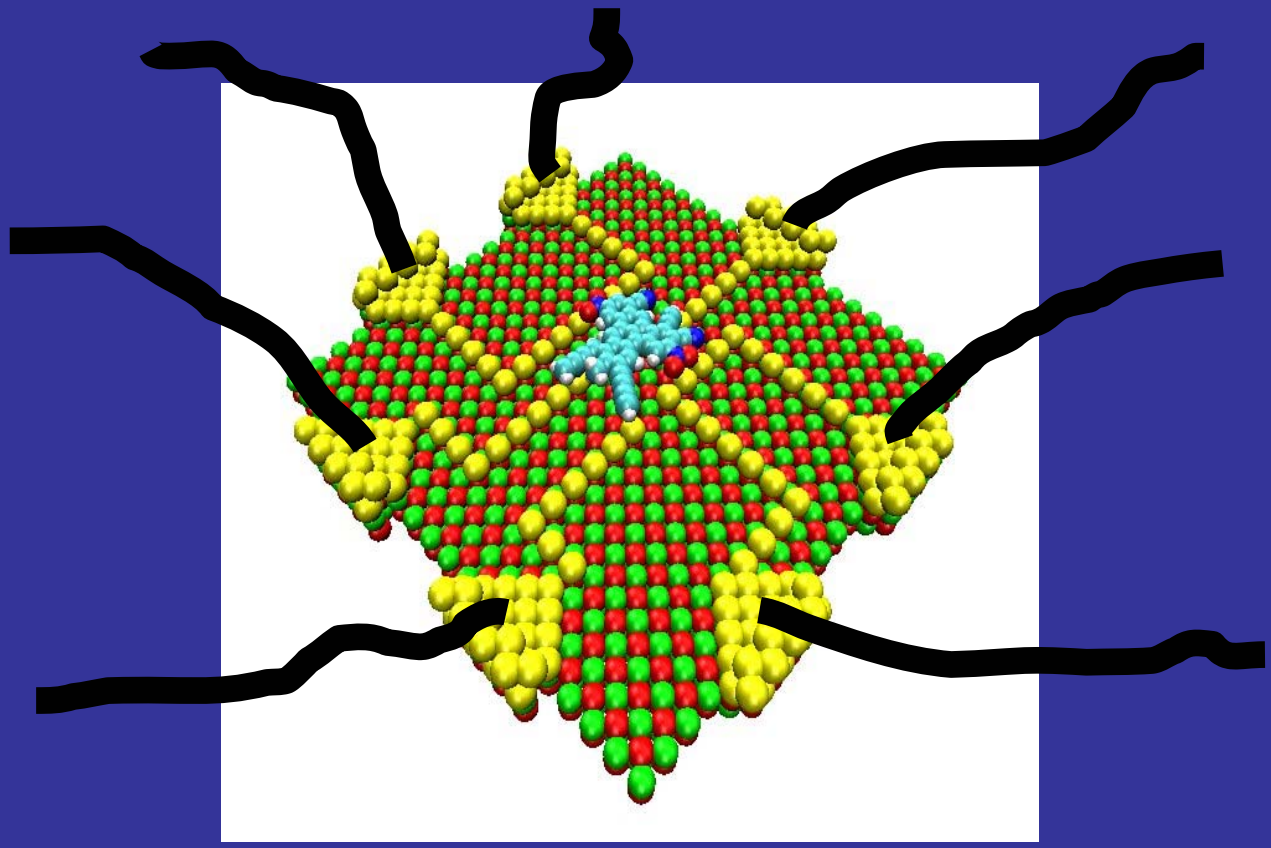






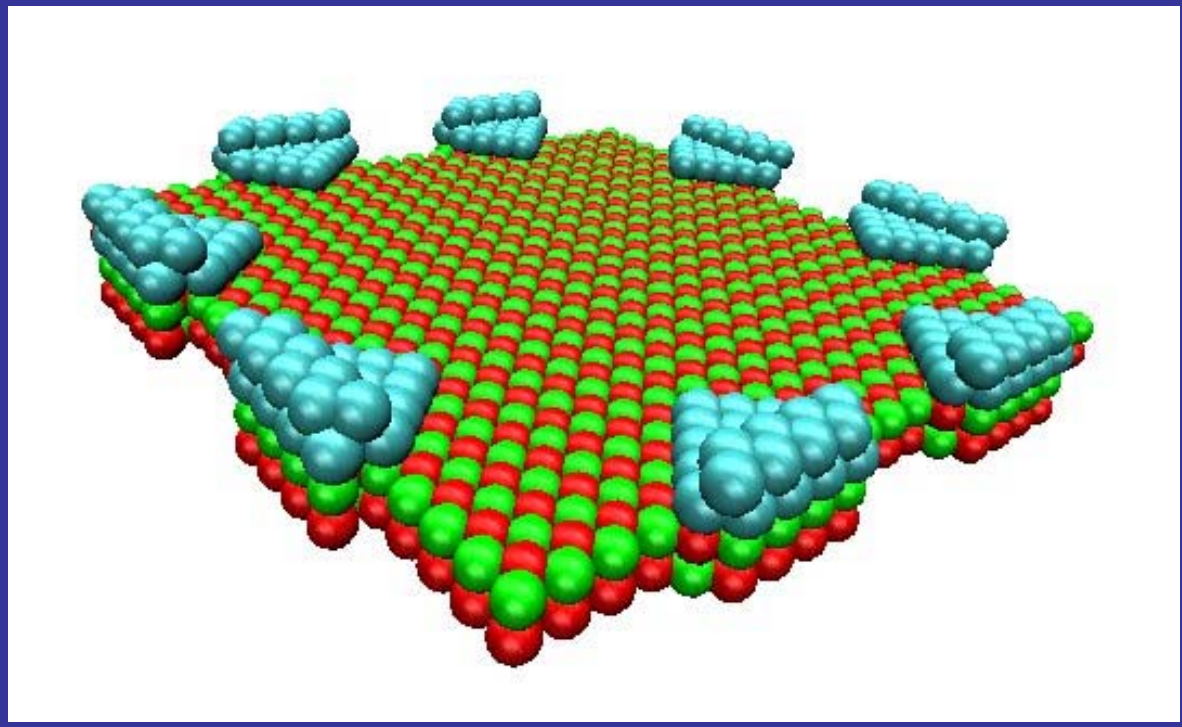
Pico-Inside

Unit 3
Atomic scale technology for surface interconnects



Pico-Inside

1st step: ultraflat nano-island
on a semi-conductor surface

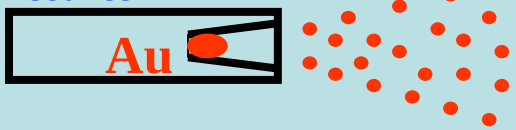


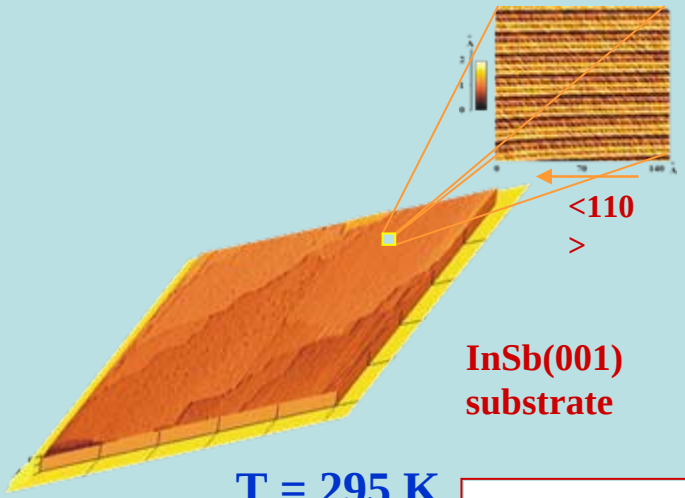
Growth and self-assembling of nanostructures on semiconductor

Au/InSb(001)

Au deposition

Evaporation source

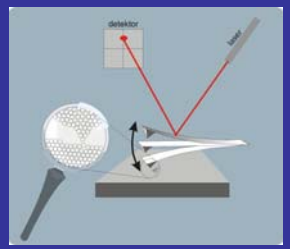




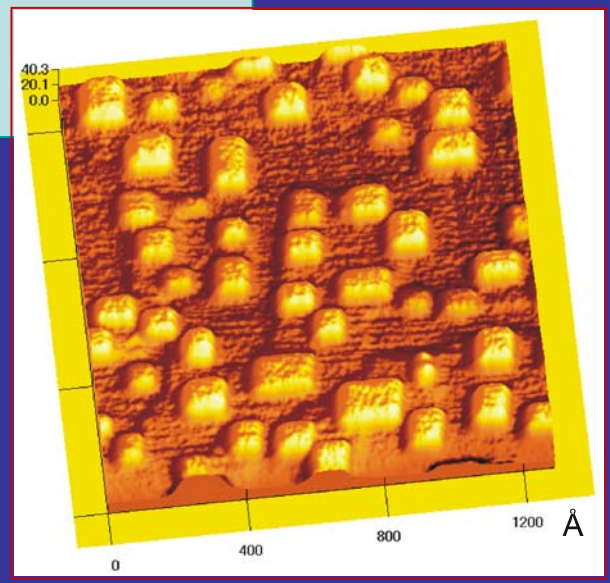
InSb(001) substrate

T = 295 K

rate 1-2 ML/min

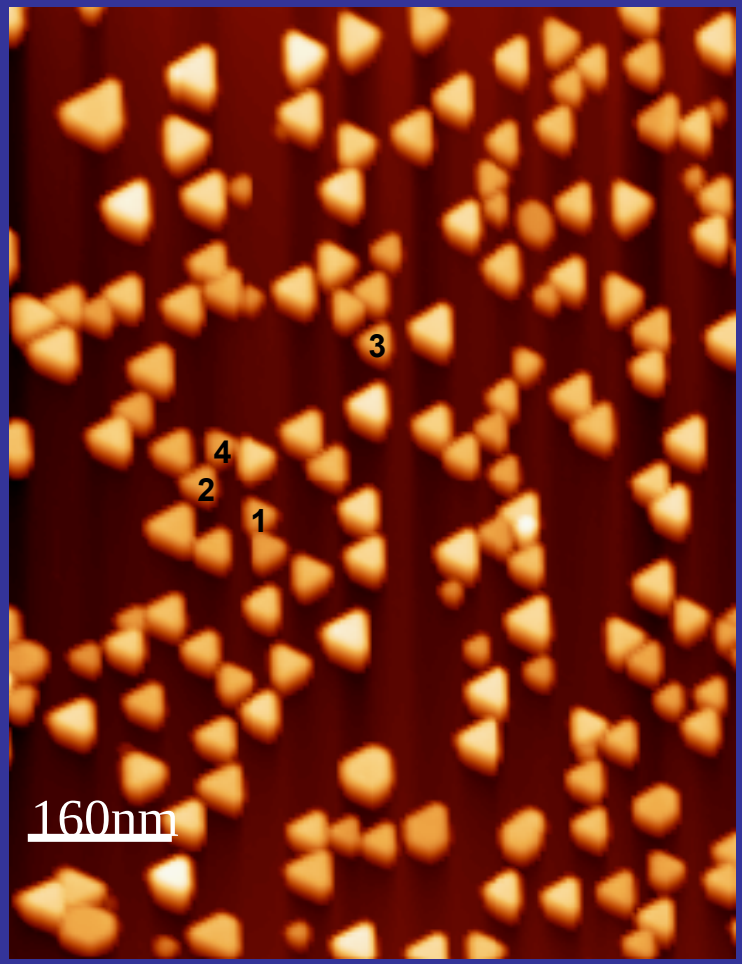


0,2 ML Au / InSb(001)

