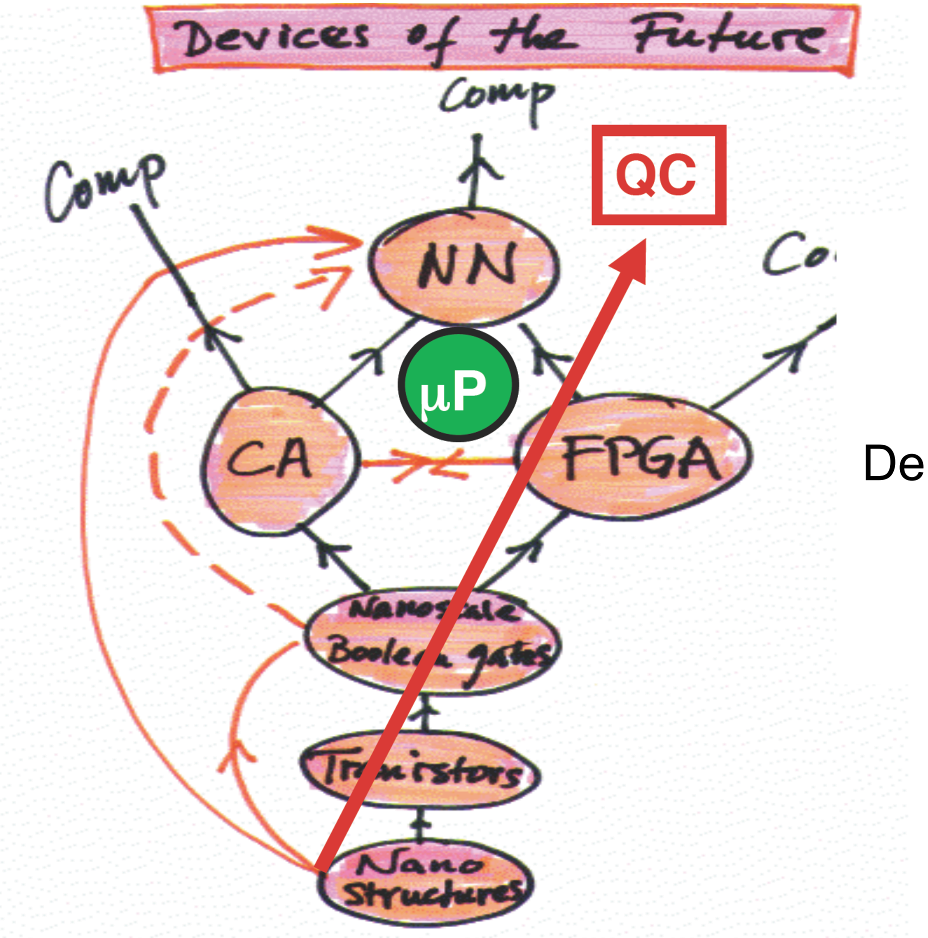
Molecular Electronics/Quantum Computers

Computing towards 2020

Identification of requirements for future ICT devices



Göran Wendin

Bionanosystems Laboratory
Dept of Microtechnology and Nanoscience
- MC2
Chalmers University of Technology
Gothenburg, Sweden

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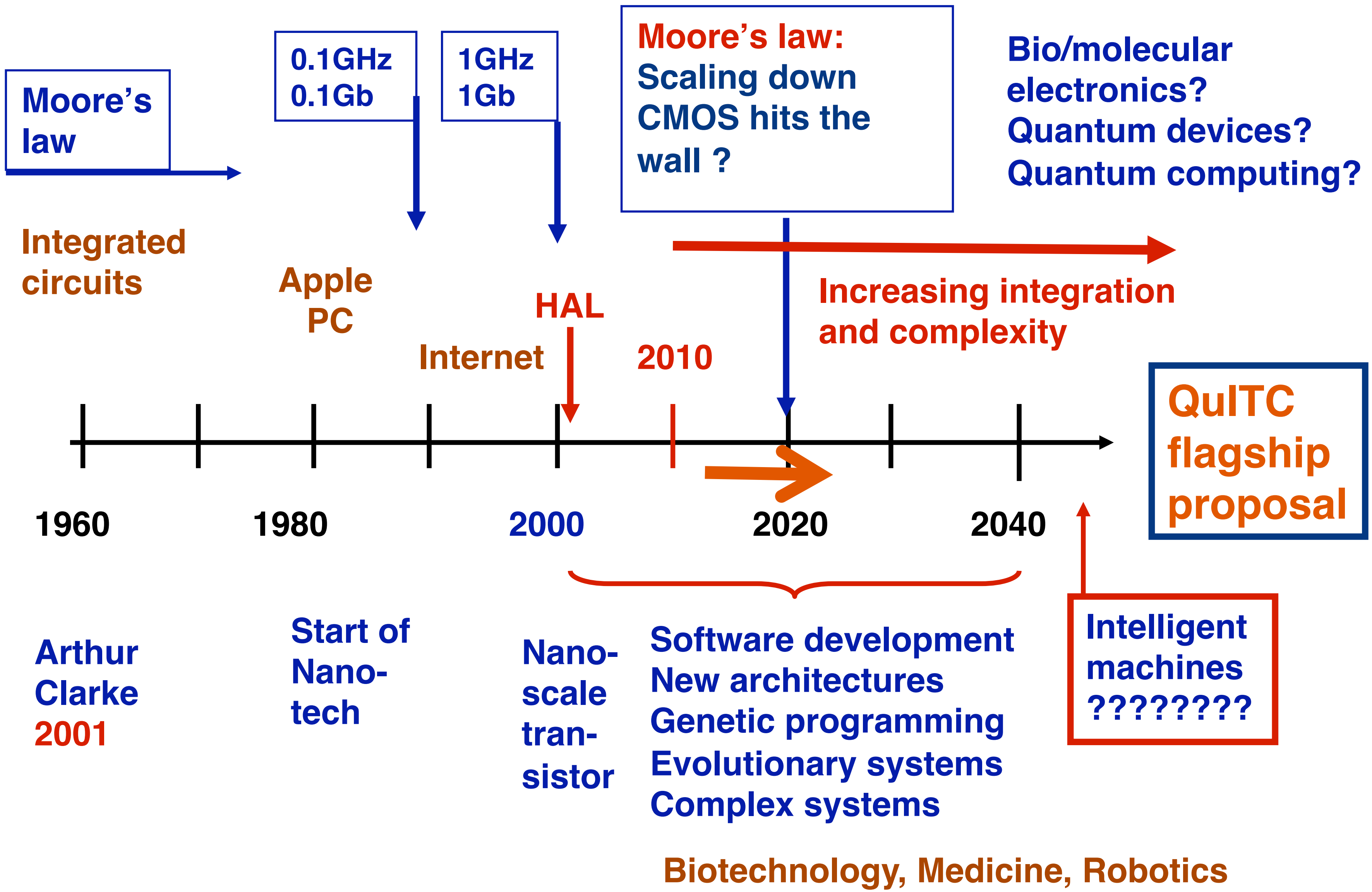
A perspective on time and development ...



Quantum IT Challenge for eScience

CIP
Classical Info Proc.

QIP
Quantum Info Proc.

High Performance Computing (HPC)
Extended CMOS
Multicore
Digital
~~Neuromorphic~~
Software

eDesign

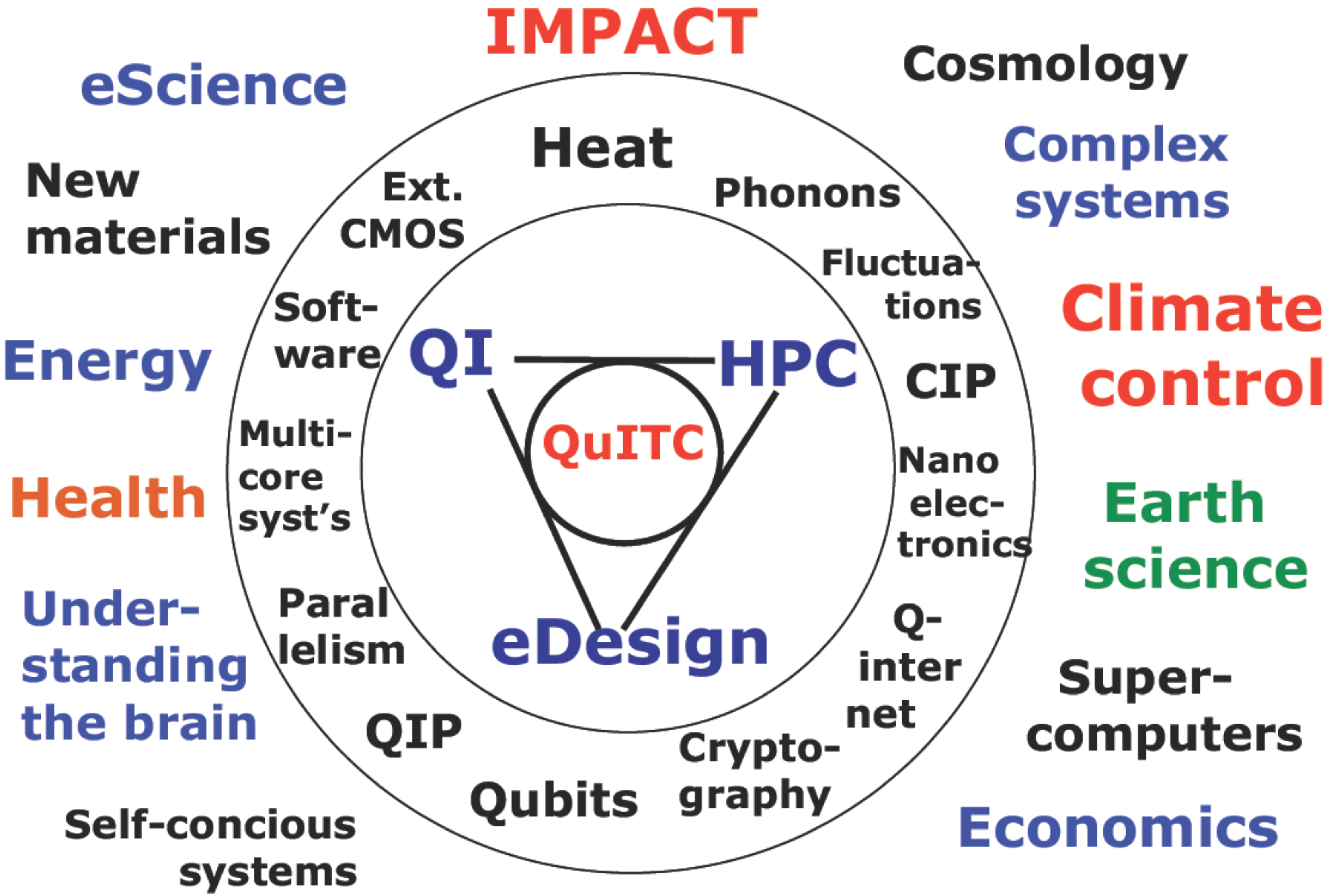
Quantum computing
Quantum Information
Quantum communication

Quantum Technologies

Low energy operation
Heat reduction
Cooling
Phonon engineering

CIP: so far only Ext. CMOS (incl. CNT, graphene). NOT Molecular Electronics

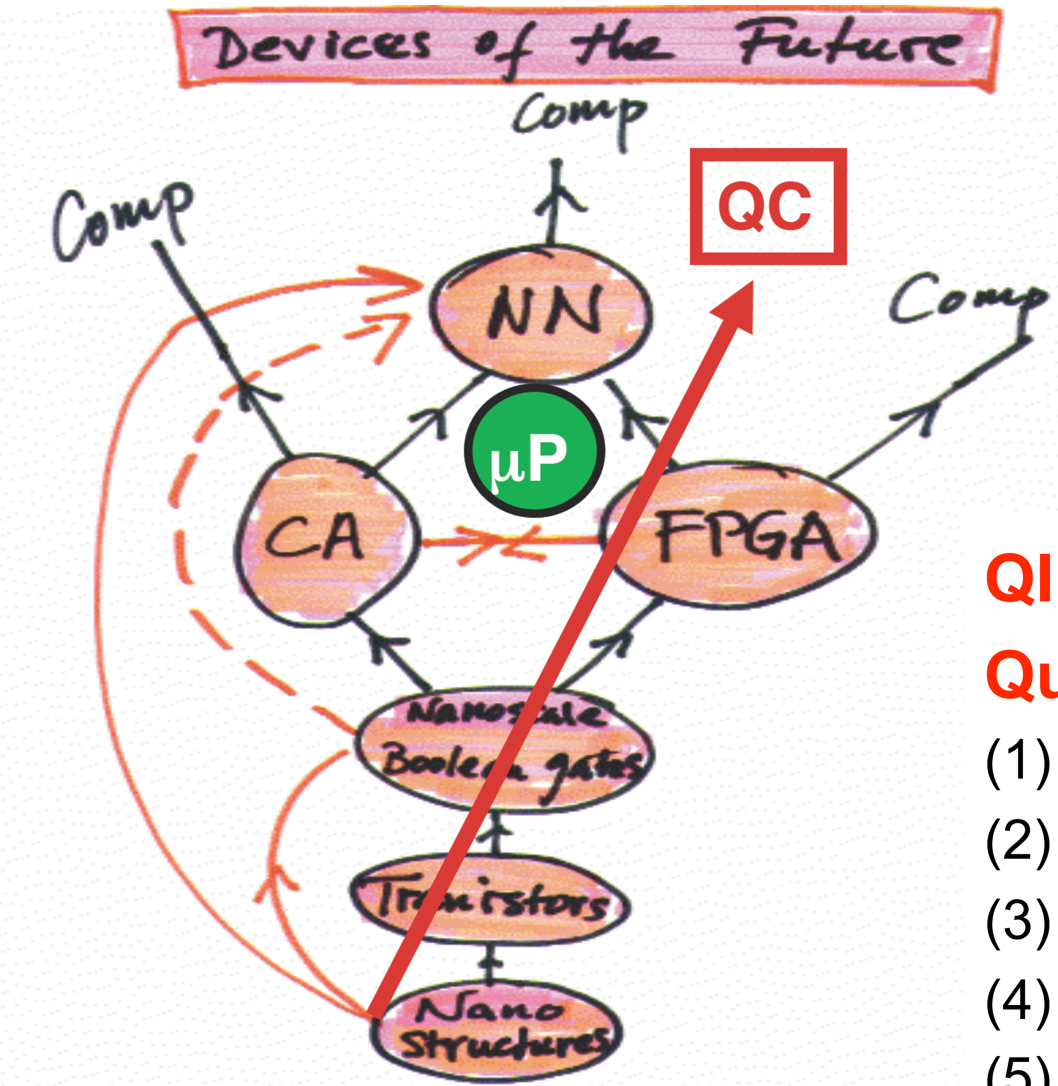
QuITC – a flagship (or at least a tug/pilot)?



Classical-quantum integration – hybrid systems

New HPC system devices within 10 years?

