Quantum-dot Cellular Automata (QCA)

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Supported by ONR, DARPA, NSF

Outline of presentation

- QCA overview
- Metal-dot QCA devices
- Molecular QCA → architectures
- Power dissipation - fundamental issues (*Lent contra Zhirnov*)

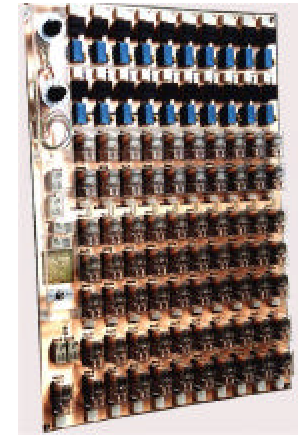
First question for molecular electronics

How is information represented physically?

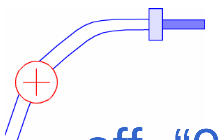
Zuse's paradigm

- Konrad Zuse (1941) Z3 machine
  - Use **binary numbers** to encode information
  - Represent binary digits as on/off state of a **current switch**

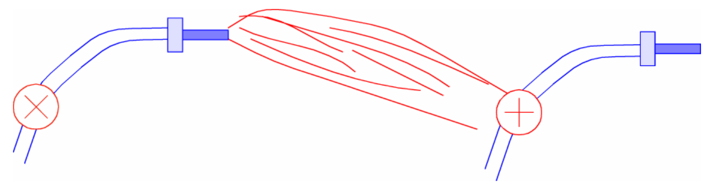
Telephone relay



Z3 Adder

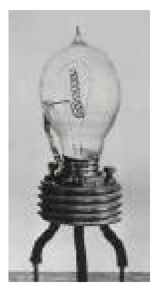


off="0"



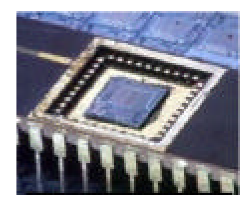
The flow through one switch turns another on or off.

Electromechanical relay



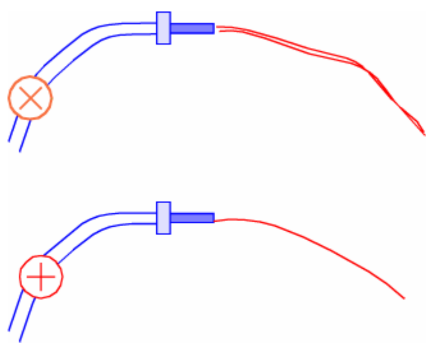
Vacuum tubes

Solid-state transistors

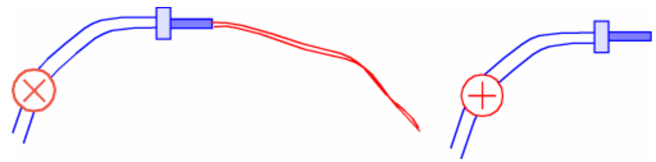


CMOS IC

Problems shrinking the current-switch



Valve shrinks also – hard to get good on/off



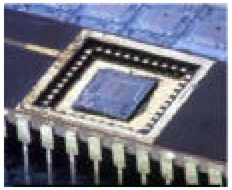
Current becomes small - resistance becomes high
Hard to turn next switch
Charge becomes quantized

Power dissipation threatens to melt the chip.

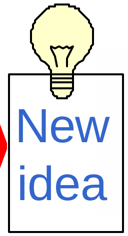
Electromechanical relay

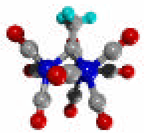
Vacuum tubes

Solid-state transistors



CMOS IC





Molecules

To reach the single-molecule level, a new approach to representing information is required.

New paradigm: Quantum-dot Cellular Automata

Represent information with molecular charge configuration.

<u>Zuse's paradigm</u>

✓ • Binary

✗ • ~~Current switch~~ → ✓ • charge configuration

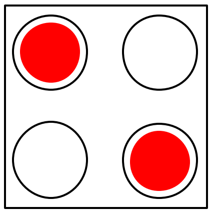
Revolutionary, not incremental, approach

Beyond transistors – requires rethinking circuits and architectures

Use molecules, not as current switches, but as **structured charge containers**.

Quantum-dot Cellular Automata

Represent binary information by charge configuration



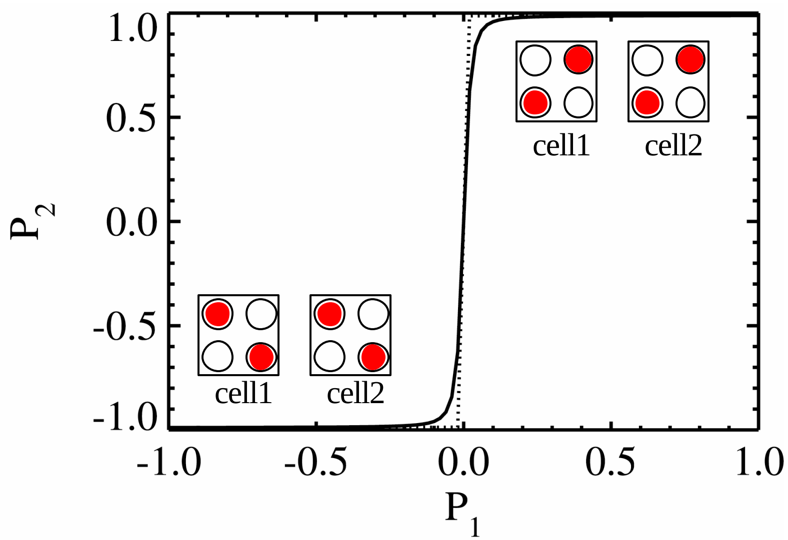
A cell with 4 dots

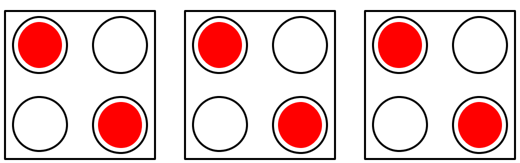
2 extra electrons

Tunneling between dots

Polarization P = -1
Bit value “0”

Cell-cell response function





Neighboring cells tend to align.
Coulombic coupling

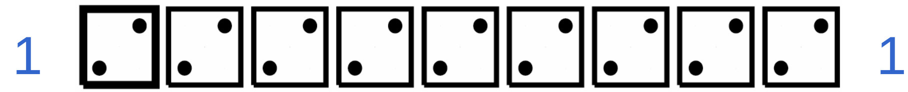
Bistable, nonlinear cell-cell response

Restoration of signal levels

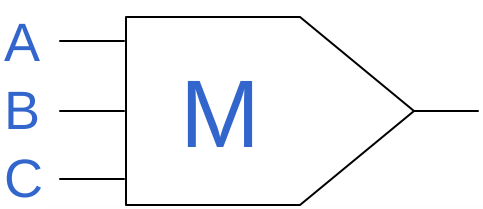
Robustness against disorder

QCA devices

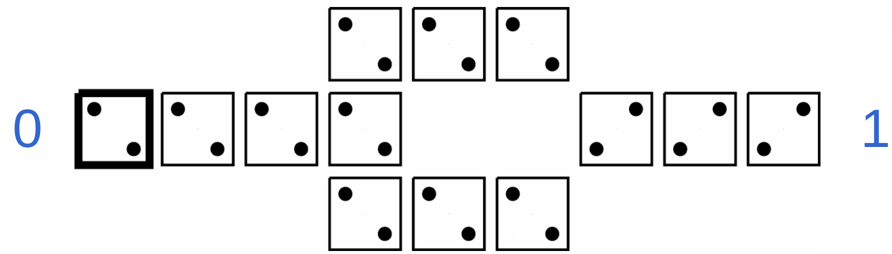
Binary wire

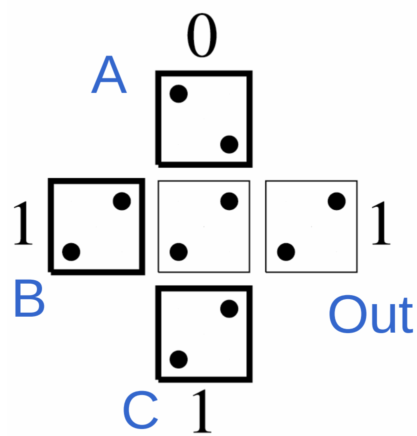


Majority gate

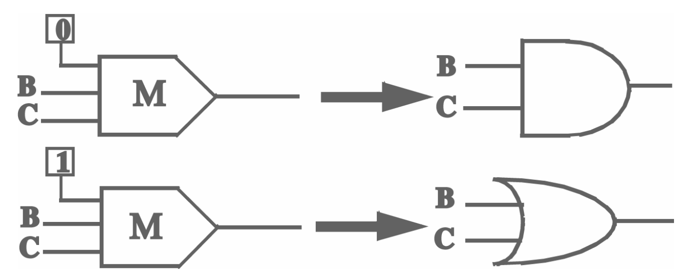


Inverter



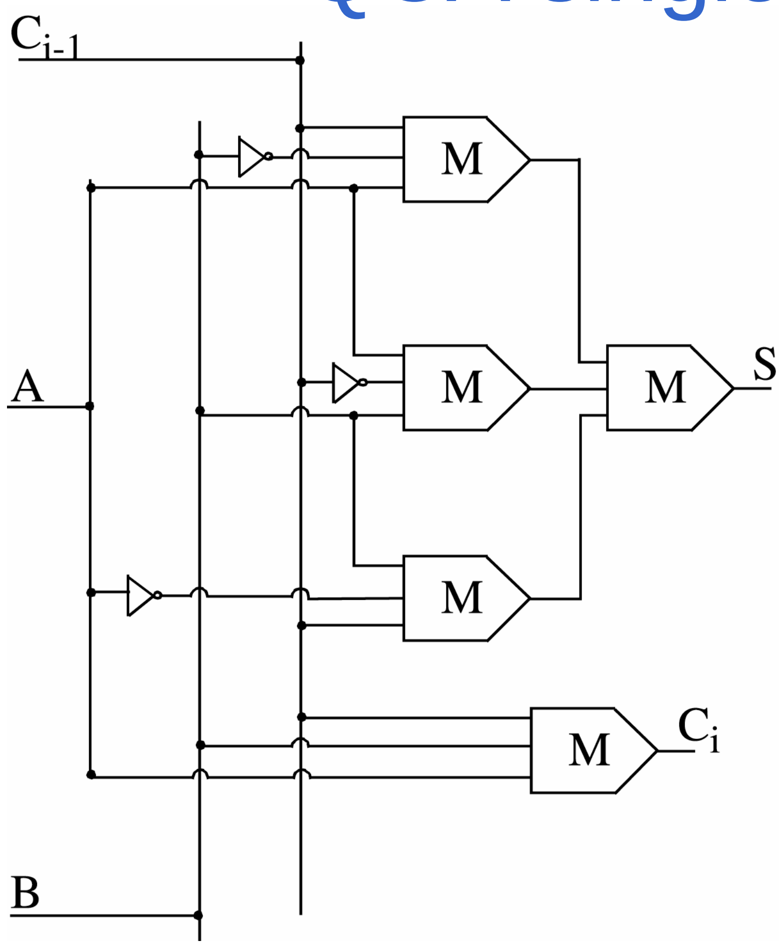


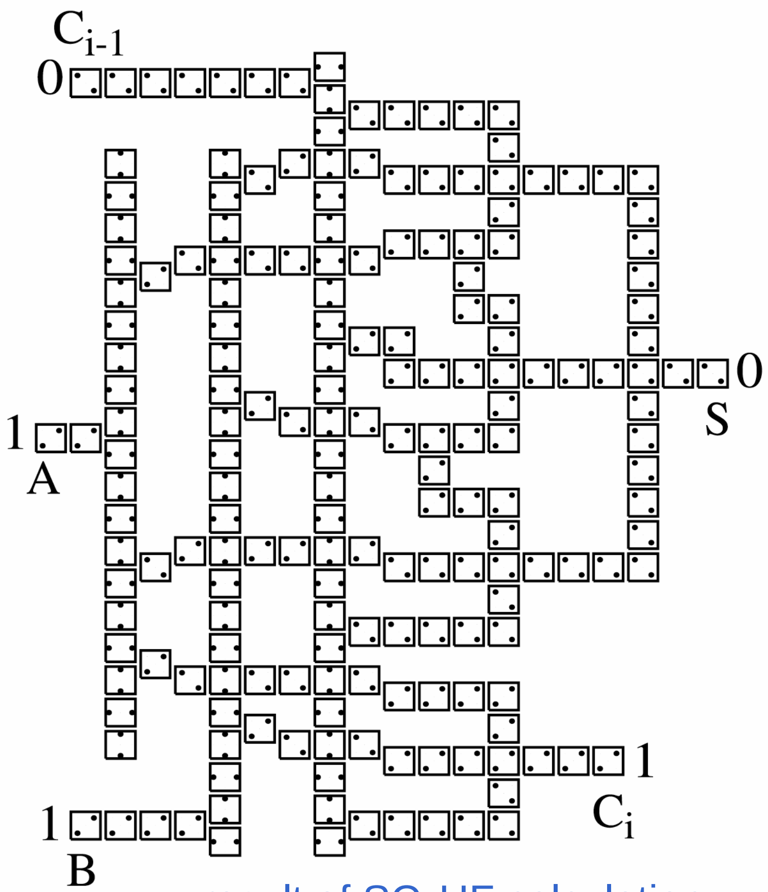
	A	B	C	Output
AND gate	0	0	0	0
	0	0	1	0
	0	1	1	1
	0	1	0	0
OR gate	1	1	0	1
	1	1	1	1
	1	0	1	1
	1	0	0	0



Programmable 2-input AND or OR gate.

QCA single-bit full adder

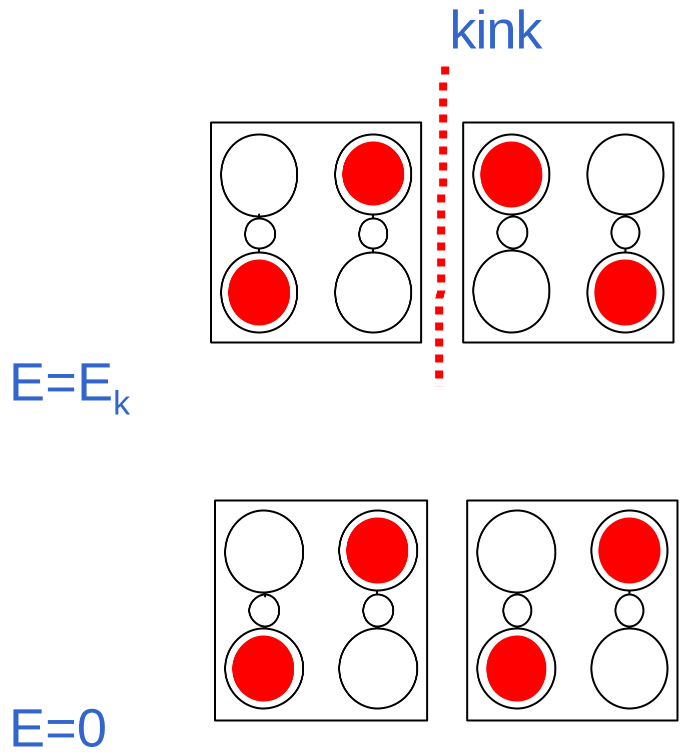




result of SC-HF calculation with site model

Hierarchical layout and design are possible.

Characteristic energy



We would like “kink energy” $E_k > k_B T$.

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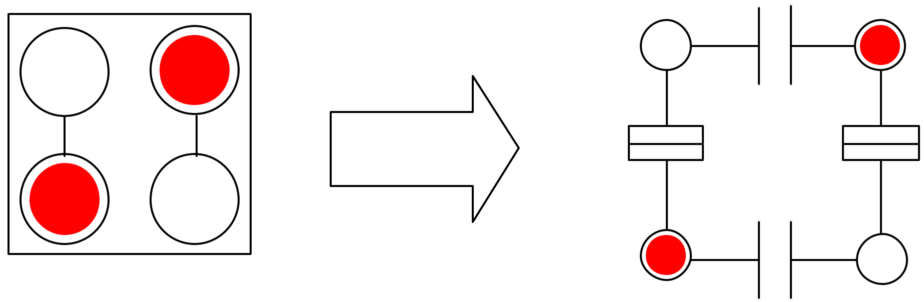
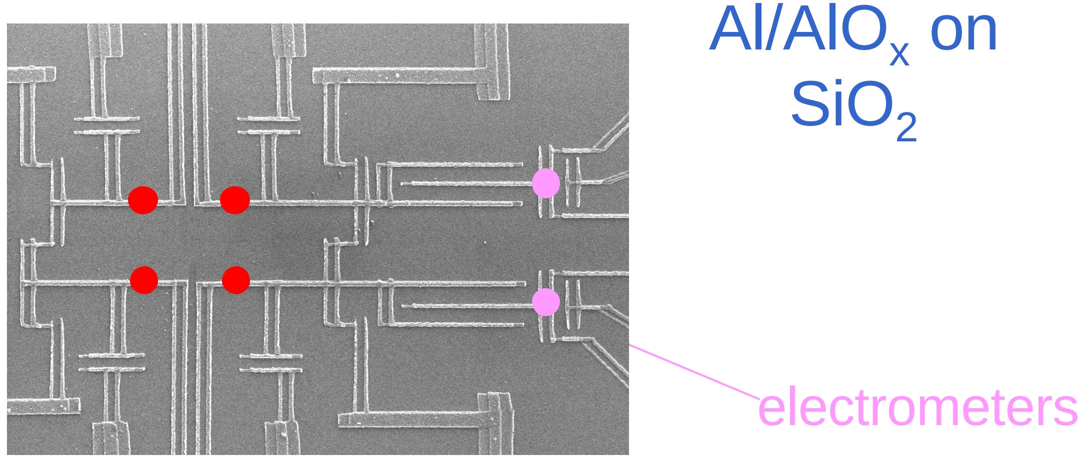
- Molecular QCA ➔ architectures
- Power dissipation - fundamental issues (*Lent contra Zhirnov*)

QCA devices exist



Metal-dot QCA implementation



Al/AlO_x on SiO_2

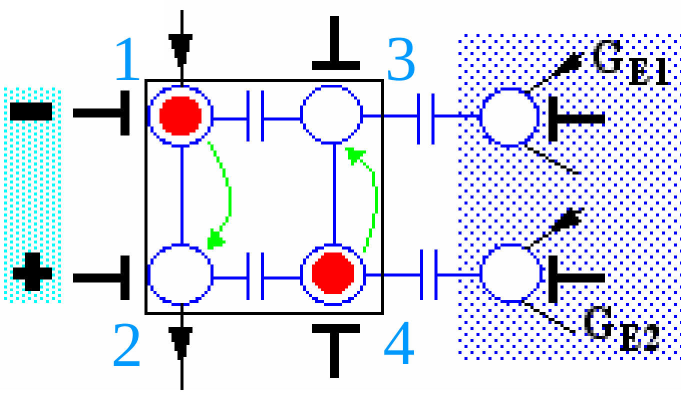
“dot” = metal island

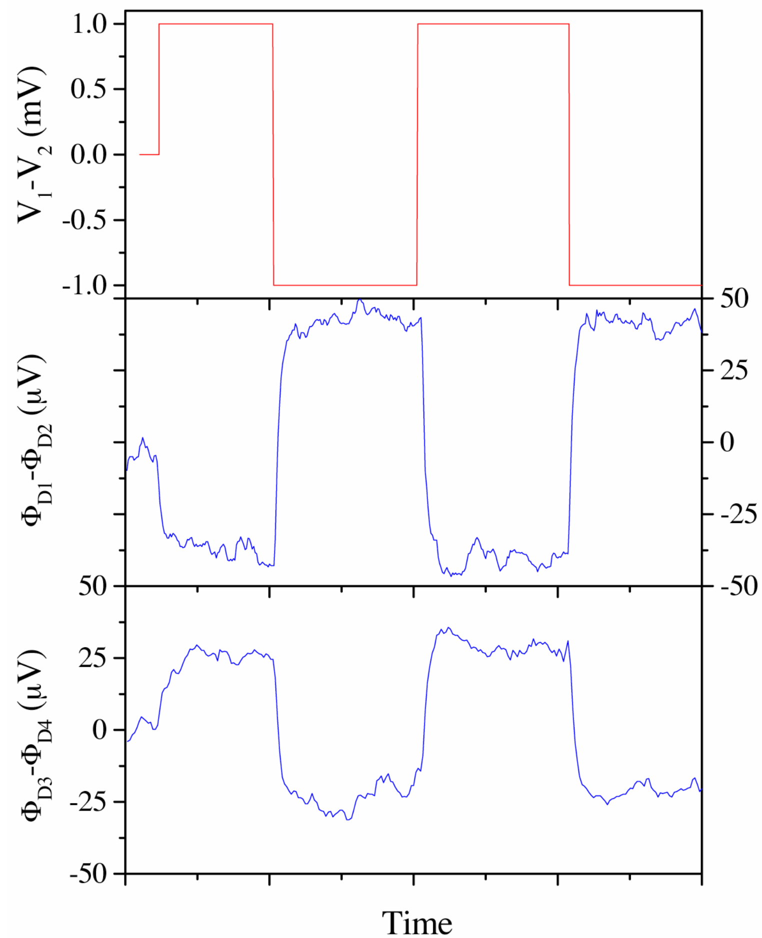
70 mK

Greg Snider, Alexei Orlov, and Gary Bernstein

Metal-dot QCA cells and devices

- Demonstrated 4-dot cell

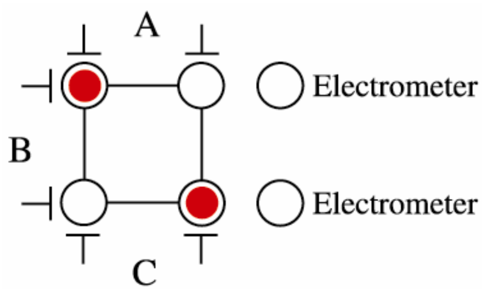


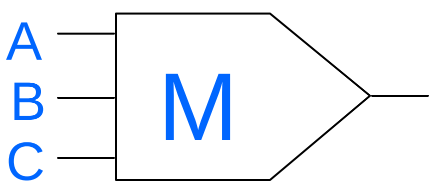


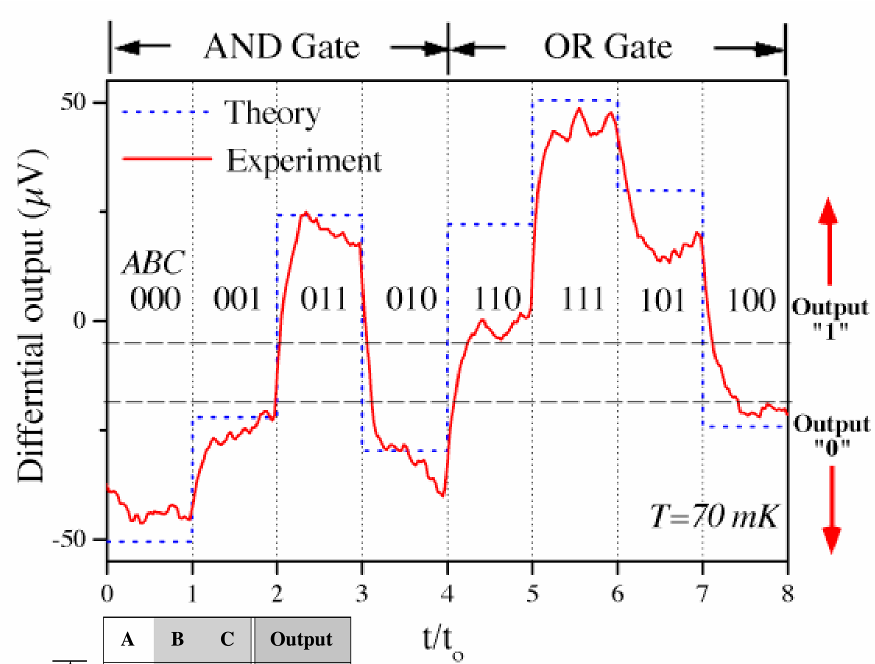
A.O. Orlov, I. Amlani, G.H. Bernstein, C.S. Lent, and G.L. Snider, *Science*, **277,** pp. 928-930, (1997).

Metal-dot QCA cells and devices

- Majority Gate







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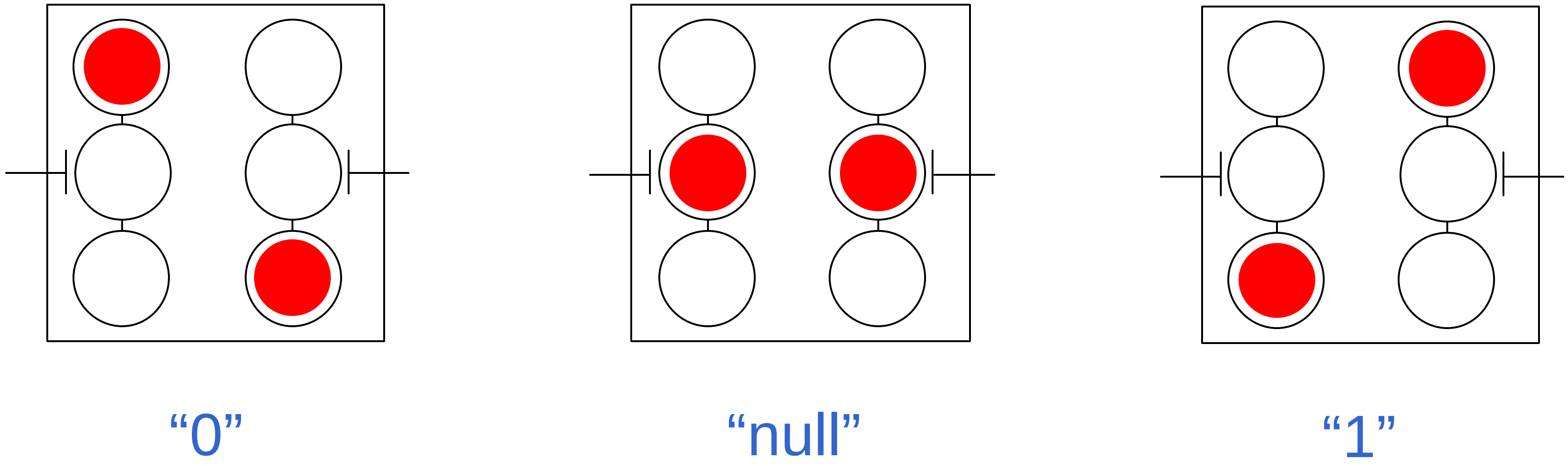
	1	0	1	1
	1	0	0	0

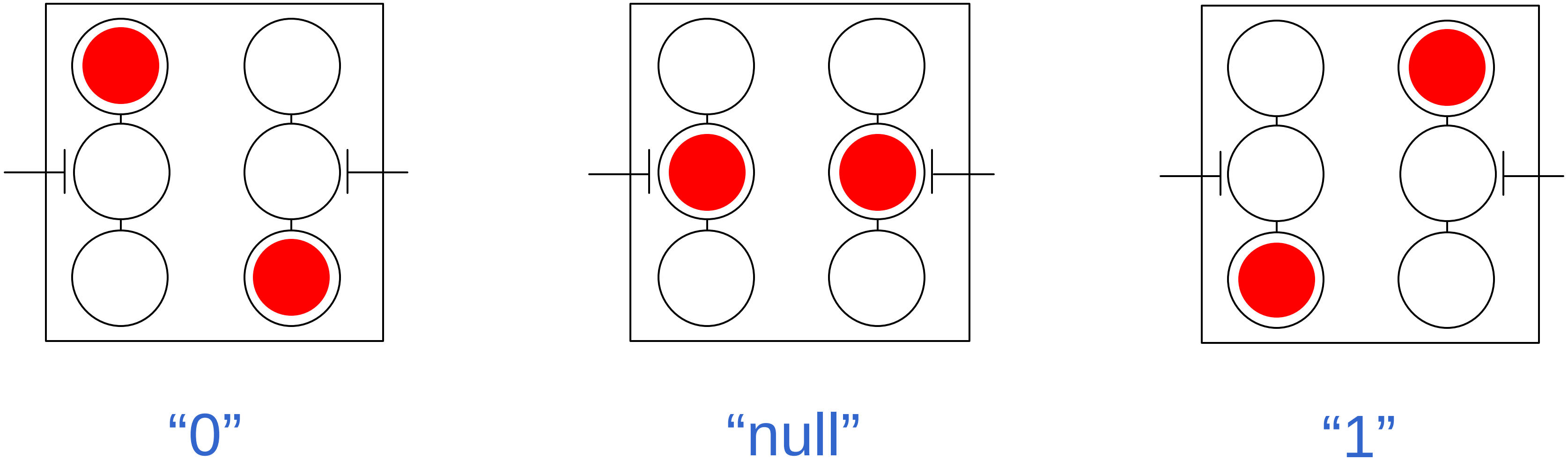
Amlani, A. Orlov, G. Toth, G. H. Bernstein, C. S. Lent, G. L. Snider, *Science* **284**, pp. 289-291 (1999).

Clocked QCA cells



- Middle dot adds "null" state to cells.
- Applied voltage (clock) alters energy of middle dots and forces charge into null or "active" dots.
- Energy from clock provides *power gain* which restores weakened signals.