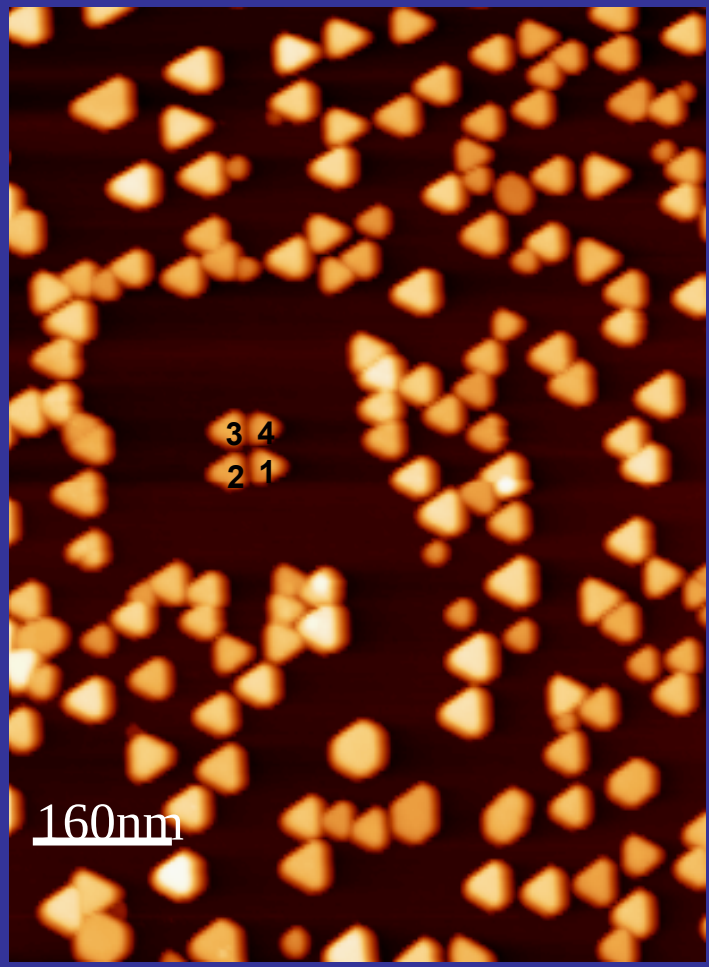


Pico-Inside

UHV-STM construction of a planar 4 nano-contacts on MoS2

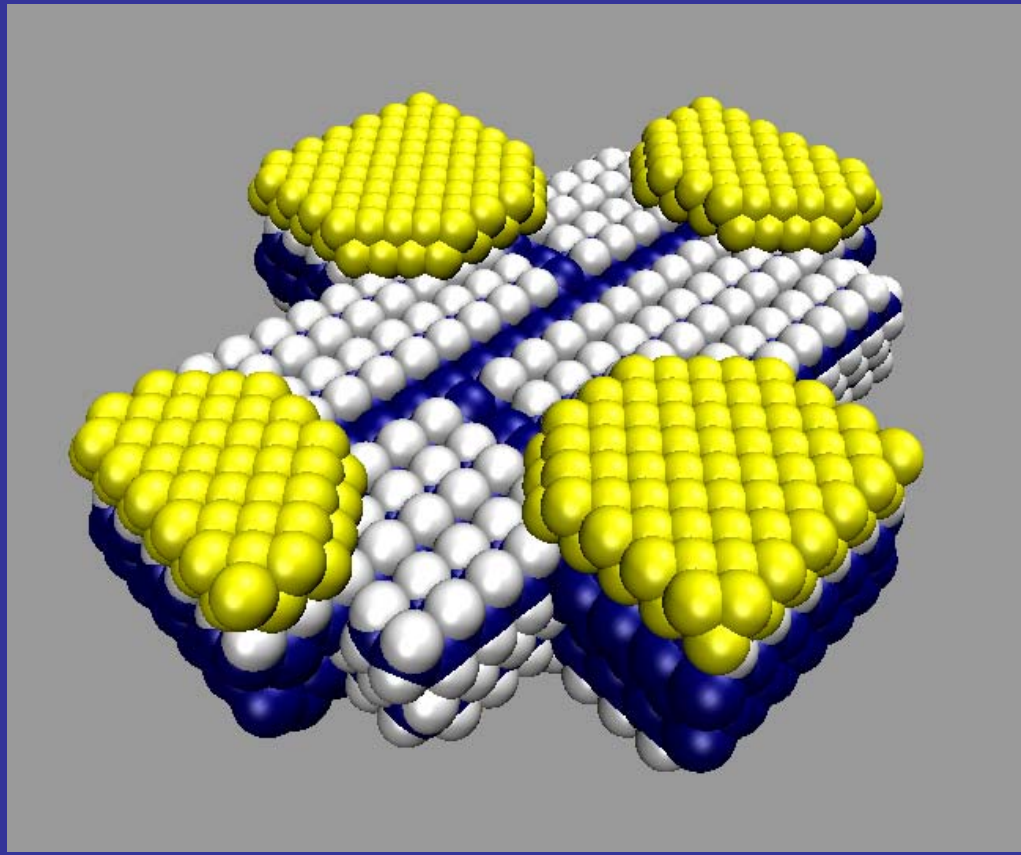


before



after

2nd step: Atomic to nanoscale interconnects

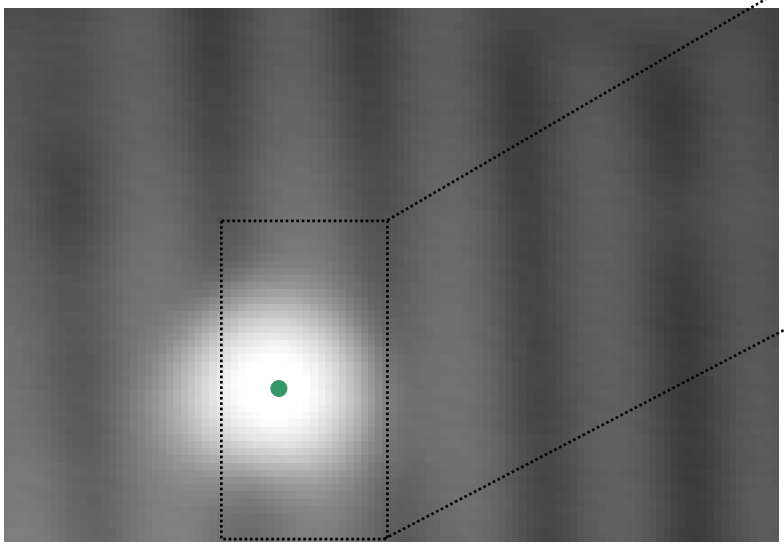


Manipulating a single H on Si(100)H

n-doped Si(100)

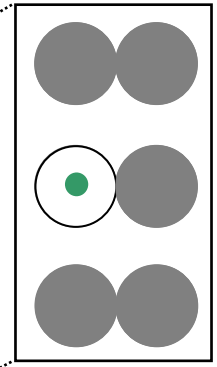
Low temperature-STM (5 K)

-1.7V 69pA



4 nm

Top view



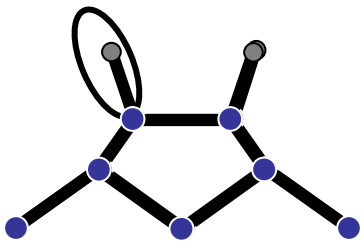
H

Si Dangling Bond

- Surface voltage pulse of **+2.5V**: Desorption of the H atom

➡ Creation of a Si dangling bond

Side view



H

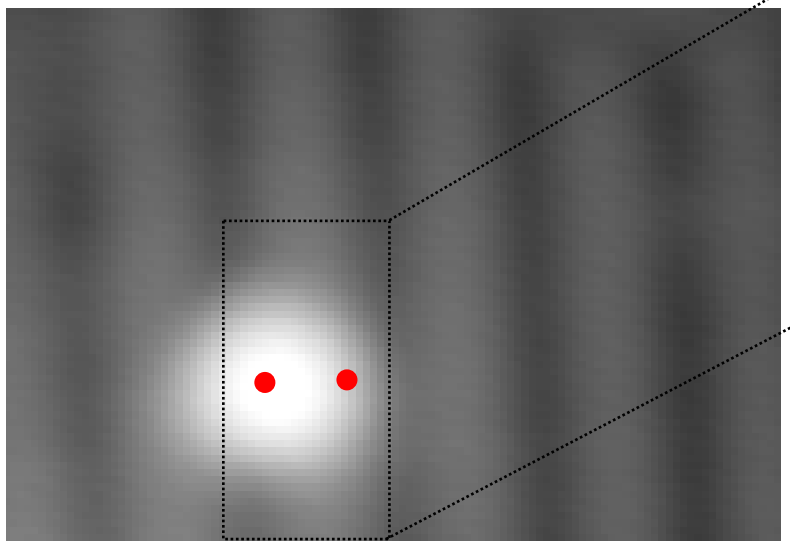
Si

Manipulating a single H on Si(100)H

n-doped Si(100)

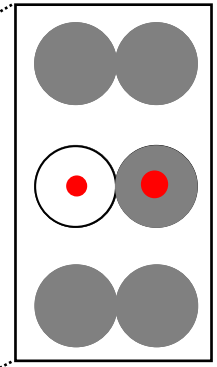
Low temperature-STM (5 K)

-1.7V 69pA



4 nm

Top view



H

Si Dangling Bond

- Surface voltage pulse of **+2.5V**: Desorption of the H atom

➡ Creation of a Si dangling bond

- Surface voltage pulse of **-2.5V**:

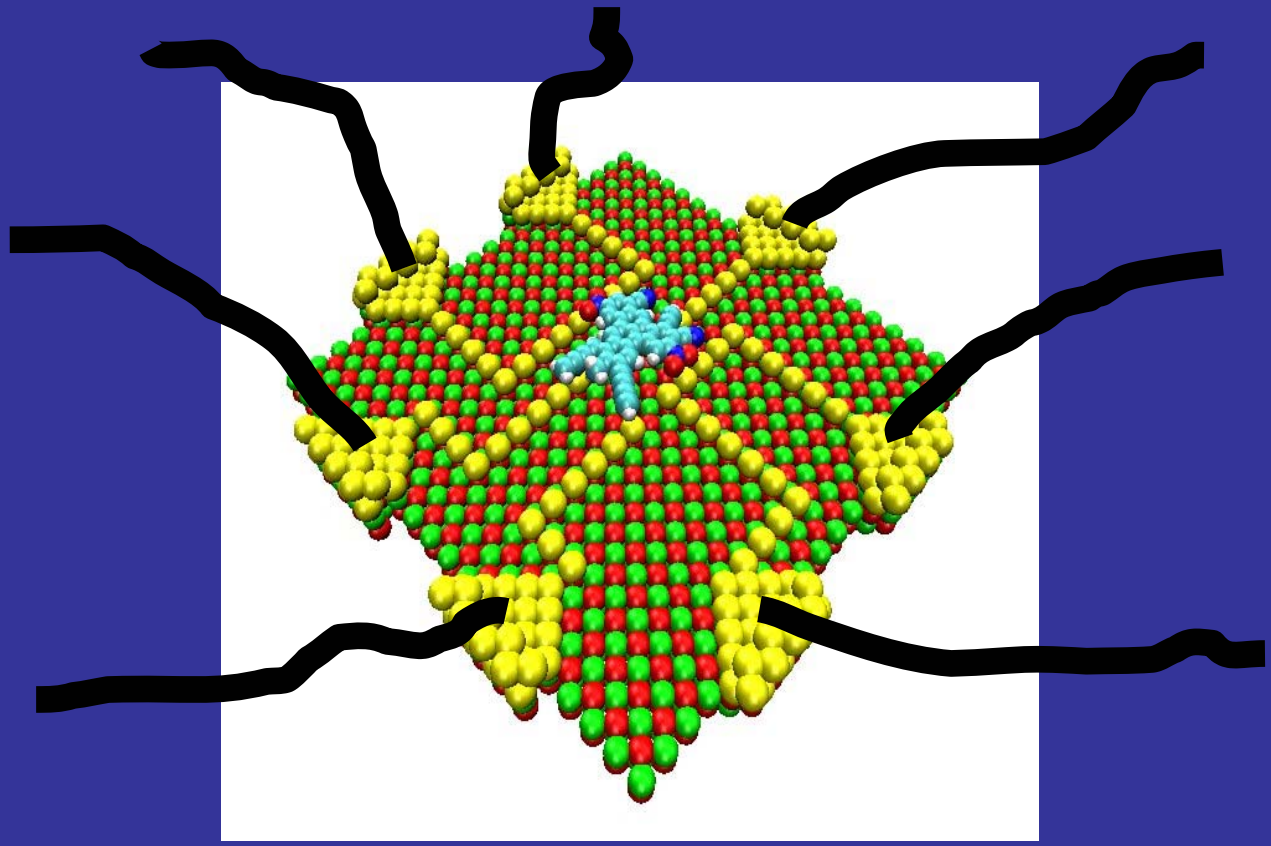
➡ H-atom lateral displacement

The H-atom lateral displacement is reversible

Pico-Inside

3rd step:

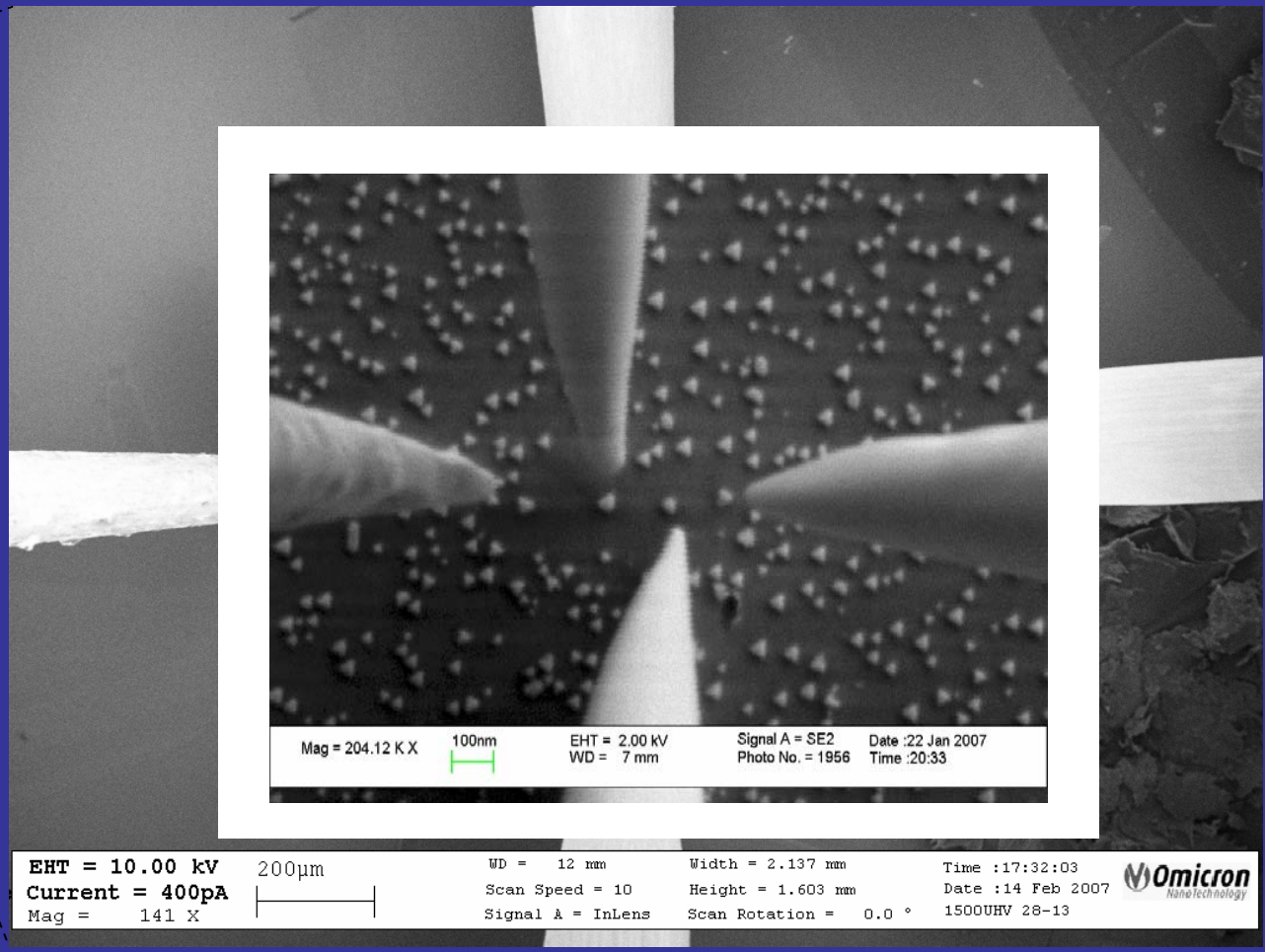
interconnects from the nano to the macroscale?



(Preserving the atomic precision)

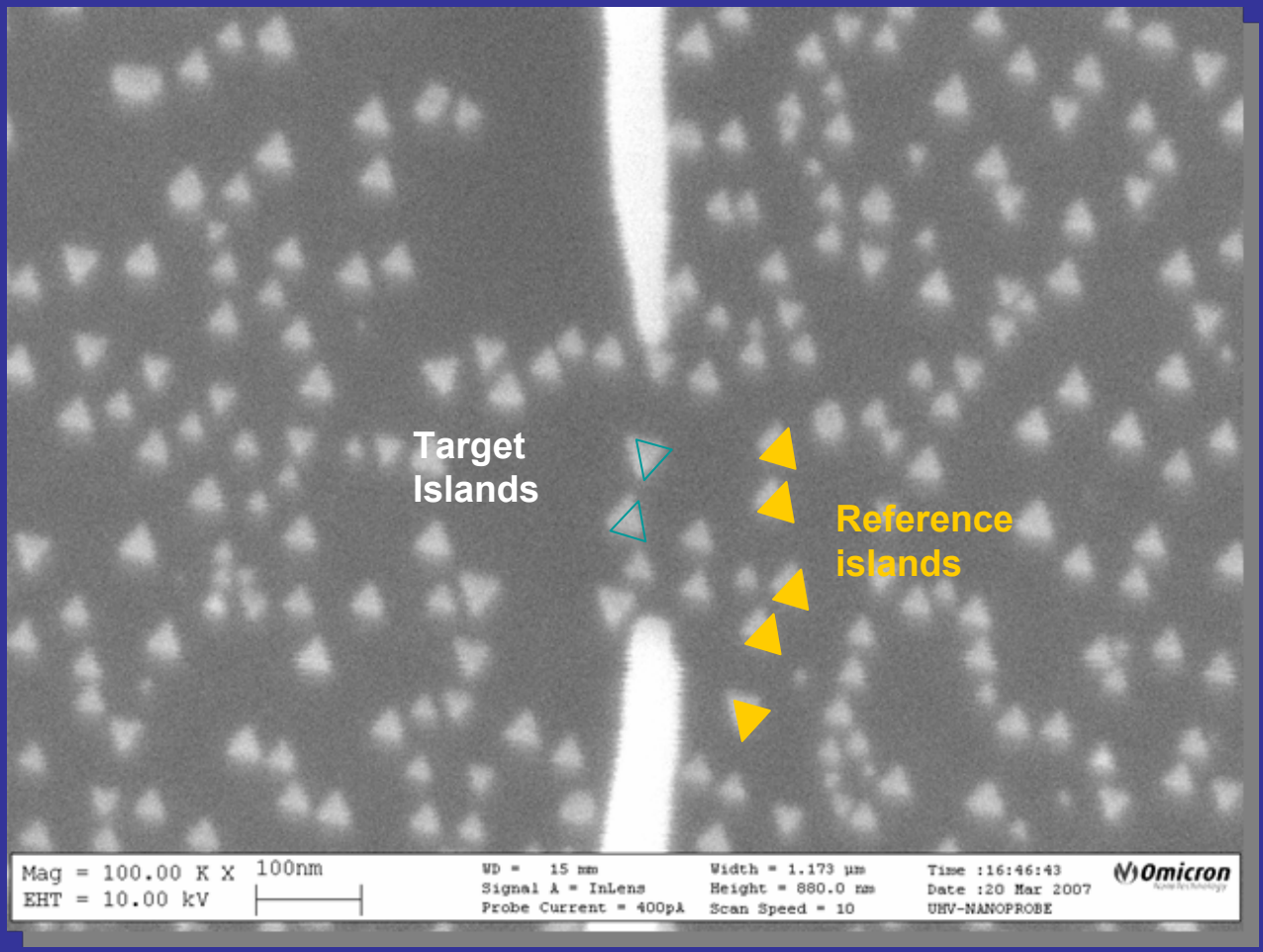
Pico-Inside

High aspect ratio tips. Bases are far apart.