- Carbon nanotube (CNT) and/or graphene electronics ☺
- Memristors, Oxide electronics ☺
- Quantum coherent electronics ☺
- Molecular Electronics (ME) ☹
- Synaptic ME/oxide networks ☹ ☺
- Neural/brain networks *in silico* ☺



Molecular CIP

Quantum *incoherent*

(1) Single-molecule devices
(2) Multi-mol SAM devices
(3) Memristors, crossbars
(4) Neuromorphic networks

QIP

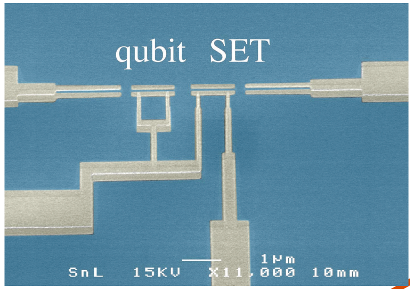
Quantum *coherent* (QC)

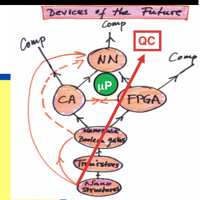
(1) Ion traps
(2) Atom traps
(3) Photonic circuits
(4) Spins in molecules
(5) Spins in solids
(6) Josephson junctions

(1)–(3): Quantum Optics

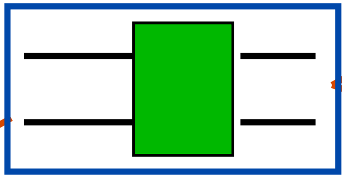
(1)–(6): Toward solid state integration

Irreversible - reversible computers





One big memory.
All information kept
all the time.
Logically reversible
(No) dissipation



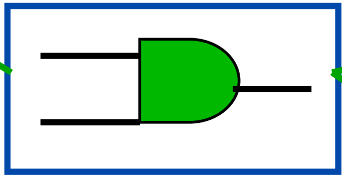
Logically reversible

Quantum computer,
COHERENT
Atom traps, nuclear spins
Josephson Junction circuits
Semicond QDs, impurities

Classical, INCOHERENT
Ballistic
Brownian

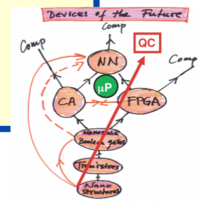
μP
Micro processors

Logically irreversible

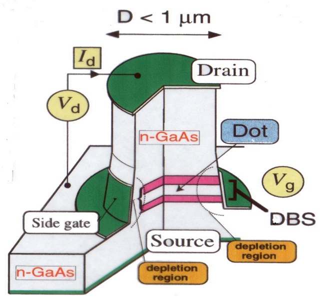


Scaled down μP, INCOH.

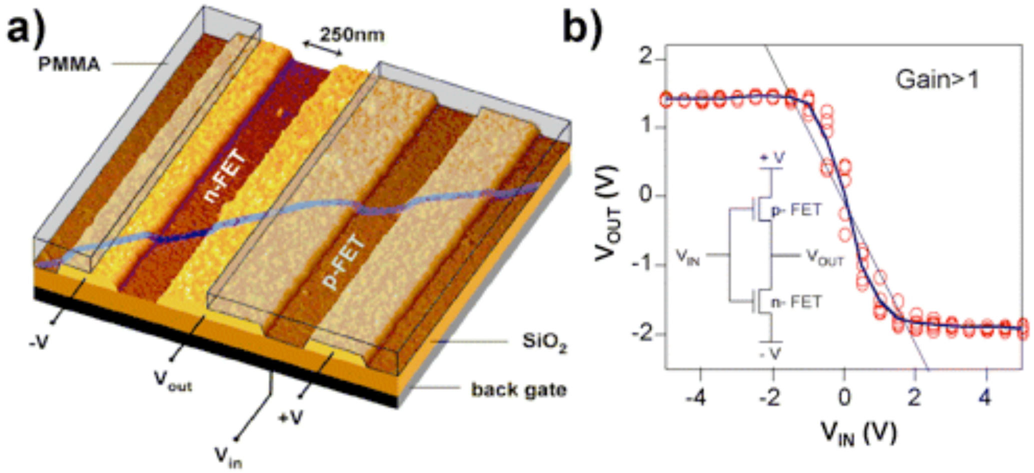
Quantum device μP,
INCOHERENT
RTD, RTT, QD, SET
RSFQ, Josephson flux circuits
Spin valves
Molecular Electronics



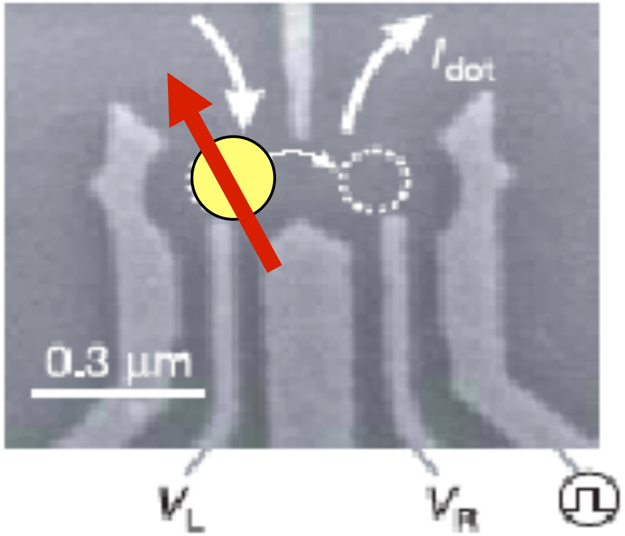
Information
destroyed
all the time.
Logically irreversible.
Dissipation

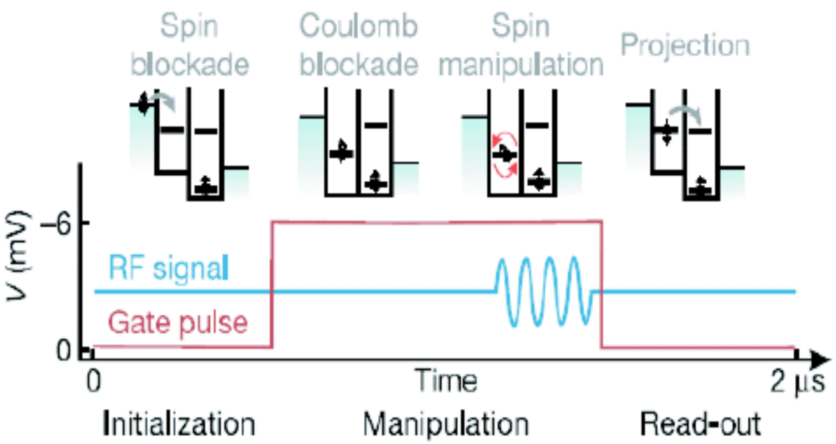


Classical vs Quantum bits



Logic levels
“0” and “1”
Low/high voltages
V0/V1





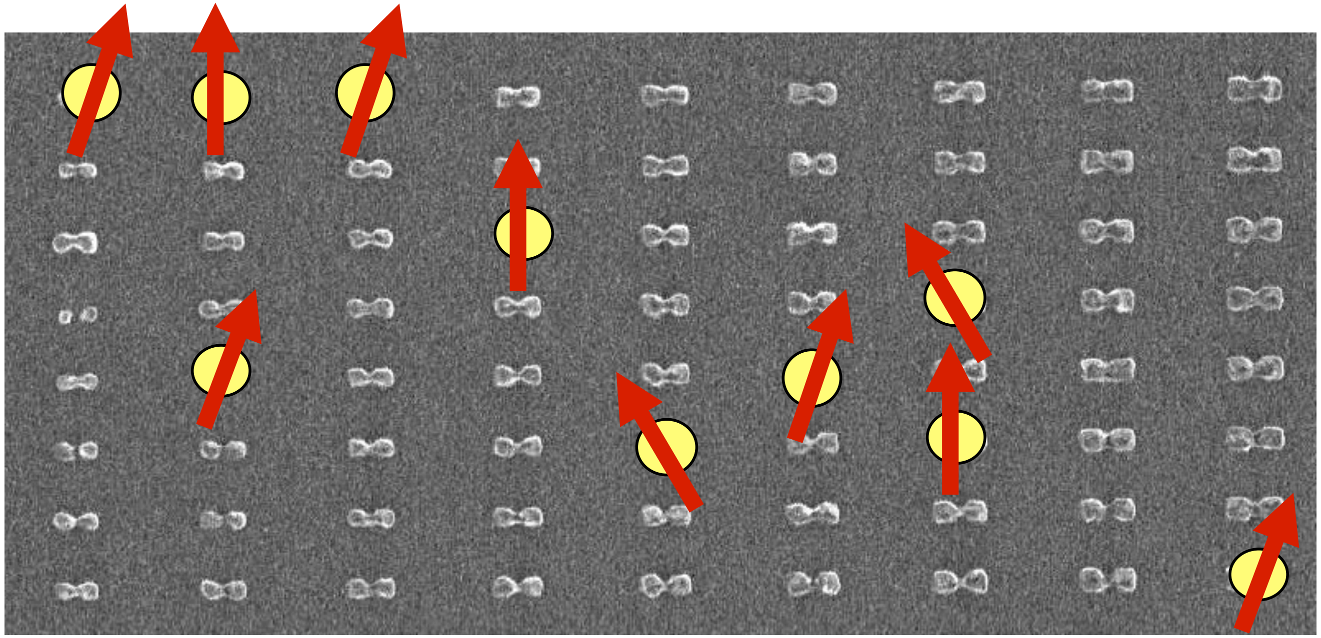
Logic levels
l0> and l1>
Quantum energy levels, states, coherence

E1, l1>

E0, l0>

Phase information

N-qubit memory register - 2^N configurations



Computing is done on a qubit memory. The circuit is a sequence of quantum gates. Operation and readout are done via DC and AC pulses (MW, opt).

$$|\psi\rangle = a_1\,|0..00\rangle + a_2\,|0..01\rangle + a_3\,|0..10\rangle + \ldots + a_{(2^N-1)}\,|11..1\rangle$$

Superposition of 2^N configurations = Parallelism

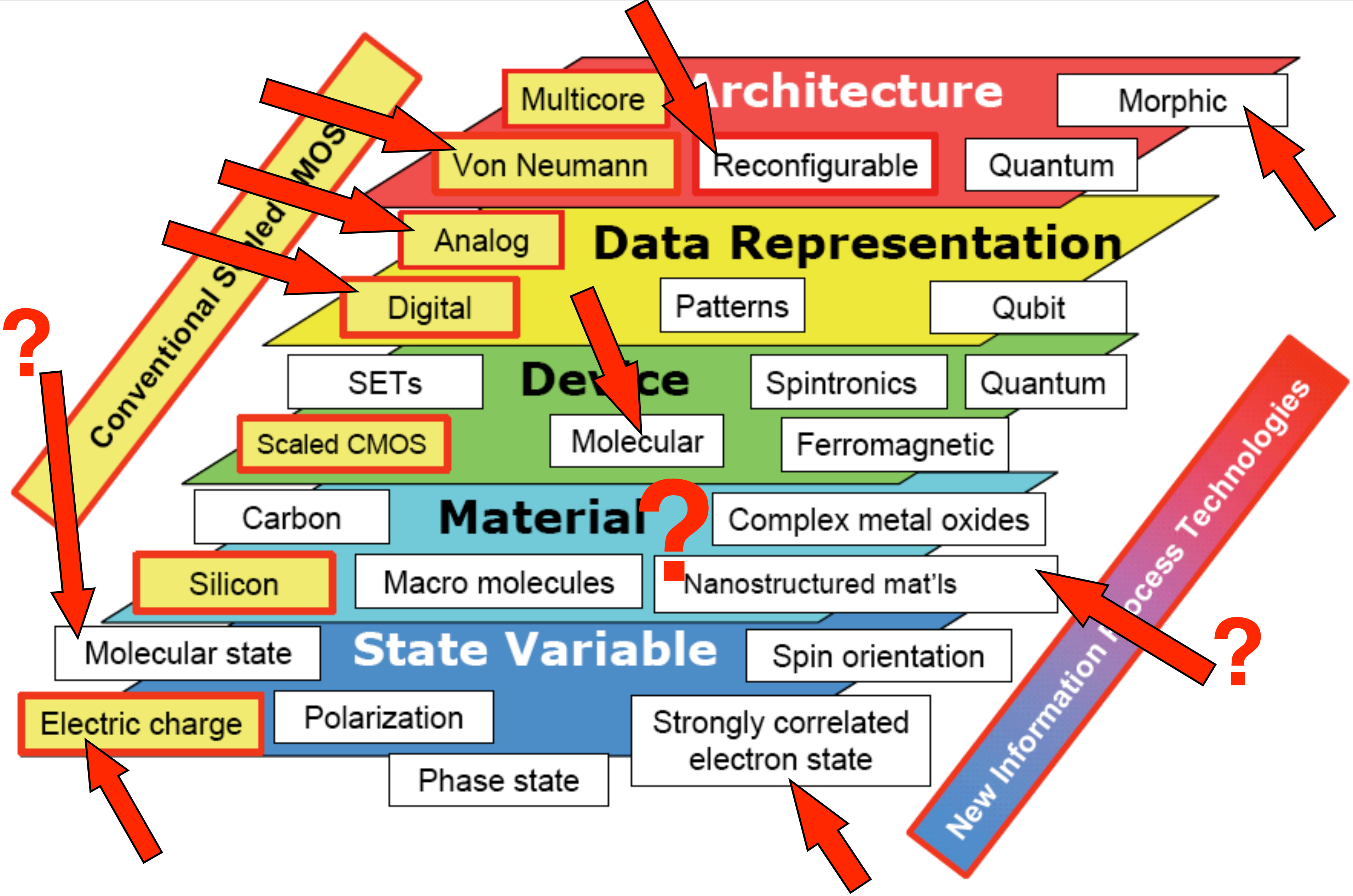
Entanglement (non-product state) = non-classical correl./information

Classically, *one at a time*: 0..00 OR 0..01 OR 0..10 OR .. 1..11

Coherence is needed for superposition and entanglement to work

→ solving some problems in polynomial rather than exponential time

Molecular CIP is a mess .....