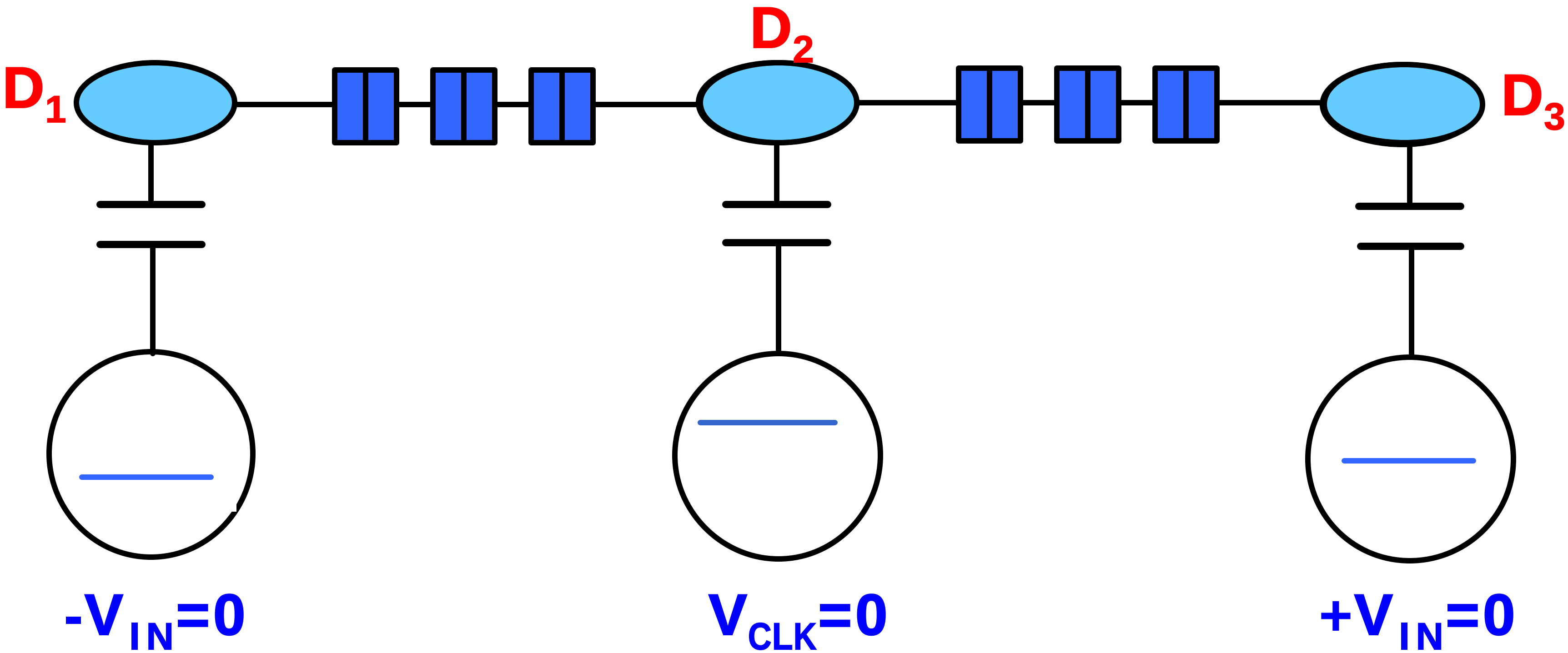
Clocked QCA cells



- Landauer – adiabatic clocking
- Lent et al. – clocked QCA
- Likharev et al. – single electron parametron
- Toth and Lent – clocked metal-dot QCA

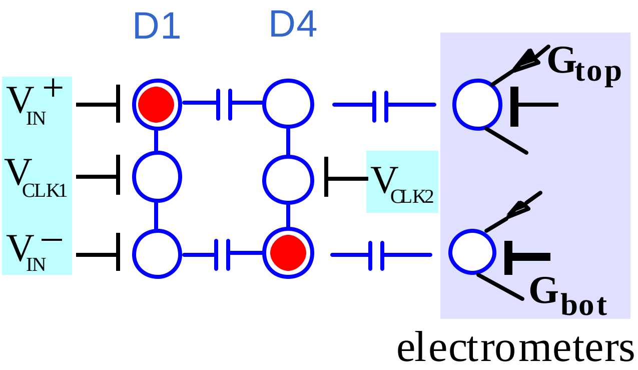
Three-dot QCA latch operation

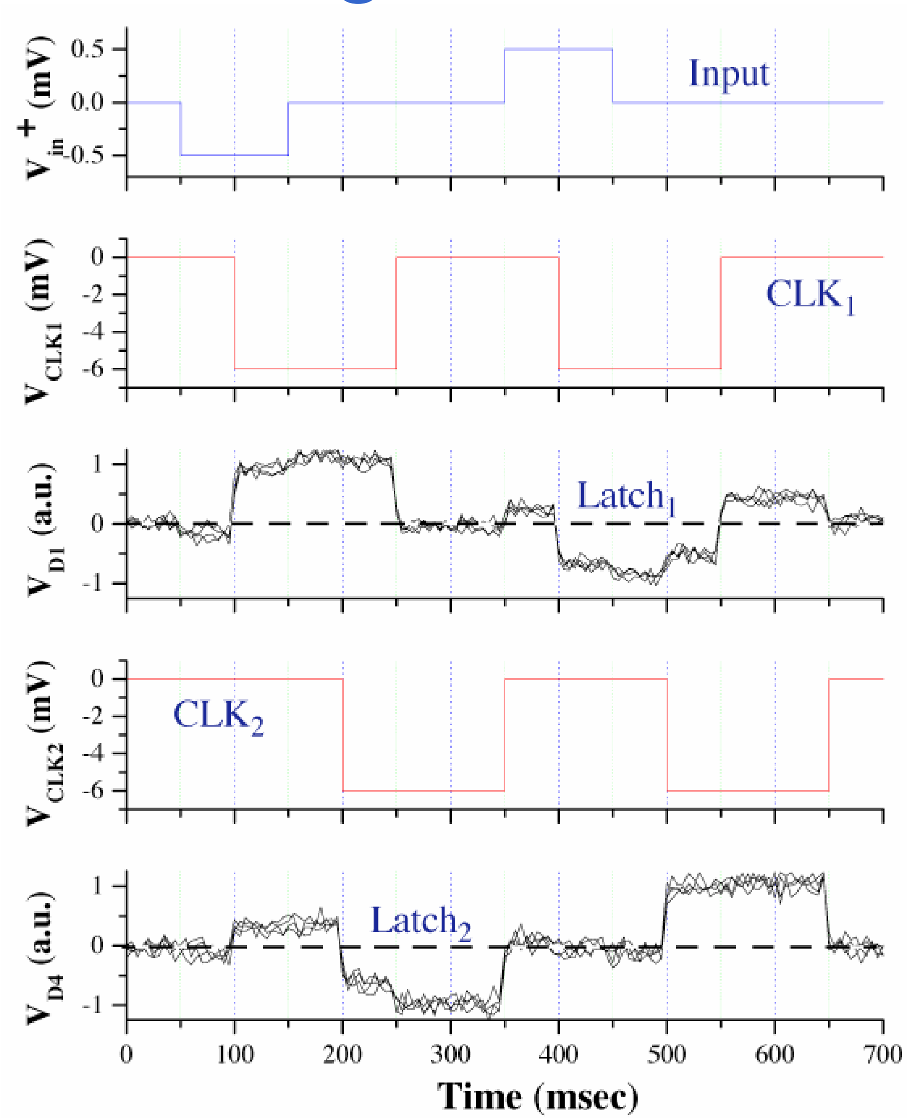
(0,0,0) ¬ (0,-1,1) back to null



- Clock supplies energy, input defines direction of switching
- Three states of the QCA latch: “0” , “1” and “null”

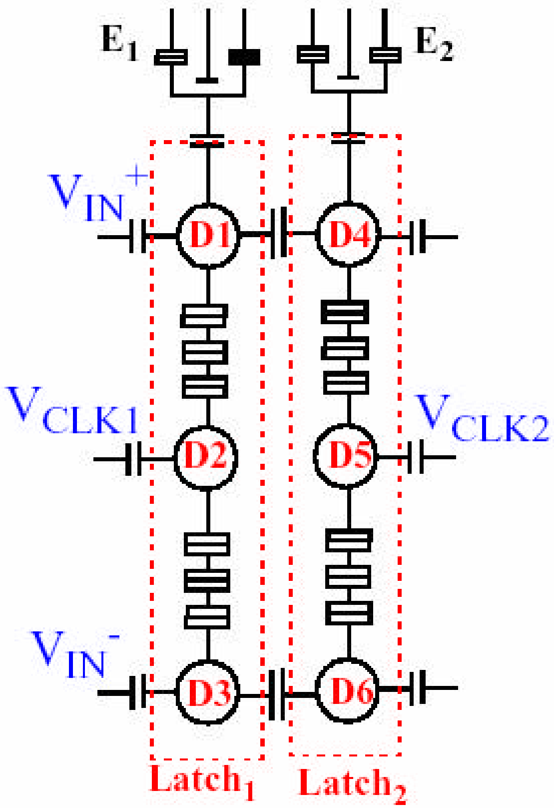
QCA Shift Register



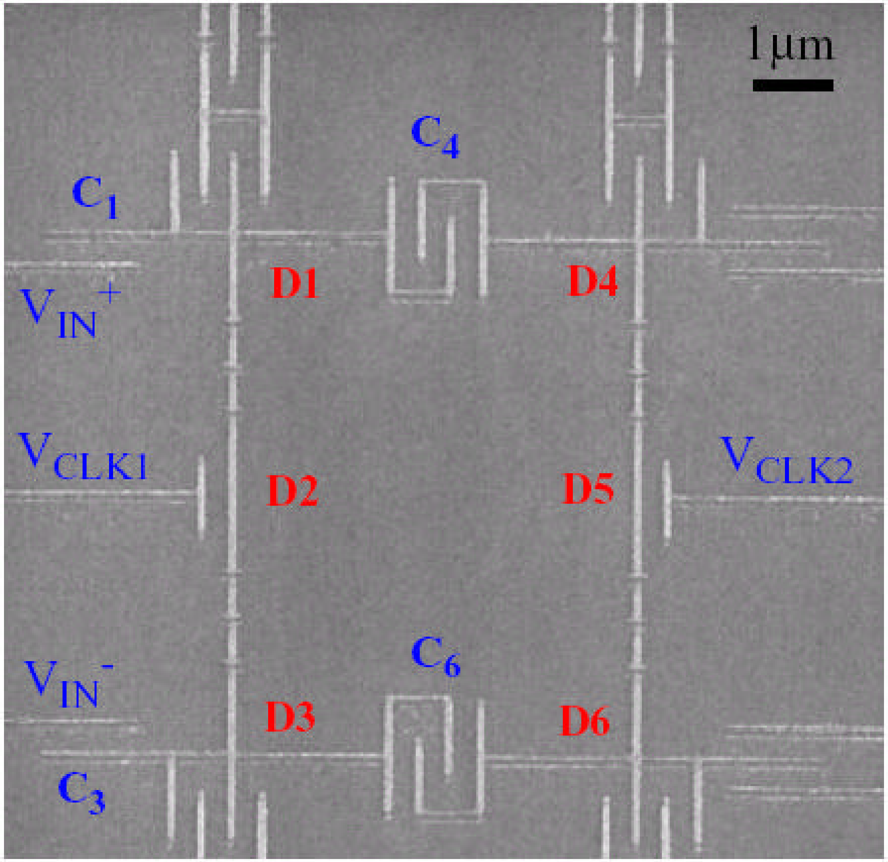


QCA Shift Register

Schematic Diagram



SEM Micrograph



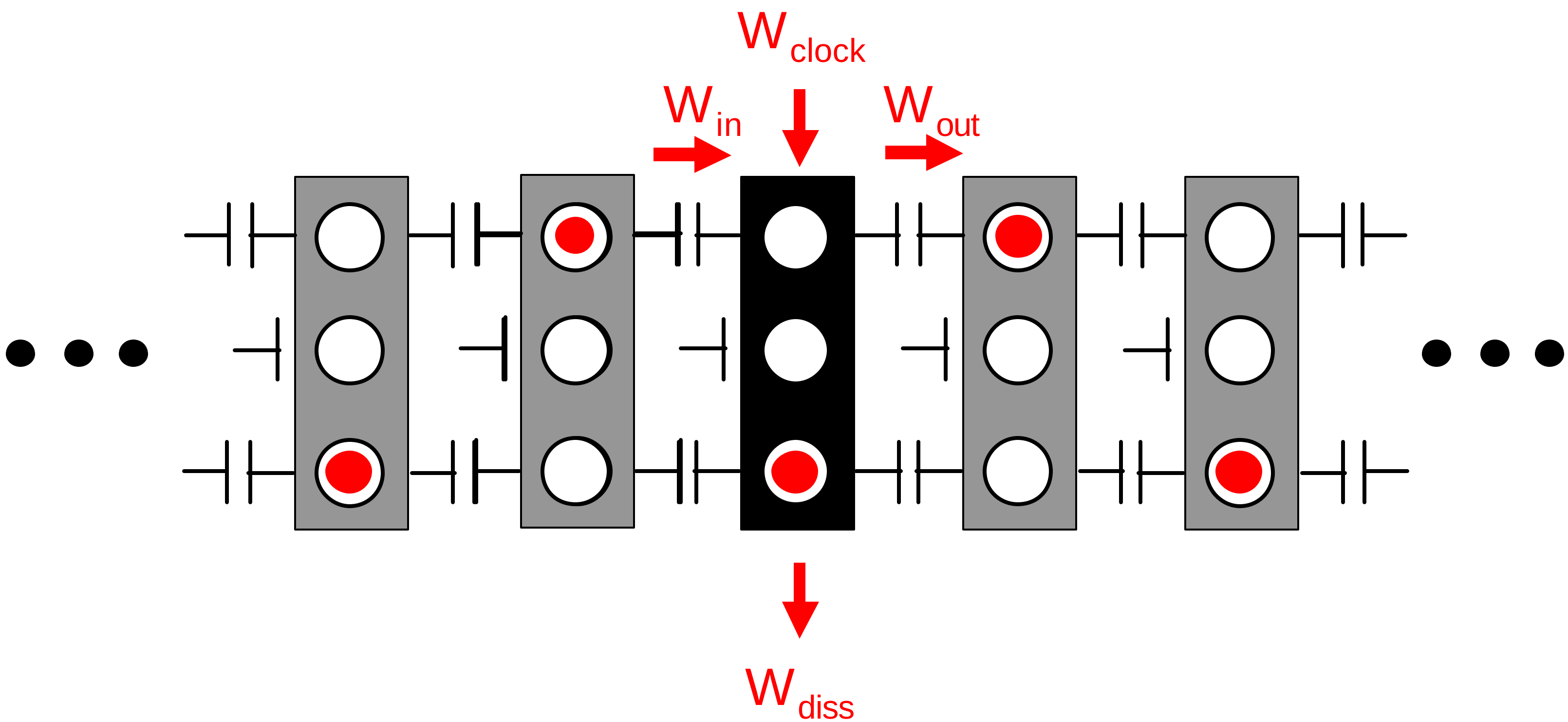
Power Gain in QCA Cells

- Power gain is crucial for practical devices because some energy is always lost between stages.

- Lost energy must be replaced.
  - Conventional devices – current from power supply
  - QCA devices – from the clock

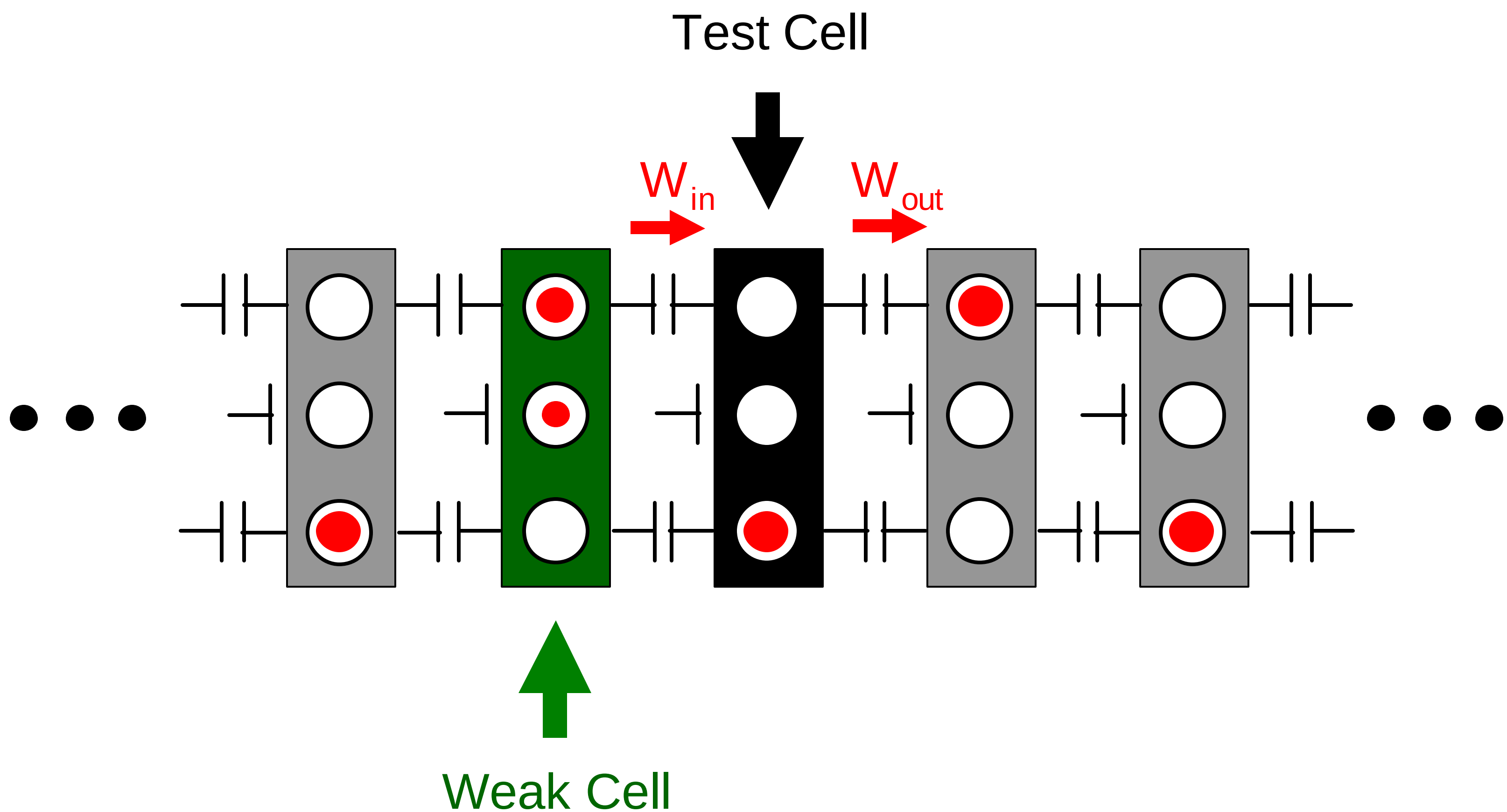
- Unity power gain means replacing exactly as much energy as is lost to environment.

Metal-dot Shift Register



When working well, $W_{diss} = W_{clock}$, $W_{in} = W_{out}$, and power gain =1

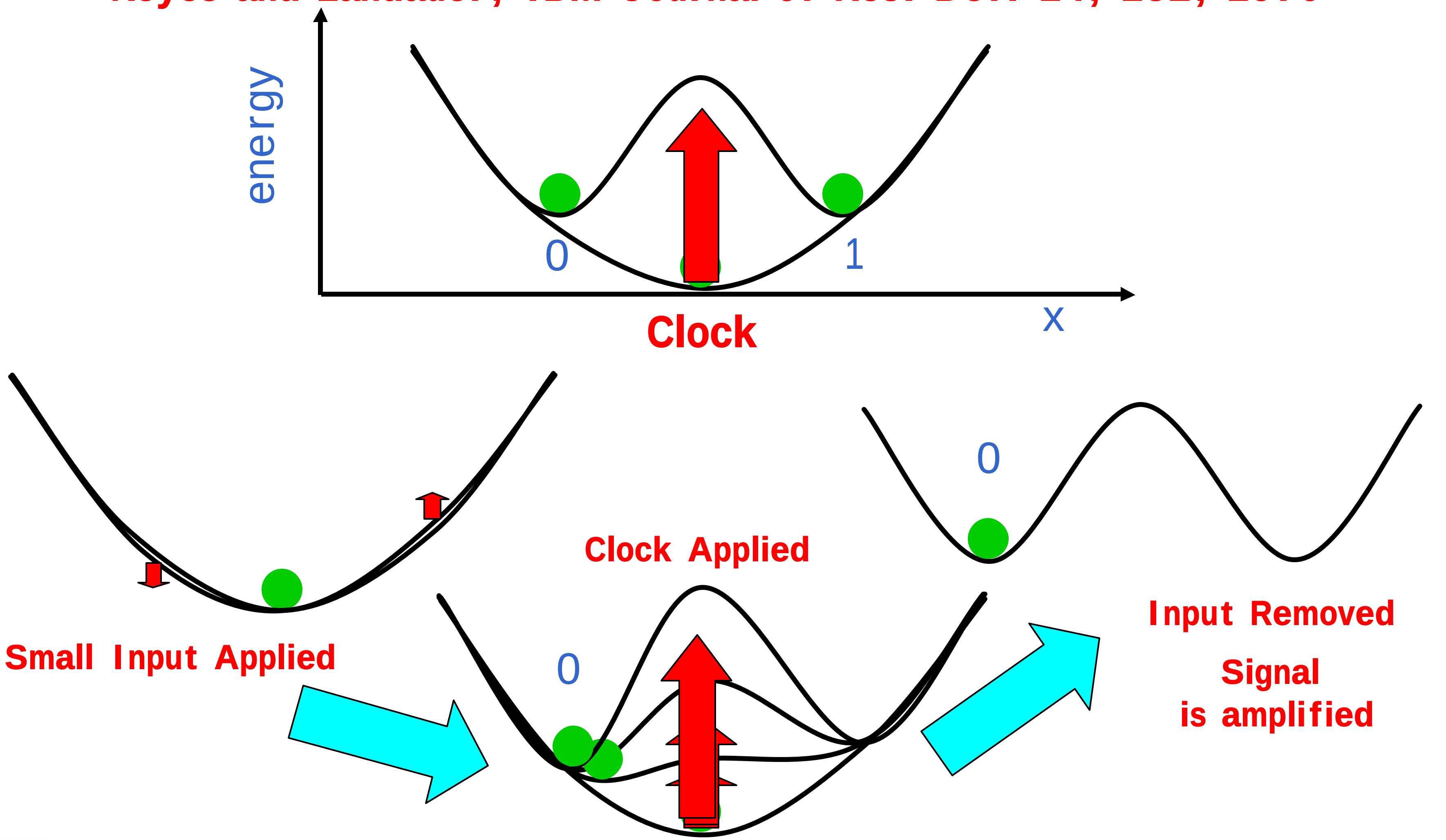
Metal-dot Shift Register with Weak Cell



Measured gain = $P_{out}/P_{in} = W_{out}/W_{in}$**=3.25**

Clocking in QCA

Keyes and Landauer, IBM Journal of Res. Dev. 14, 152, 1970



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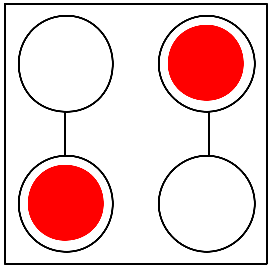
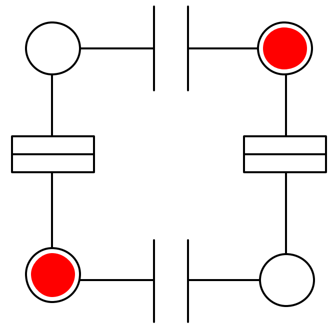
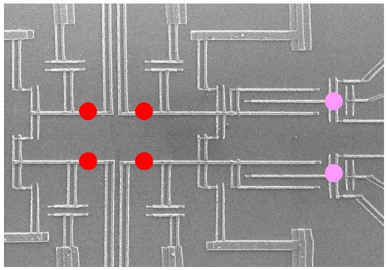
From metal-dot to molecular QCA

Metal tunnel junctions

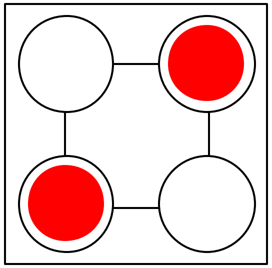


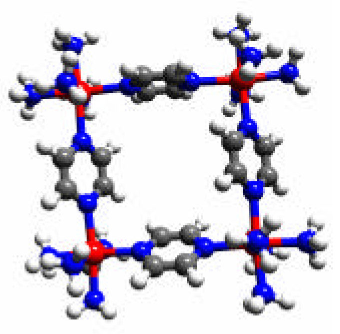




"dot" = metal island

70 mK





"dot" = redox center

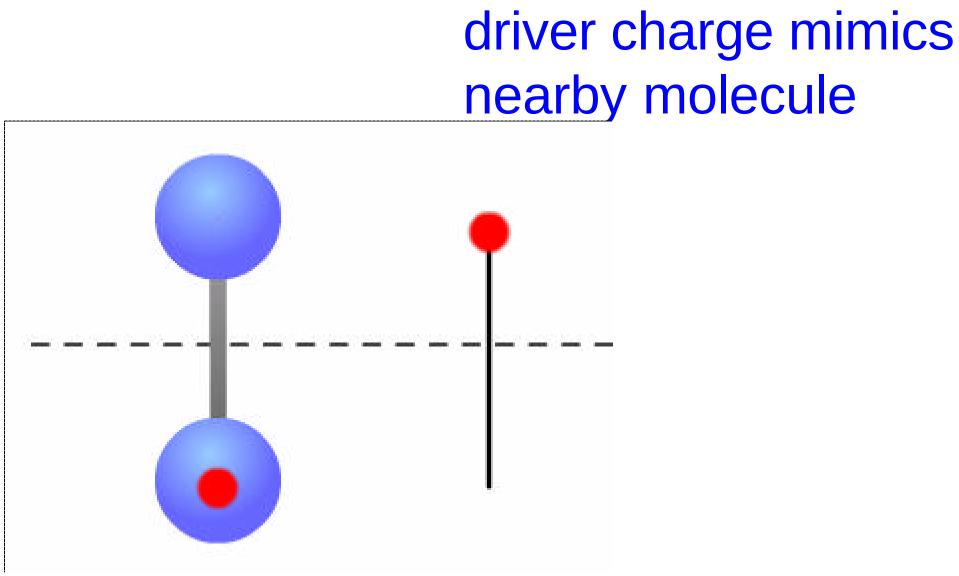
Mixed valence compounds

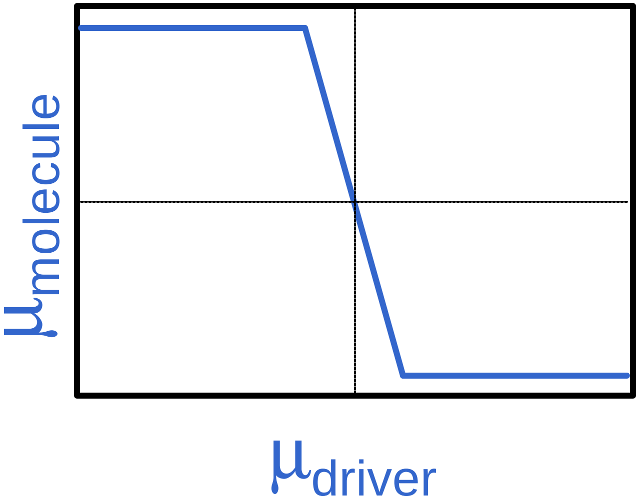
room temperature+

Key strategy: use *nonbonding* orbitals (π or d) to act as dots.

Theory of molecular QCA bistability

The first step:

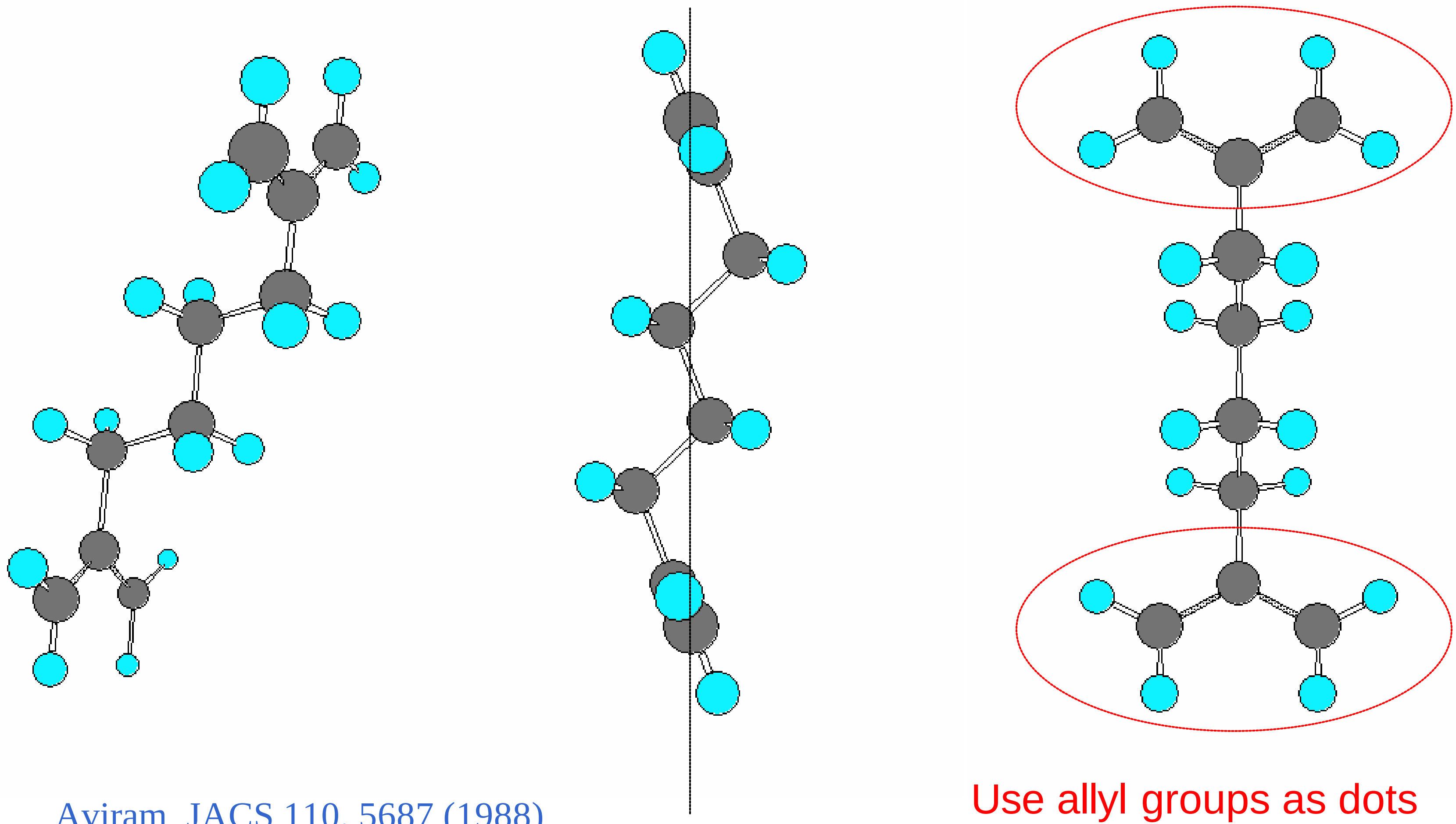




Look for systems that exhibit
nonlinear bistable, “clicky” behavior.