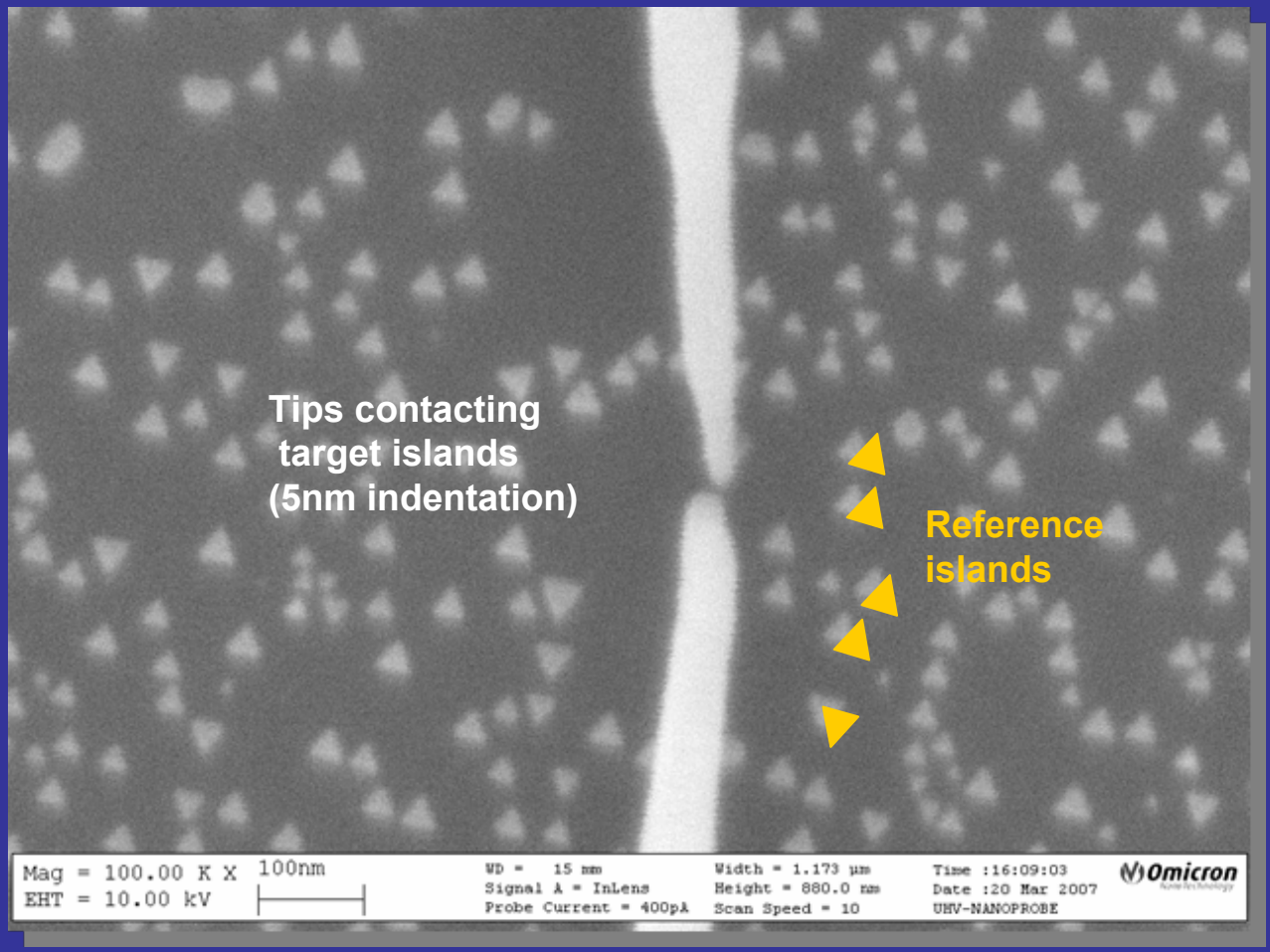
Omicron 4 probes UHV 50 K + SEM Gemini (10 KeV, 400 pA)

Fine Navigation under the SEM



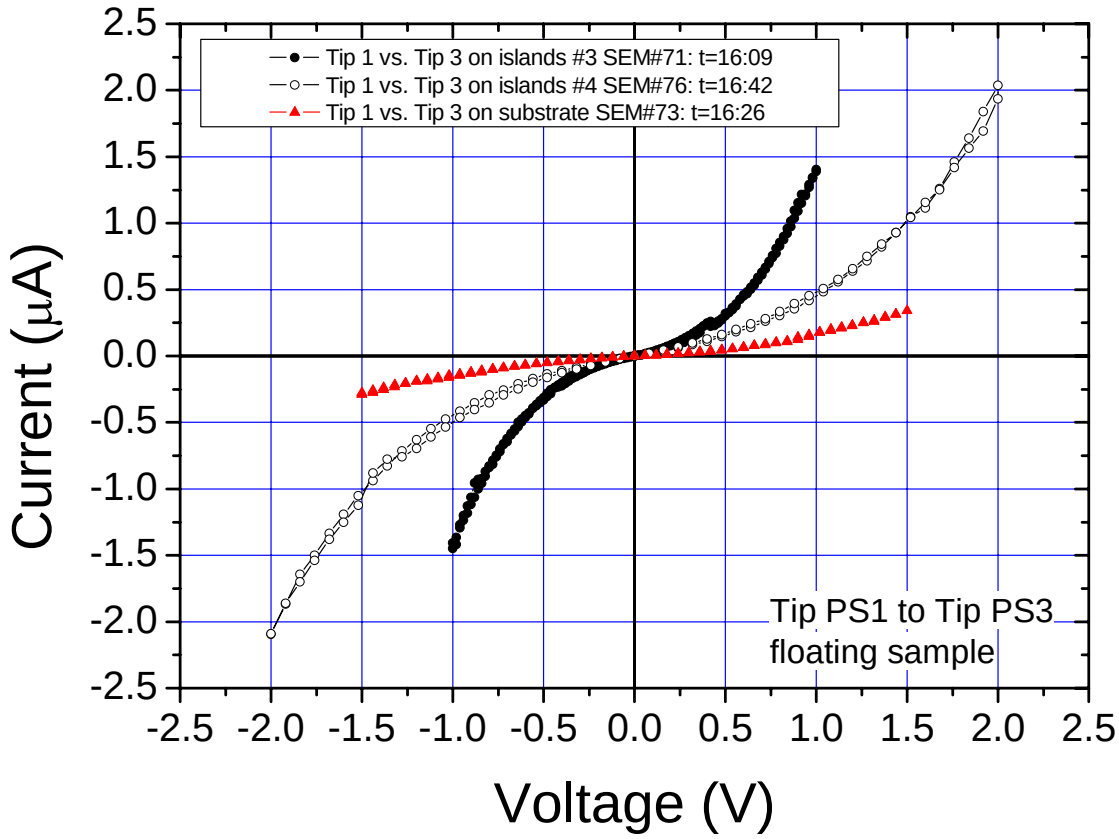
- Two target islands (green)
- Reference islands (yellow) marked for visual identification

Fine Navigation

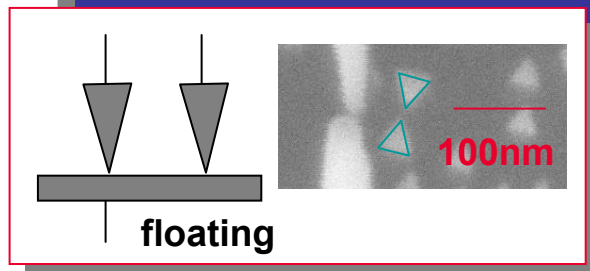


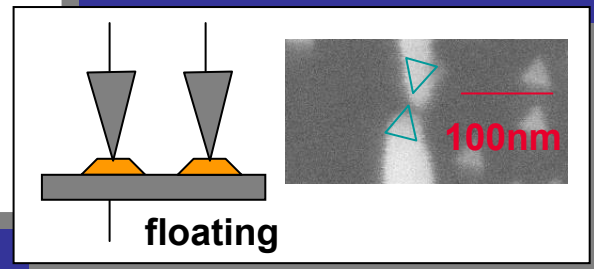
- Two tips on target islands
- Electrical contact, 5nm indentation
- Transport measure-ment between two islands

Surface Transport Measurement between two islands



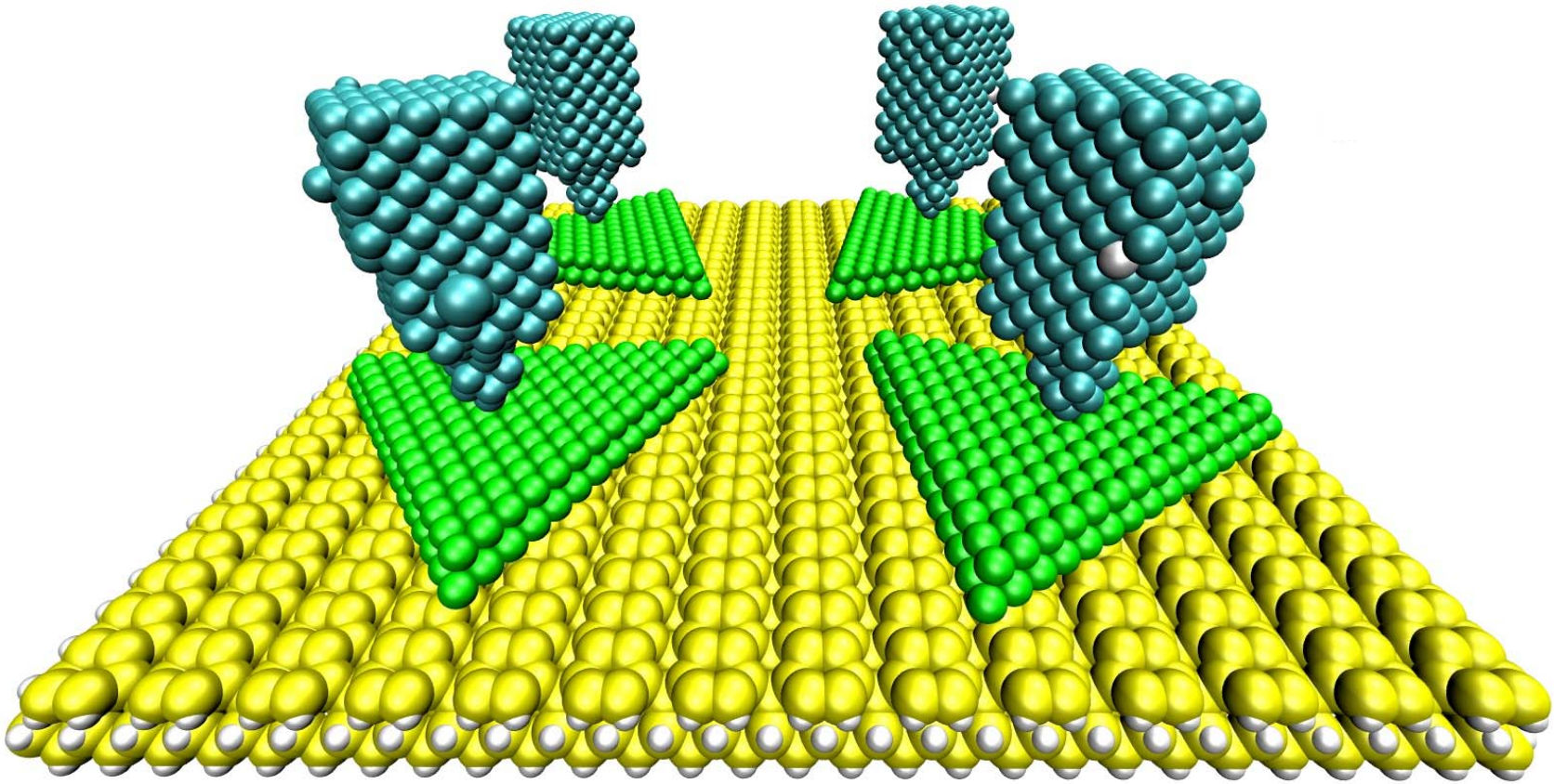
- 2-point measurements between tips on islands and substrate
- Higher conductance for islands due to larger contact area