Molecular CIP concepts

- Conventional architecures
- Molecular memories
- Crossbar structures
- Memristors
- Synapses
- CMOL (Cmos + "MOLecules")
- Biologically inspired computing
- Neuromorphic computing

Single-molecule gates -- 1970's →

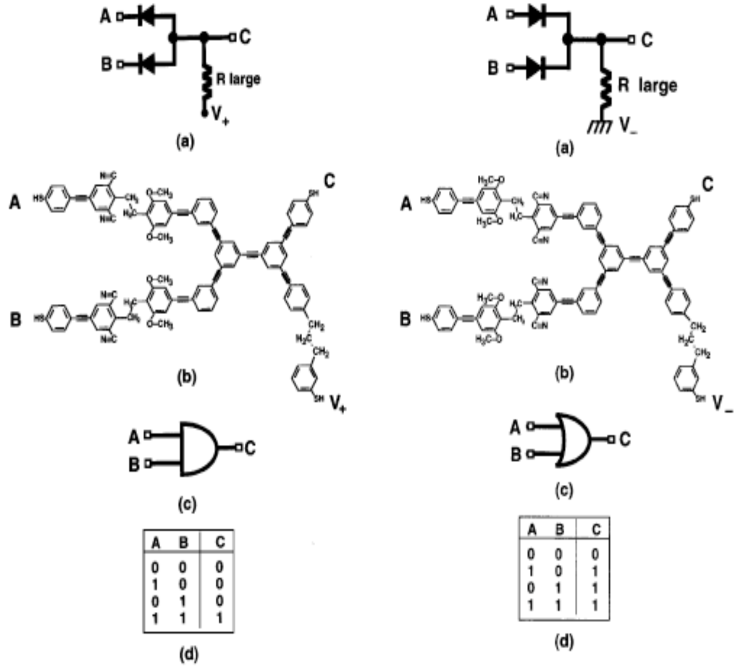
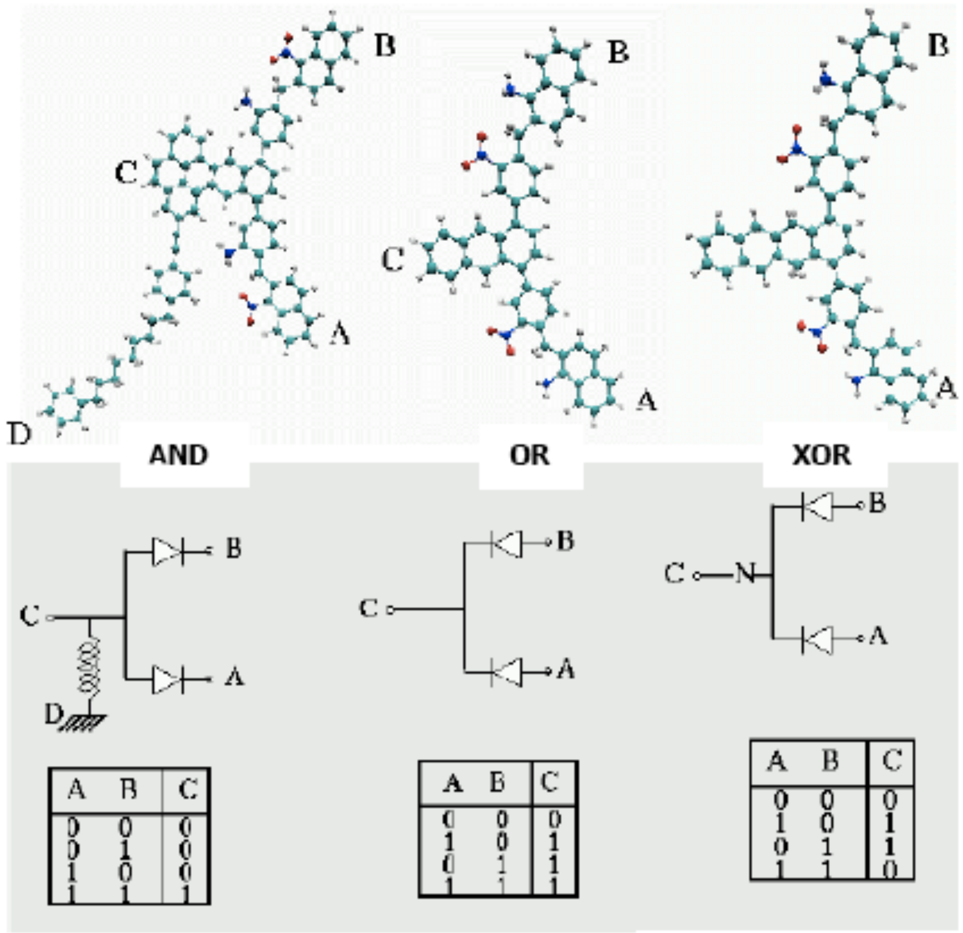


Figure 3.3: An early example of design of purely molecular AND and OR diode-resistor logic. Ellenbogen and Love [181].

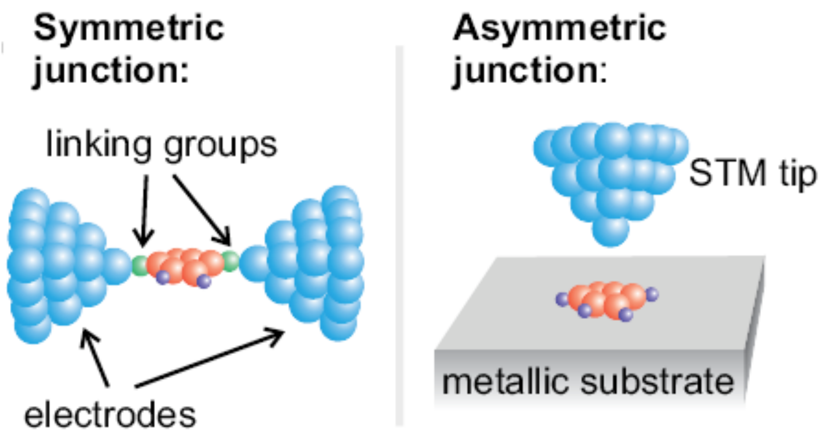
From Mitre Corp. (2000)



From Pico Inside (2009)

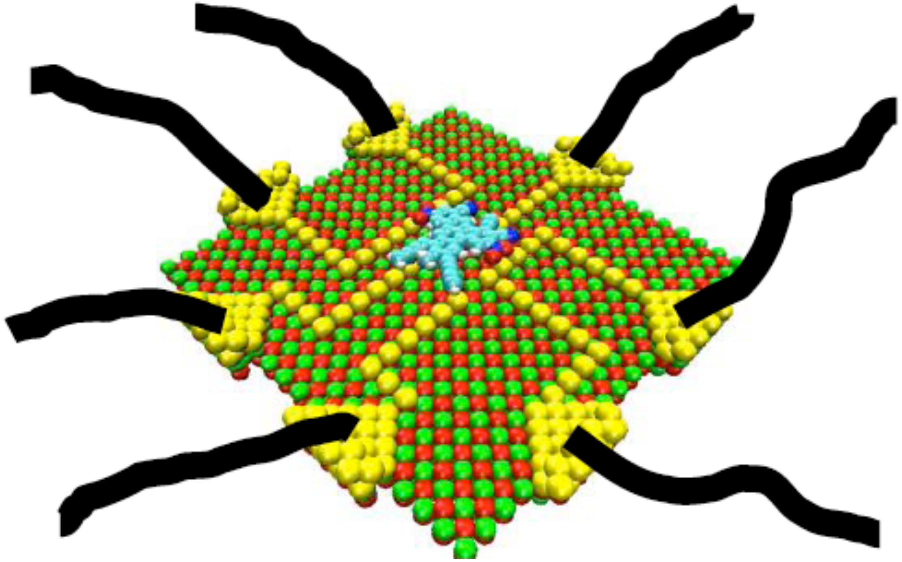
No exp proofs of concept

Contacting single molecules

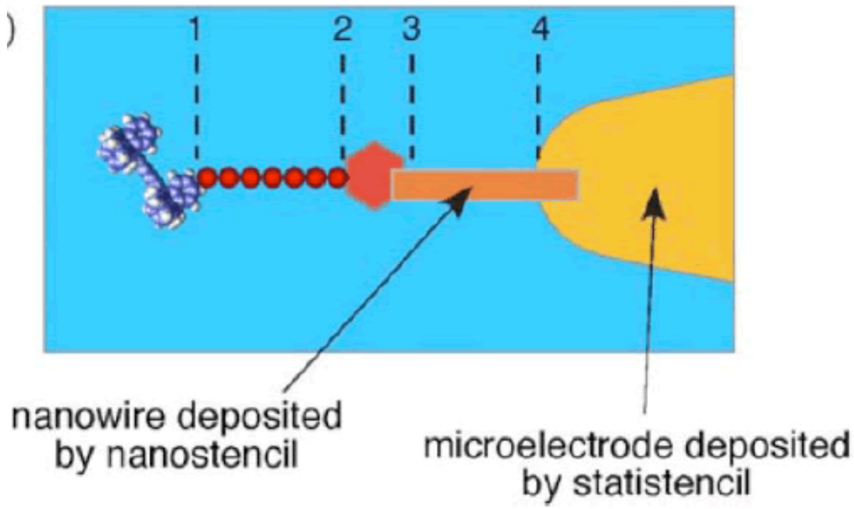


Two different approaches

- Put down wiring, add molecules
- Put down molecules, add wiring



From Pico Inside



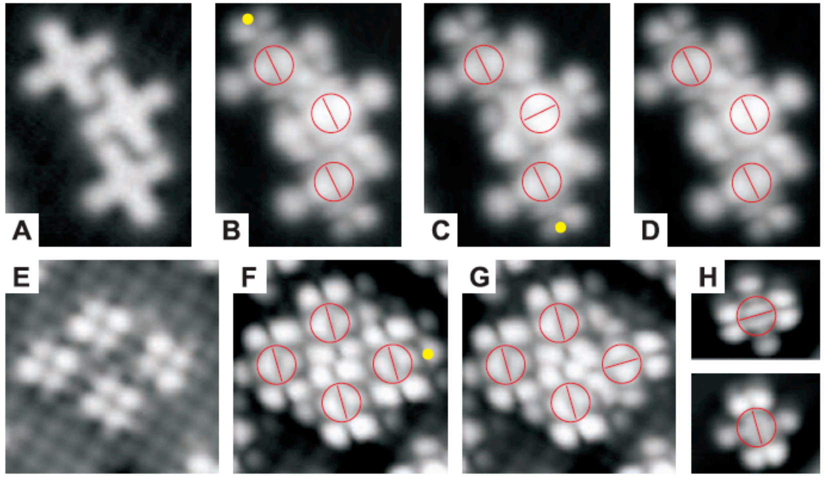
From Pico Inside

Molecular switches (experiment)

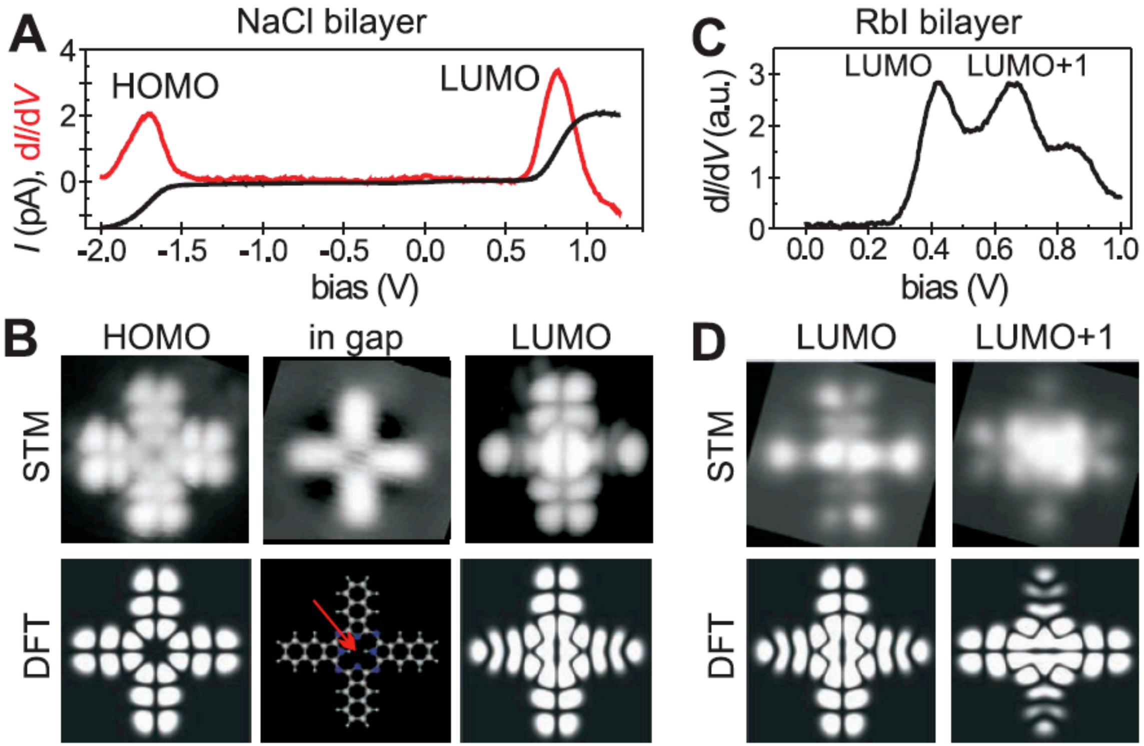
Current-Induced Hydrogen Tautomerization and Conductance Switching of Naphthalocyanine Molecules

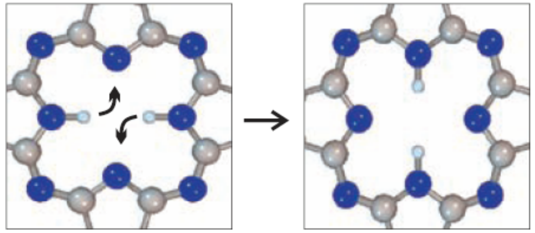
Peter Liljeroth,[1*] Jascha Repp,[1,2] Gerhard Meyer[1]

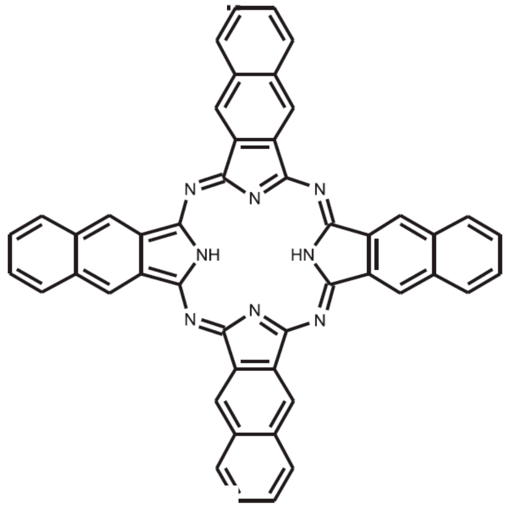
SCIENCE VOL 317 31 AUGUST 2007



STM: IVC and orbital mapping

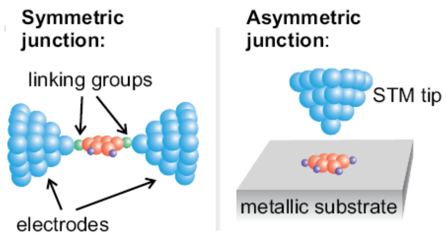






Single-molecules/CMOS - SWOT .....