Beth Isaksen

Aviram molecule: simple model system

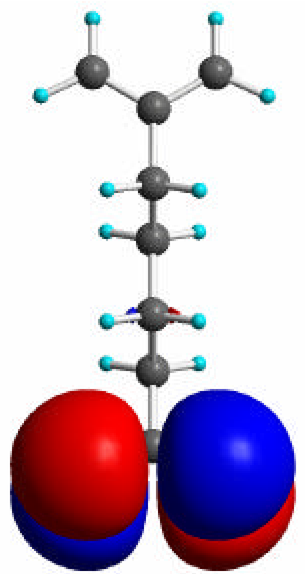


Use allyl groups as dots

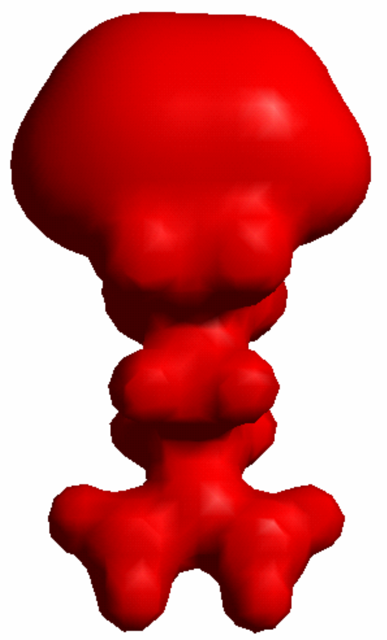
Aviram JACS 110, 5687 (1988)
Hush *et al.* JACS 112, 4192 (1990)

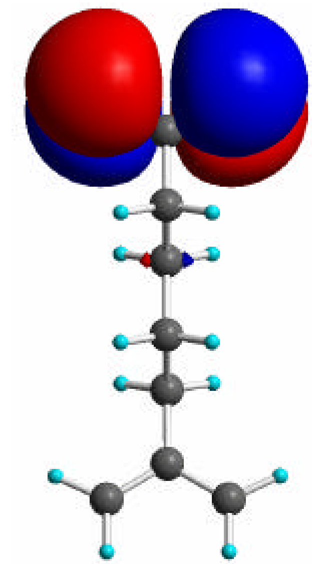
Charge configuration represents bit

HOMO

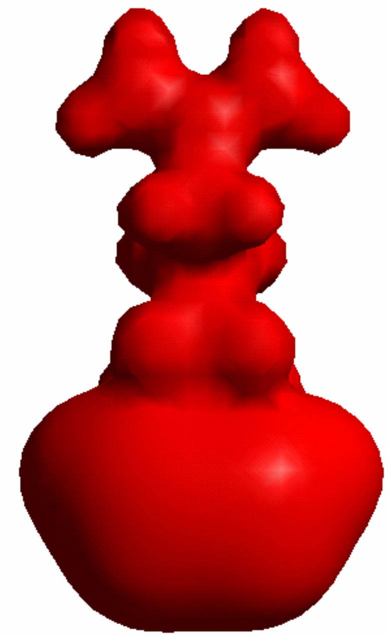


"1"





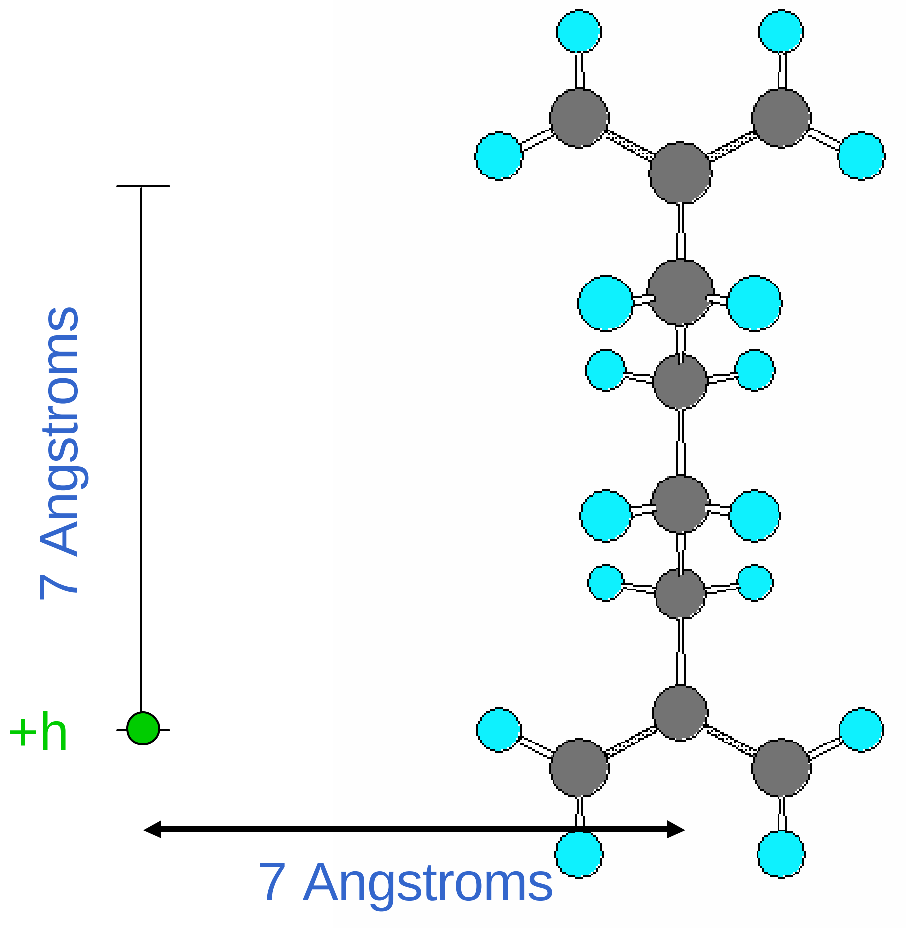
"0"



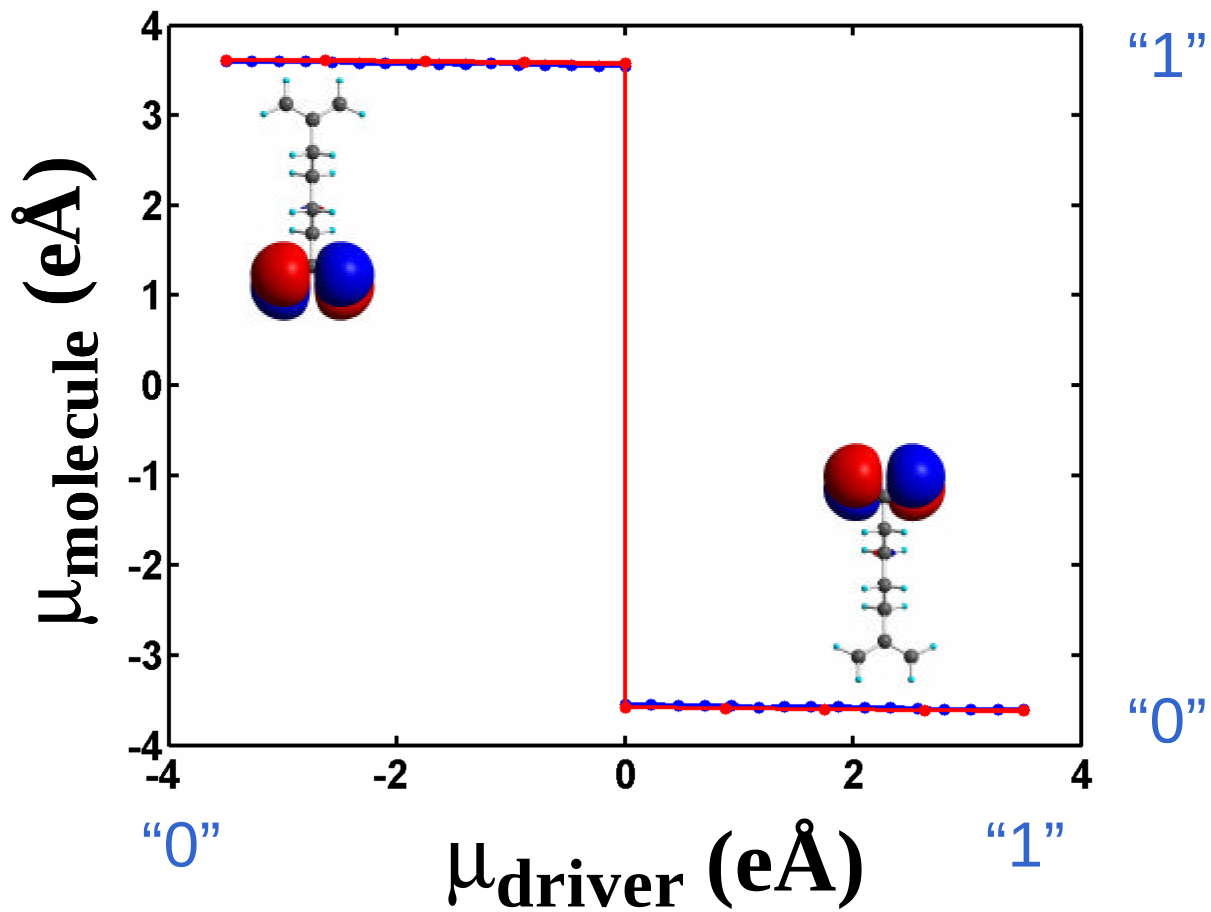
isopotential
surface

Gaussian 98 UHF/STO-3G

Driver mimics another molecule



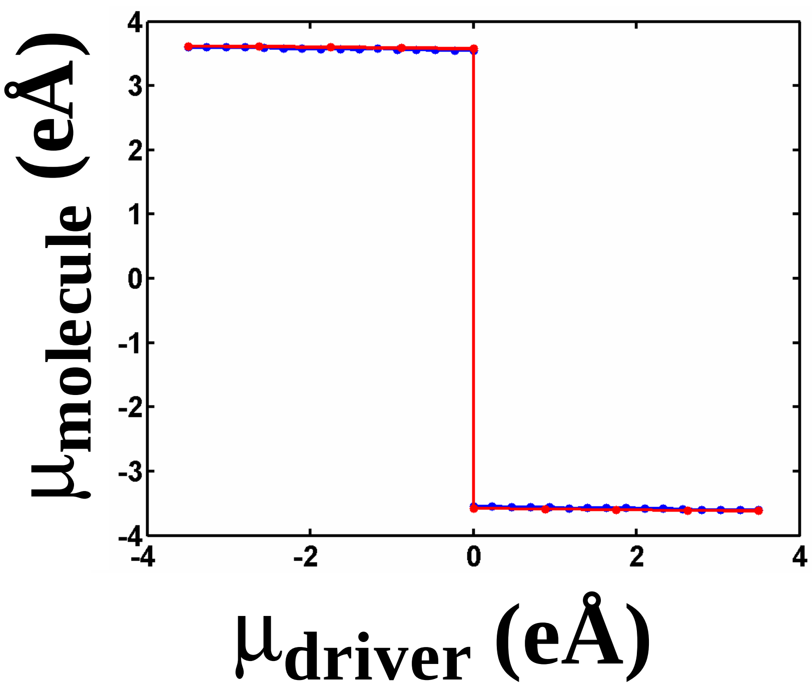
Cell-cell response

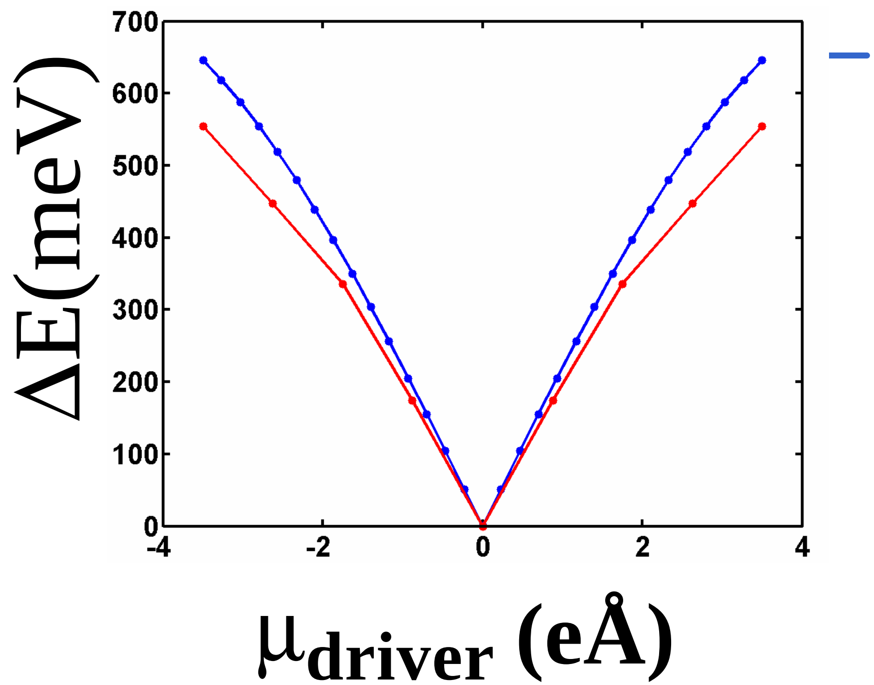


frozen nuclear positions   relaxed nuclear positions

Cell-cell response

E_k=635 meV





frozen nuclear positions

relaxed nuclear positions

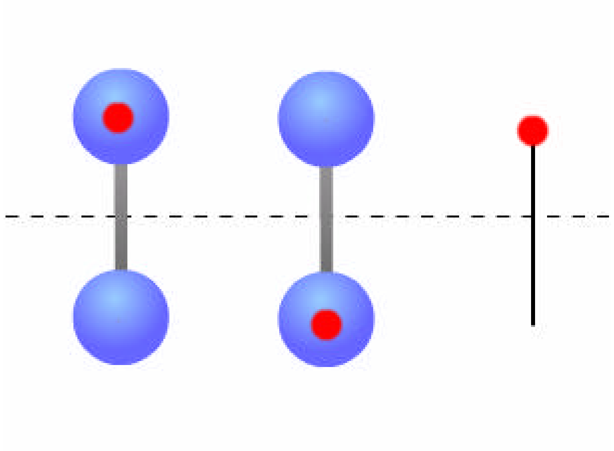
Excellent QCA cell-cell response function

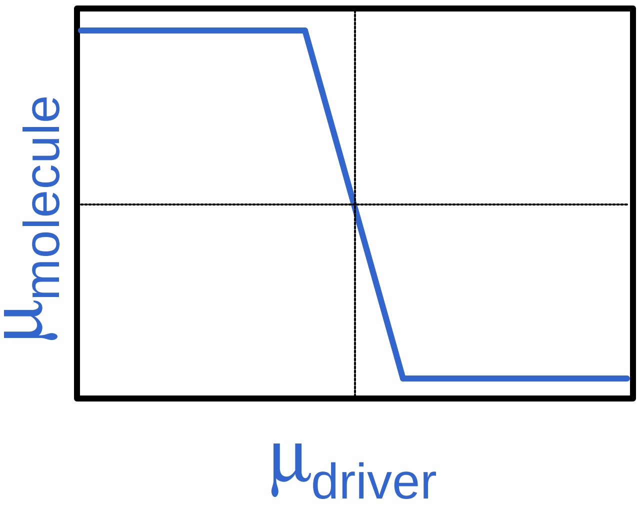
High kink energy

Theory of molecular QCA bistability

The second step:

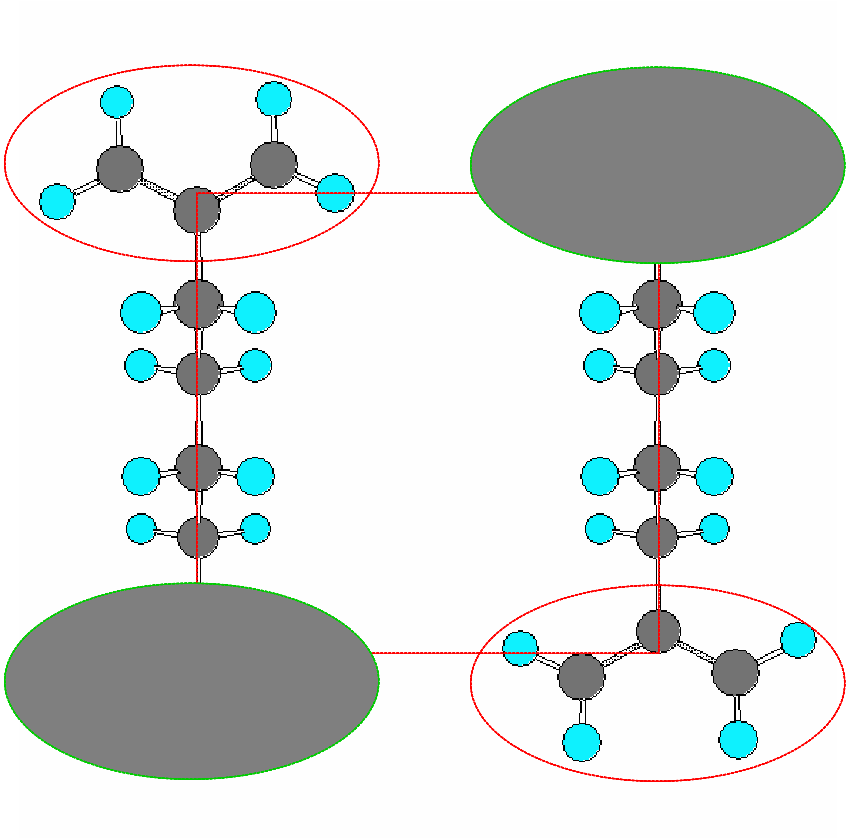
driver charge mimics
nearby molecule





Can one molecule switch another molecule?

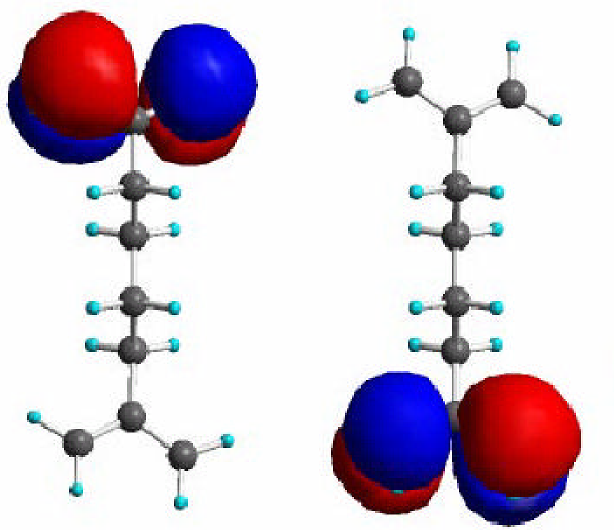
Double molecule



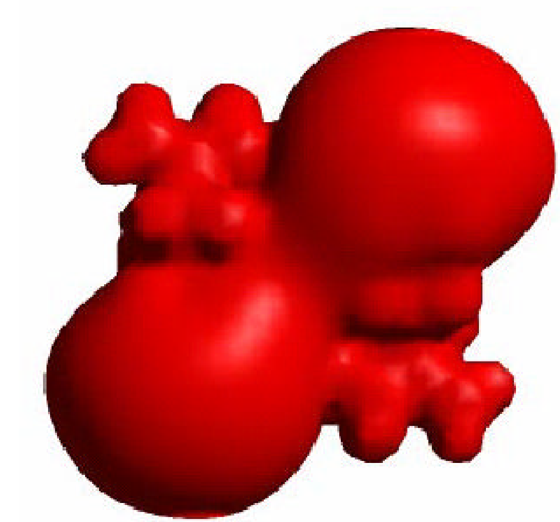
Considered as a single cell, bit is represented by quadrupole moment.

Alternatively: consider it a dipole driving another dipole.

Double molecule

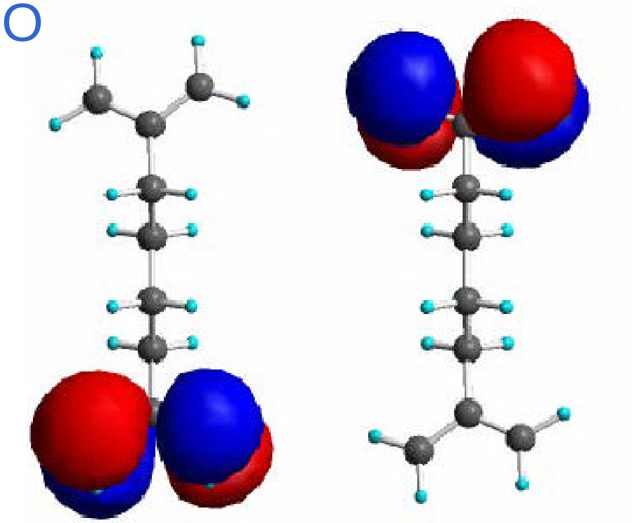


"1"

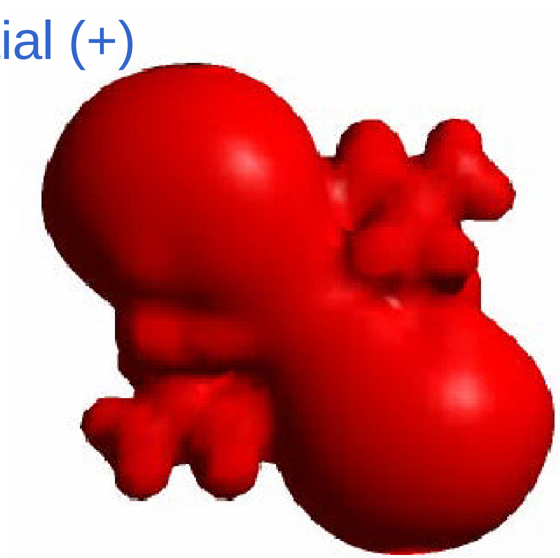


HOMO

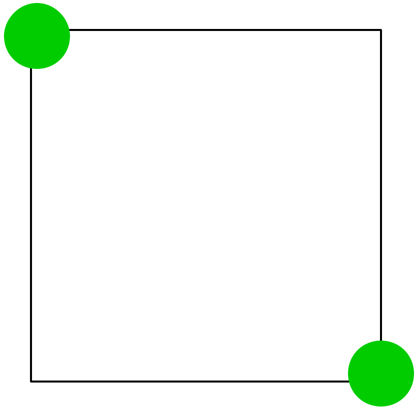
Isopotential (+)

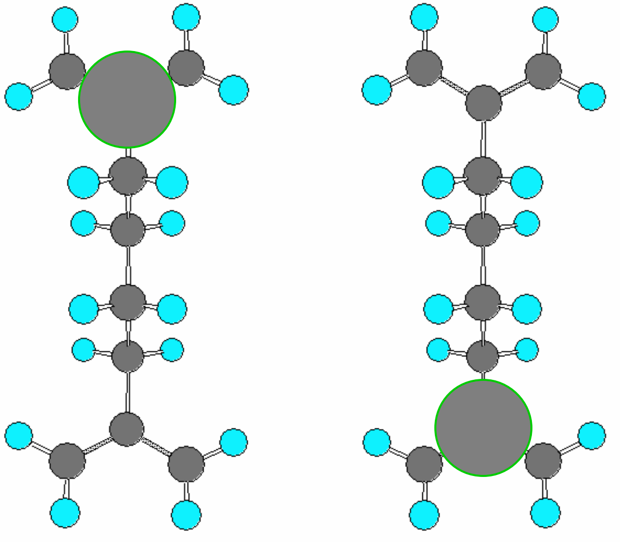


"0"

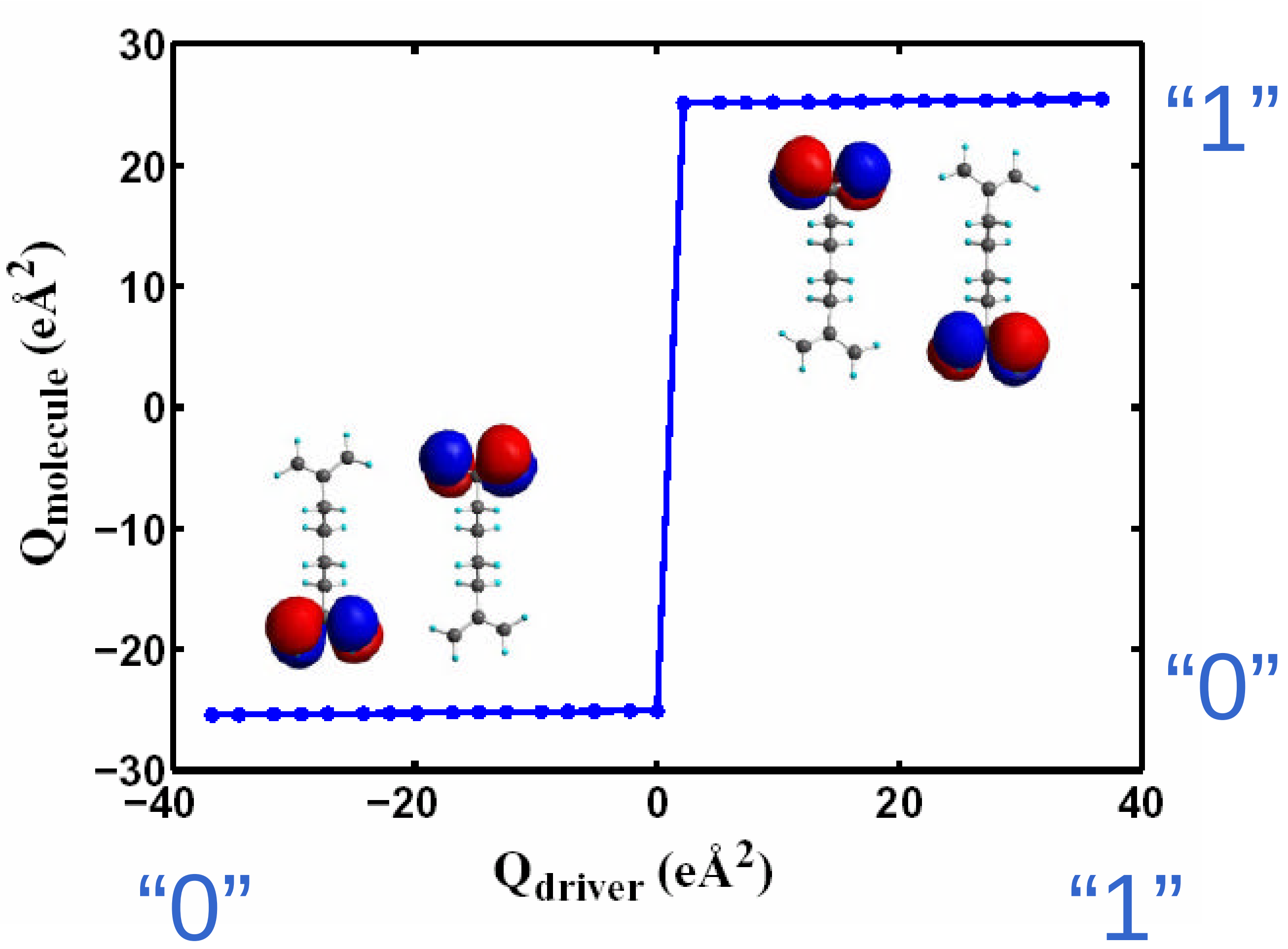


Driver for double molecule

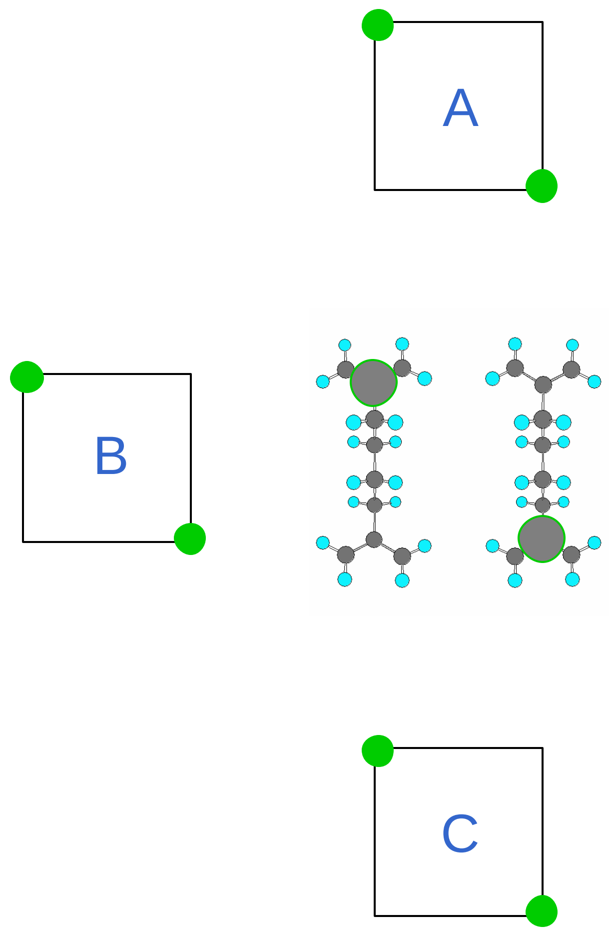




Double molecule cell-cell response



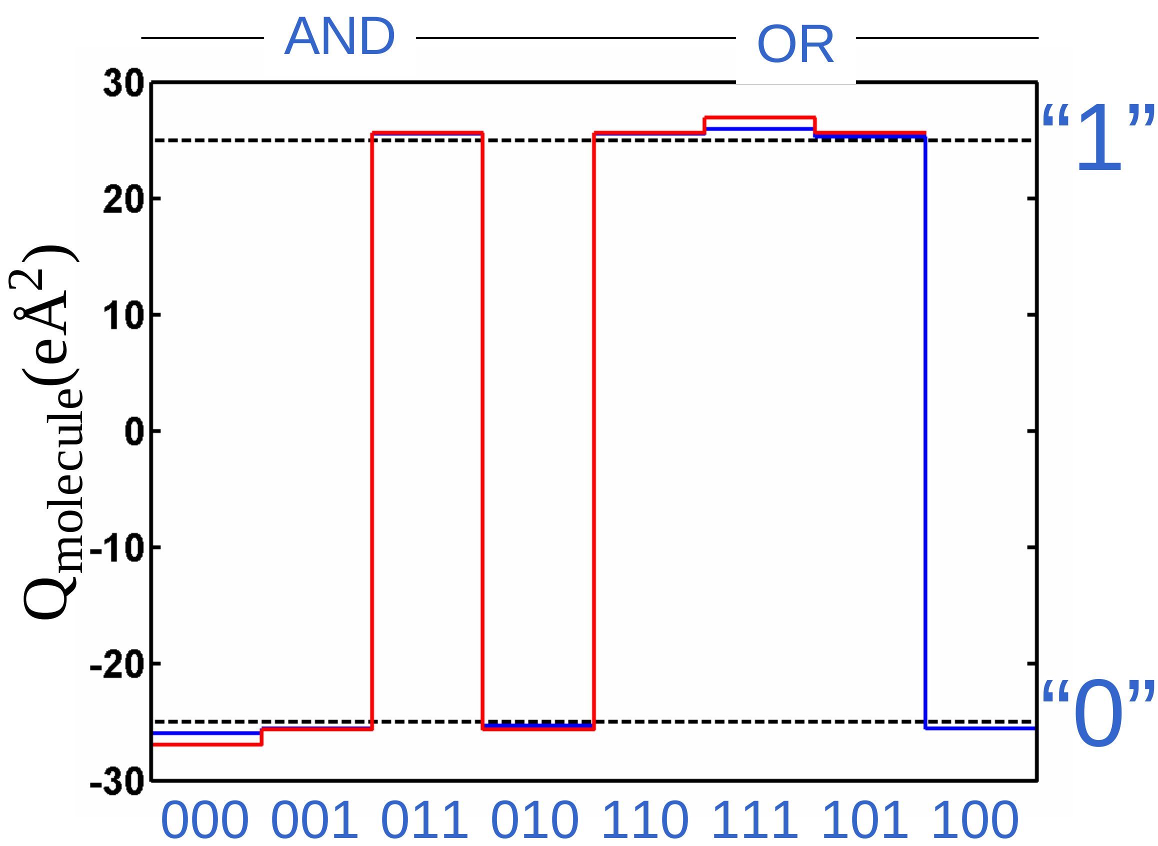
Molecular QCA majority gate



Inputs are quadrupoles mimicking other QCA molecules.