Pico-Inside

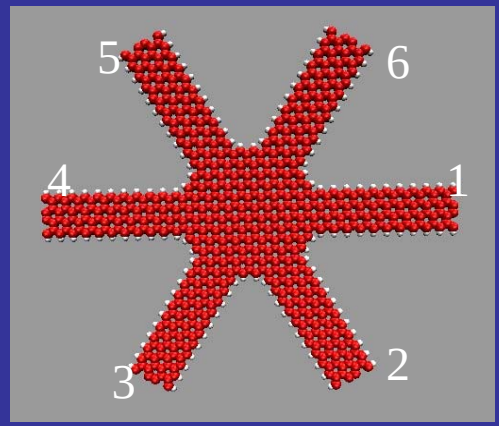
Theory of surface interconnect using N-ESQC



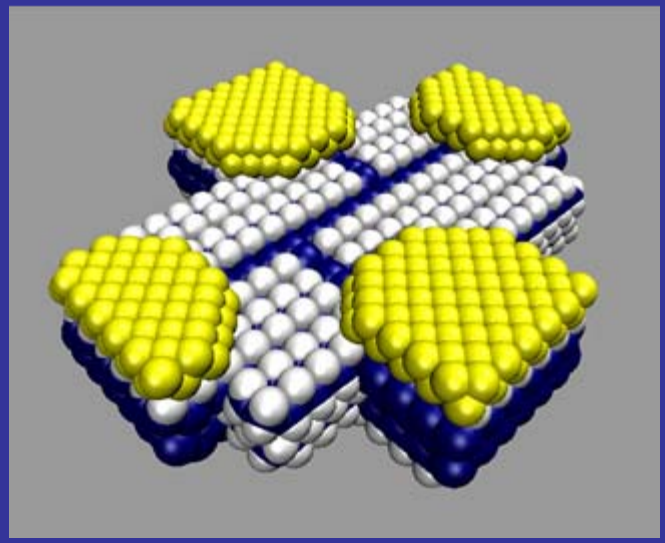
6112 Surface atoms, 225 Au atoms per nano-island
& 284 per metallic tip

N-ESQC test

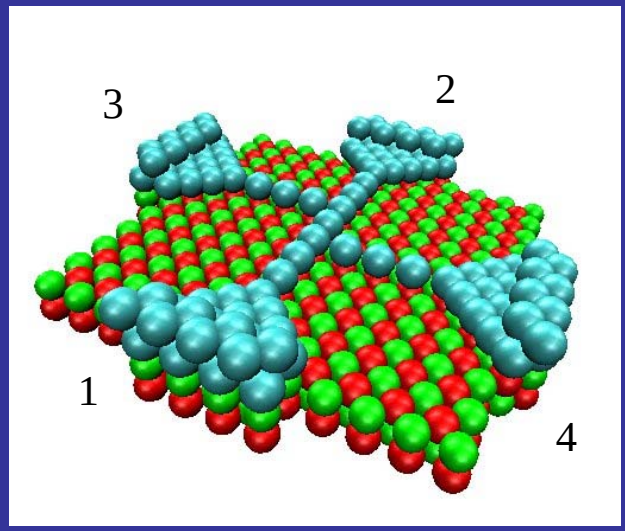
NATOM atoms	NDIMOL orbitals	SIZE nm	NATOM dimensions	NDIMOL maximum	Virtual Mem Gb	Res Mem Gb	Solver Time (s)	1 point Time (s)
96	378	1.72	1000	2000	1.9	0.074	120	60
228	876	2.7	1000	2000	2	0.128	284	76
408	1560	3.68	1000	2000	2.1	0.242	1607	103
636	2436	4.67	1000	3000	3.4	0.536	6021	125
912	3504	5.65	1600	5000	6.5	1	19589	143
1236	4764	6.63	1600	5000	7.1	1.8	45186	200
1608	6216	7.61	1800	6500	10.1	3.1	108412	289
2028	7860	8.6	2100	7900	14.3	5.4	222645	415
2496	9696	9.58	2500	10000	20.8	7.3	440000	570
4188	16356	14,48						



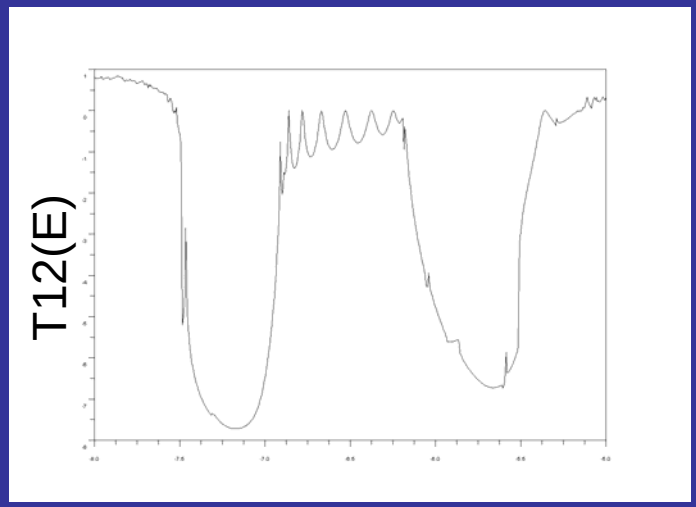
Theory of surface atomic scale circuit electronic transport