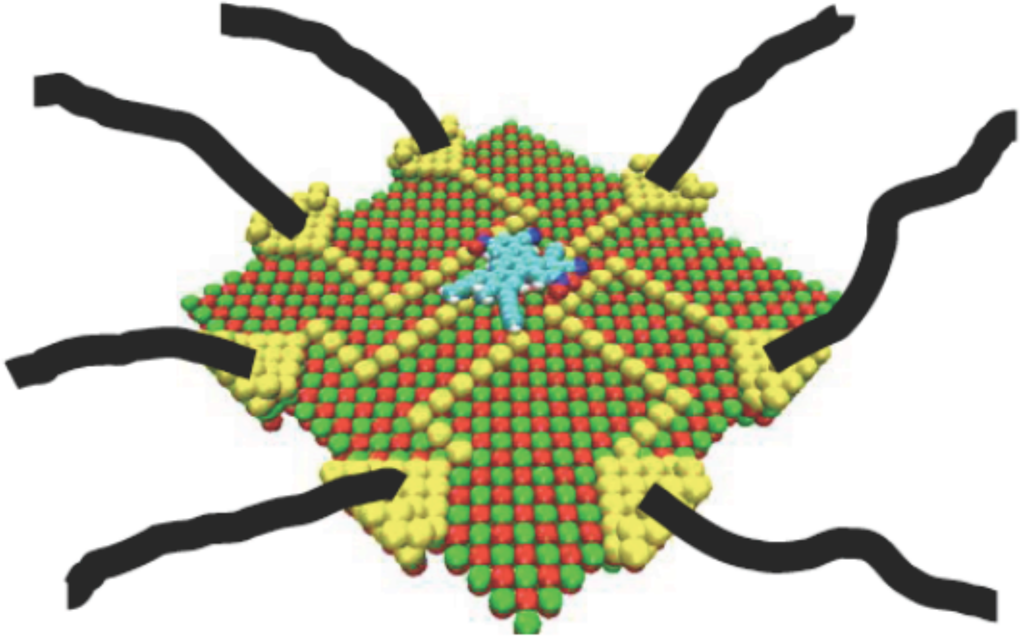
S	W
Nanoscale High density Exp proofs of concepts of diodes and transistors	Poor reproducibility Wiring and contacts difficult No exp circuits implemented Slow Not really smaller than Si-CMOS
O	**T**
Great for basic research Development of nano/ multiscale technologies from atomic to lab levels Development of self-assembly	May/will never become a practical competitive technology

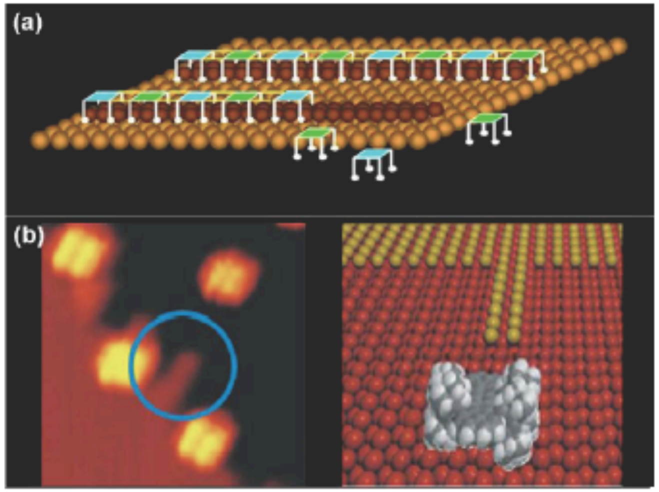


Molecular circuits, Pico-Inside

Hamiltonain Logic Gates: computing inside a molecule.

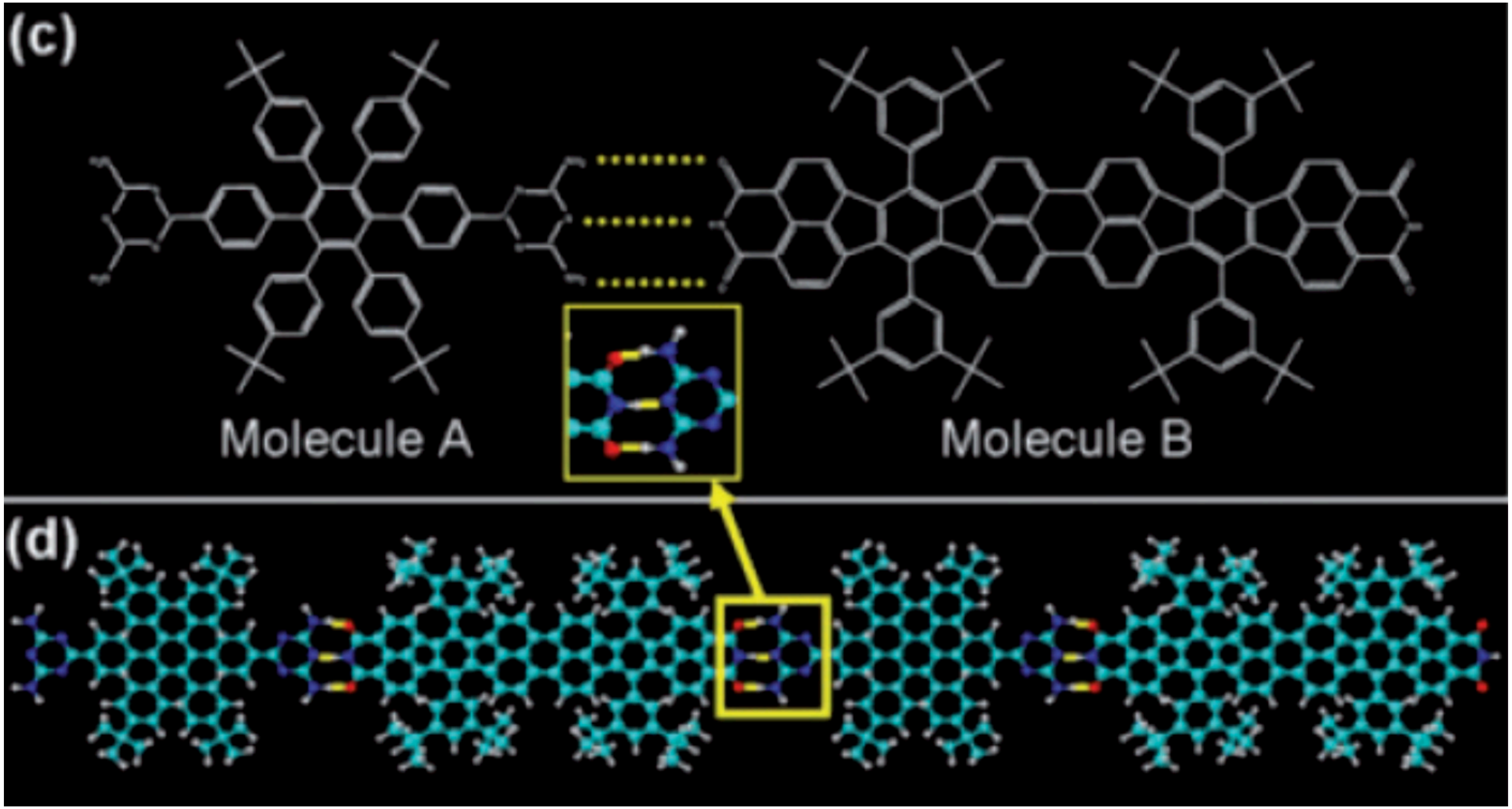
Pico Inside – C. Joachim et al.





1. J. Furjasek, N. Cerf, I. Duchemin, C. Joachim. Hamiltonain Logic Gates: computing inside a molecule. International Journal of Nanoscience 24, 161-172, 2005
2. I. Duchemin, C. Joachim. A quantum digital half adder inside a single molecule. Chem. Phys. Letter, 406, 167-172, 2005
3. C. Joachim. The diving Power of the superposition principle for molecules-machines. J. Phys. Condensed Matter, 18, S1935-S1942, 2006

Molecular circuits, Pico-Inside



Towards Self-assembly of Molecular Moulds by Complementary Hydrogen-bonding

Wei Xu[a], Miao Yu[a], Régis Barratin[b], André Gourdon[b], Flemming Besenbacher[a], and Trolle R. Linderoth[a]

E nano newsletter December 2007

EU-FP6 Integrated Project Pico-Inside

Exp. contacting single-molecule devices

Y. Okawa, M. Aono *Nature* **2001**, *409*, 683.
Y. Okawa, M. Aono *J. Chem. Phys.* **2001**, *115*, 2317.
Y. Okawa, D. Takajo, S. Tsukamoto, T. Hasegawa, M. Aono *Soft Matter* **2008**, *4*, 1041.

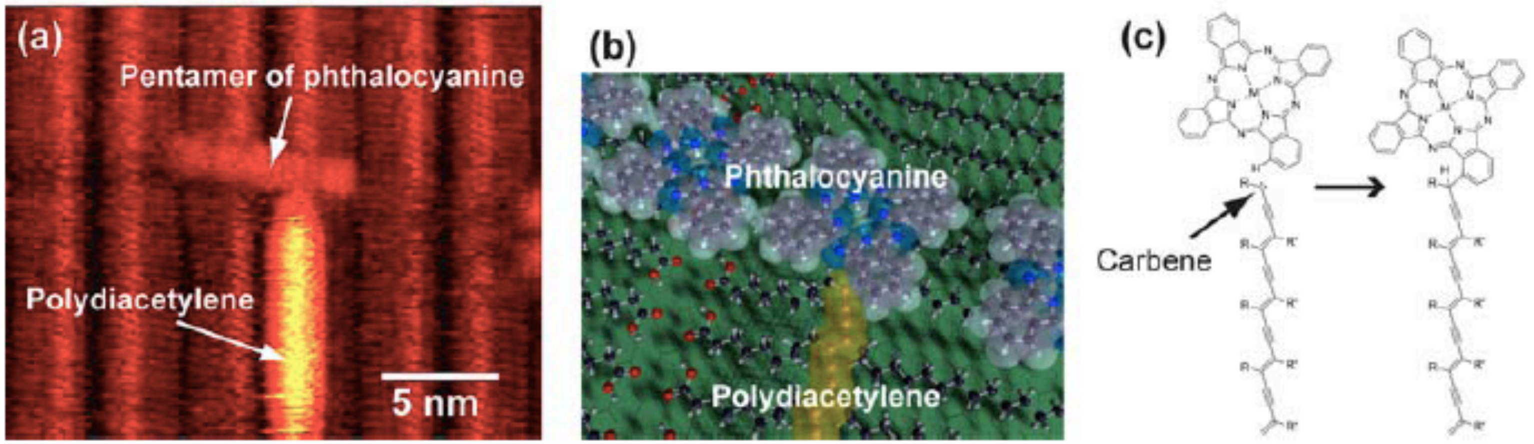


Figure. (a) STM image showing the connection of a single polydiacetylene chain to a single phthalocyanine molecule in a pentamer. (b) Structure model of the connection. (c) Insertion reaction of carbene at the end of polymer to a C–H bond of phthalocyanine.

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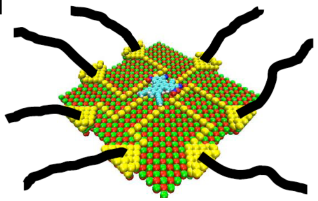
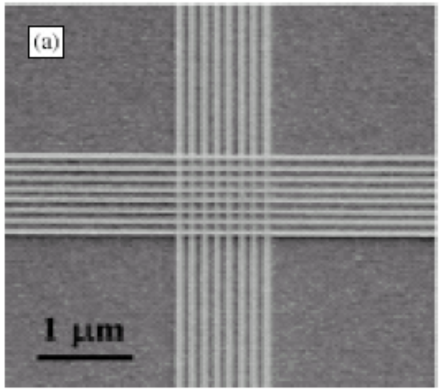
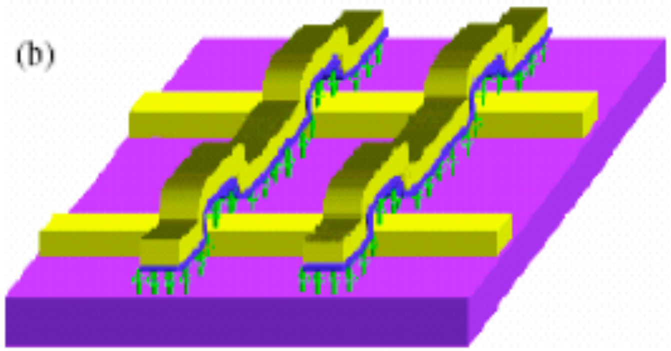
Single-molecule logic gates - SWOT .....

S Nanoscale Complex logic Hamiltonian gates in a single molecule Theoretical proof of concept for model systems 	W No exp proof of concept Wiring and contacts difficult Experiments to test the principles may take years....??
O Great for basic research Development of nano/ multiscale technologies from atomic to lab levels Development of self-assembly	T May never become a practical competitive technology

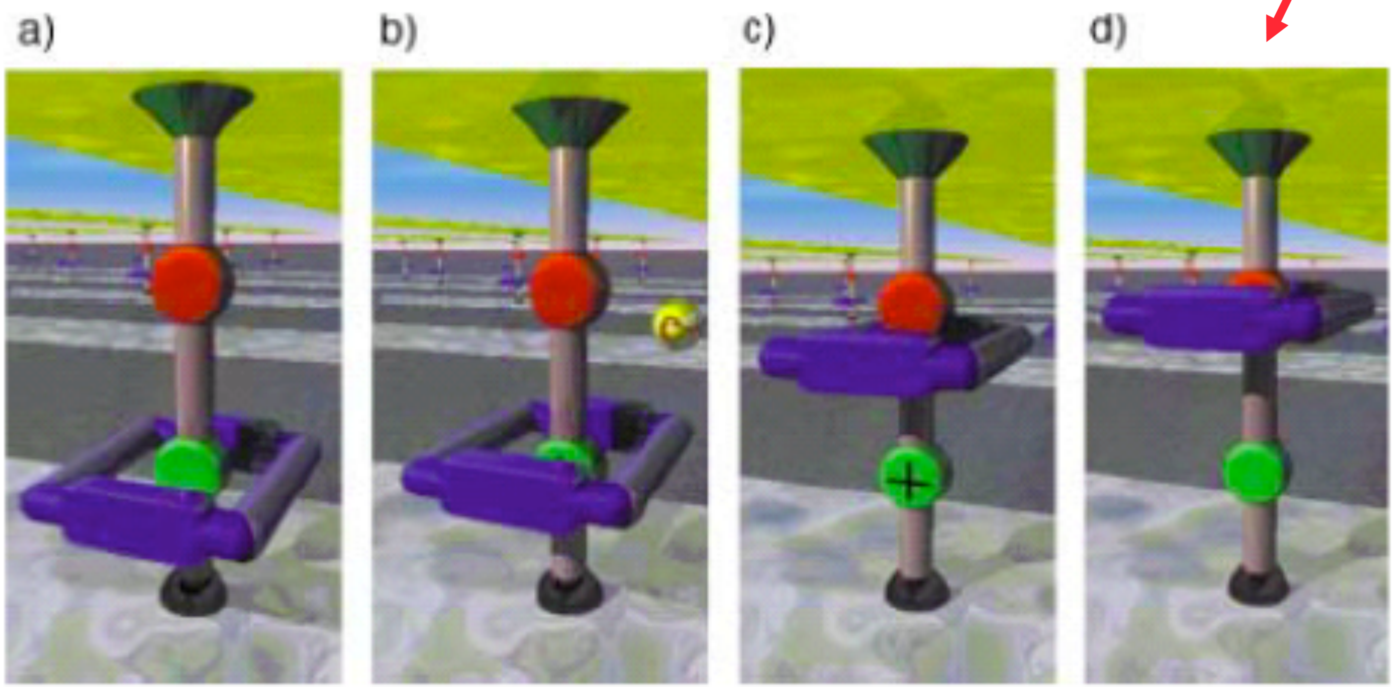
Molecular memory cells/switches

(Hewlett Packard, 2002-2007)