Molecular QCA majority gate

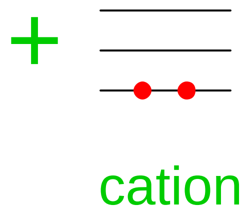
	A	B	C	Output
AND gate	0	0	0	0
AND gate	0	0	1	0
AND gate	0	1	1	1
AND gate	0	1	0	0
OR gate	1	1	0	1
OR gate	1	1	1	1
OR gate	1	0	1	1
OR gate	1	0	0	0

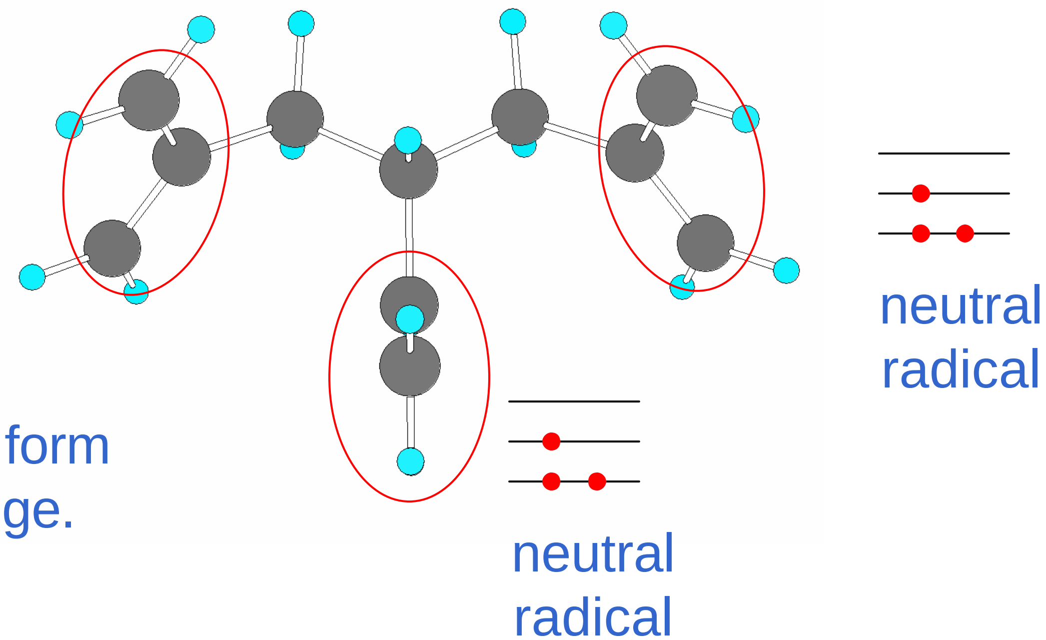


relaxed nuclear positions
frozen nuclear positions

Molecular logic gate.

Molecular 3-dot cell

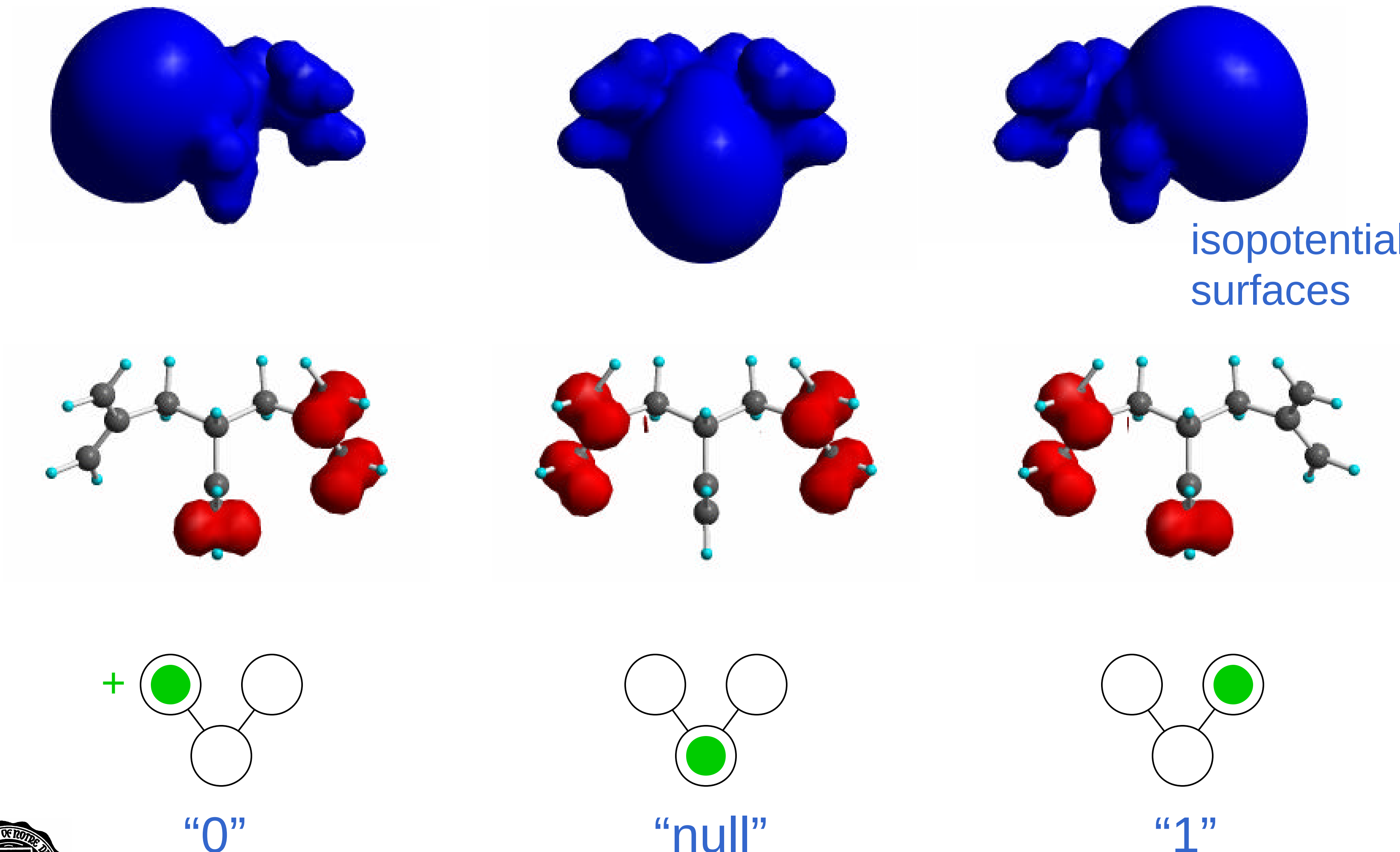




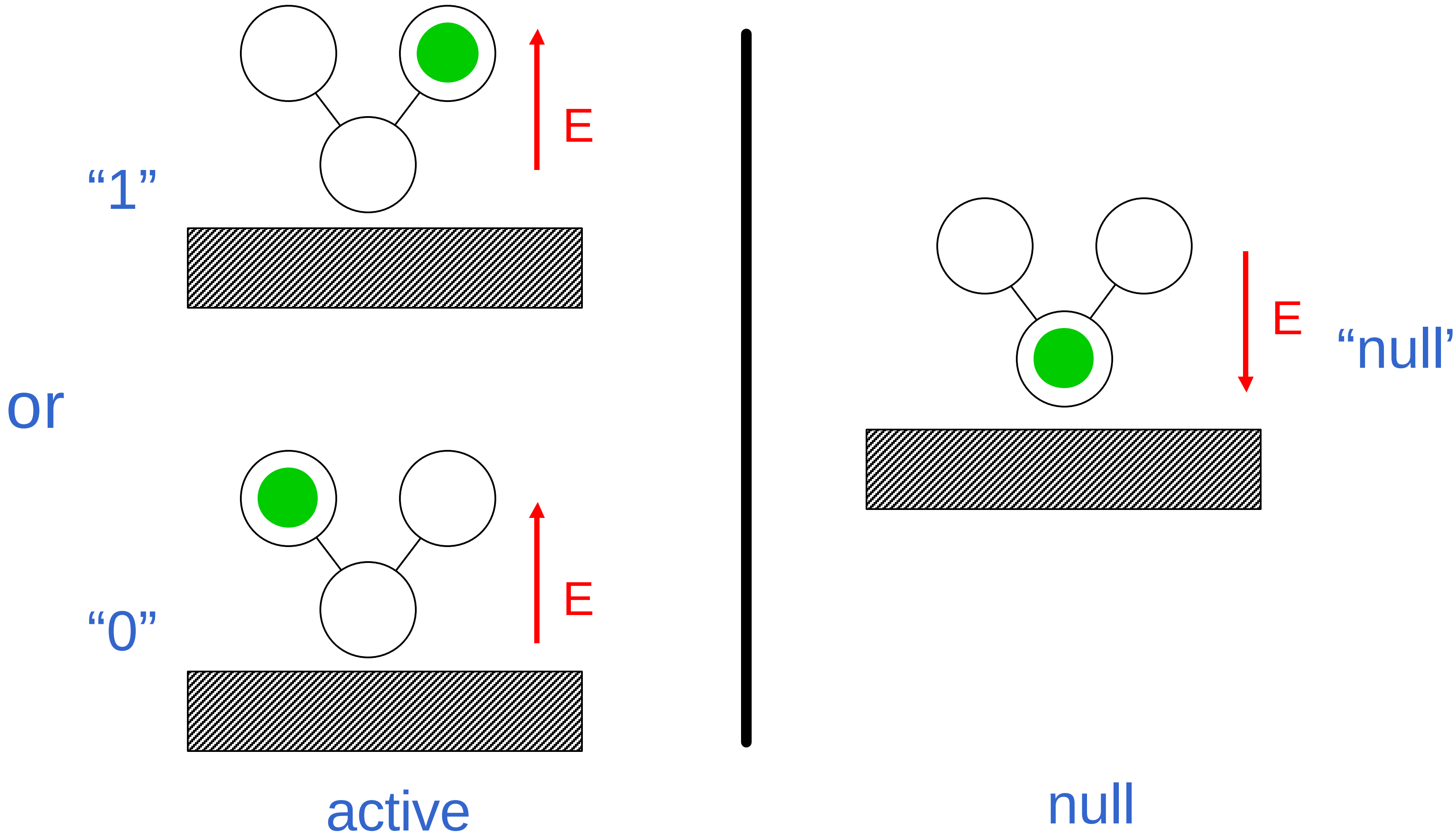
Three allyl groups form "dots" on alkyl bridge.

For the molecular cation, a hole occupies one of three dots.

Charge configuration represents bit



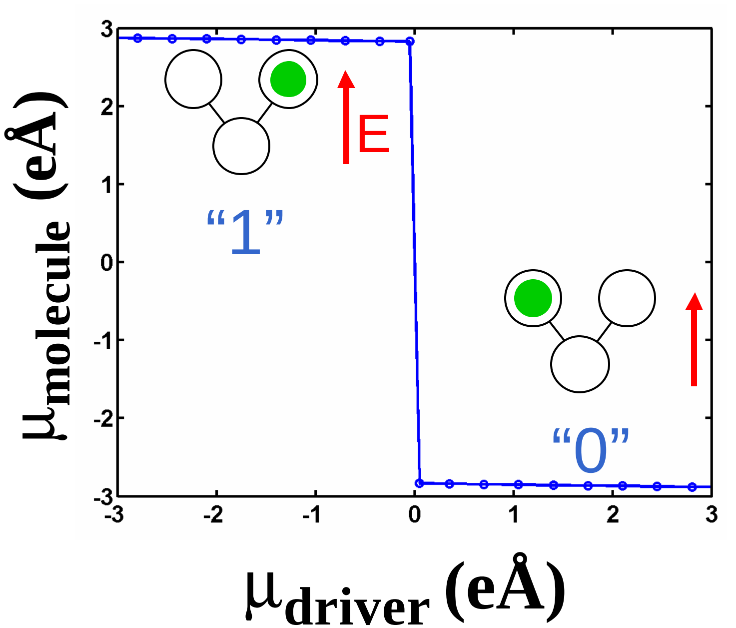
Clocking field

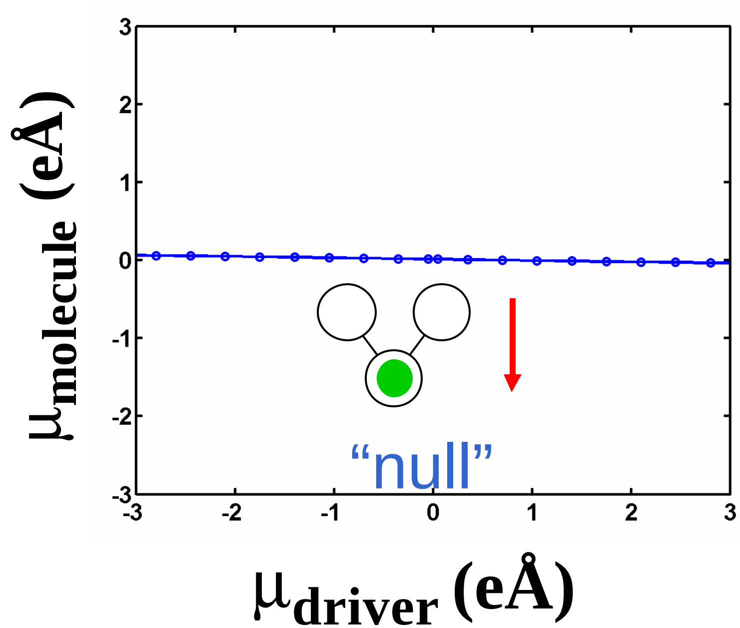


Use local electric field to switch molecule between active and null states.

similar to Likharev & Korotkov – metal tunnel junction single-electron parametron

Clocking field alters response function

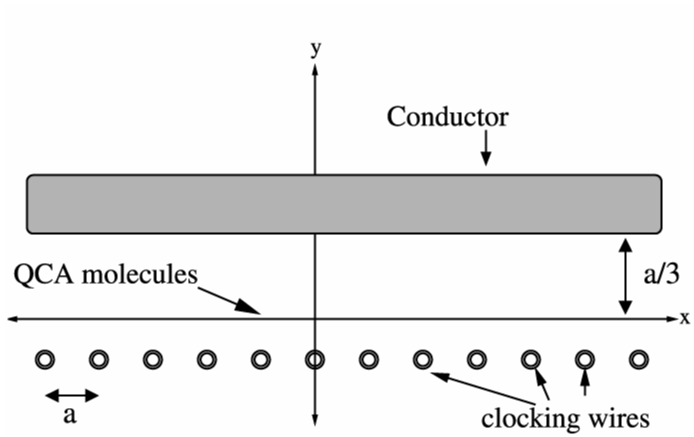




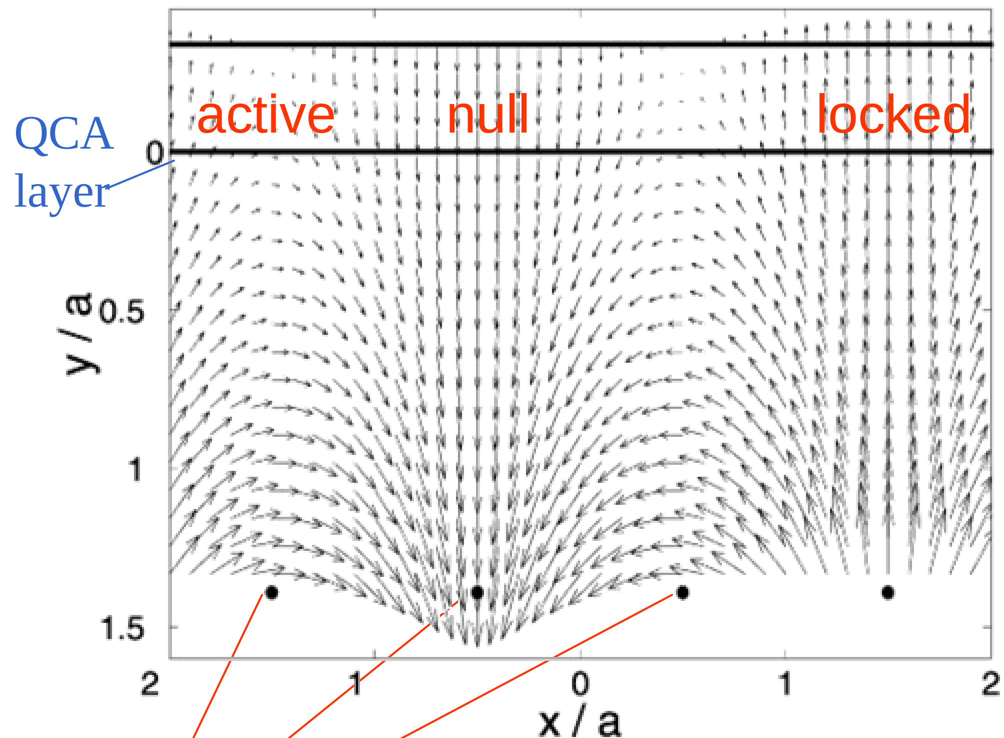
- Clocking field positive (or zero)
- Positive charge in top dots
- Cell is active – nonlinear response to input

- Clocking field negative
- Positive charge in bottom dot
- Cell is inactive – no response to input

Molecular clocking



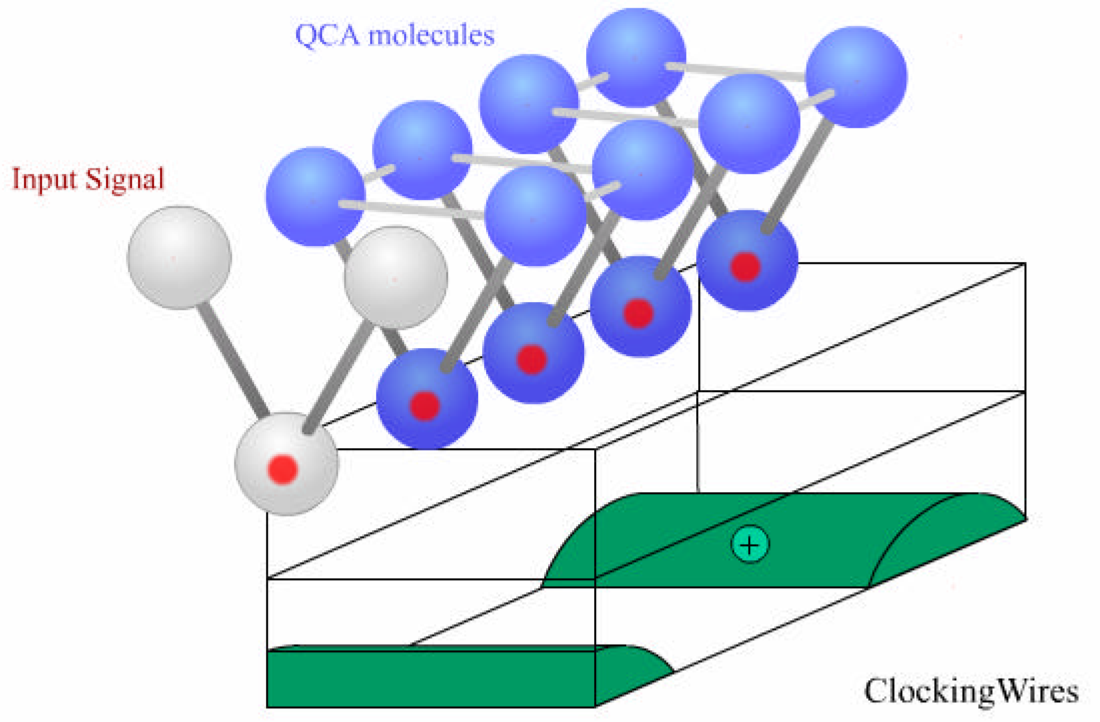
Hennessey and Lent, JVST (2001)



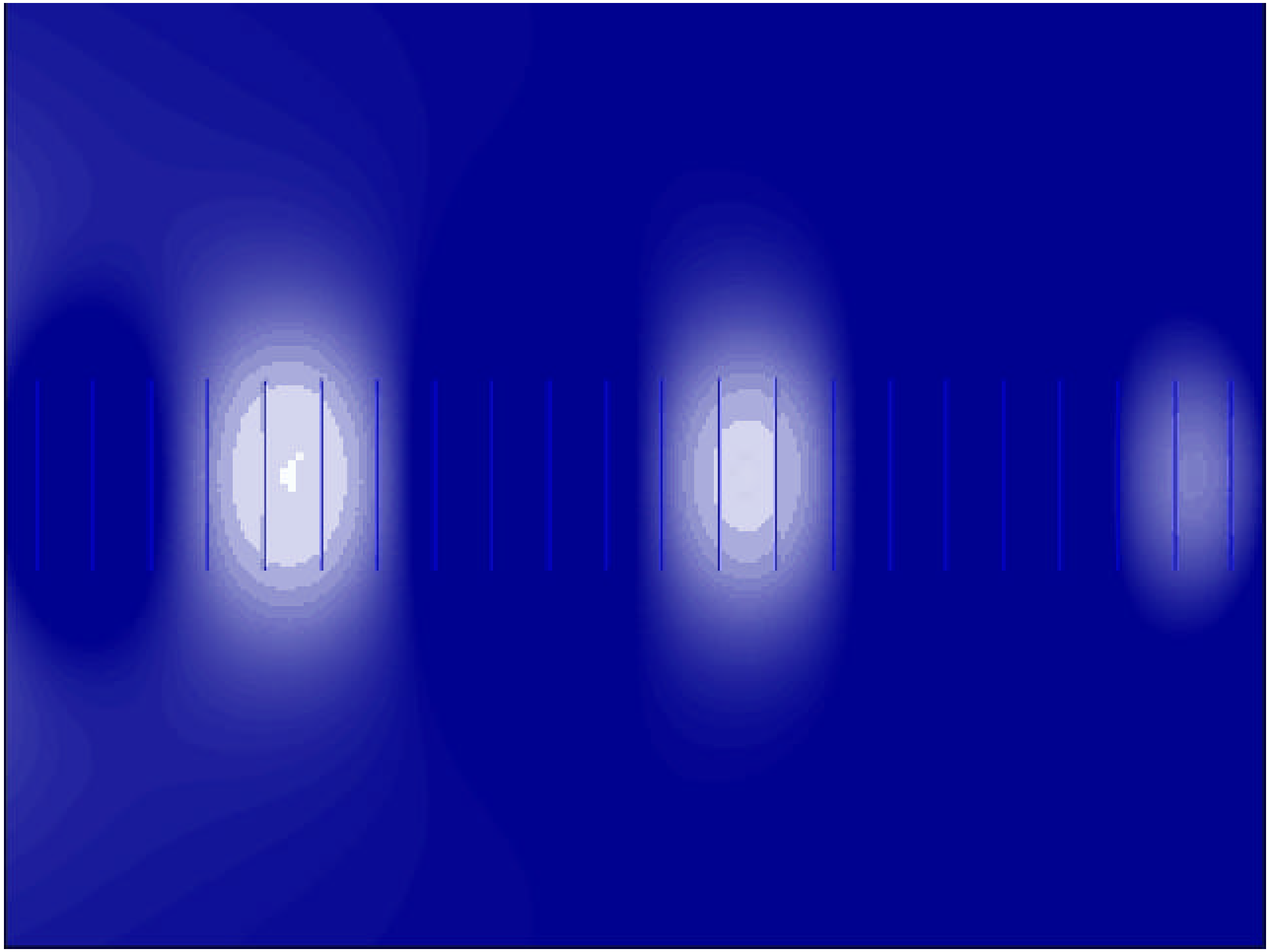
Clocking field is provided by buried wire electrodes (CMOS controlled).

Wire sizes can be 10-100 times larger than molecules.