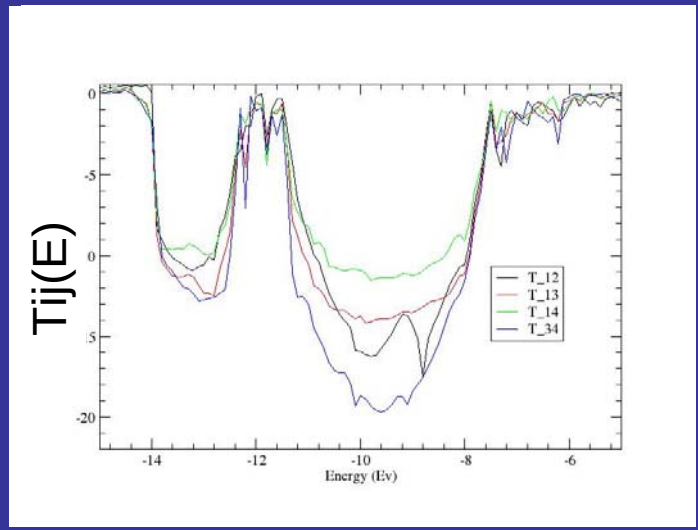


N-KESQC on Si(100)H



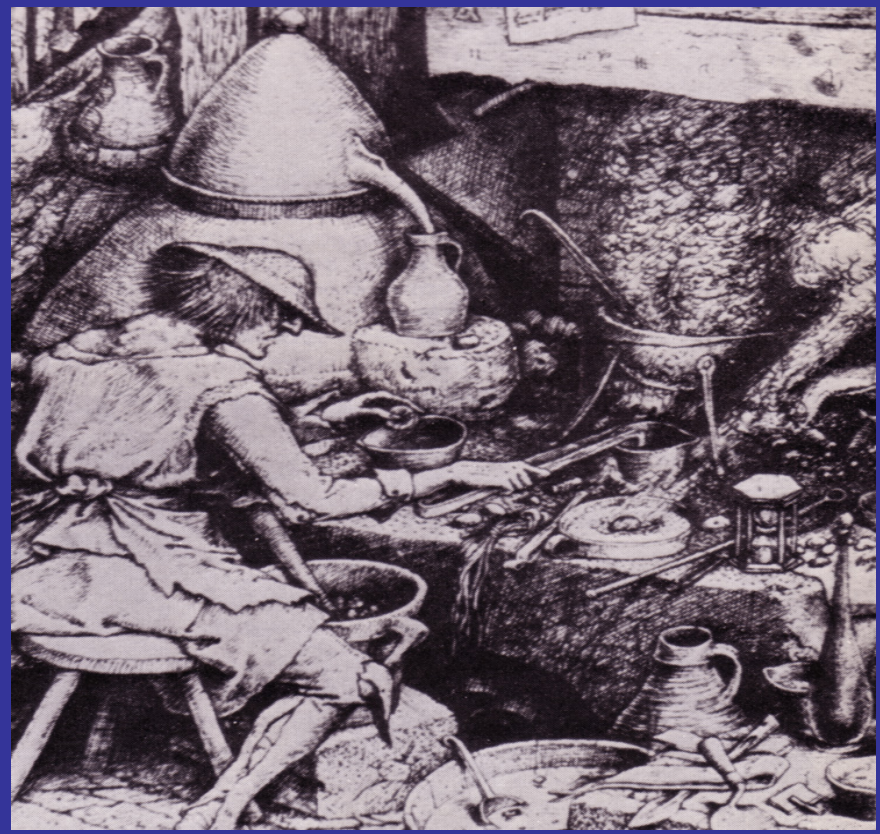
N-ESQC on MgO



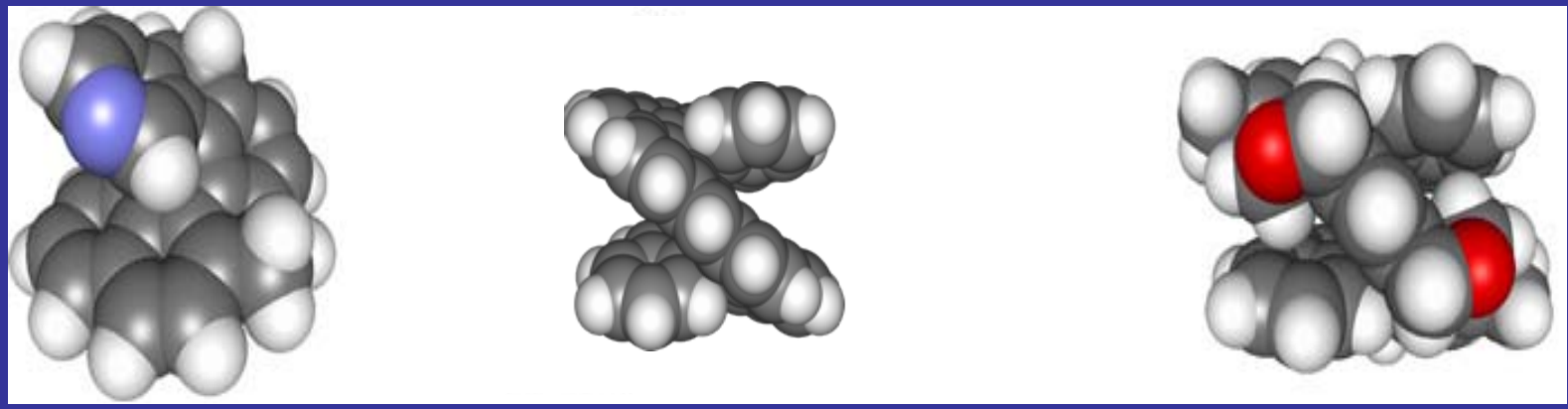


Pico-Inside

Unit 4
The Chemistry

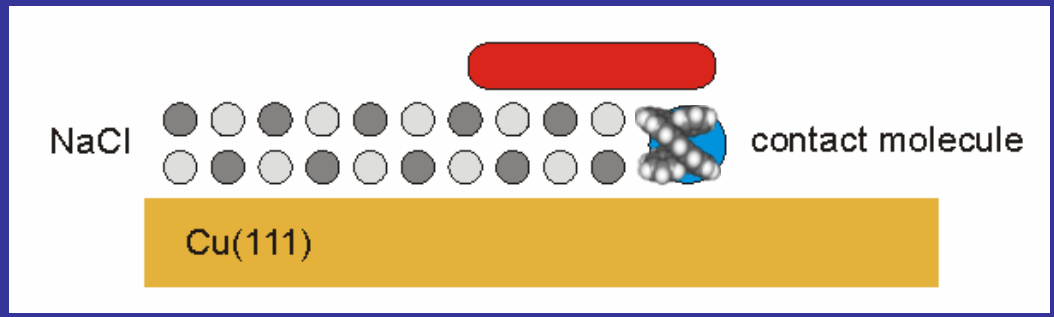


The Helicene series for interconnects

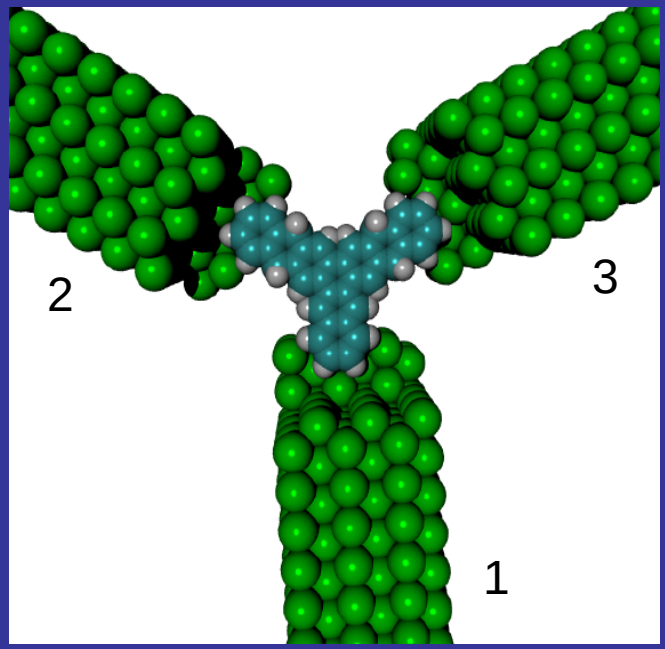


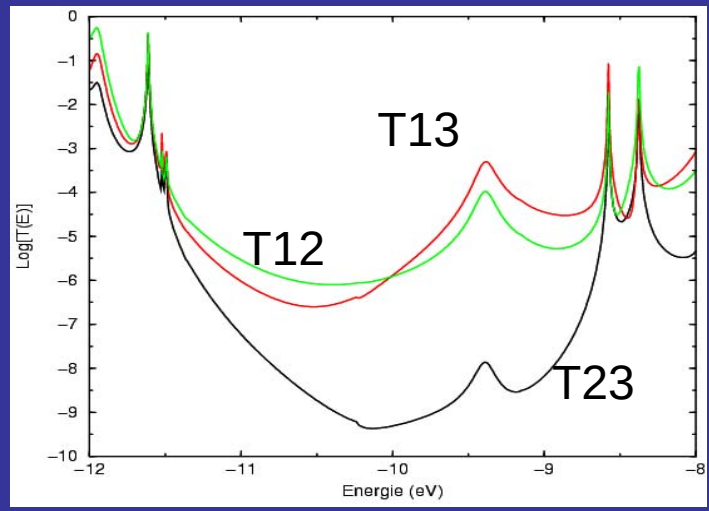
Hetero-helicenes

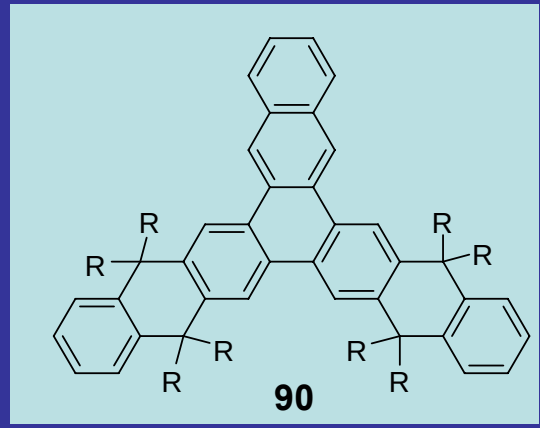
extended helicenes



A semi-classical OR gate based on tunnel exponential decay







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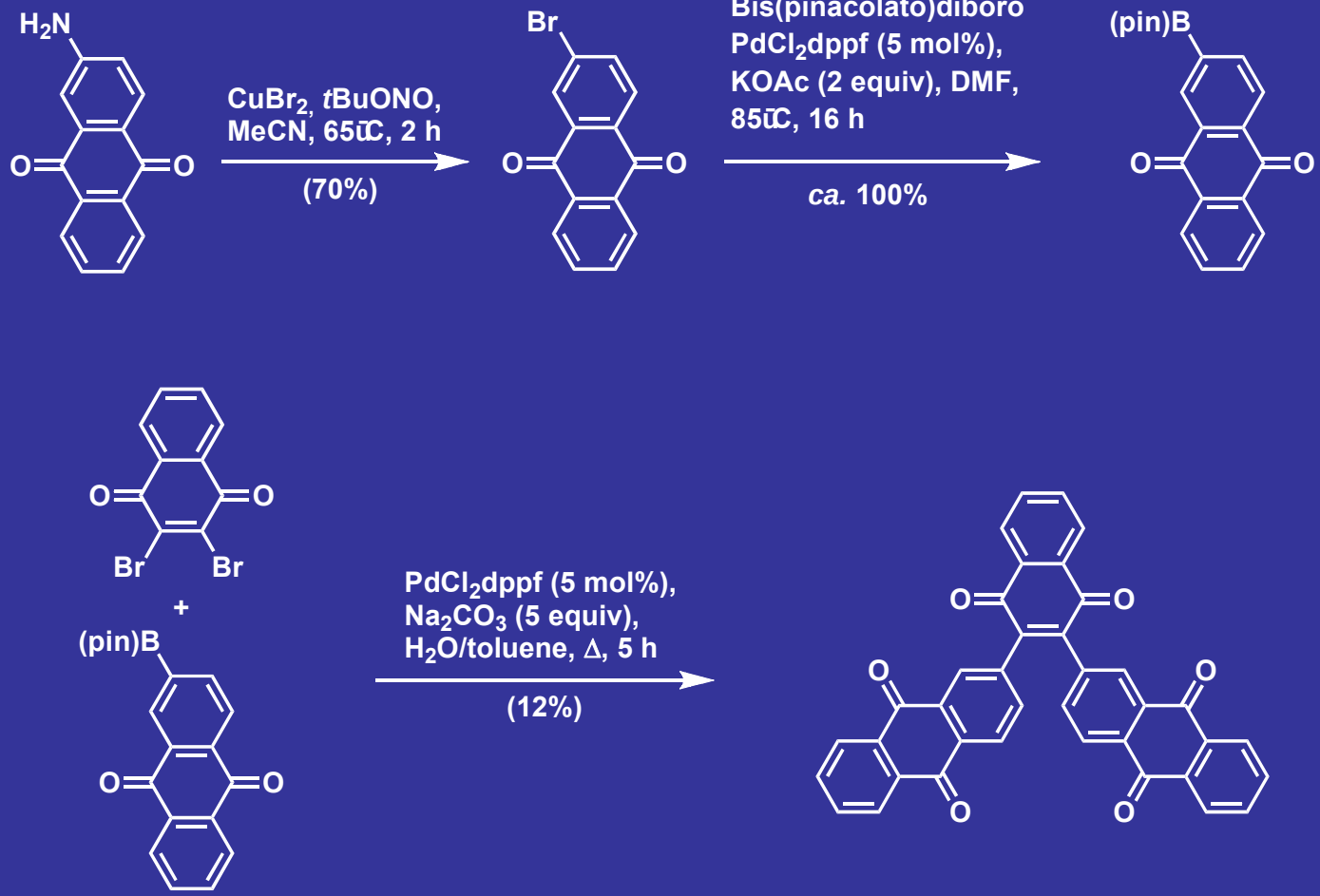
Molecule OR Polyaromatic Hydrocarbons