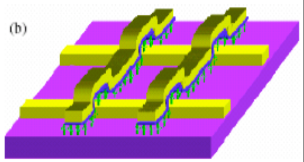
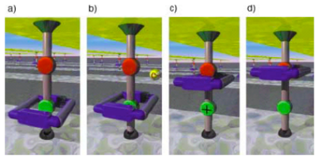




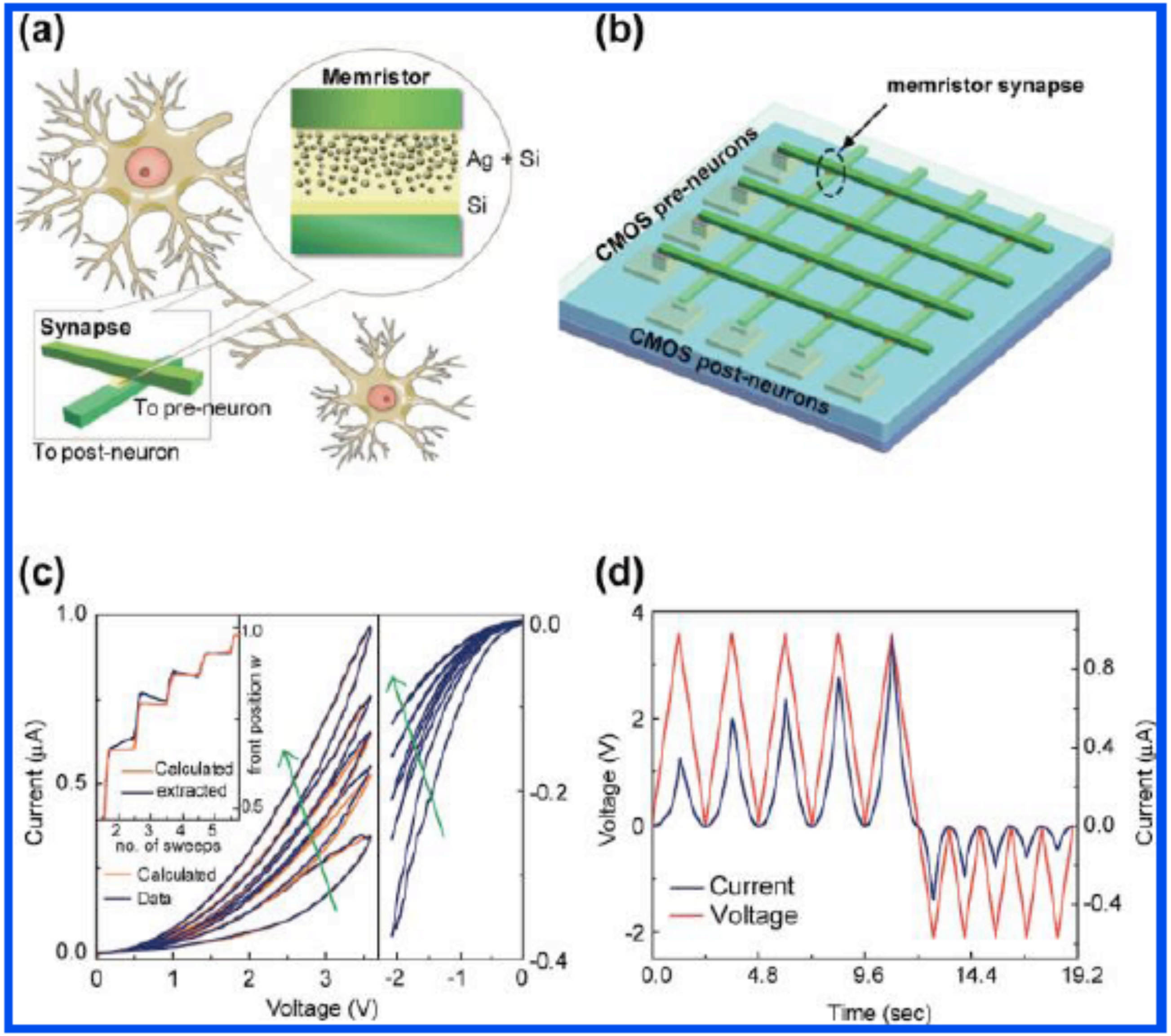
2-terminal voltage switch



Molecular thin film memristors - SWOT

S Exp nanoscale switches and memory Logic gates (also conditional) Reconfigurable devices Conventional and neuromorphic architectures  	W Exp results debated (filamentary conduction) Research stage
O Great for basic research Development of self-assembly May become a working technology	T May never become a competitive technology

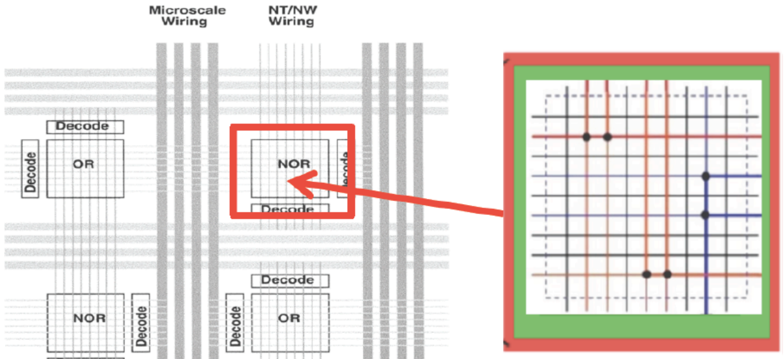
Non-molecular memristors



Nanoscale Memristor Device as Synapse in Neuromorphic Systems

Jo et al., Nano Lett. **10**, 1297 (2010)

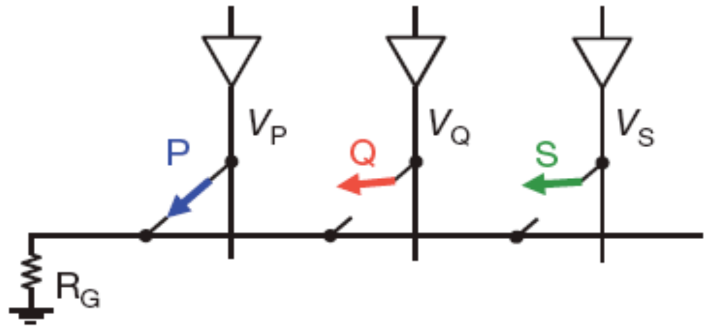
HP: crossbars, conditional logic



(a) (b)

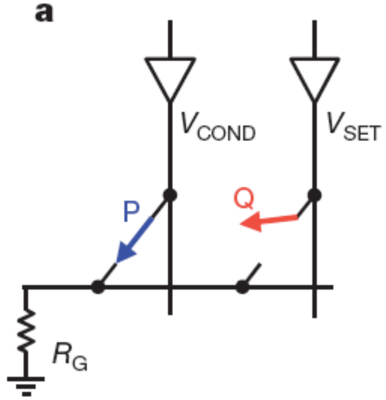
a

	Clocking voltages	
Step 1: $s = 0$		$V_S = V_{CLEAR}$
Step 2: pIMPs	$V_P = V_{COND}$	$V_S = V_{SET}$
Step 3: qIMPs	$V_Q = V_{COND}$	$V_S = V_{SET}$



Borghetti et al., Nature **464** (8 April 2010)

a



b

$q' \leftarrow p$IMPq

In p	In q	Out q'
0	0	1
0	1	1
1	0	0
1	1	1

b

Step 1	Step 2			Step 3				Steps 1, 2, 3		
$s = 0$	$s' \leftarrow p$IMPs			$s'' \leftarrow q$IMPs'				$s'' \leftarrow p\overline{\mathrm{NAND}q}$		
s	p	s	s'	q	s'	s''		p	q	s''
0	0	0	1	0	1	1	=	0	0	1
0	0	0	1	1	1	1		0	1	1
0	1	0	0	0	0	1		1	0	1
0	1	0	0	1	0	0		1	1	0

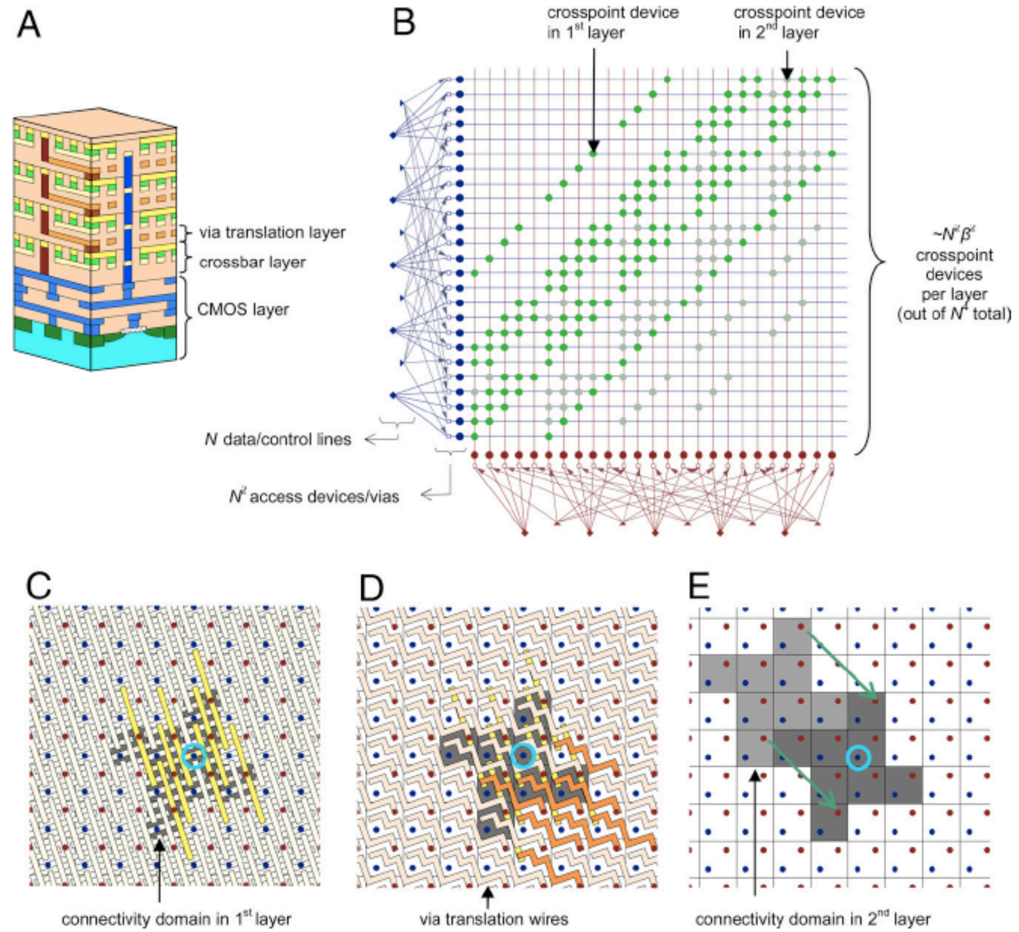
Memristor crossbar

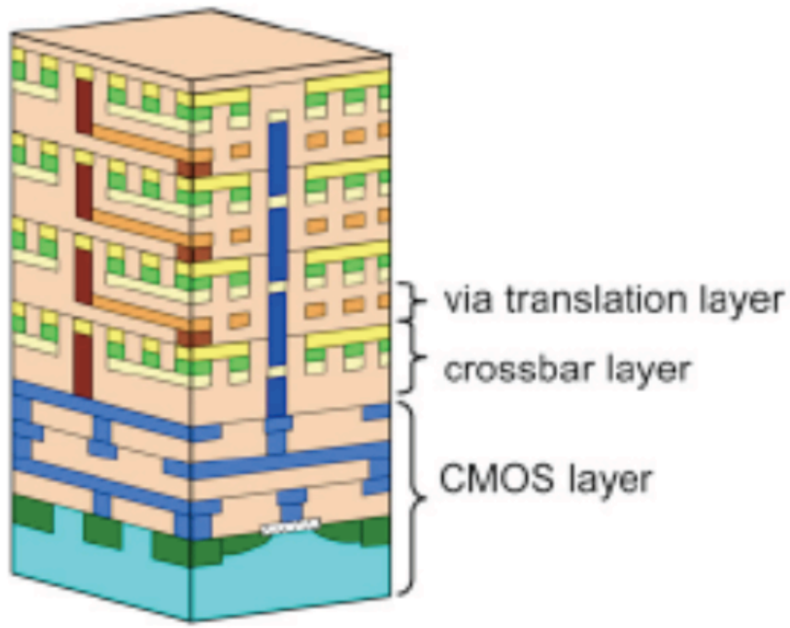
Four-dimensional address topology for circuits with stacked multilayer crossbar arrays

Dmitri B. Strukov[1] and R. Stanley Williams

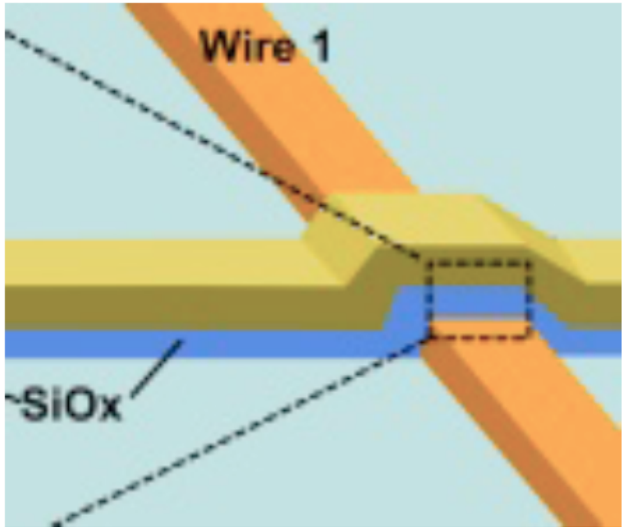
PNAS | December 1, 2009 | vol. 106 | no. 48 | 20157