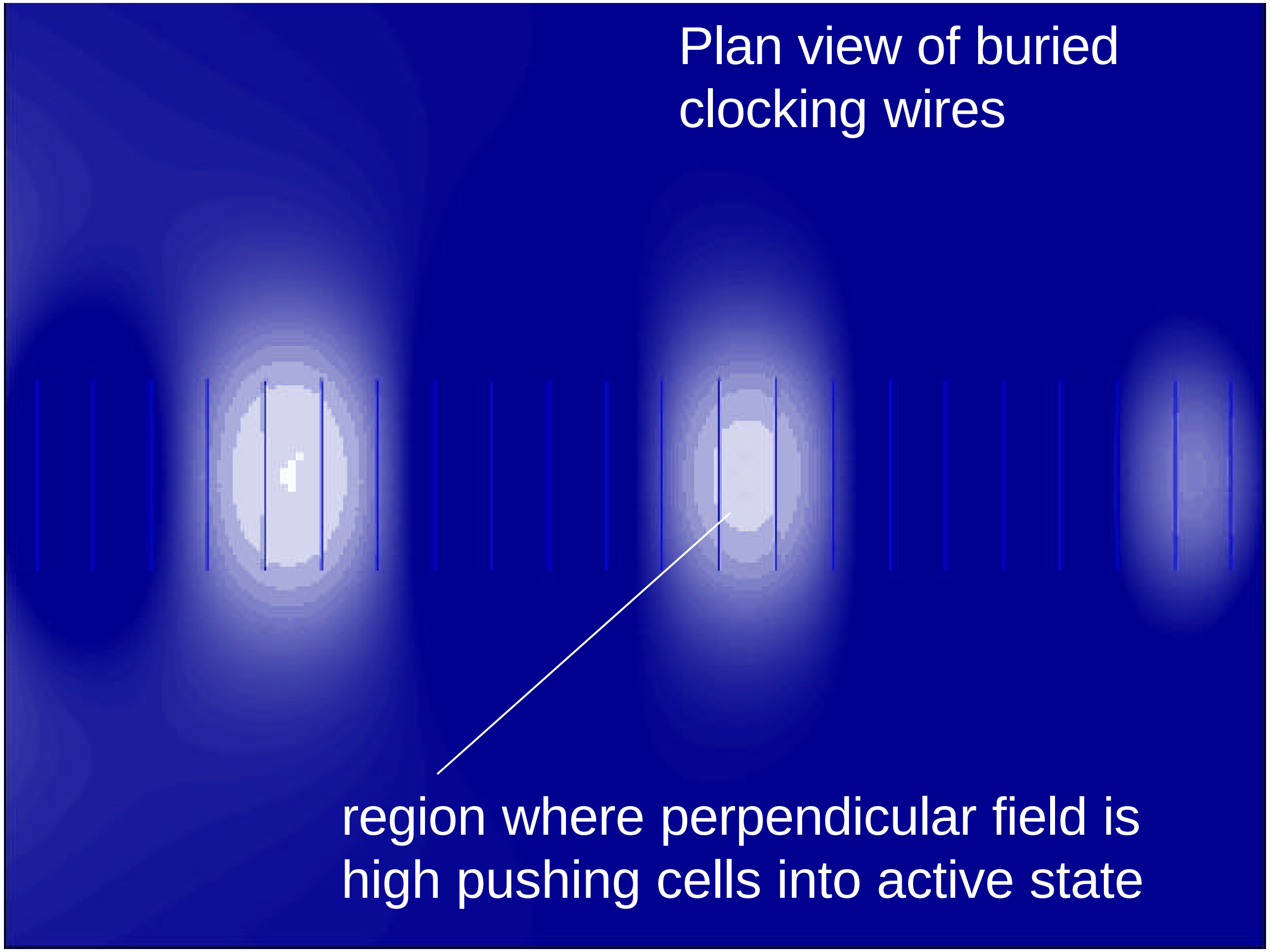
Clocked molecular QCA



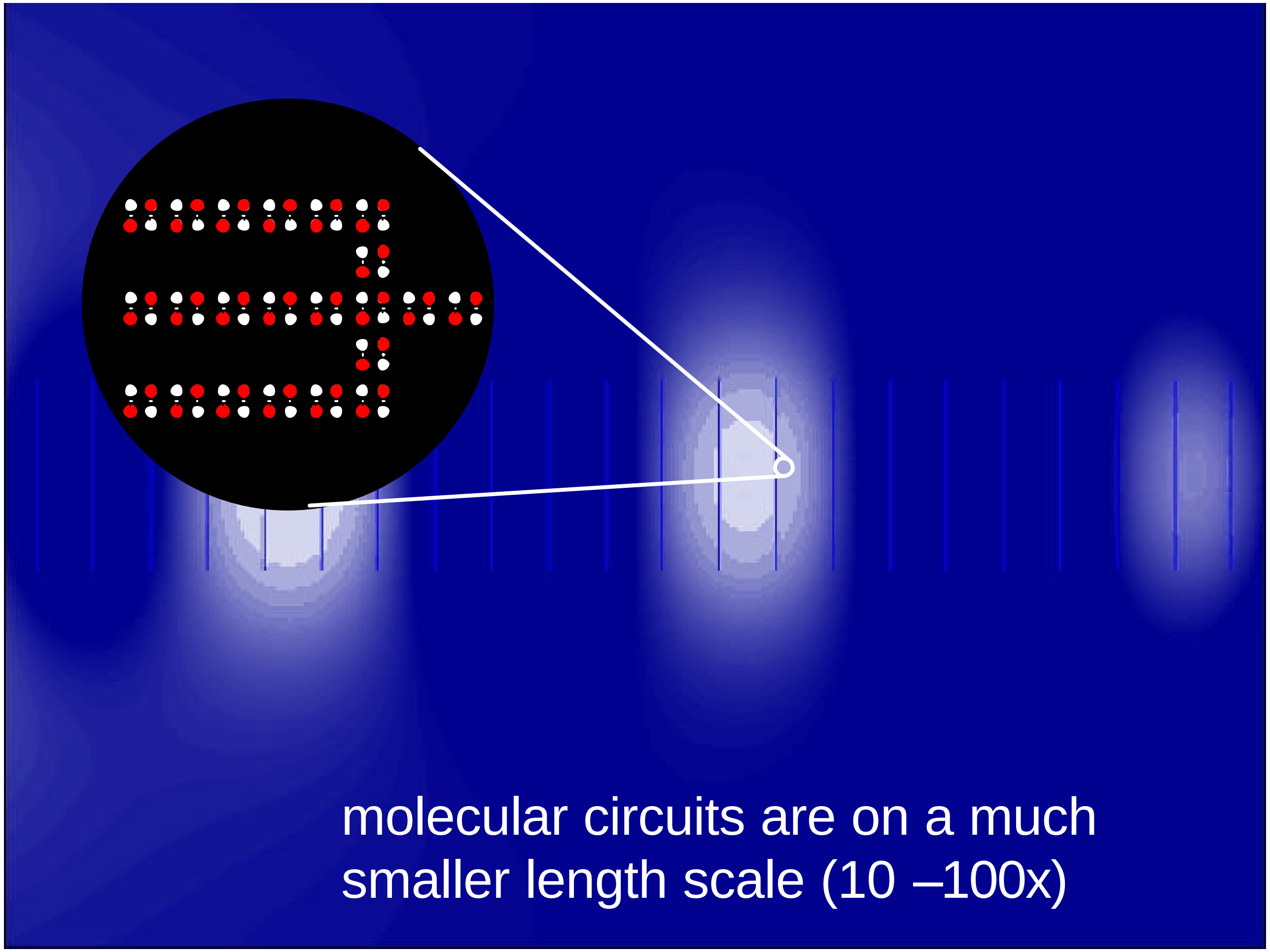
Clocking field: linear motion



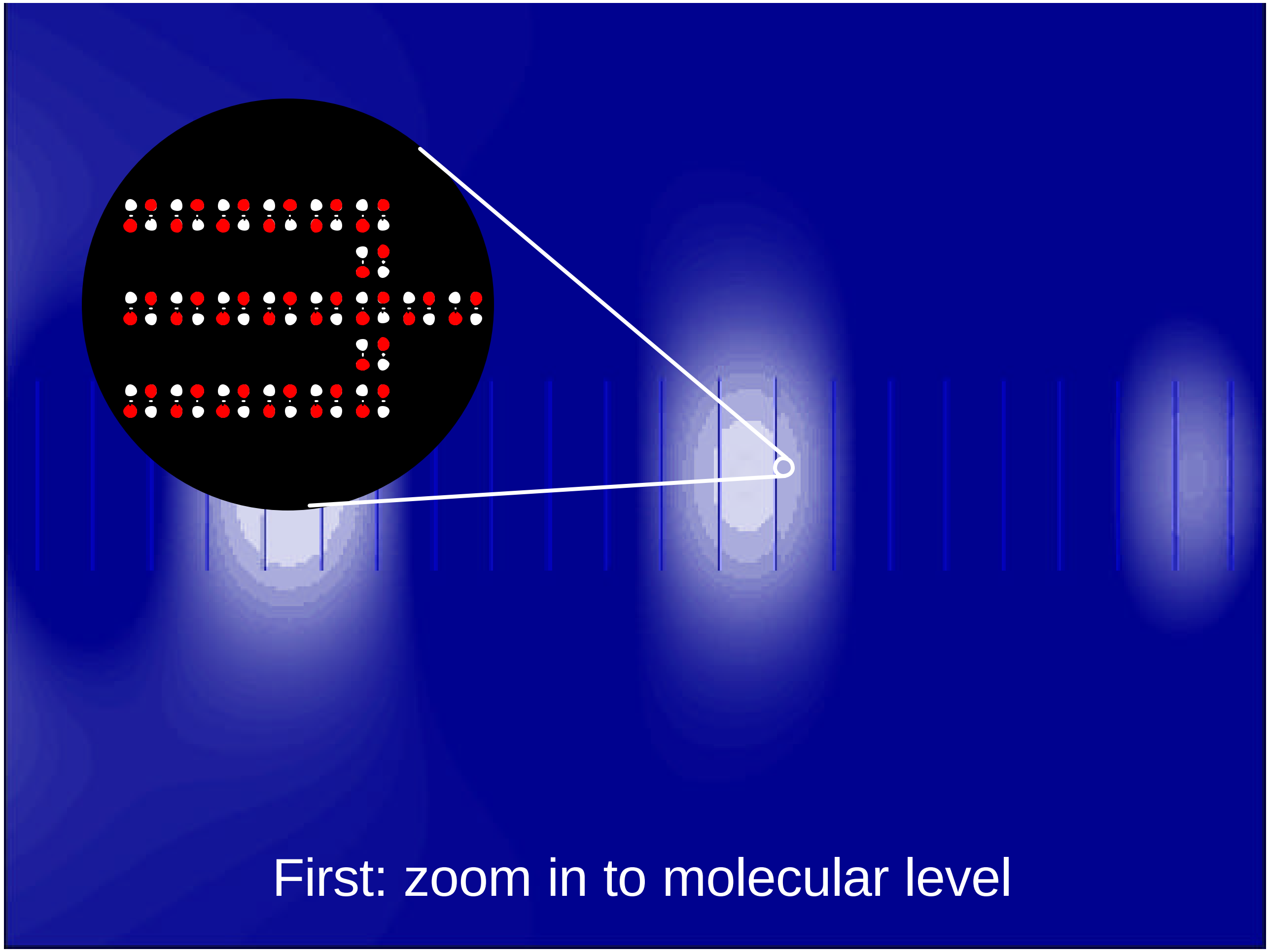
Molecular circuits and clocking wires



Molecular circuits and clocking wires



Molecular circuits and clocking wires



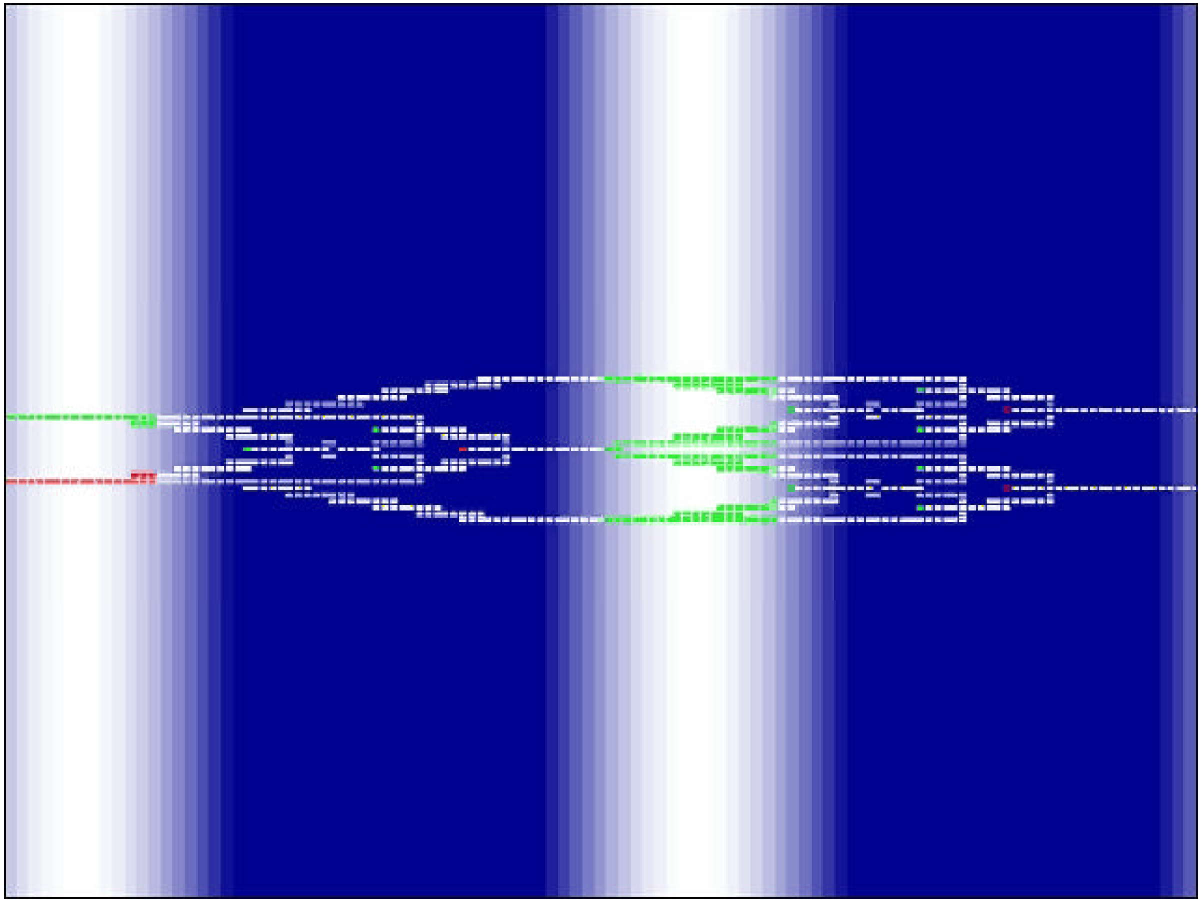
Field-clocking of QCA wire: shift-register

Computational wave: majority gate

Computational wave: adder back-end

XOR Gate

Permuter



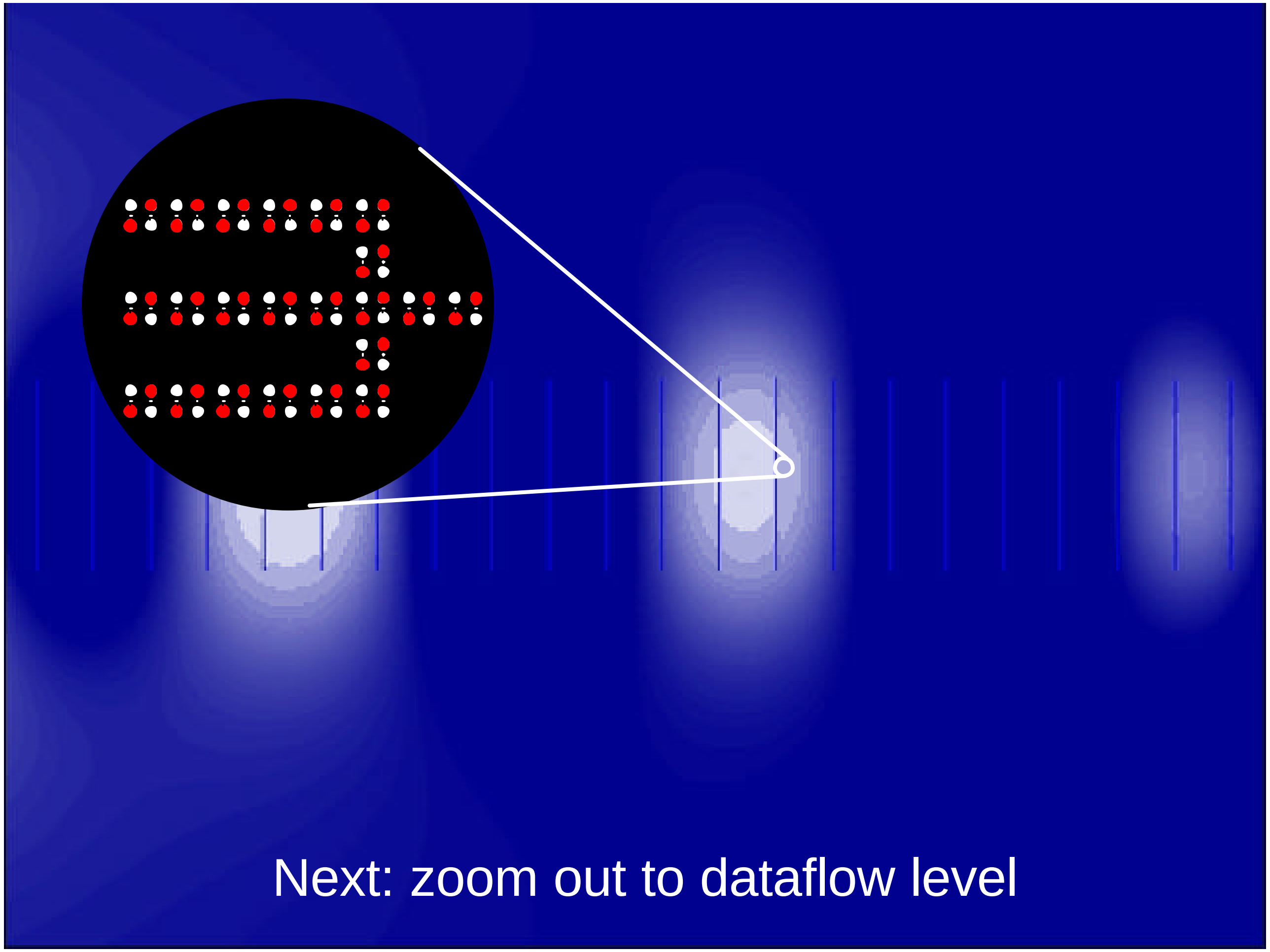
Triple-Wide Wire

Advantages: easier fabrication, works at higher temperatures

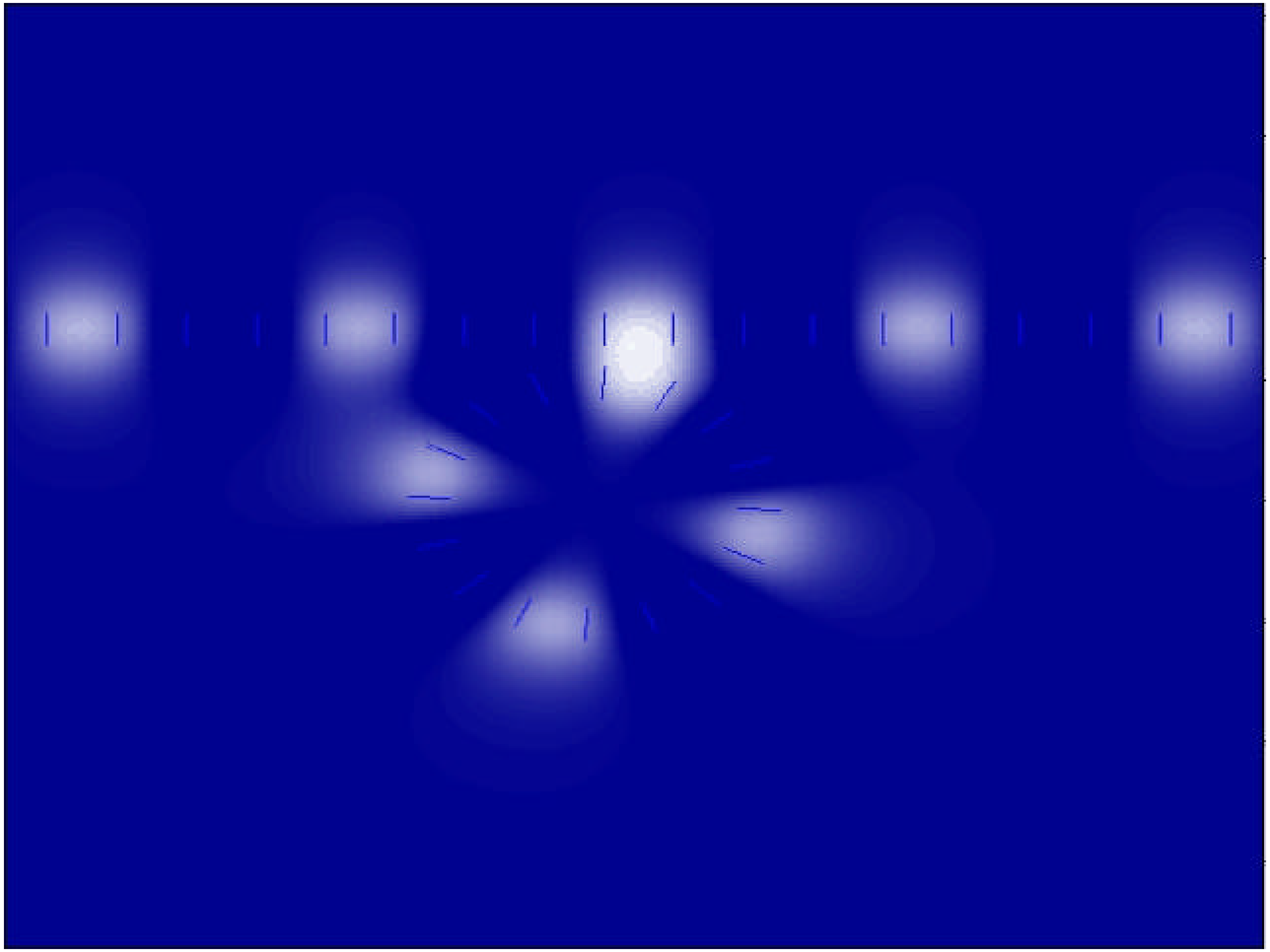
Disordered wire

Redundancy results in defect tolerance.

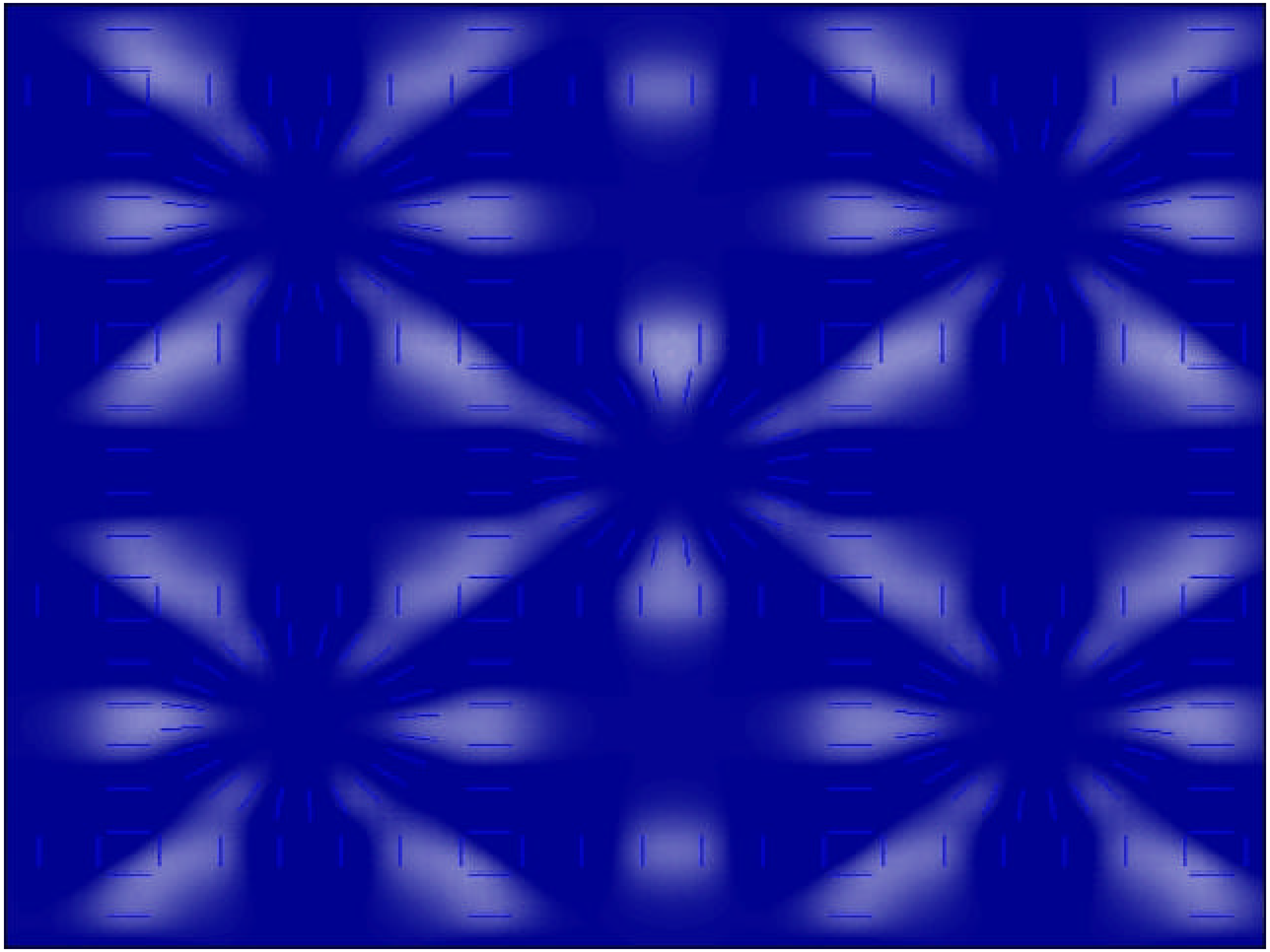
Molecular circuits and clocking wires



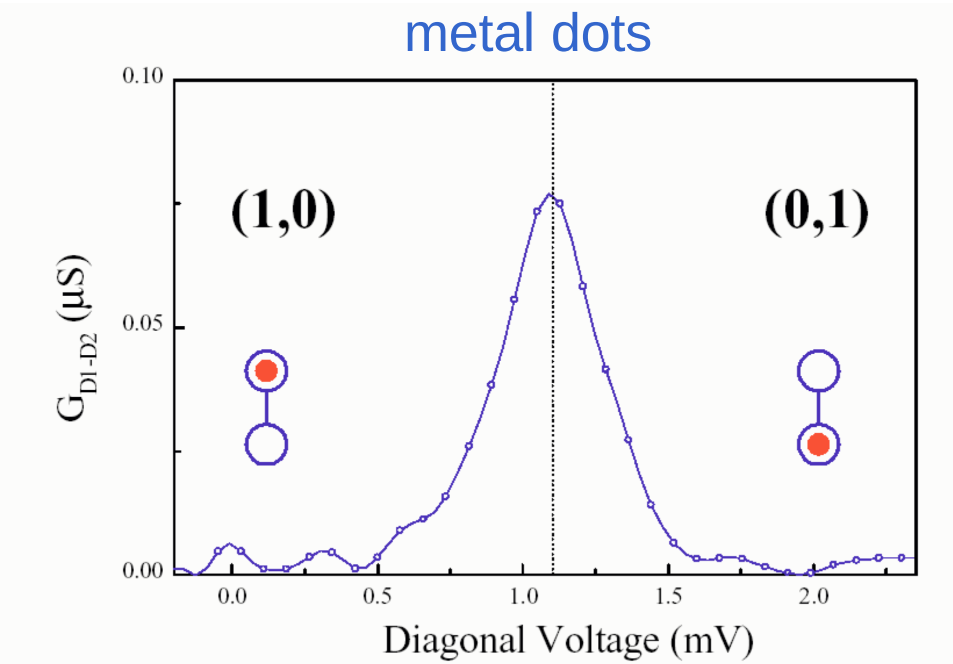
Clocking field: propagation + loop

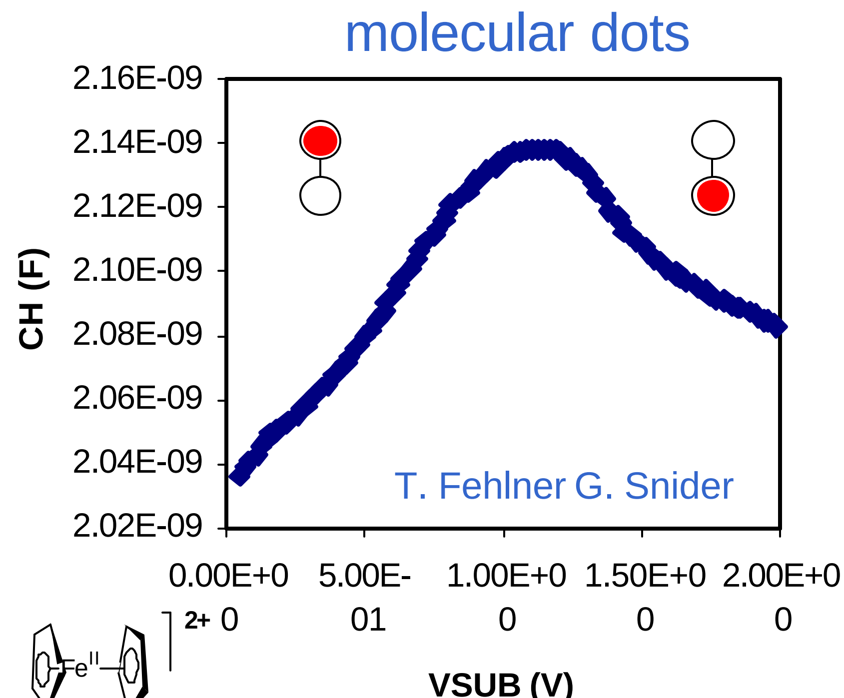


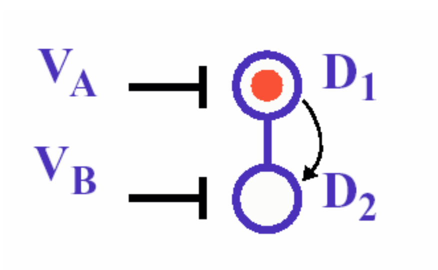
Computational grid with loops

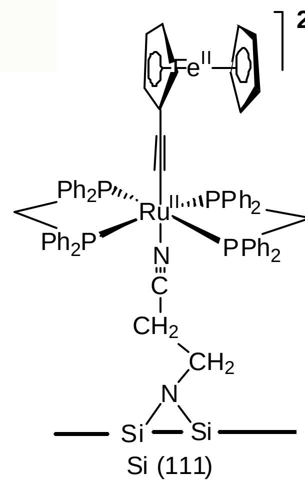


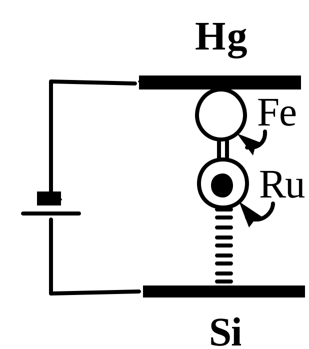
Experiments on molecular double-dot



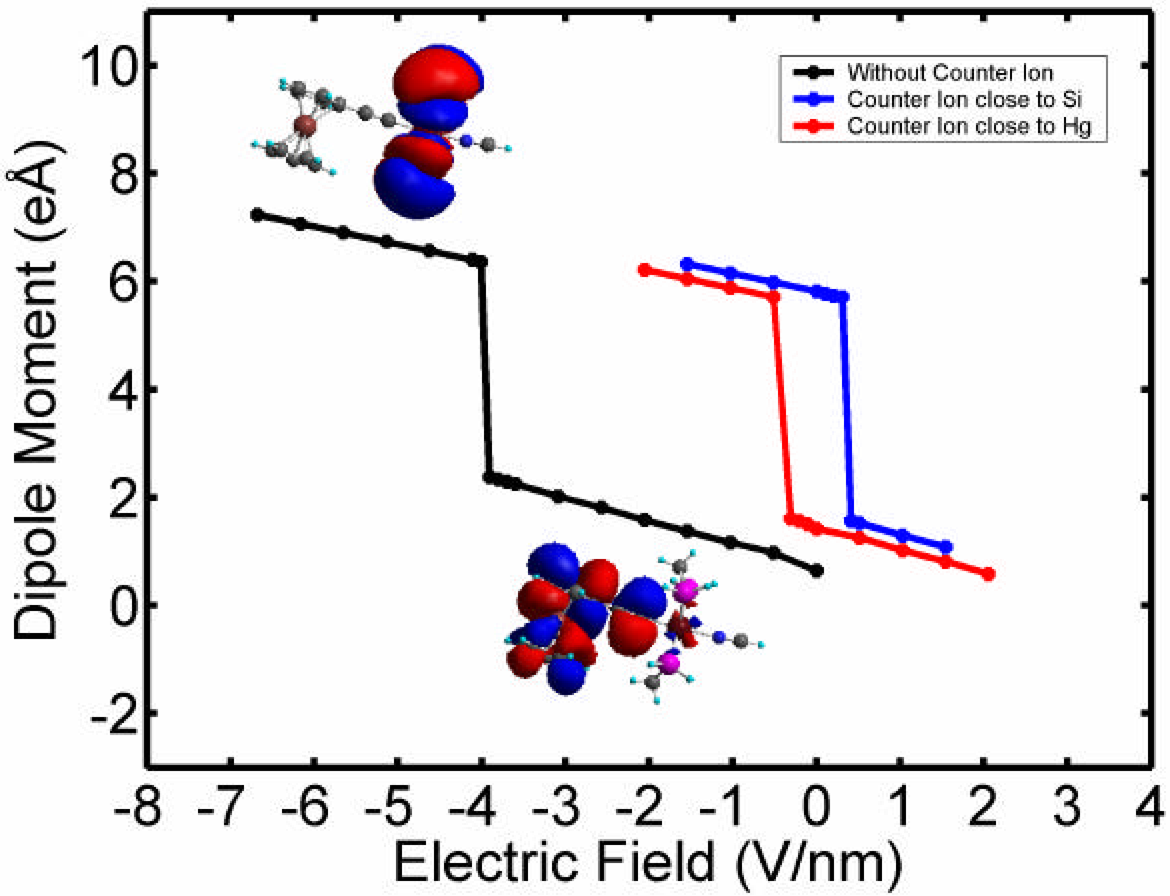








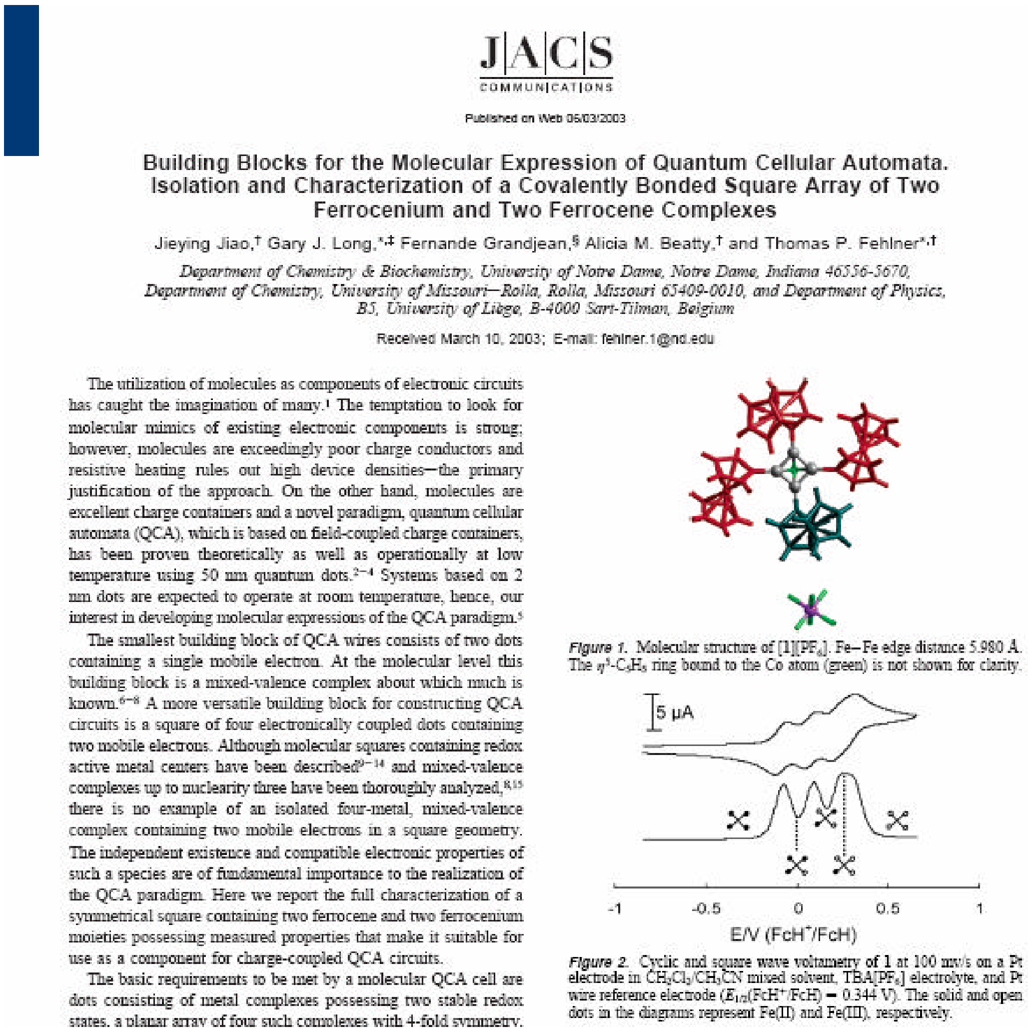
Switching of molecular double-dot



Gaussian 98

Electric field switches biased double dot.