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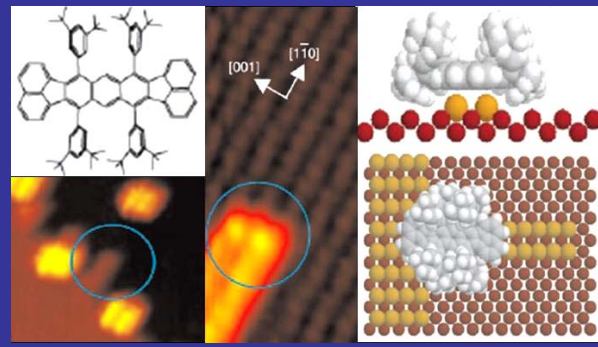
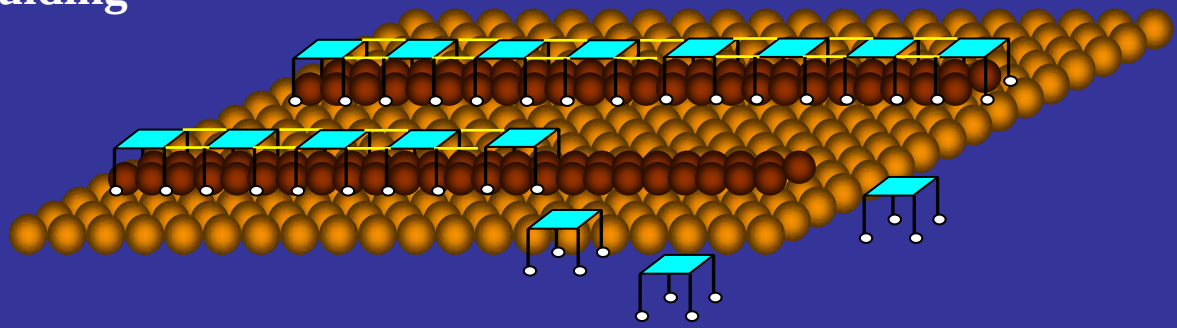
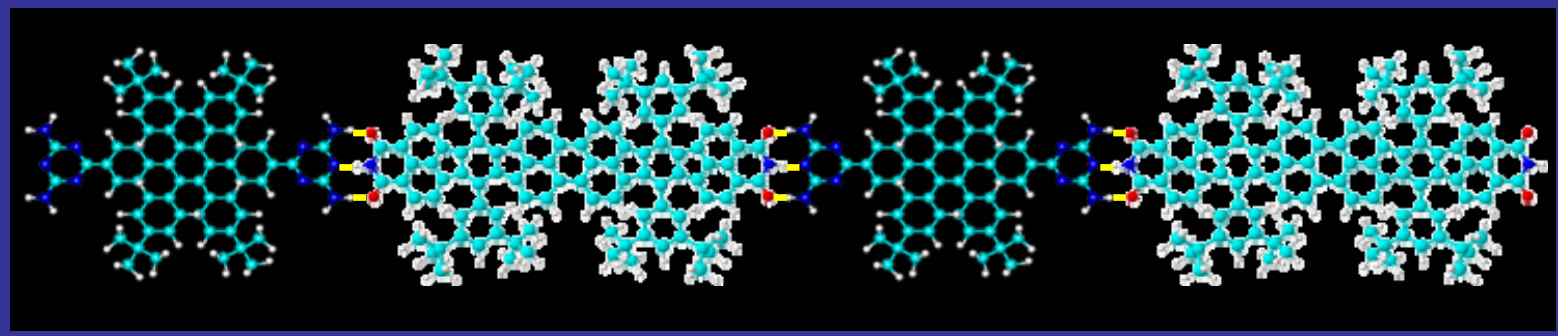
Molecular templates for the formation of atomic nanostructures



Science 296, 328 (2002)

Molecular moulding





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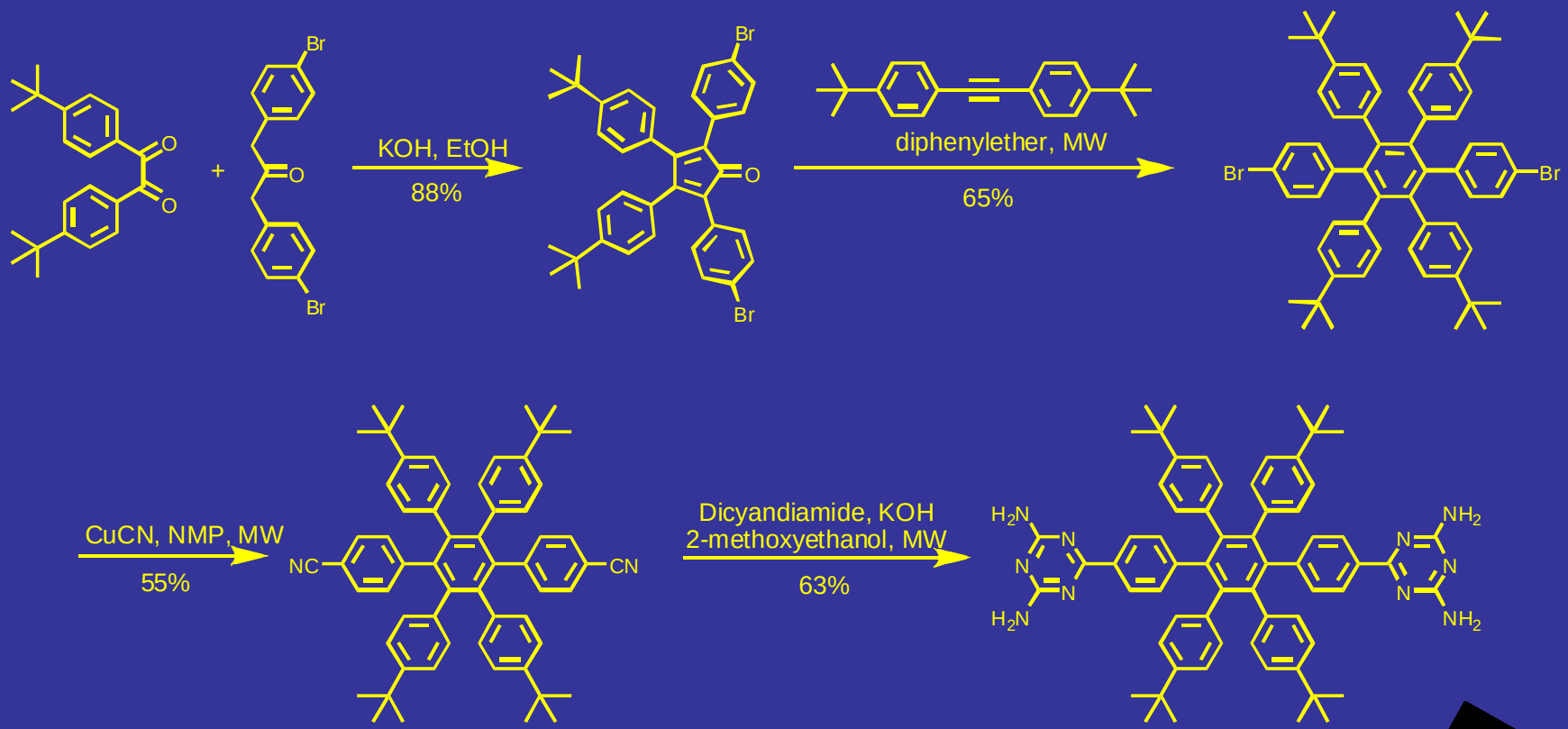
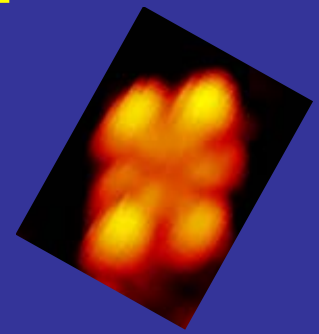
IST-FET IP project n° 015847

First molecule (A) : bis(diaminotriazine)lander





on Cu(110)

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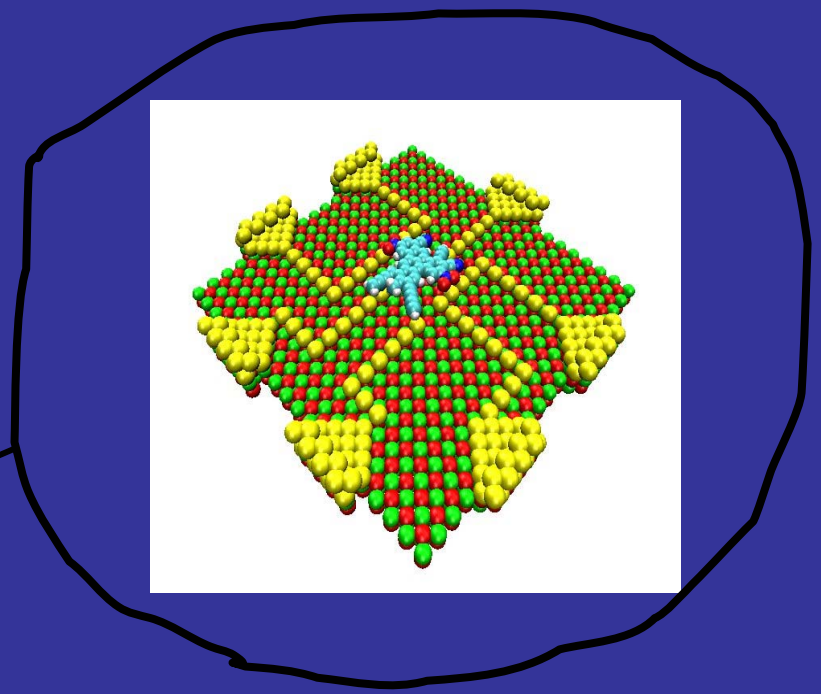
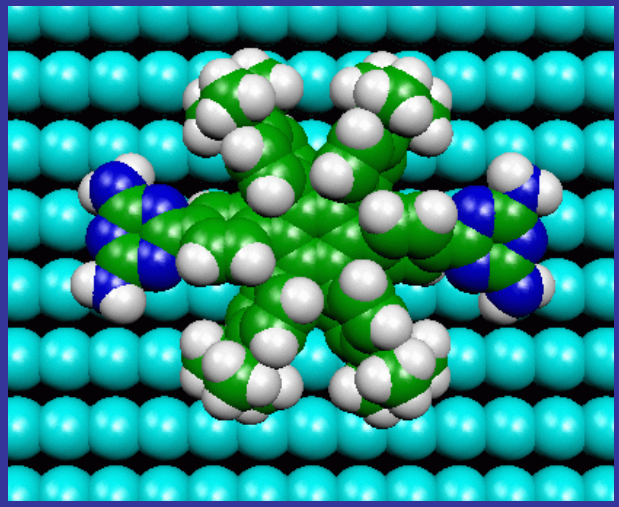
Unit 5
Theory of molecule on surface



