Quantum-dot Cellular Automata: beyond transistors to extreme supercomputing

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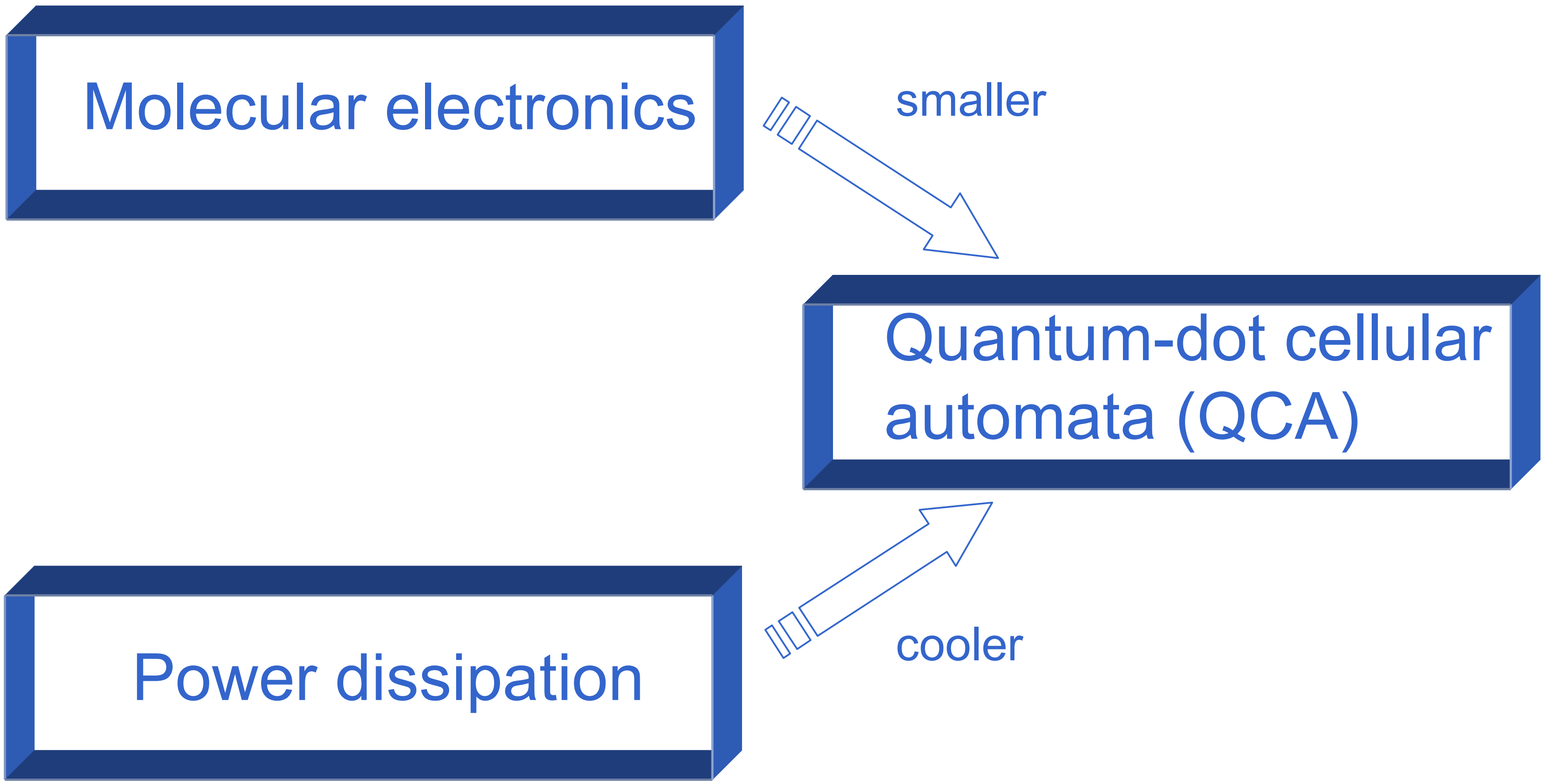
Converging problems

- How can we make the most powerful computer?
  - Binary
  - Most processing elements/cm^2 – high functional density
  - ➔ molecules as devices

- How can we solve the “heat problem”?
  - Power dissipation is limiter
  - Understand the fundamentals of the issue
  - Need to go beyond transistors
  - Practical way to do “reversible computation”

There is an approach than may solve both these problems and provide a path forward: QCA