Square 4-dot QCA molecules



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COMMUNICATIONS

Published on Web 05/03/2003

Building Blocks for the Molecular Expression of Quantum Cellular Automata. Isolation and Characterization of a Covalently Bonded Square Array of Two Ferrocenium and Two Ferrocene Complexes

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The utilization of molecules as components of electronic circuits has caught the imagination of many.[1] The temptation to look for molecular mimics of existing electronic components is strong; however, molecules are exceedingly poor charge conductors and resistive heating rules out high device densities—the primary justification of the approach. On the other hand, molecules are excellent charge containers and a novel paradigm, quantum cellular automata (QCA), which is based on field-coupled charge containers, has been proven theoretically as well as operationally at low temperature using 50 nm quantum dots.[2−4] Systems based on 2 nm dots are expected to operate at room temperature, hence, our interest in developing molecular expressions of the QCA paradigm.[5]

The smallest building block of QCA wires consists of two dots containing a single mobile electron. At the molecular level this building block is a mixed-valence complex about which much is known.[6−8] A more versatile building block for constructing QCA circuits is a square of four electronically coupled dots containing two mobile electrons. Although molecular squares containing redox active metal centers have been described[9−14] and mixed-valence complexes up to nuclearity three have been thoroughly analyzed,[8,15] there is no example of an isolated four-metal, mixed-valence complex containing two mobile electrons in a square geometry. The independent existence and compatible electronic properties of such a species are of fundamental importance to the realization of the QCA paradigm. Here we report the full characterization of a symmetrical square containing two ferrocene and two ferrocenium moieties possessing measured properties that make it suitable for use as a component for charge-coupled QCA circuits.

The basic requirements to be met by a molecular QCA cell are dots consisting of metal complexes possessing two stable redox states, a planar array of four such complexes with 4-fold symmetry.

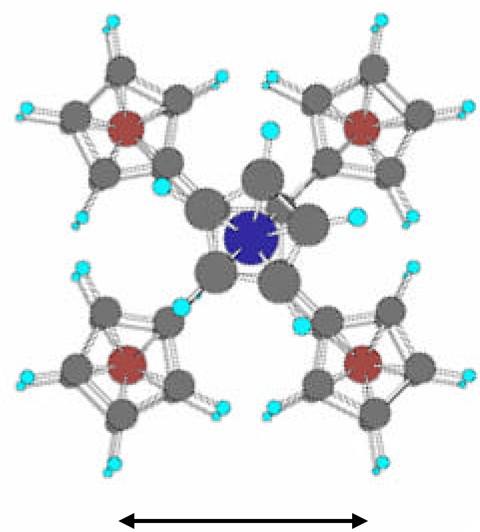
Figure 1. Molecular structure of [1][PF_6]. Fe−Fe edge distance 5.980 Å. The η^5-C_5H_5 ring bound to the Co atom (green) is not shown for clarity.

5 µA

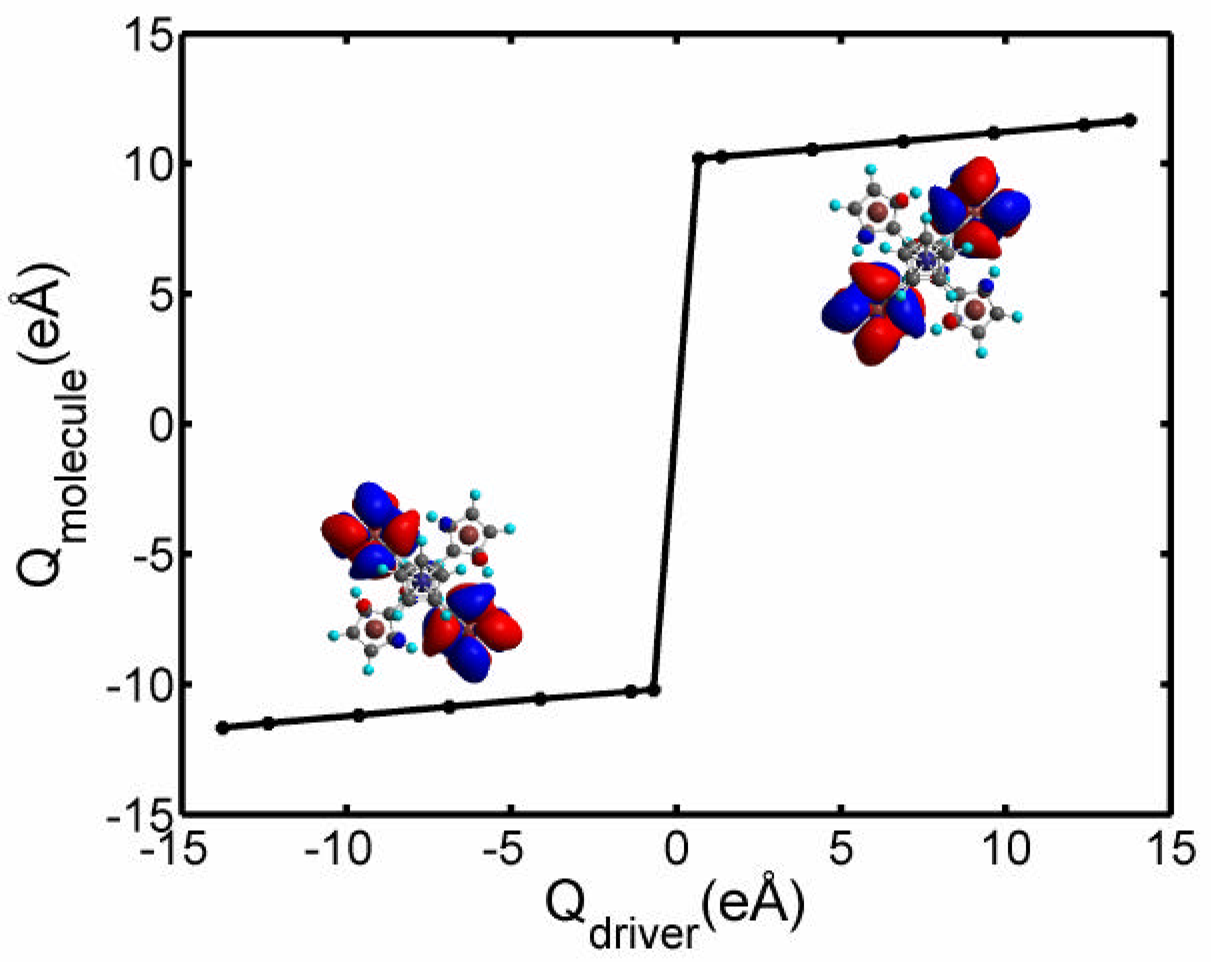
-1 -0.5 0 0.5 1

E/V (FcH^+/FcH)

Figure 2. Cyclic and square wave voltametry of **1** at 100 mv/s on a Pt electrode in CH_2Cl_2/CH_3CN mixed solvent, TBA[PF_6] electrolyte, and Pt wire reference electrode ($E_{1/2}$(FcH^+/FcH) = 0.344 V). The solid and open dots in the diagrams represent Fe(II) and Fe(III), respectively.



Calculation of driven 4-dot molecular cell

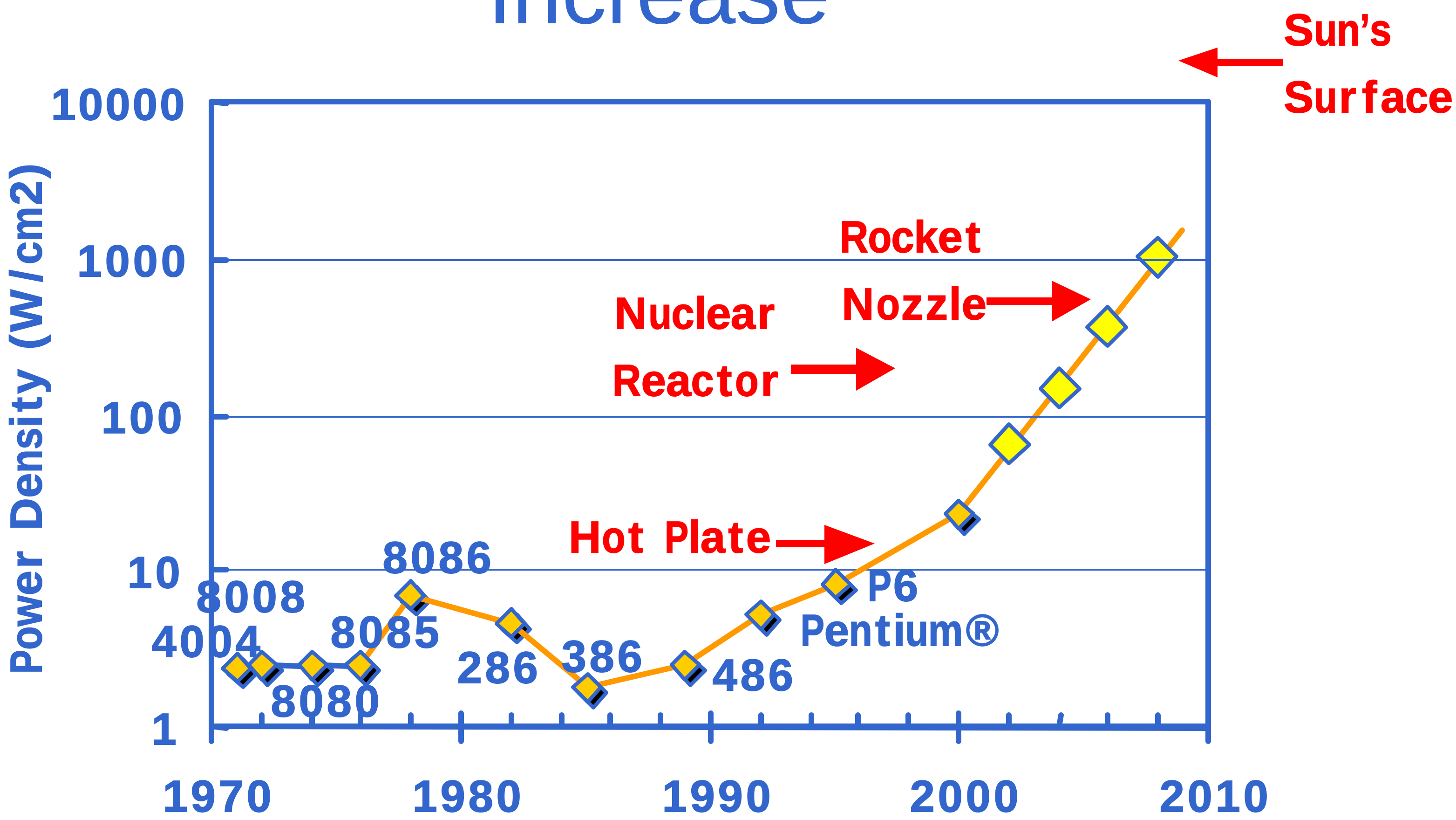


Quadrupole driver switches 4-dot cell.

Outline of presentation

- QCA overview
- Metal-dot QCA devices
- Molecular QCA ➔ architectures
- Power dissipation - fundamental issues (*Lent contra Zhirnov*)
  - History and fundamental analysis
  - QCA as concrete example
  - Double wells and limits

Power Density will Increase



Power densities too high to keep junctions at low temps

Slide author: Mary Jane Irwin, Penn State University

Source: Borkar & De, Intelâ

Physics of computation

- Is there a fundamental lower limit on energy dissipation per bit?
- What is the distinguishability criterion in thermal environment?
- What limits switching speed?
- Is there a fundamental limit on size of bit?
- Are there other, practical limitations?

Landauer

Question: Is there a fundamental lower limit to the amount of energy that must be dissipated to compute a bit?

Answer: No.

Question: Isn't it $k_B T \ln(2)$?

Answer: No, it isn't.

There is no fundamental lower limit on the amount of energy that must be dissipated to compute a bit.
Landauer (1961)

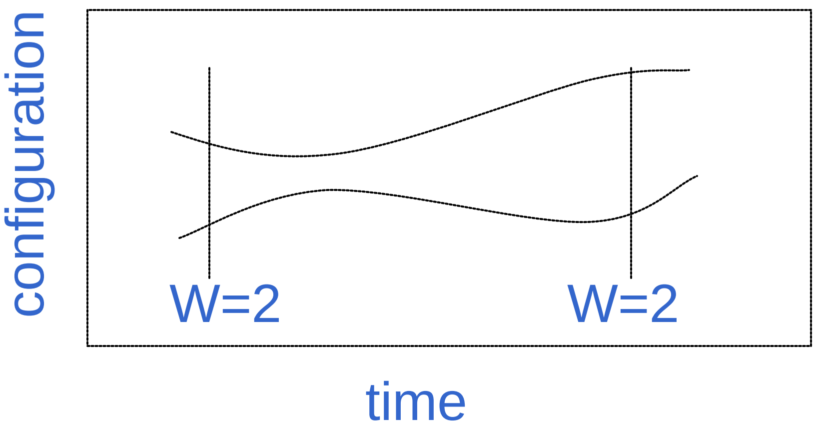
Minimum energy for computation

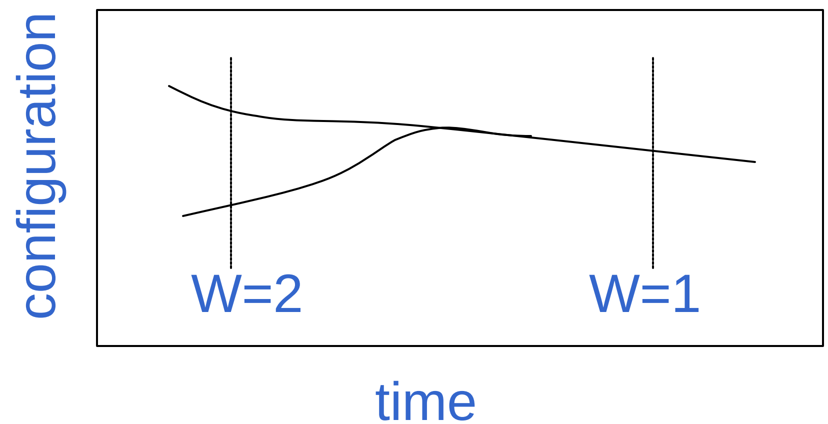
- Maxwell's demon (1875) – by first measuring states, could perform reversible processes to lower entropy
- Szilard (1929), Brillouin (1962): *measurement* causes $k_B T \ln(2)$ dissipation per bit.
- Landauer (1961,1970): only *erasure* of information causes dissipation of $k_B T \ln(2)$ per bit.
- Bennett (1982): full computation can be done without erasure.

logical reversibility ⇔ physical reversibility

See Timler & Lent "Maxwell's demon and quantum-dot cellular automata" JAP (2003).

Physical reversibility ⇔ logical reversibility

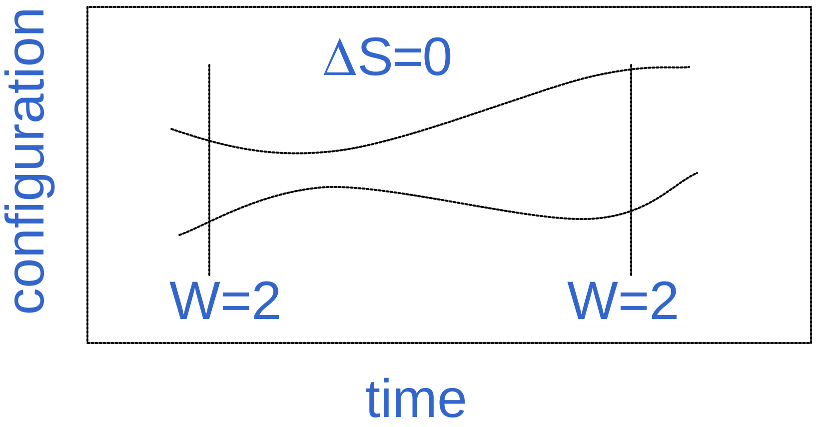


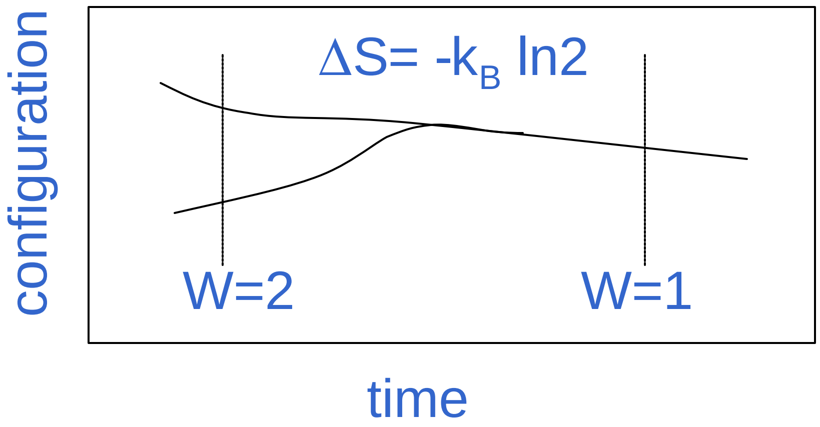


Entropy $S=k_B \ln(W)$

Boltzmann's tombstone

Physical reversibility ⇔ logical reversibility





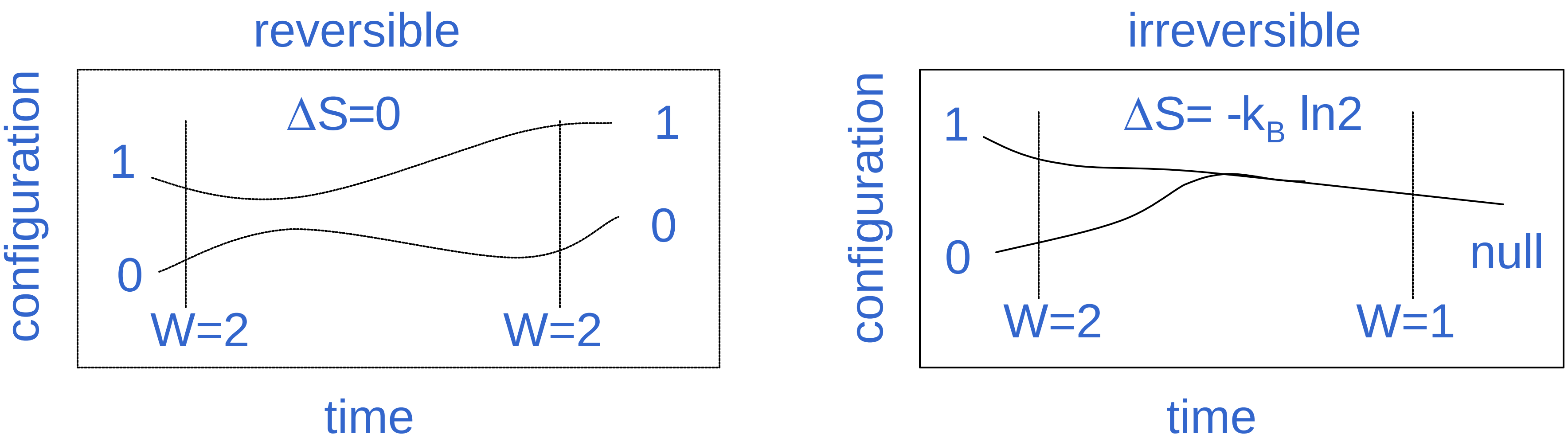
Entropy $S=k_B \ln(W)$
Total $\Delta S > 0$. (2nd Law of Thermodynamics)

Reduction of entropy in system must be accompanied by transfer of entropy elsewhere.

Either:

1) information transfers to another system, or
2) free energy $\Delta F = T\Delta S = k_B T \ln(2)$ transfers to environment.

Physical reversibility ⇔ logical reversibility



Logical reversibility means that inputs are logically determined by outputs.

Logically reversible computation *can* be implemented by physically reversible processes.

Logically irreversible computation cannot be implemented by physically reversible process. Example: erasure.

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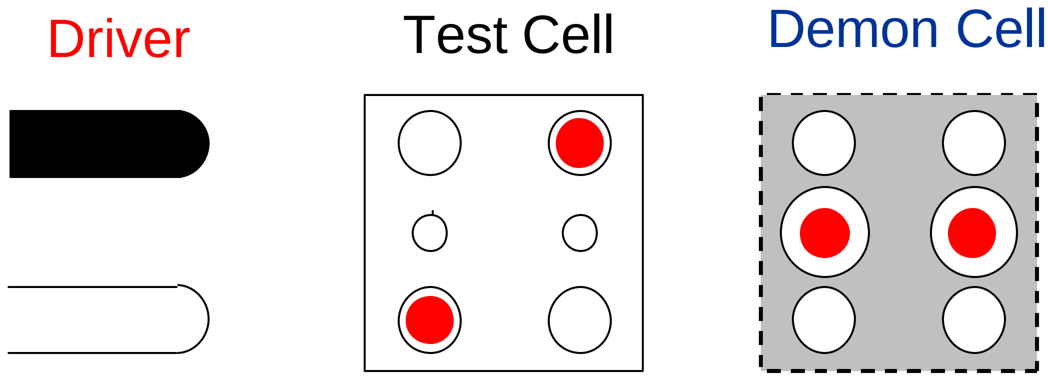
  - Double wells and limits

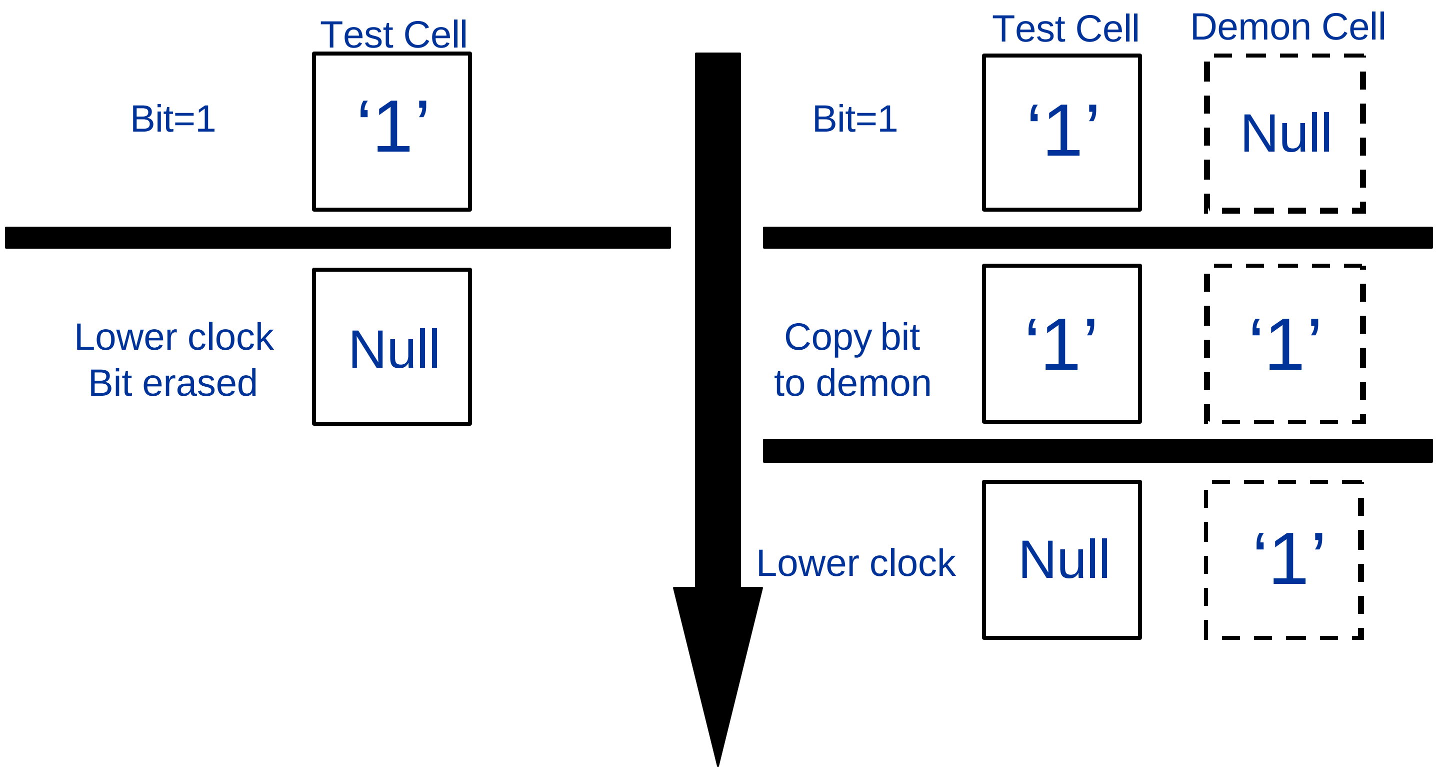
QCA system considered



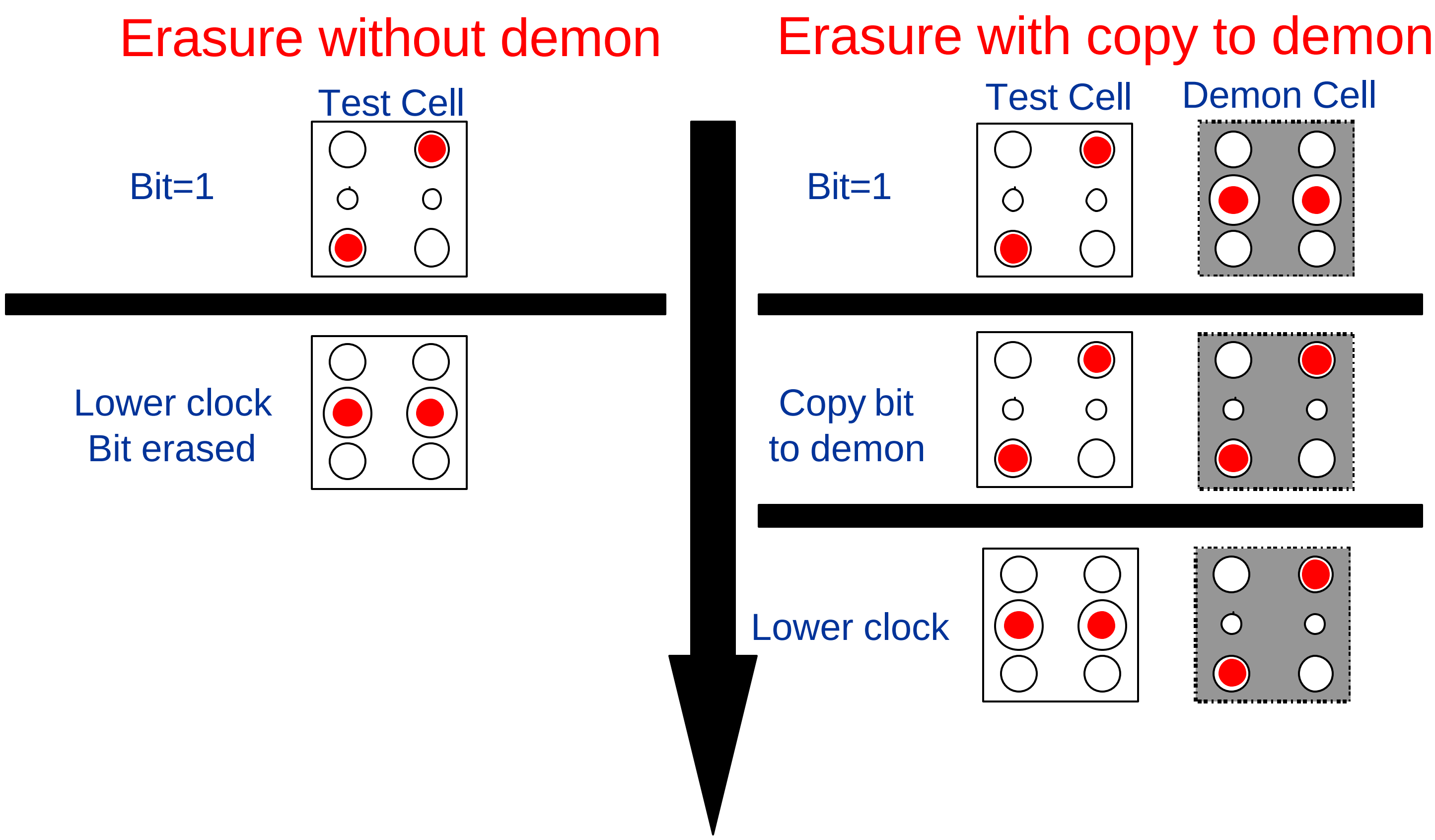
- Driver- provides input bit
- Demon cell (after Maxwell's Demon)- measures and copies the polarization of the test cell