With Fujitsu Europe

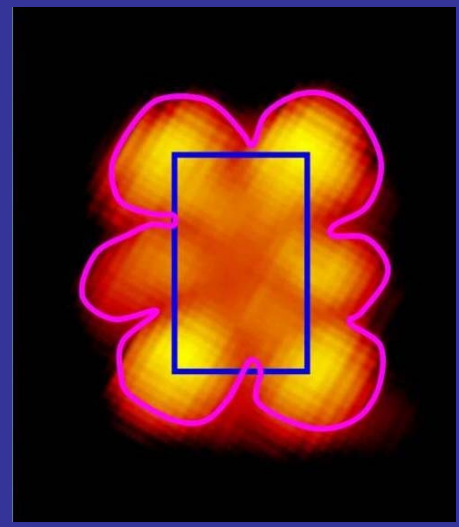
STM calculations Molecule on a metallic surface

Molecule A



26 Å× 30 Å

ESQC image

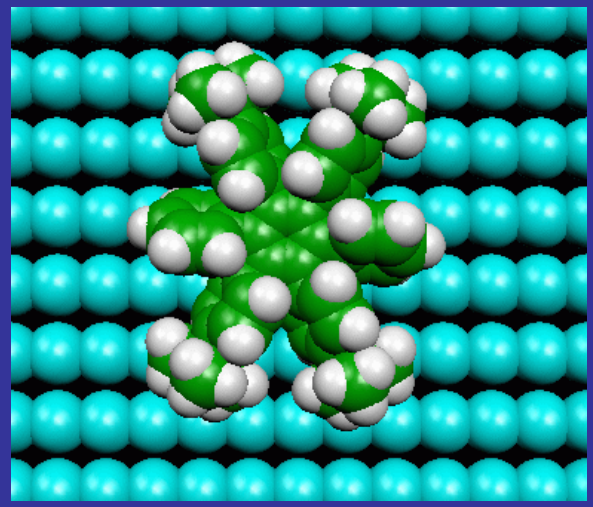


22 Å× 16 Å

Experiment (Aarhus)

Molecule A’

on Cu(110)



AFM calculations CaO(001) surface

Atomic-scale contrast obtained with vAFM

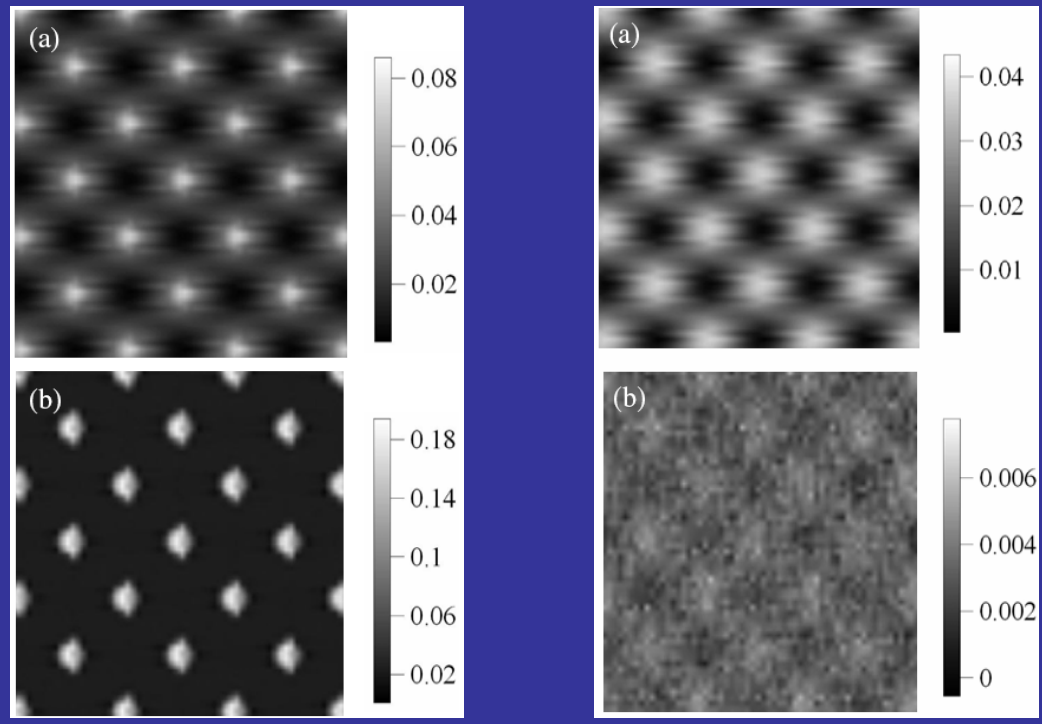
MgO tip

Mg-terminated tip

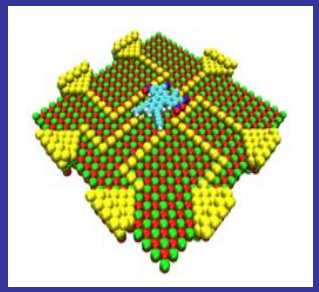
O-terminated tip

Topography

Dissipation

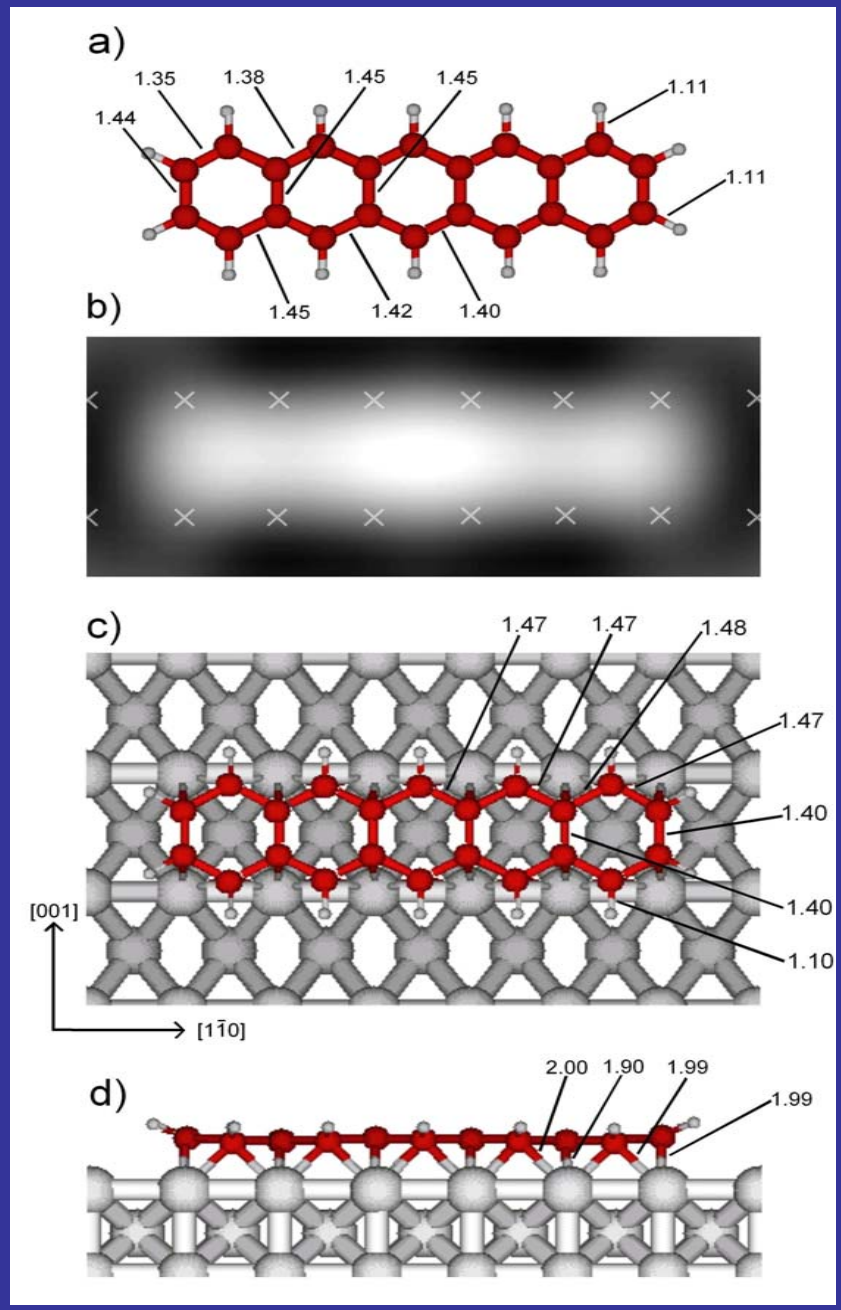


Frequency shift: - 279 Hz

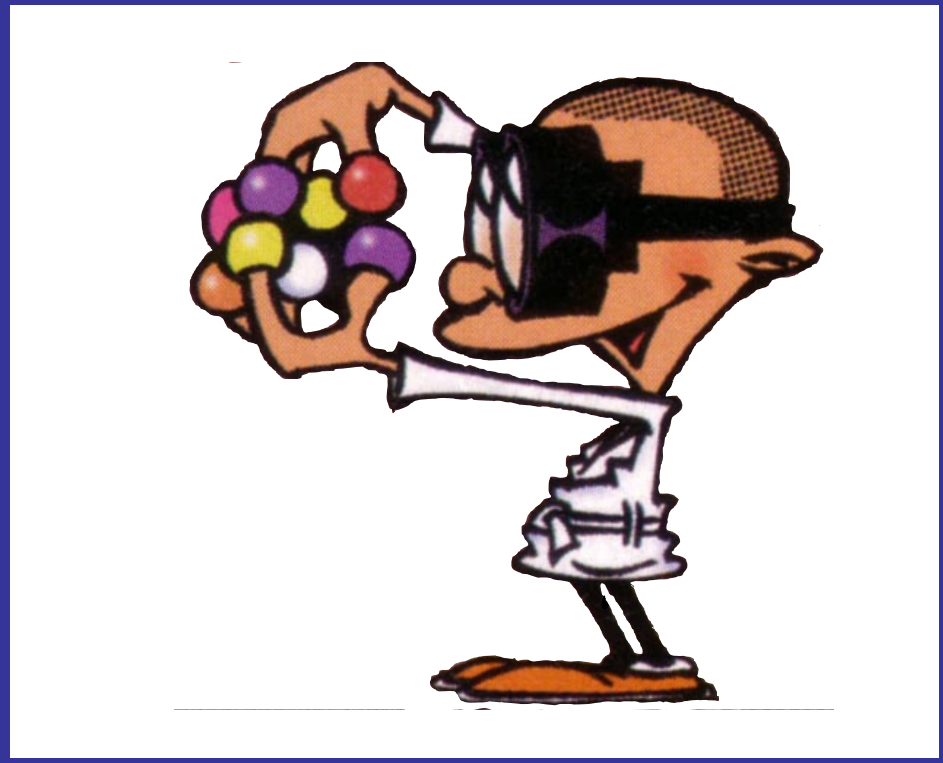


Large molecule:
Full geometry optimisation using the new ASED+ semi-empirical method & STM constant current STM images

Small molecule:
Full geometry optimisation using the new DFT technique



Emerging nano-electronics



Welcome in Pico-Inside

Unit 6: The Phantom Foundation