Hewlett-Packard Laboratories, 1501 Page Mill Road, MS1123, Palo Alto, CA 94304





Rice memristor crossbar



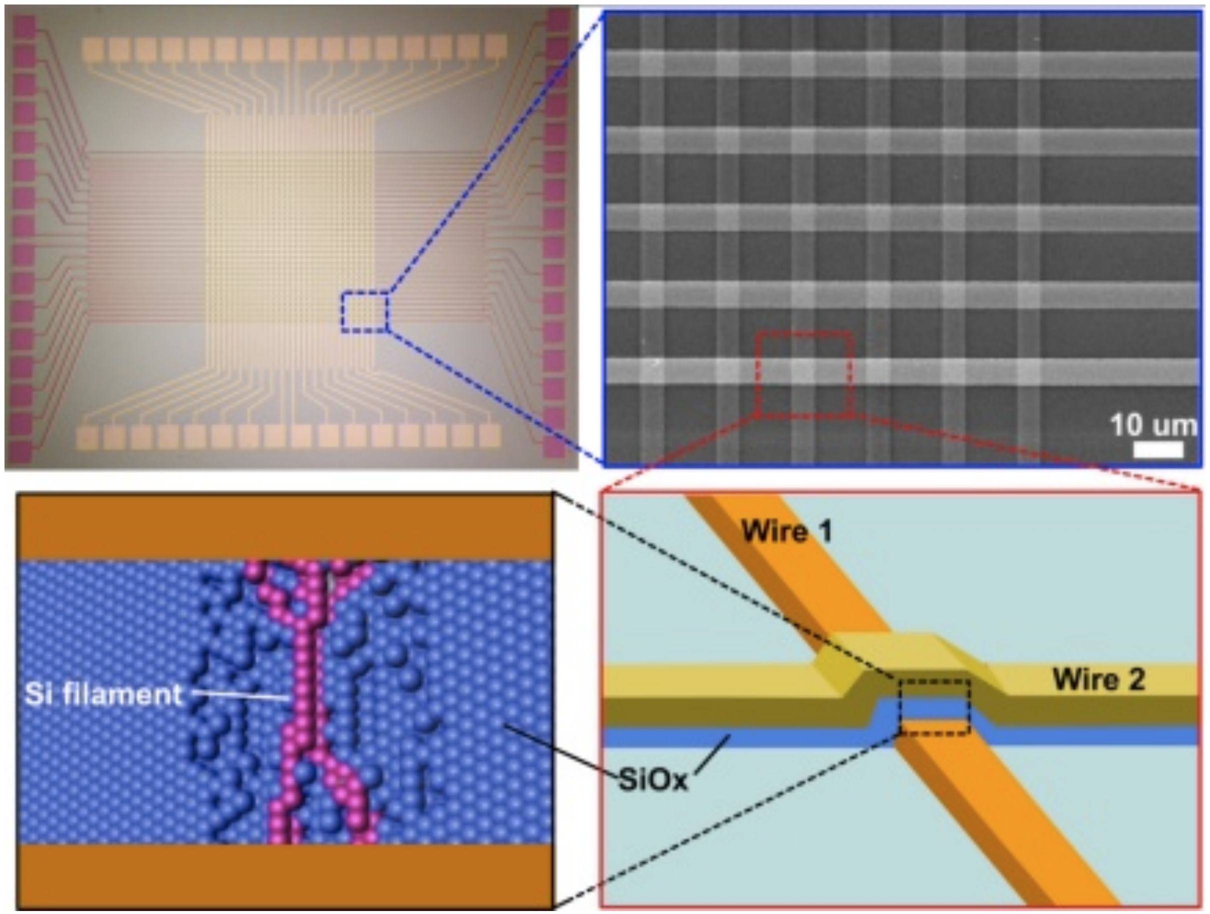
R. Colin Johnson

9/1/2010 5:32 PM EDT

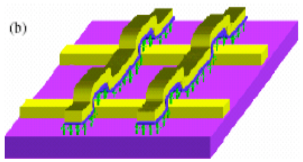
Memristors made from pure silicon could enable resistive random access memory that are simpler and cheaper to manufacture than Hewlett-Packard's titanium-based formulation, according to researchers at Rice University. PORTLAND, Ore. — Memristors made from pure silicon could enable resistive random access memory (ReRAM) that are simpler and cheaper to manufacture than Hewlett-Packard Co.'s titanium-based formulation, according to researchers at Rice University. In collaboration with fabless chip design house PrivaTran Inc. the team demonstrated a proof-of-concept ReRAM that packs only 1-kbit, but which they claim can be scaled beyond the densities of flash.

"Our memristors are made out of silicon instead of titanium like HPs," said Tour. "In its patent application, HP listed many oxides, but not silicon-oxide, which we have now turned into a bit cell for resistive RAMs."

Rice memristor crossbar

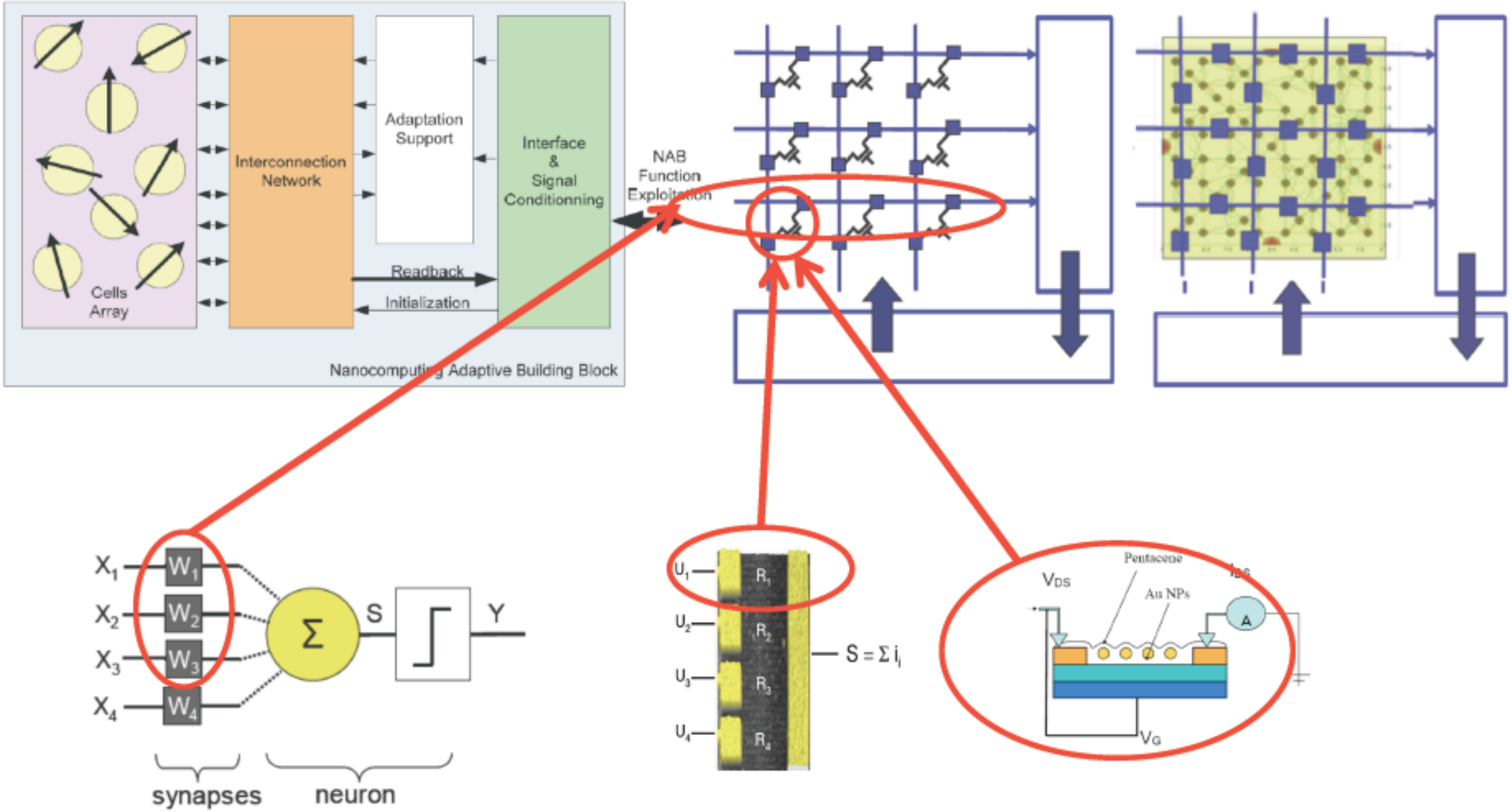


Oxide/.... thin film memristors - SWOT

S Exp nanoscale switches and memory Logic gates (also conditional) Reconfigurable devices Conventional and neuromorphic architectures  	W Research stage
O Development of self-assembly Development of a working technology	T May not become a competitive technology

Molecular neuromorphic concepts and devices

The NABAB concept



OG-CNTFET

Optically Gated
Carbon Nano Tube FET

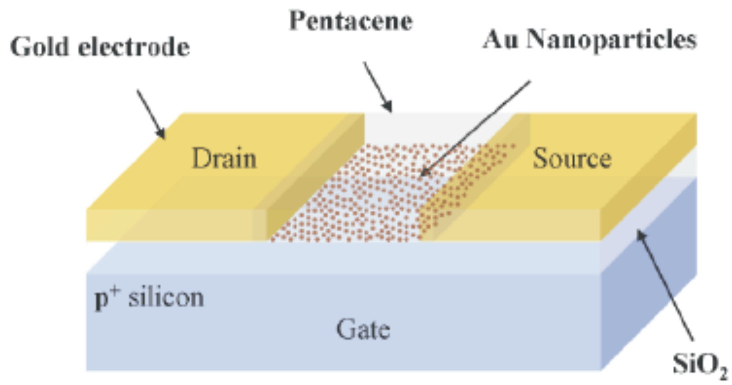
NOMFET

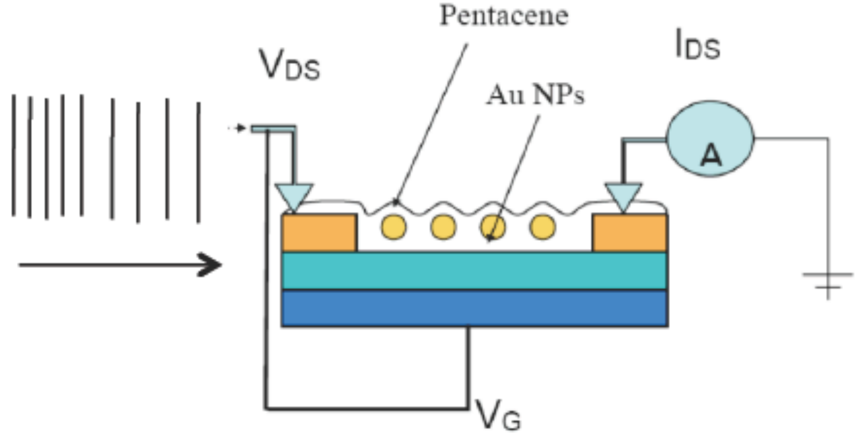
Nano Organic Memory FET

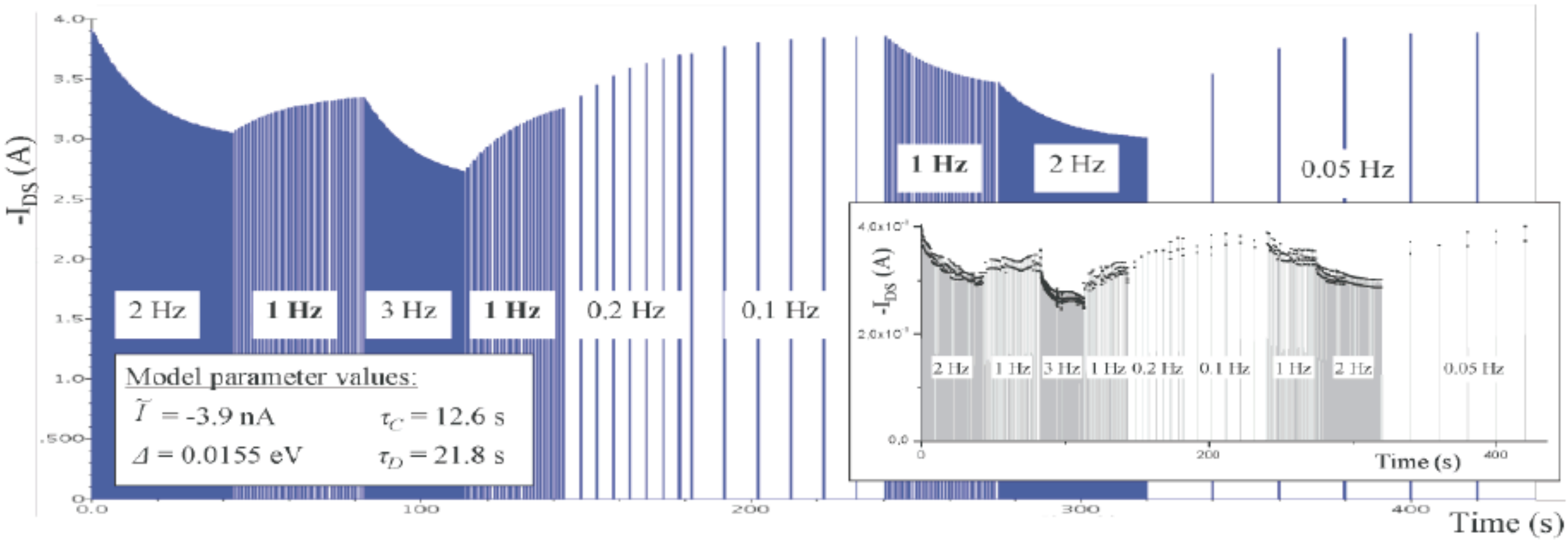
Molecular neuromorphic concepts and devices

http://www.google.se/search?hl=sv&source=hp&q=nomfet+synaps&aq=f&aqi=&aql=&oq=&gs_rfai=
http://en.wikipedia.org/wiki/NOMFET

Input pulse rate determines the effective charge (balance between charging and leakage), controlling the conductance of the NOMFET.