Bit erasure

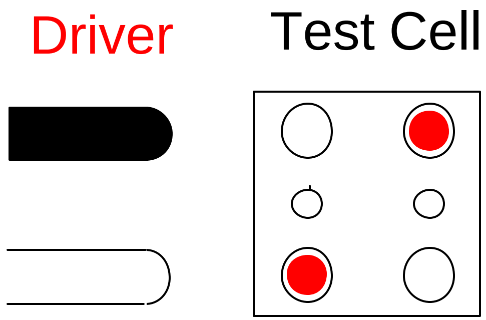
Erasure without demon | **Erasure with copy to demon**

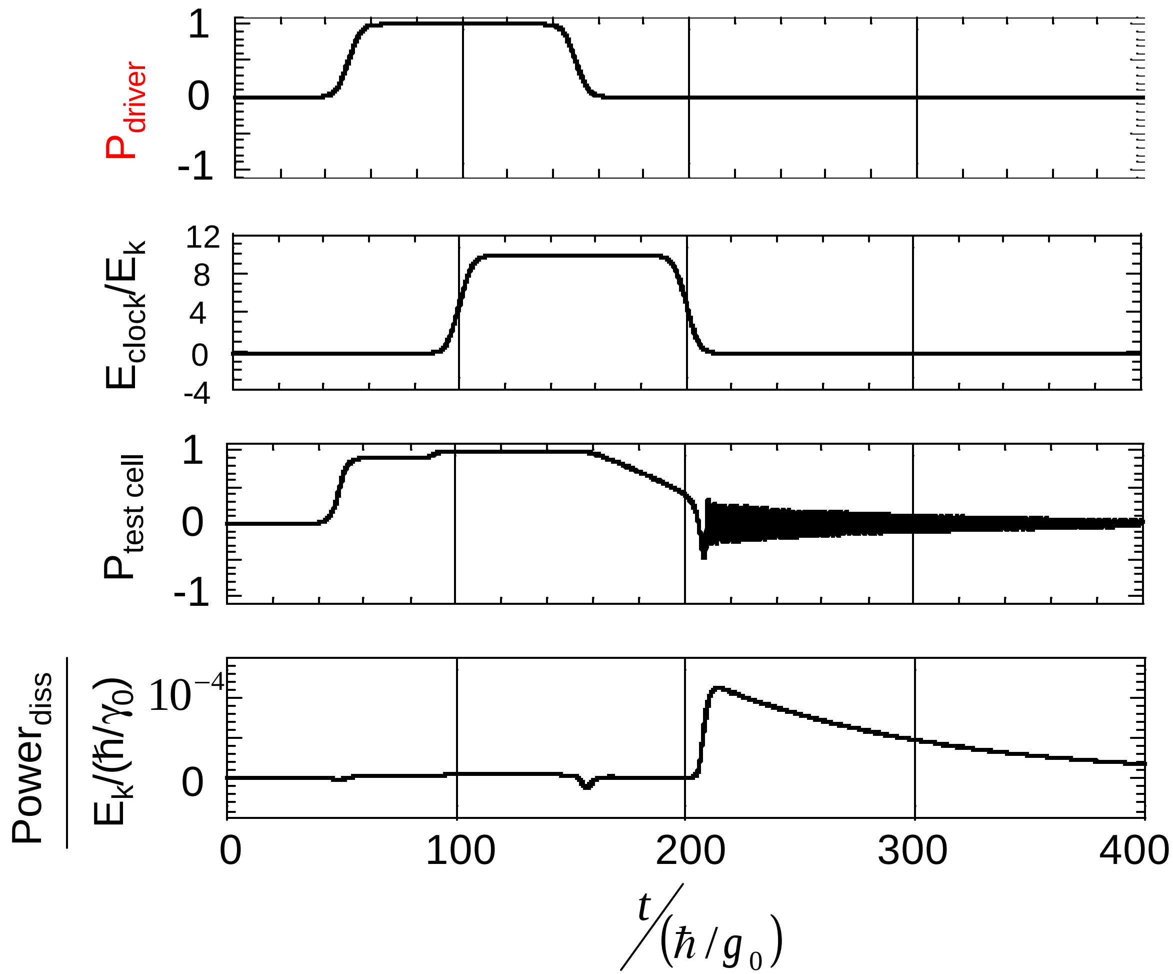


Bit erasure in a QCA cell



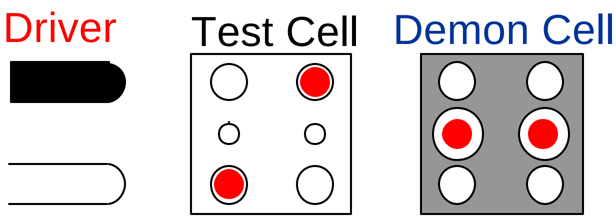
Erasure dynamics without demon cell

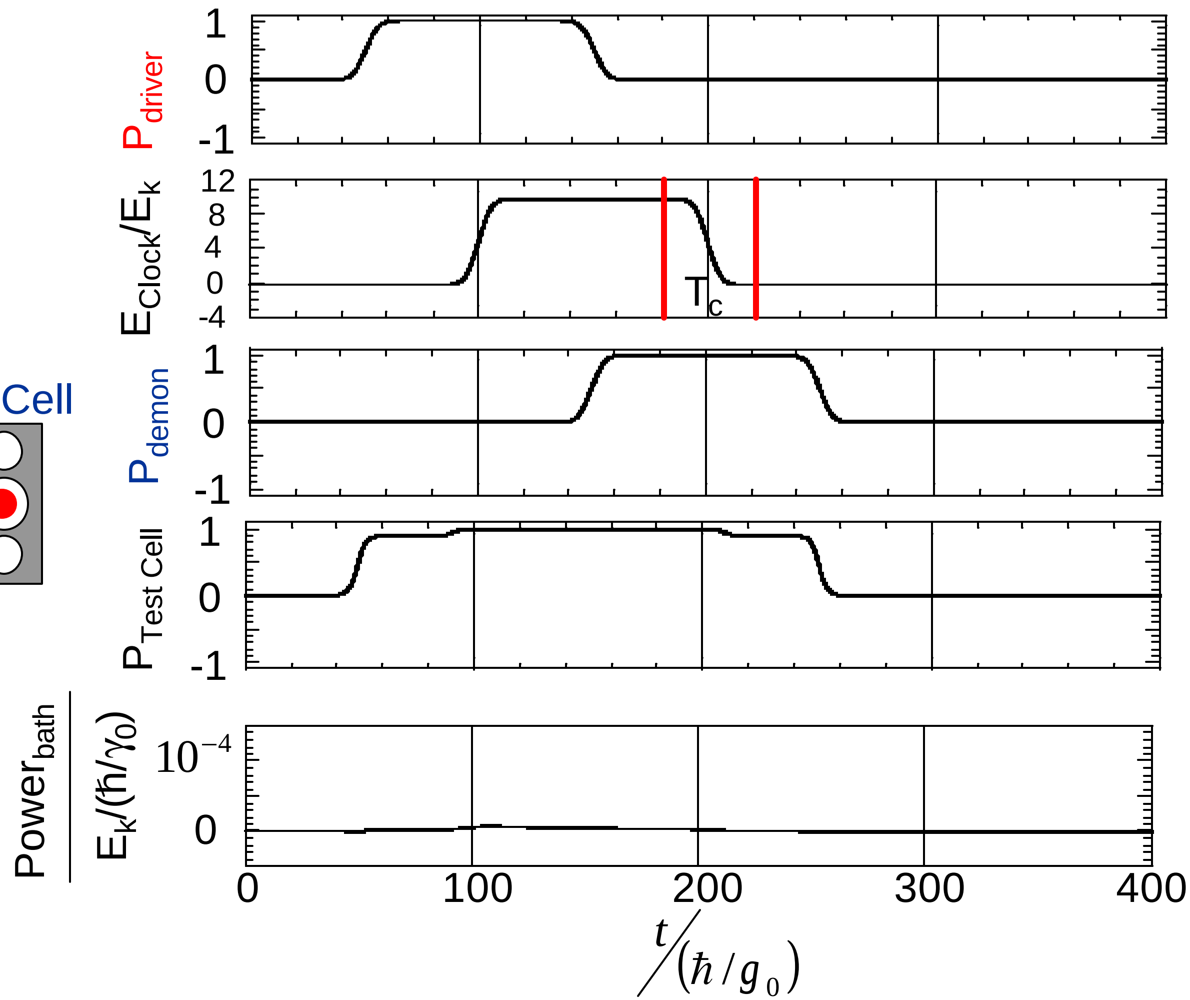




Without a demon cell, erasing the bit results in considerable energy dissipation.

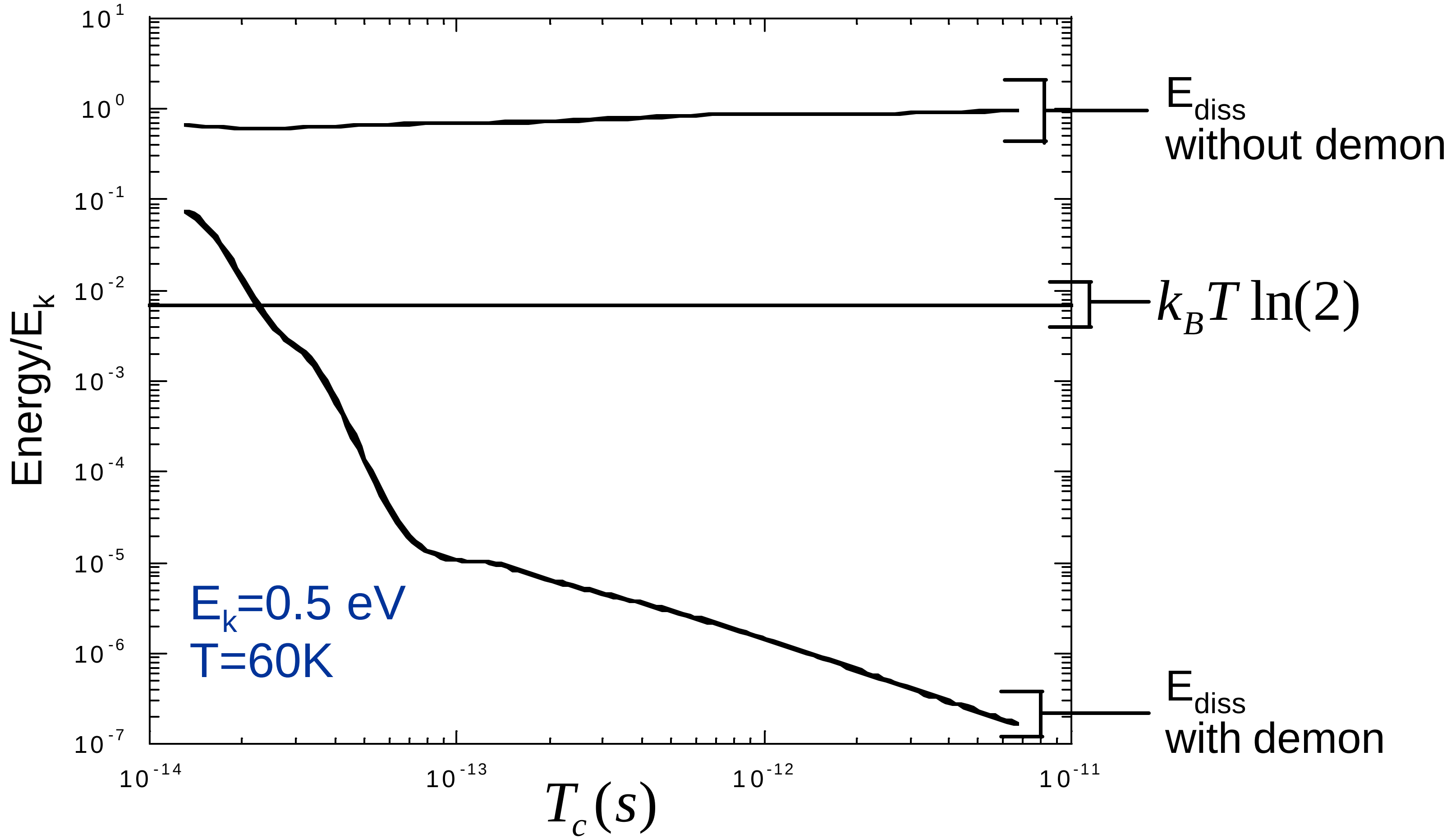
Erasure dynamics with copy to the demon cell





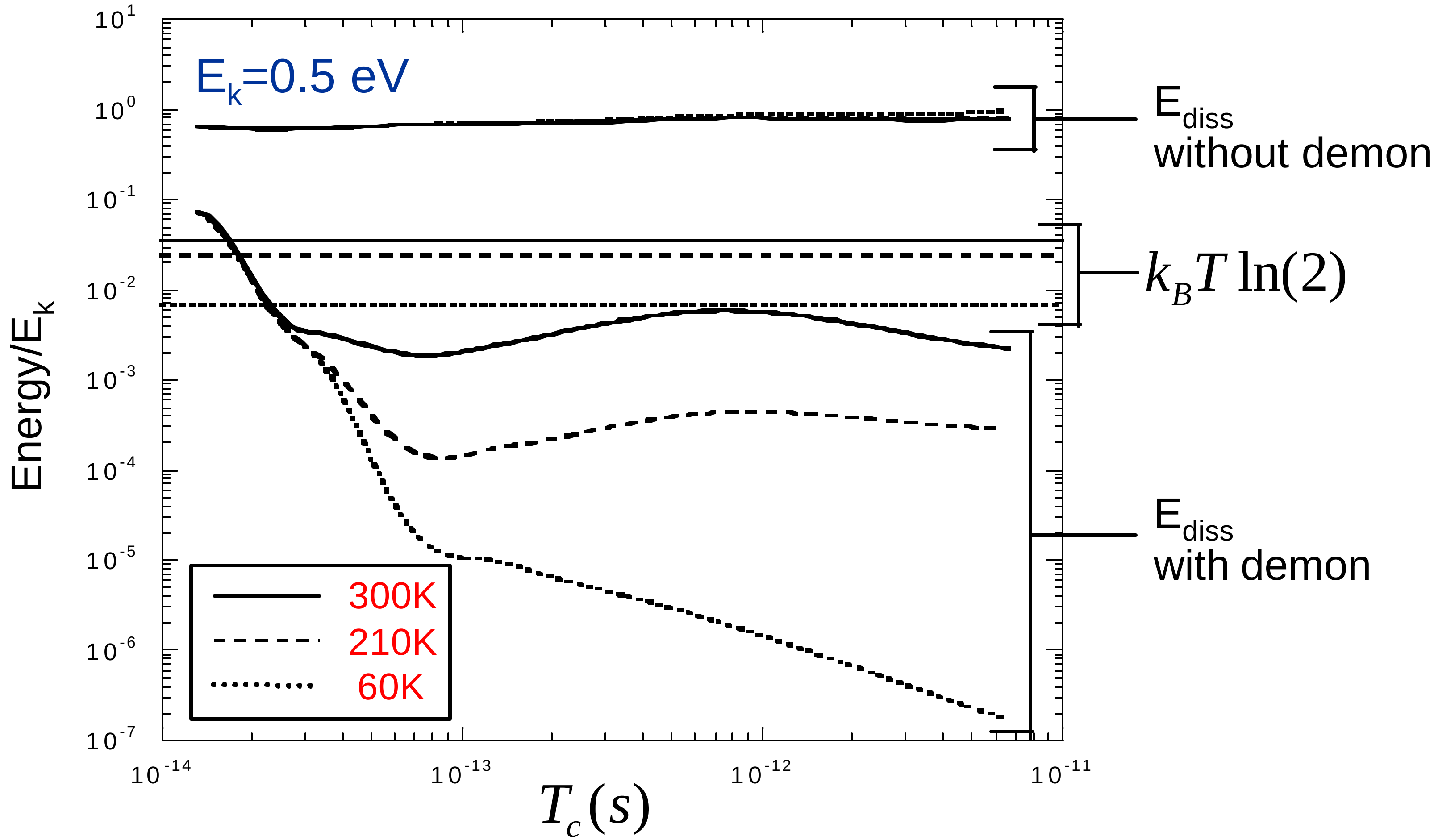
Erasing the bit with a copy to the demon cell, results in very little energy dissipation.

Energy loss for erasing a single bit



The demon cell makes the erasure reversible, so energy loss can be much less than $k_B T\ln(2)$.

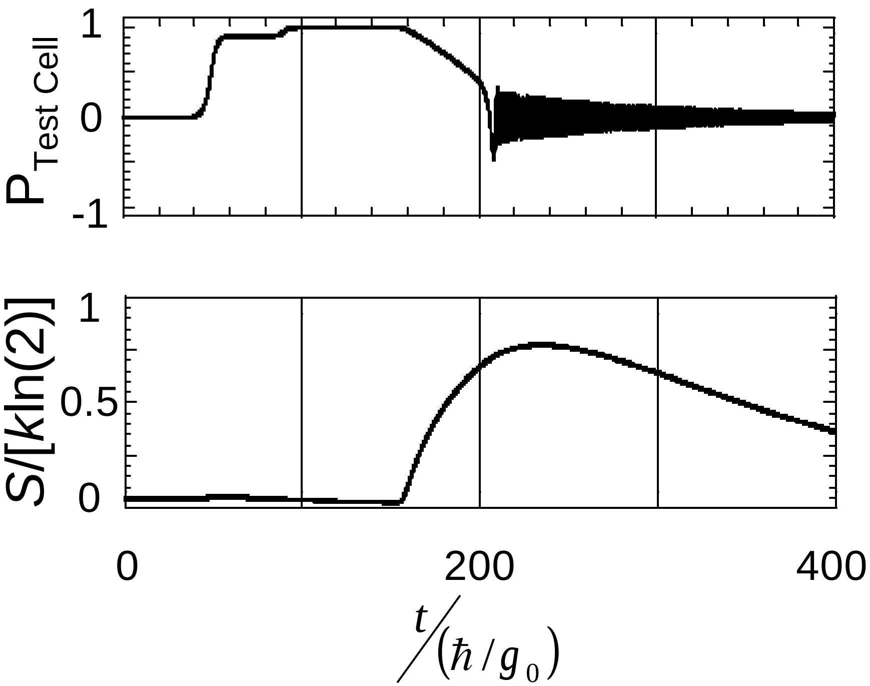
Energy loss for erasing a single bit



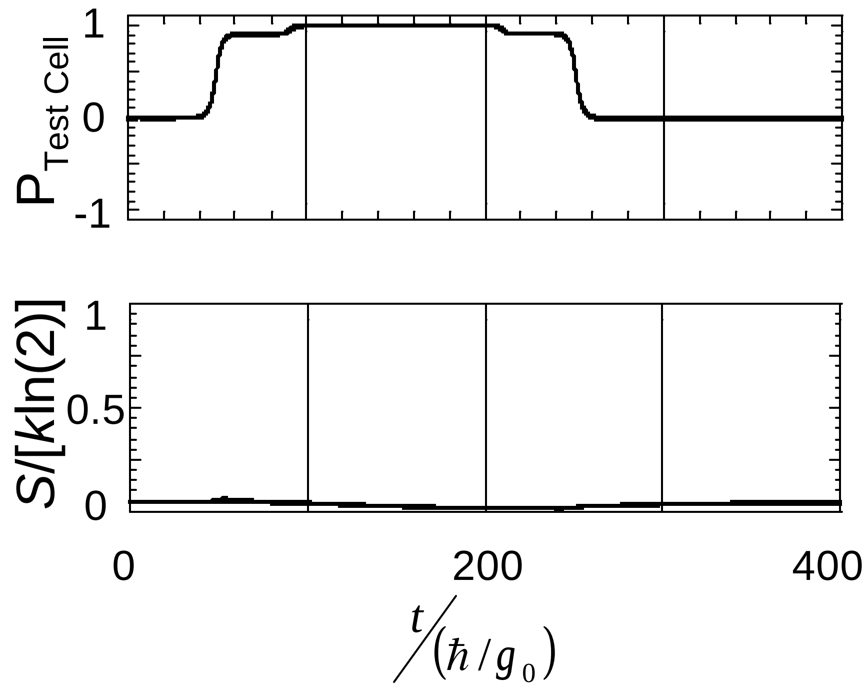
The demon cell makes the erasure reversible, so energy loss can be much less than $k_B T\ln(2)$.

Entropy during erasure

Erasure Without Demon Cell



Erasure With Copy to Demon Cell

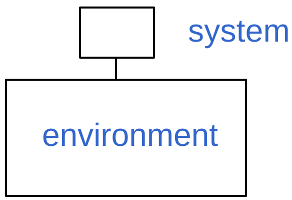


(Von Neumann) $$S = -k \cdot Tr\{ r \ln(r)\}$$

Erasure without the demon cell generates entropy.

Quantum description

Coherence vector formalism



Extract the real degrees of freedom from the density matrix

real vector $\vec{l}$

$$l_i = Tr(?\,\hat{l}_i)$$

$\hat{l}_i$ are the $n^2 - 1$ generators of SU(n), n=2,3

Equation of motion

$$\frac{d\,\vec{l}}{dt} = \mathbf{O}\,\vec{l} + \frac{\vec{l} - \vec{l}_{ss}}{t}$$

$$\mathbf{O}_{ik} = \sum_j f_{ijk}\Gamma_j$$

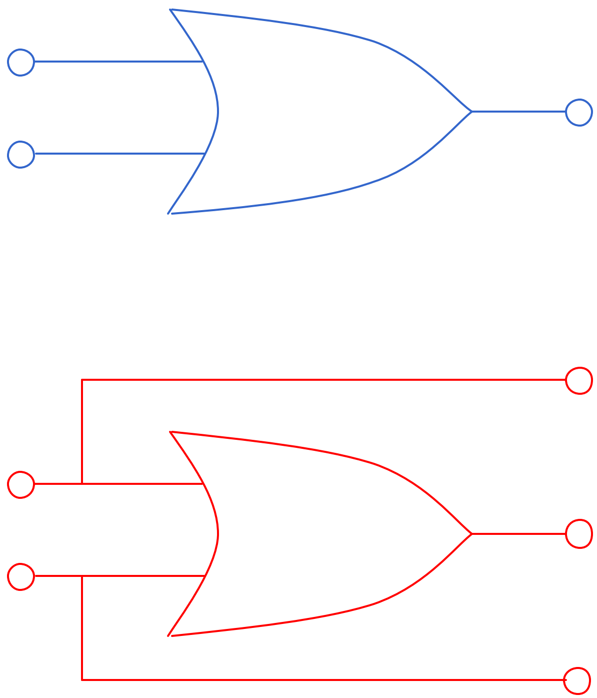
$$\Gamma_j = \left(\frac{1}{\hbar}\right) tr(H\,\hat{l}_i)$$

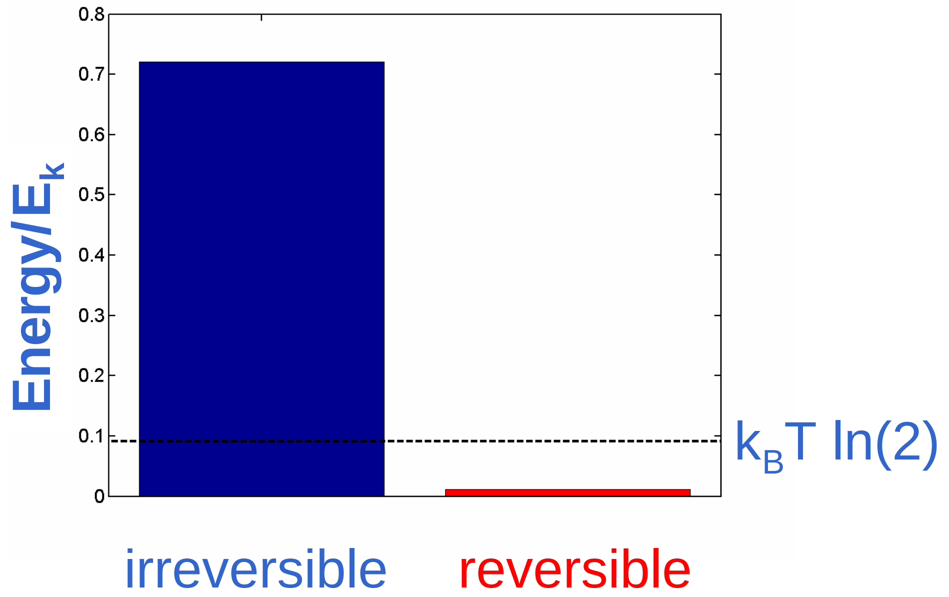
$$\vec{l}_{ss} = tr(?^{eq}\,\hat{l}_i)$$

f_{ijk} : structure constants of SU(n)

$$?^{eq} = \frac{e^{-bH}}{tr(e^{-bH})}$$

QCA gate: reversible/irreversible

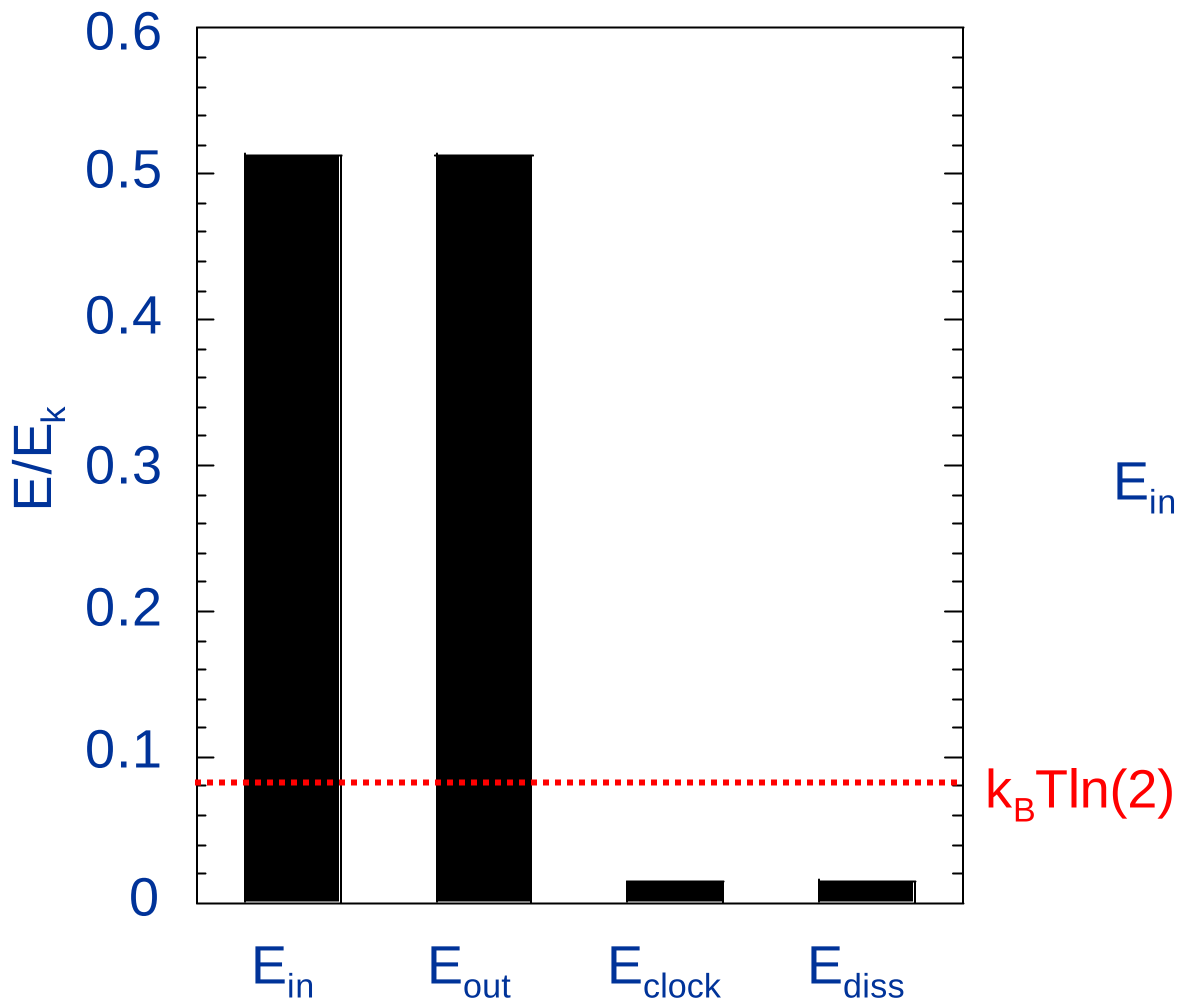


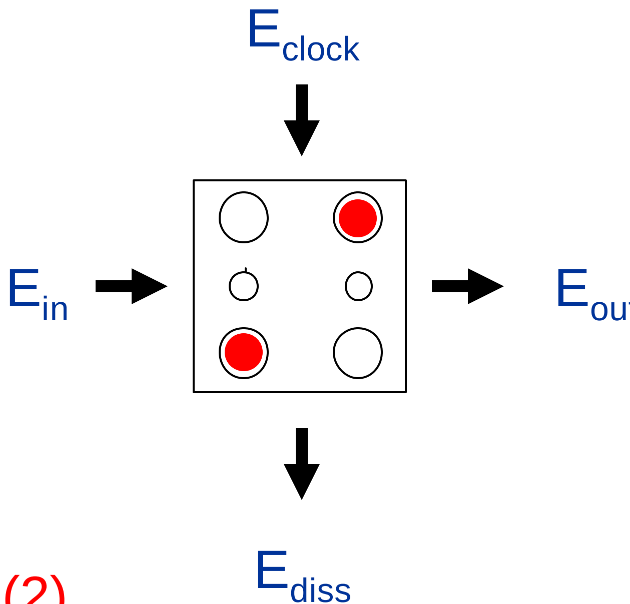


Direct time-dependent calculations shows: Logically reversible circuit can dissipate much less than $k_BT \ln(2)$.

Field-clocking of QCA wire: shift-register

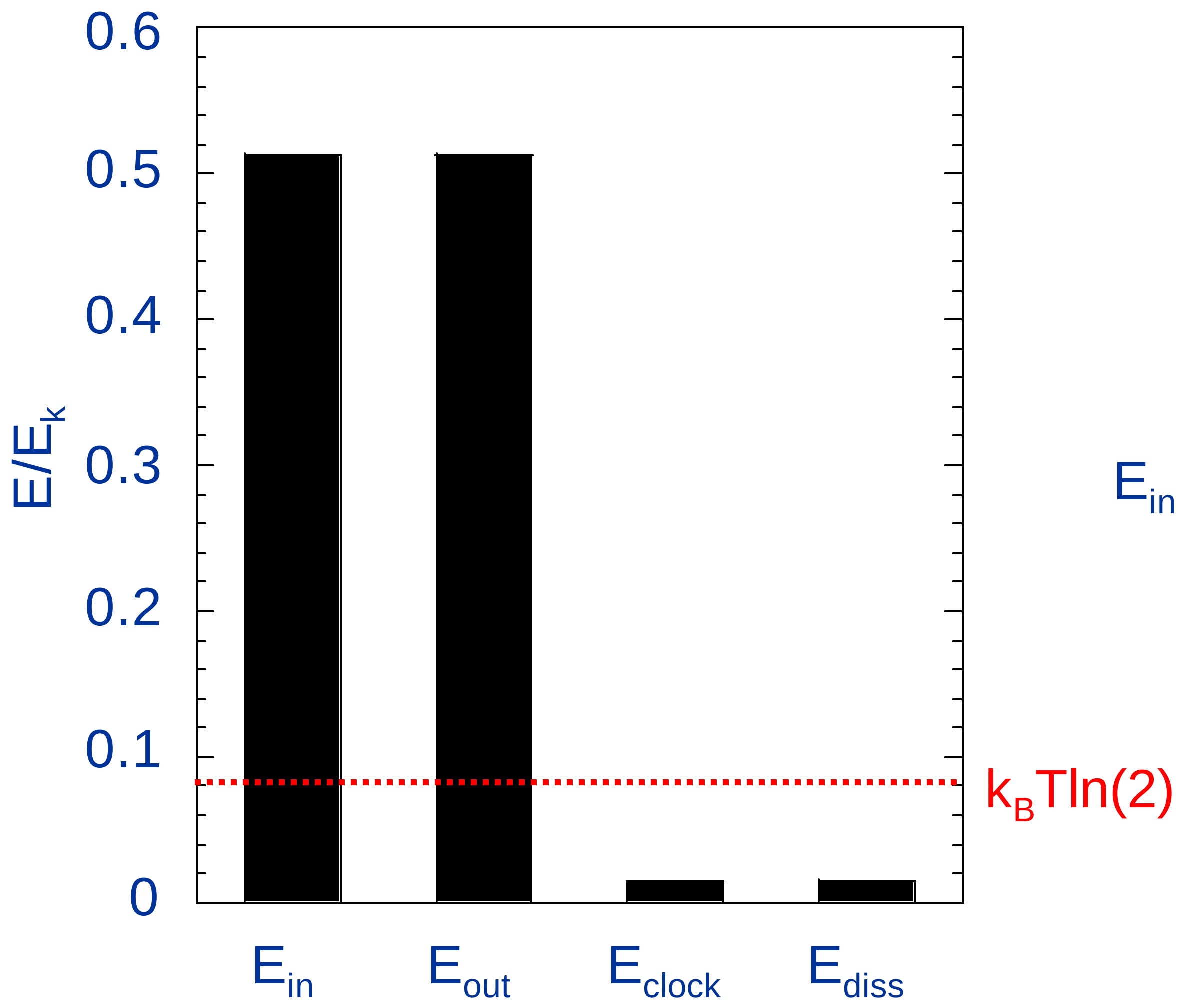
Energy flow in QCA cell

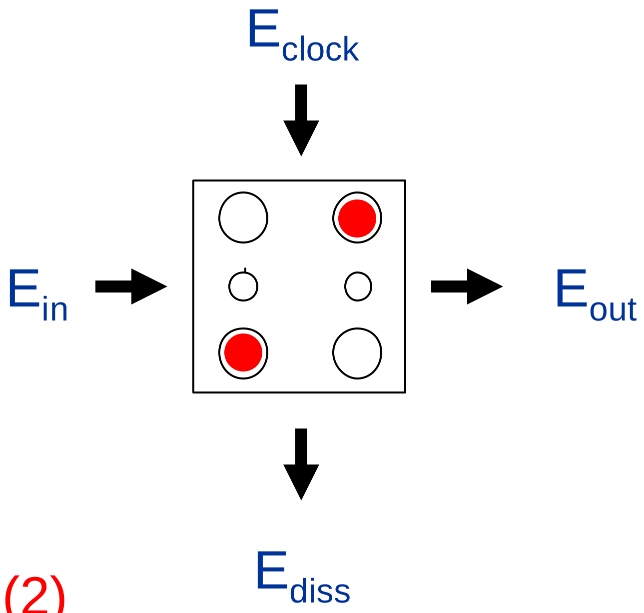




Switching events in QCA cells can dissipate much less than $k_B T\ln(2)$

Energy flow in QCA cell





Distinguishability requires $E_{in} > k_BTln(2)$. E_{diss} can be much less.

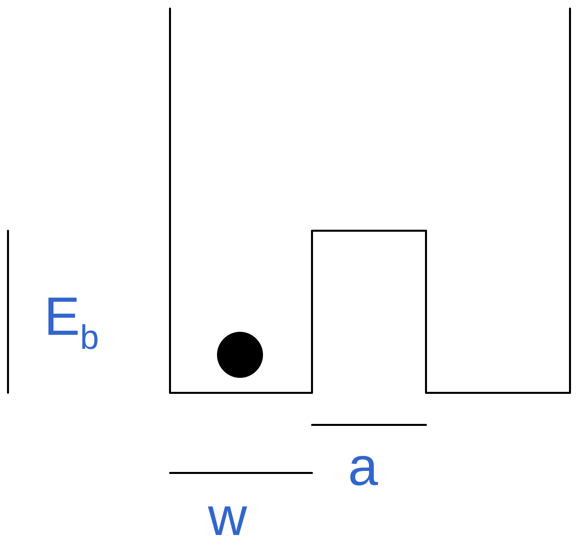
Distinguishability

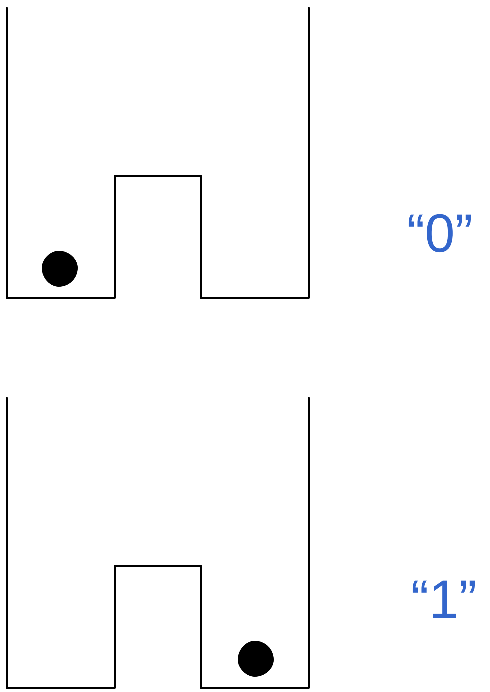
- Information is physical
- *Signal energy* must be greater than $k_B T \ln(2)$ for next stage to be able to distinguish it from thermal fluctuation. (a “read” criterion)
- The signal energy need not be dissipated.
- What to do with it?
  - Bennett: Never throw away information. Reverse computation to return all energy to inputs.
  - Modestly reversible computation. Don’t erase information needlessly.

Outline of presentation

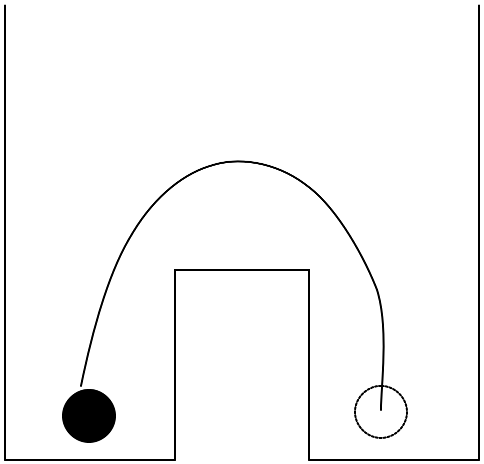
- QCA overview
- Metal-dot QCA devices
- Molecular QCA ➔ architectures
- Power dissipation - fundamental issues (*Lent contra Zhirnov*)
  - History and fundamental analysis
  - QCA as concrete example
  - Double wells and limits

Double well represents bit

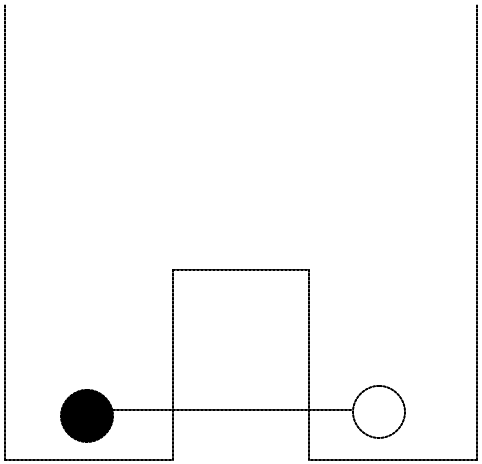




Bit switching



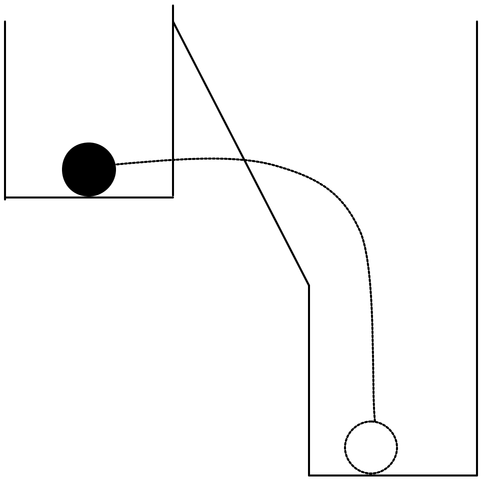
Thermal hop over barrier
dissipates no energy.



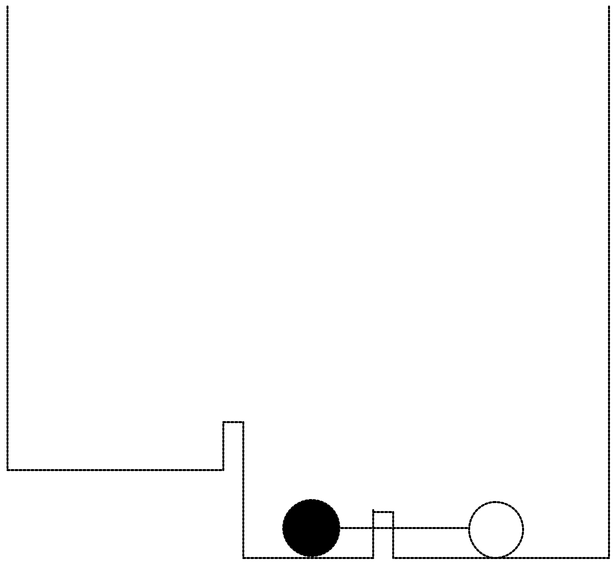
Tunneling through barrier
dissipates no energy.

Note: Traversing an energy barrier dissipates no energy.

Dissipation: falling down hill



QCA adiabatic switching

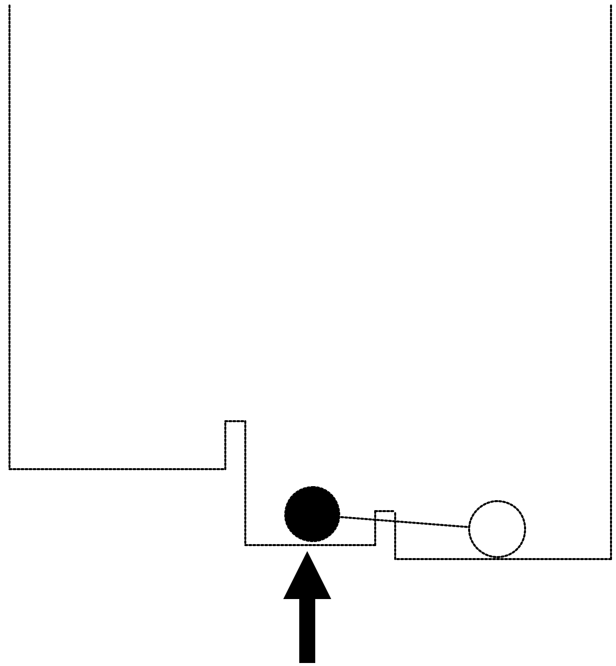


Remove input bias

Raise clocking potential

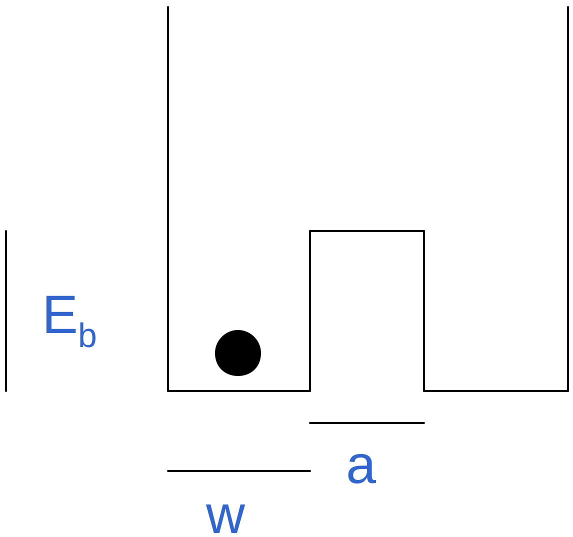
Keep system always very close to ground state.
Don't let it fall downhill.

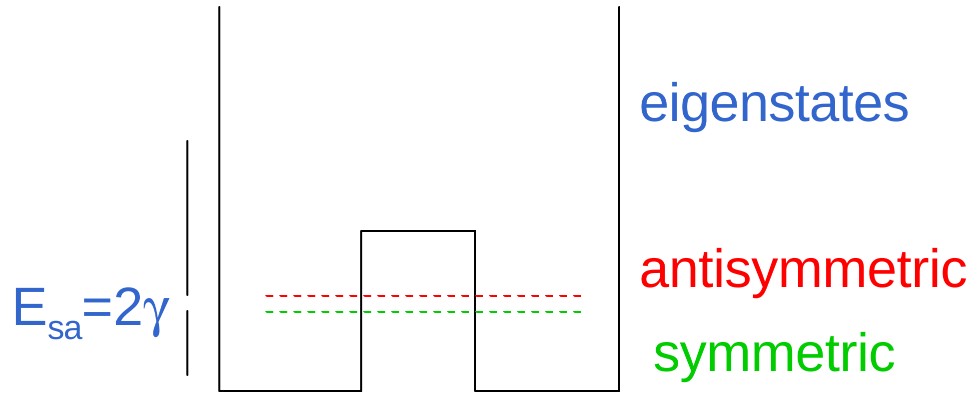
Breakdown of adiabaticity



If clock moves up too fast, system cannot get to ground state without some dissipation.

Switching time

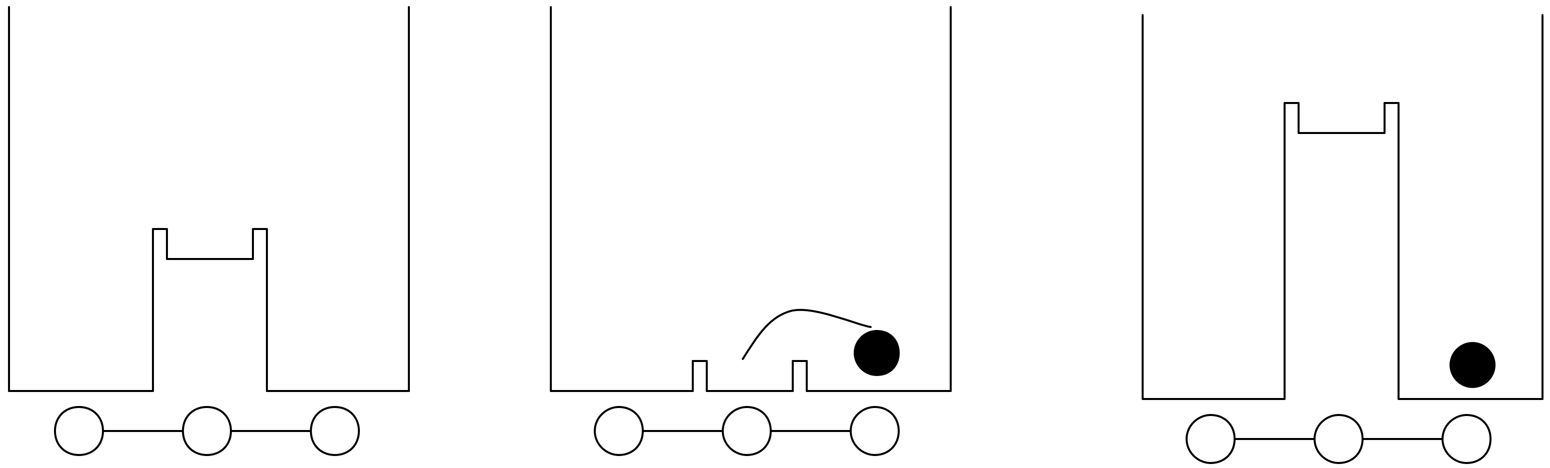




$$t_{switching} \sim \frac{\hbar}{\gamma}$$

High or wide barrier ➔ small γ, longer $t_{switching}$

QCA approach: modulate barrier



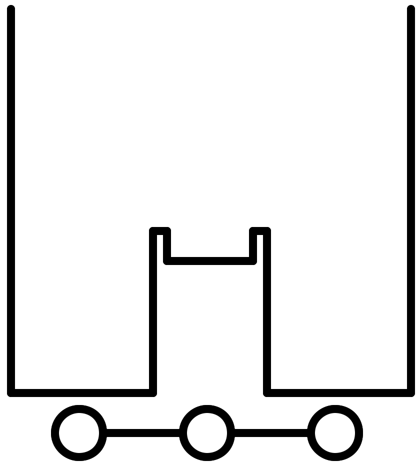
switch when
barriers are low

distinguish (read)
when barriers are high

- Barriers that limit switching speed can be small.
- Barriers that limit distinguishability can be large.
- Important speed limitation is adiabaticity.

Distinguishability criterion is unrelated to switching speed.

Is there a thermodynamic *smallest* size?

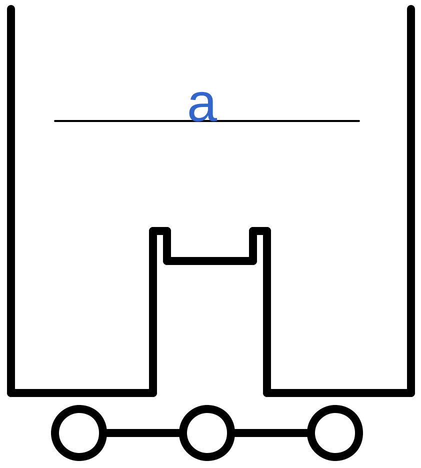


Scale ~a^2V

- Smaller structure has larger potential barriers, but same barrier transparency.
- Coulomb effects are stronger (1/r) ➔ E_k greater.
- Smaller structure works at higher temperature.

Thermodynamics imposes no lower limit to size. Smaller is better.

Uncertainty argument



$$\Delta x \Delta p \geq \hbar/2$$

$$\Delta x \approx a$$

$$\Delta p \approx \sqrt{2mE_{min}} = \sqrt{2m(kT\ln(2))}$$

$$p = \sqrt{2m(E - V)}$$

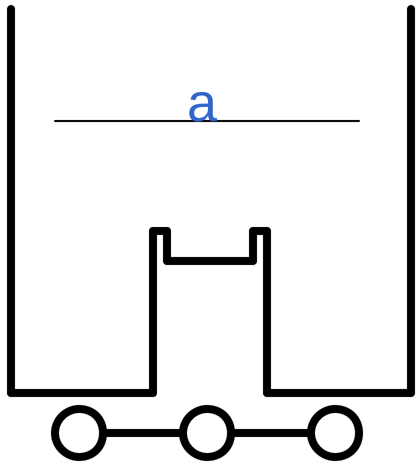
$$\frac{p^2}{2m} + V = E$$

Momentum cannot be simply related to energy except when V=0.

$$E = \frac{p^2}{2m} \approx \frac{\left(\frac{\hbar}{2\Delta x}\right)^2}{2m} = \frac{\hbar^2}{8ma^2}$$

Merely gives an estimate for the ground state of an infinite square well with width a.

Uncertainty argument



$$\Delta x \Delta p \geq \hbar / 2$$

$$\Delta x \approx a$$

$$\Delta p \approx \sqrt{2mE_{min}} = \sqrt{2m(kT\ln(2))}$$

(both expressions for Δp are struck through in red)

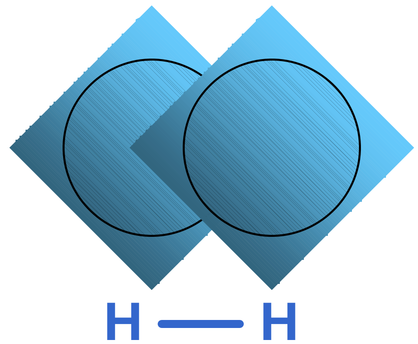
$$p = \sqrt{2m(E-V)}$$

$$\frac{p^2}{2m} + V = E$$

Momentum cannot be simply related to energy except when V=0.

Neither Heisenberg nor Boltzmann provide a lower limit to device size.

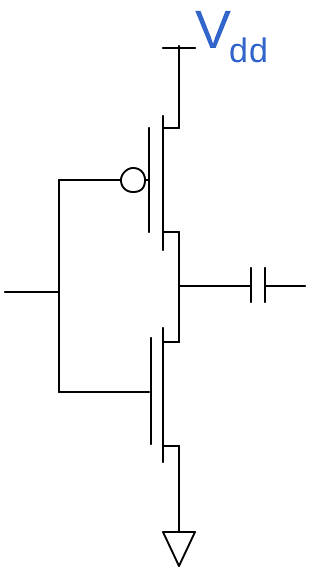
Lower limit to device size

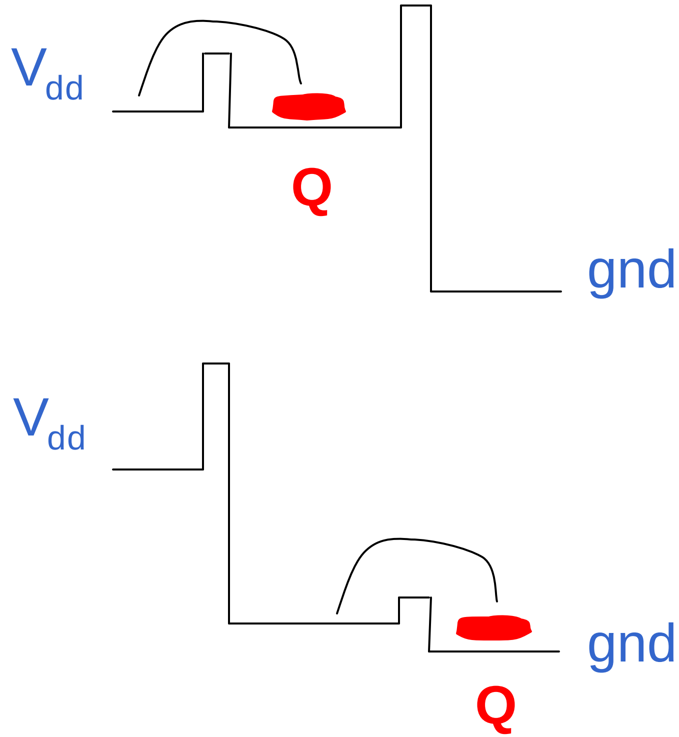


- Cannot structure matter smaller than single molecules.
- We cannot construct potential landscapes smaller than H_2.
- Limited by values of e, h, m_e: $$a_{Bohr} = \frac{4p\hbar^2}{me^2}$$

Bohr does provide lower limit on device size.

What’s wrong with transistors?



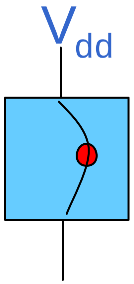


Net transport of charge from V_{dd} to ground (*falling downhill*).

Energy dissipated each cycle is at least QV_{dd}.

Energy is dissipated even for logically reversible operations.

Transistors at molecular densities



Suppose in each clock cycle a *single* electron moves from power supply (1V) to ground.

Transistors at molecular densities

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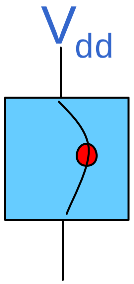
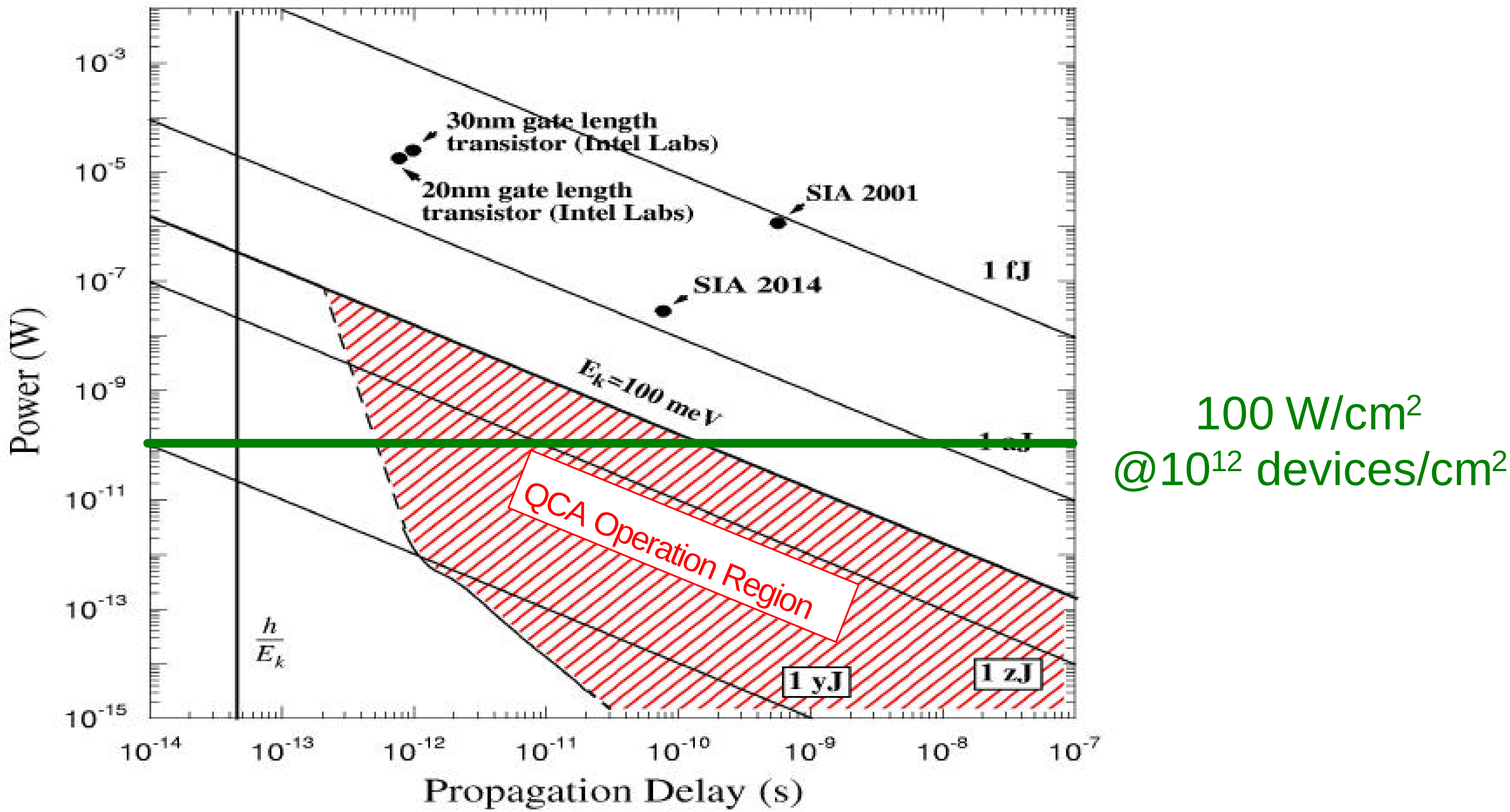


Power dissipation (Watts/cm^2)

Frequency (Hz)	10^{14} devices/cm^2	10^{13} devices/cm^2	10^{12} devices/cm^2	10^{11} devices/cm^2
10^{12}	16,000,000	1,600,000	160,000	16,000
10^{11}	1,600,000	160,000	16,000	1,600
10^{10}	160,000	16,000	1,600	160
10^{9}	16,000	1600	160	16
10^{8}	1600	160	16	1.6
10^{7}	160	16	1.6	0.16
10^{6}	16	1.6	0.16	0.016

ITRS roadmap:
9nm gate length, 10^9 logic transistors/cm^2 @ 3×10^{10} Hz for 2016

QCA Power Dissipation



QCA architectures could operate at densities 10^{12} devices/cm^2 and 100GHz without melting the chip.

Power dissipation at molecular densities

- Cannot afford to dump charge to ground.
- Must use some version of adiabatic switching.
  - Keep system always near ground state (*e.g.* clocked QCA).
  - No fundamental lower limit on energy dissipation per bit provided information is not erased. (Landauer)
  - Must dissipate at least $k_B T \ln(2)$ for each erasure.
    Radical architecture with no erasure is possible but perhaps not practical (Bennett).

Future directions for QCA

- Metal-dots: more complex circuits at higher T
- Molecules: just at start
  - Attachment to surface
  - Neutral molecules ("self-doping")
  - Clocked systems
  - Patterning into circuits
  - Detection of single molecule states with electrometers (= output at edges of device)
- Architecture:
  Need new architecture to exploit "processing-in-wire"
  - Bad news: no instant, long-range transport of information. Shift registers are everything
  - Good news: Shift registers are everything! massive pipelining

Thank you for your attention