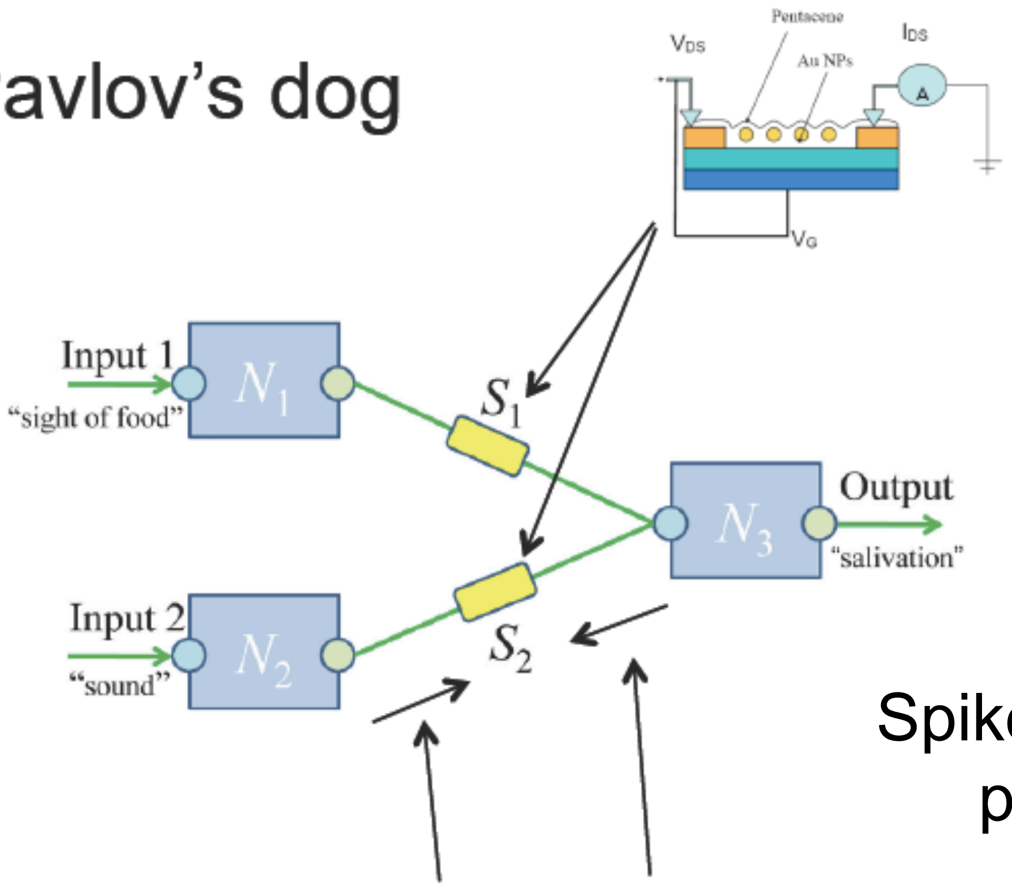






Pavlov's dog

NOMFET

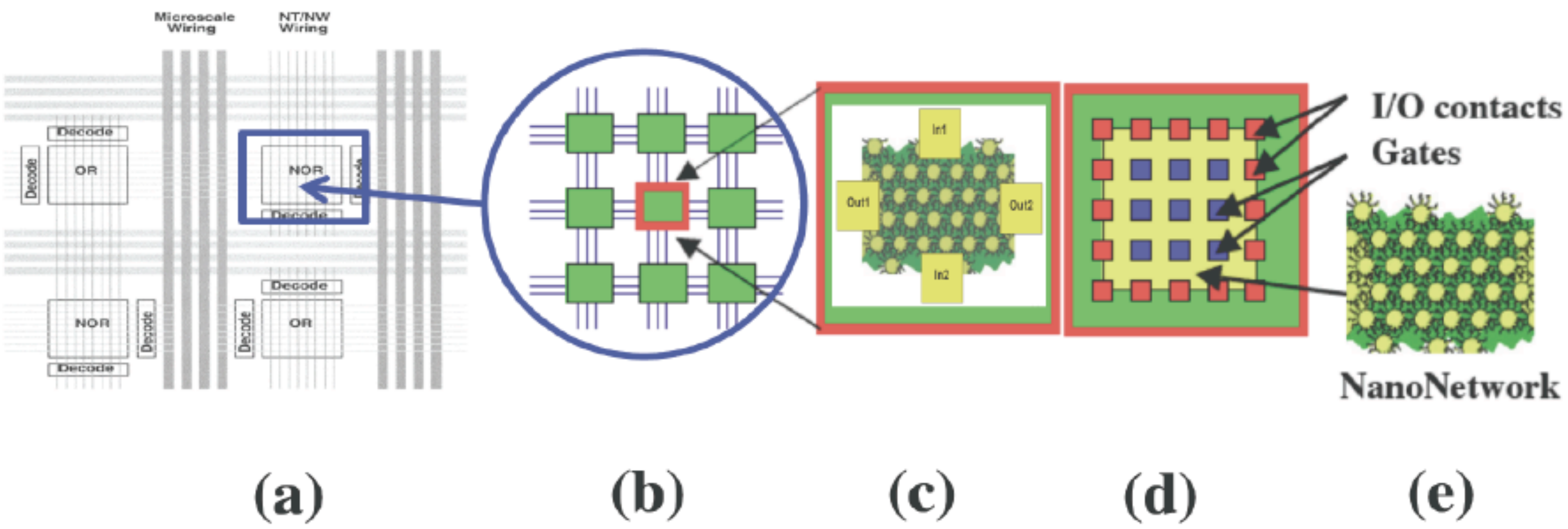


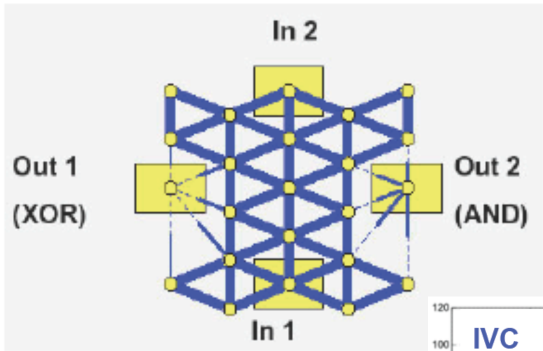
Spike-timing dependent plasticity (STDP)

Forward Backward propagating pulses.

If the forward and backward pulses coincide in time, the voltage sum will exceed the threshold of the memristor synapse and cause the conductance to increase, until the sound of the bell can induce salivation on its own.

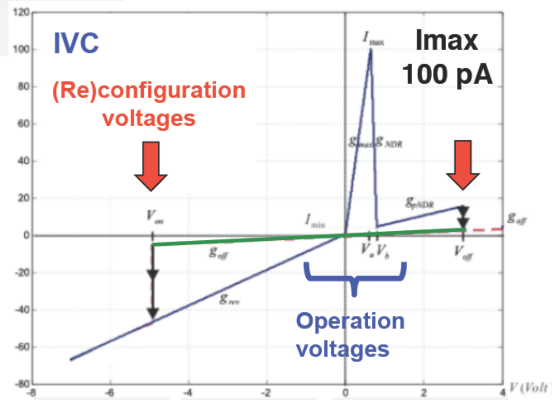
Molecular neuromorphic concepts and devices





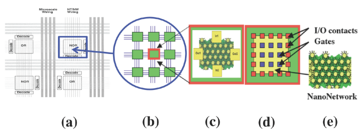
J. Sköldberg and G. Wendin,
Reconfigurable logic in nanoelectronic switching networks,
Nanotechnology **18**, 485201 (2007)

J. Sköldberg, C. Önnheim and G. Wendin,
Nanocell Devices and Architecture for Configurable Computing
With Molecular Electronics, IEEE Trans. Circ. Syst. I, **54** (11), 2461 (2007)



CHALMERS

Molecular neuromorphic networks - SWOT

S Logic gates Reconfigurable devices Synaptic devices Conventional and neuromorphic architectures  	W Embryonic Research stage
O Great for basic research Development of self-assembly May become a working technology	T May never become a competitive technology

QIP main device concepts

(1) Ion qubits in elctrostatic/dynamic traps (8)

(2) Atom qubits in crossed-laser traps (?)

(3) Photonic flying qubit circuits (4)

(4) Spin qubits in molecules (12) (NMR)

(5) Spin qubits in solids (3) (NV centres in diamond)

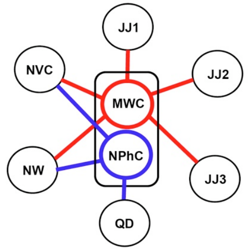
(6) Superconducting Josephson junction qubits and circuits (3)

The numbers refer to the **# of qubits** in working **coherent** quantum devices

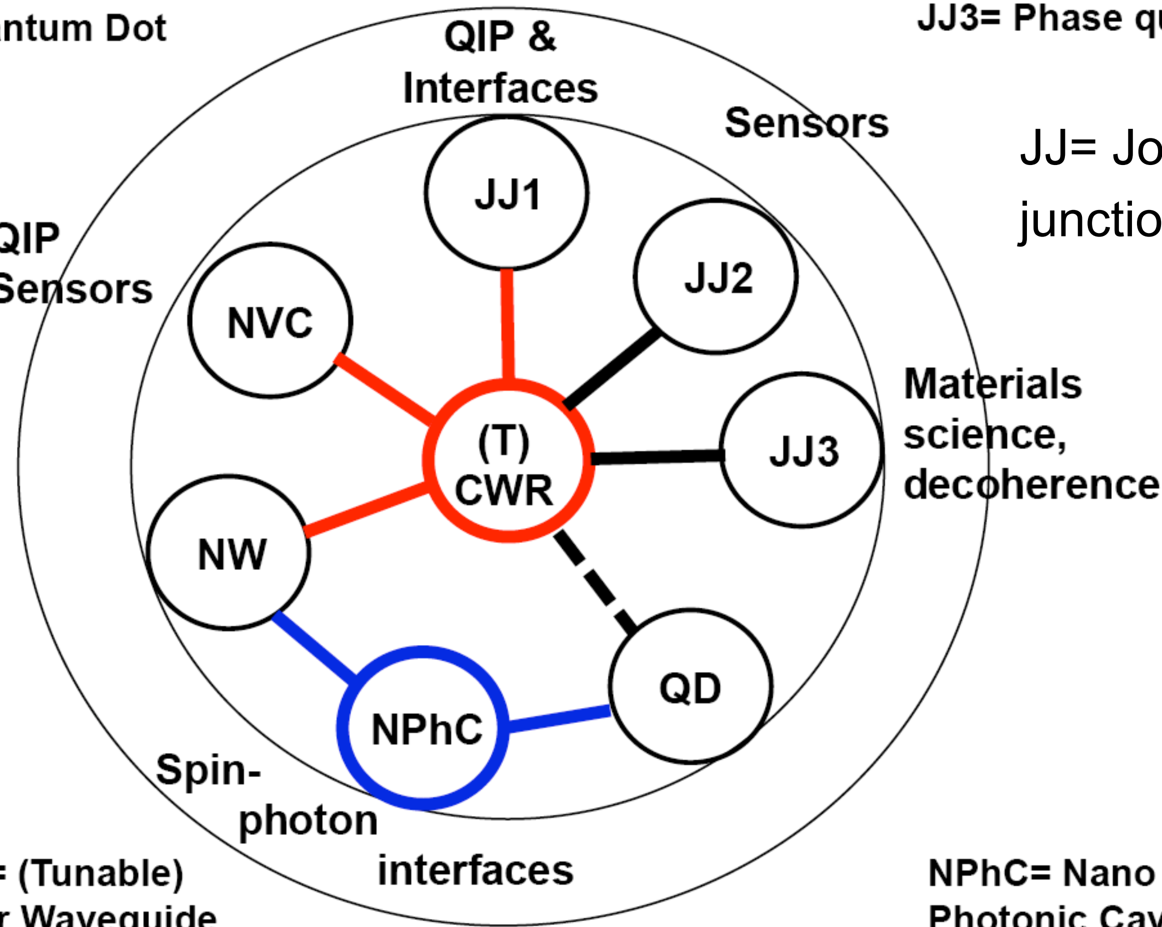
Hybrid QIP - SOLID (2010-2013)

NVC= N-V Centre
NW= Nanowire
QD= Quantum Dot

JJ1= Transmon
JJ2= Flux qubit
JJ3= Phase qubit



JJ= Josephson junction



Hybrid systems

1) JJ-JJ
2) JJ-QD/spin
3) JJ-NVC/spin
4) Microwave-optical
5) Static-flying qubits
6) …….

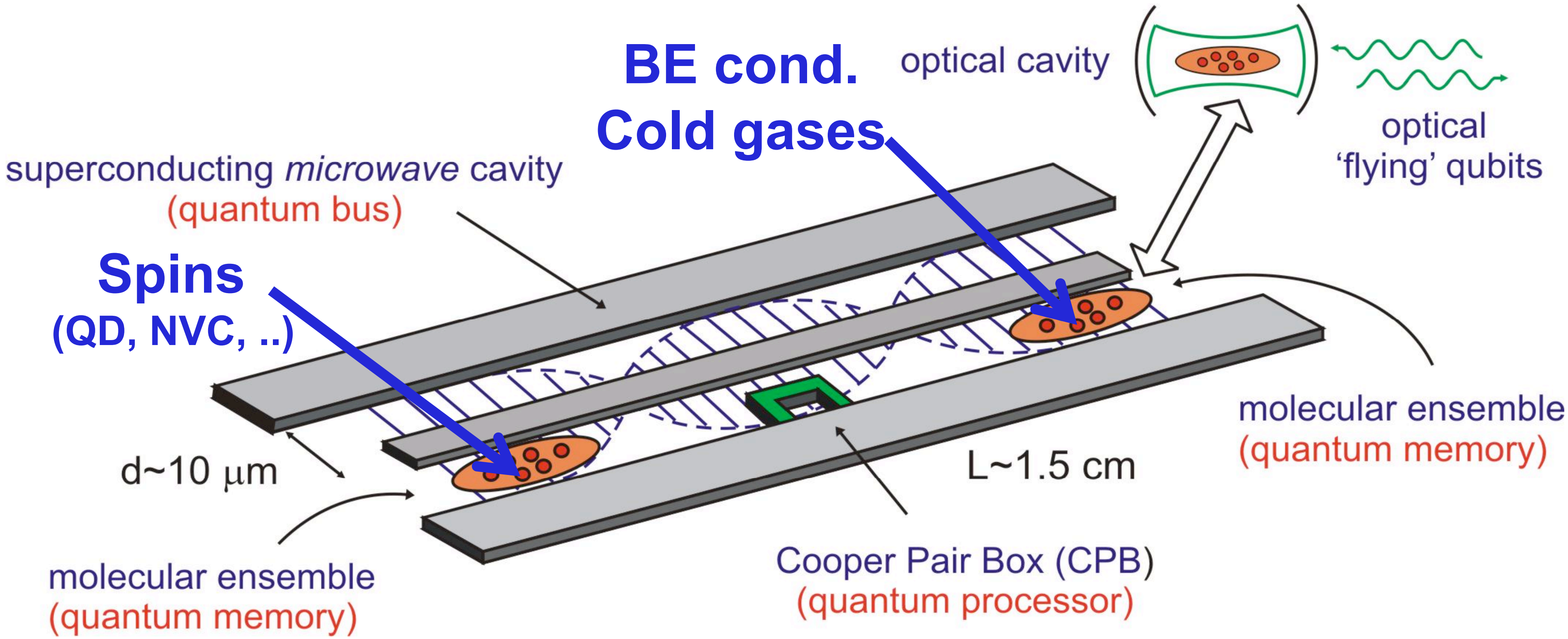
(T)CWR= (Tunable) Coplanar Waveguide Resonator

NPhC= Nano Photonic Cavity

Hybrid devices

Processing - memory - communication – collaboration

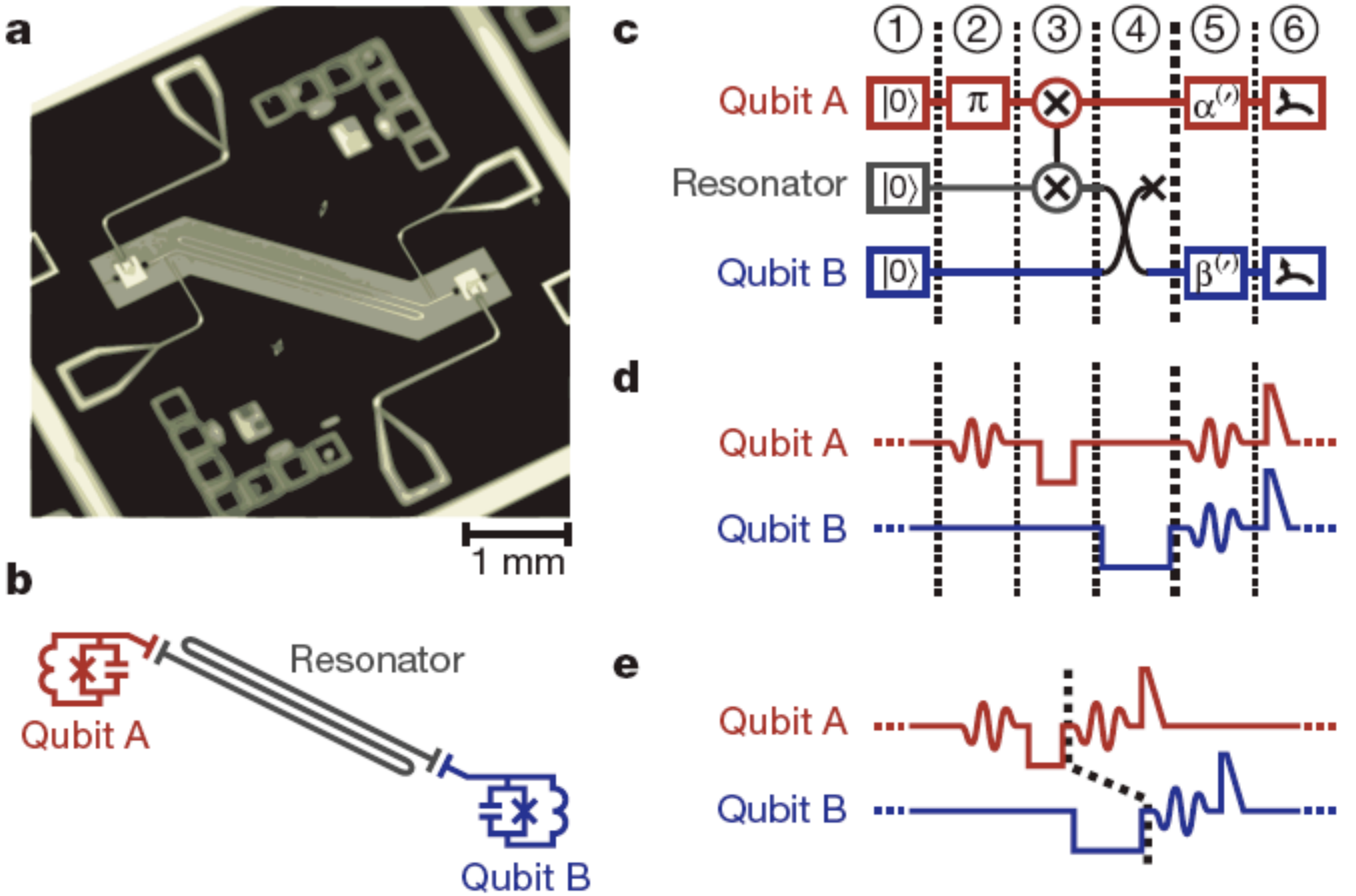
The only realistic option for non-toy QIP ?



Josephson junctions (JJ)

Picture adapted from Peter Zoller et al.

Bell state (Martinis group)



QIP algorithms, state of the art

From October 2009. To be updated.

	JJ Tmon Transmon	JJ Fx Flux	JJ Phs Phase	QD spin GaAs	NVC spins diamond	Ion trap [11]
Hybrid devices	None	None	None	None	None	None
SOLID goal	Tmon-MWC-NVC, QD; T-NVC-NPhC	Fx-MWC-Phase	Phs-MWC -Fx	QD-NPhC-QD; QD - MWC- Tmon	NVC -NPhC-NVC; NVC - MWC- Tmon	
Scalability	Unknown	Unknown	Unknown	Unknown	Unknown	Unknown
SOLID goal	Proof of concpt hybrid QIPC	Proof of cpt hybrid QIPC	Proof cpt hybr. QIPC	Proof of cpt hybrid QIPC	Proof of cpt hybrid QIPC	
Bell state	Yes [27]	Yes [2]	Yes [37]	No	Yes [10]	Yes
Tomography	Yes [27]	No	Yes [37]	No	Yes [10]	Yes
Bell inequalities	No	No	Yes! [38]	No	No	Yes
GHZ, W states	No	No	No	No	Yes [10]	Yes
Deutsch-Jozsa	Yes [36]	No	No	No	No	Yes
Teleportation	No	No	No	No	No	Yes
Grover	Yes [36]	No	No	No	No	Yes
Shor	No	No	No	No	No	QFT
QEC	No	No	No	No	No	Yes

State of the art – JJ (exp)

Universal gate operation

Bell states

State tomography

QED with 3 qubits

Bell inequalities

GHZ states

Deutsch-Jozsa

Grover

Martinis' group,, UC Santa Barbara:

Ansmann et al.: "Violation of Bell's inequality in Josephson phase qubits", Nature 461, 504-506 (2009).

Matthew Neeley et al.: "Generation of Three-Qubit Entangled States using Superconducting Phase Qubits Nature 467, 570-573 (2010).

Shoelkopf's group, Yale

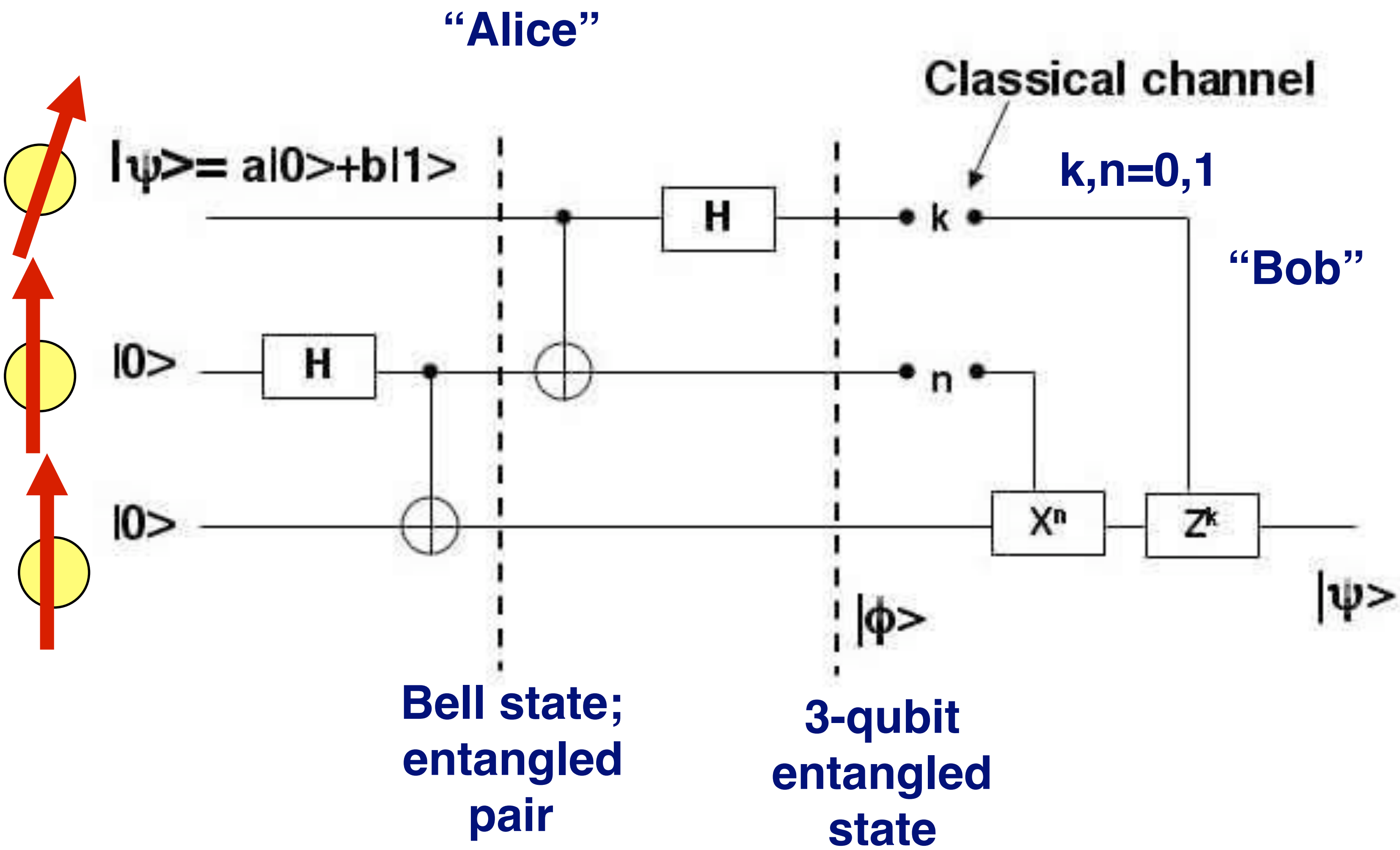
DiCarlo et al.: "Demonstration of Two-Qubit Algorithms with a Superconducting Quantum Processor" Nature 460, 240-244 (2009).

Preparation and measurement of three-qubit entanglement in a superconducting circuit
L. DiCarlo et al.. Nature, 467, 574-578 (2010).

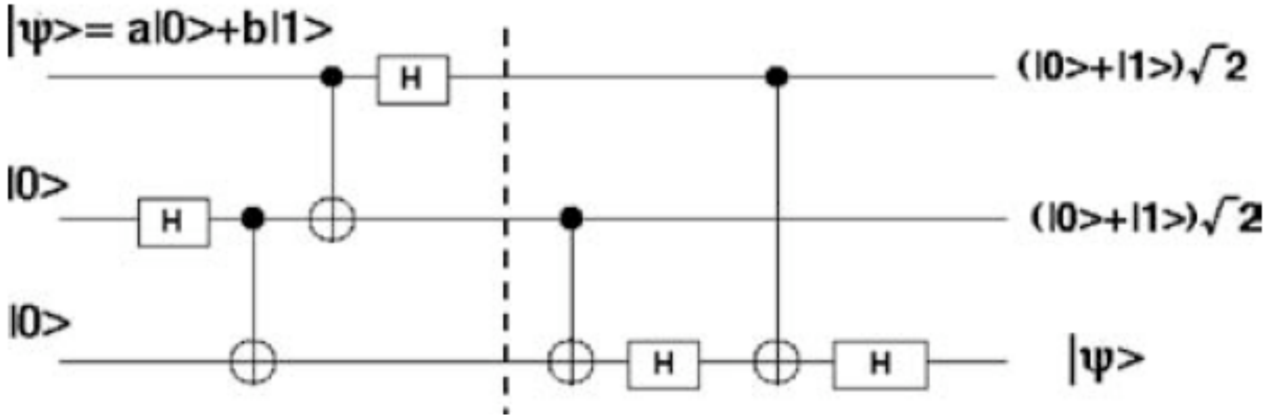
Challenges for solid-state QIP systems

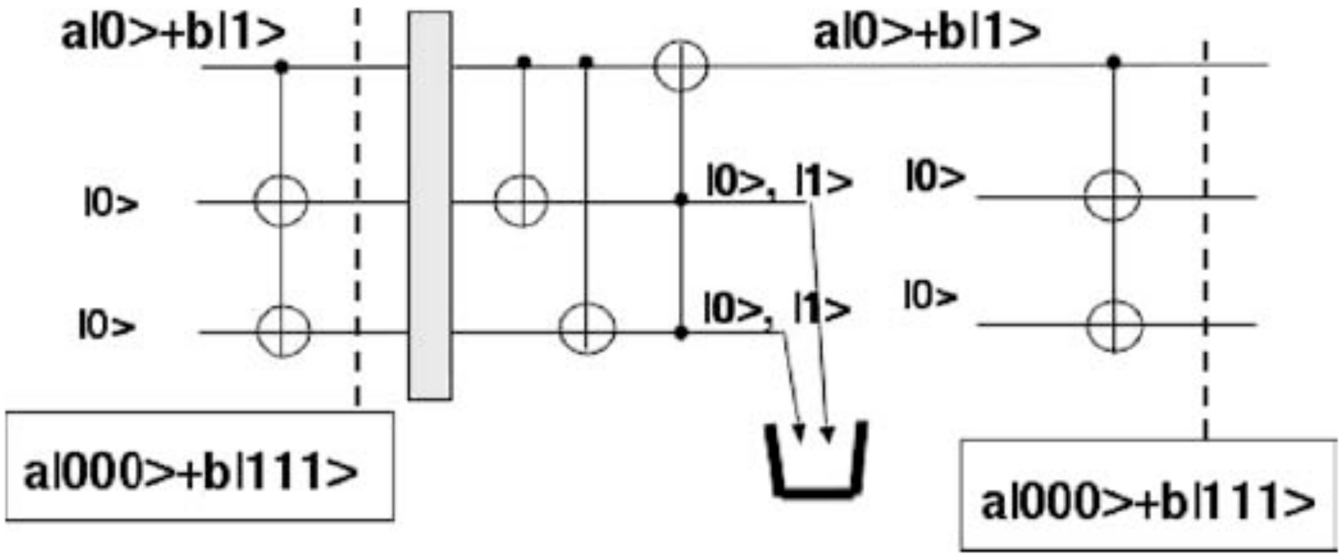
- Teleportation
- Error correction
- Simulation of quantum system

Teleportation



Teleportation and Error Correction





SOLID core technologies

Microwave engineering

- Parametric Amplifier
- Josephson Metamaterials
- Microwave photon detectors with qubit clusters
- Propagating quantum microwave fields and qubit clusters

Materials science

- Improving coherence times of qubits
- Epitaxial superconducting and tunnel barrier layers for high Q resonator and phase qubits
- Minimization of dielectric losses
- Quantum manipulation of individual two-level fluctuators in Josephson qubits
- Theoretical investigation of two-level fluctuators as quantum resource

Simulation of quantum systems – some examples

Using Quantum Computers for Quantum Simulation
K.L. Brown, W.J. Munro and V.M. Kendon, arXiv:1004.5528 **Exp+Theory**

Quantum simulation of the Dirac Equation, Nature 463, 68-71 (2010)

A Quantum-Quantum Metropolis Algorithm. *Man-Hong Yung and Alán Aspuru-Guzik Submitted (2010).*

Characterization and quantification of the role of coherence in ultrafast quantum biological experiments using quantum master equations, atomistic simulations, and quantum process tomography . *arXiv:1012.3451.*

Simulating chemistry using quantum computers
Ivan Kassal, James D. Whitfield, Alejandro Perdomo-Ortiz, Man-Hong Yung, and Alan Aspuru-Guzik. Annual Reviews of Physical Chemistry. Volume 62 In Press (2011) . arxiv:1007.2648

Quantum Computing Resource Estimate of Molecular Energy Simulation, James D. Whitfield, Jacob Biamonte and Alán Aspuru-Guzik . Molecular Physics. In press Preprint Available at arXiv:1001.3855.

Quantum devices and networks - SWOT

S	W
Exp proofs of concepts Working devices Architectures Logic gates Algorithms Schemes for scaling up	Embryonic Research stage Small numbers of qubits 50-100 needed for competitive applications Scaling up involves huge challenges
O	**T**
Basic research Quantum few-qubit appl. Develop working technologies Paradigm shift in computing Quantum internet	No killer aplications May never become a competitive technology