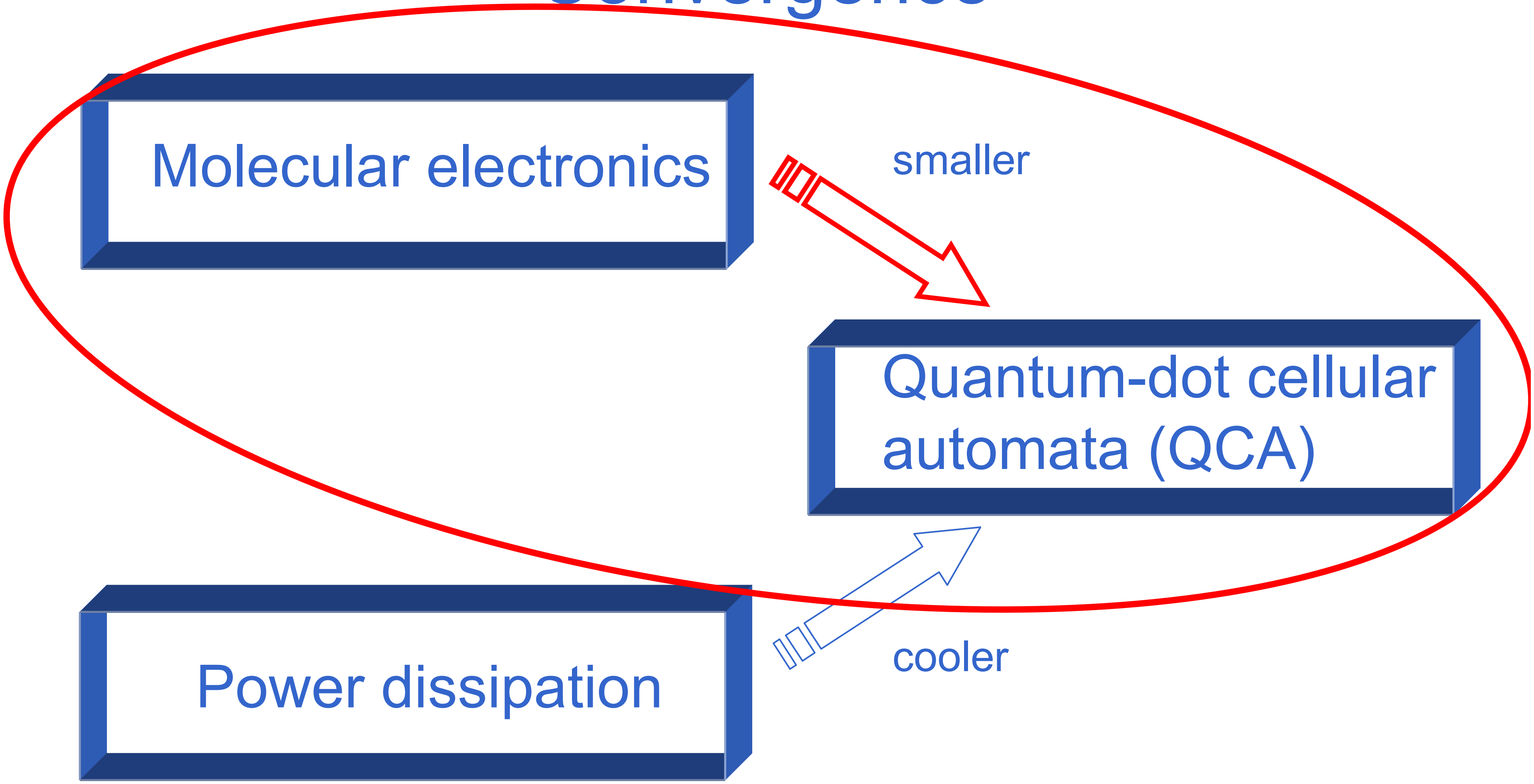
Convergence



Outline of presentation

- Shrinking electronics & QCA
- The heat problem & QCA
- A path forward

Convergence

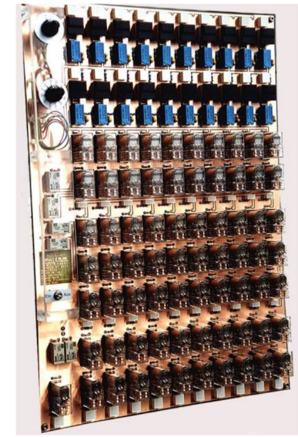


How is information represented physically?

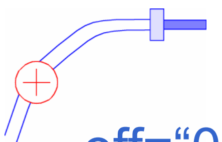
Zuse's paradigm

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

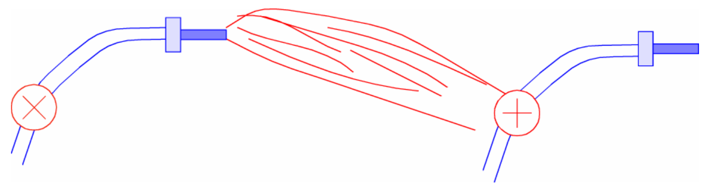
Telephone relay



Z3 Adder



off="0"

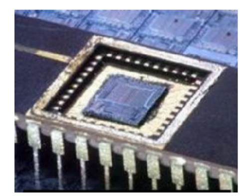


The flow through one switch turns another on or off.

Electromechanical relay

Vacuum tubes

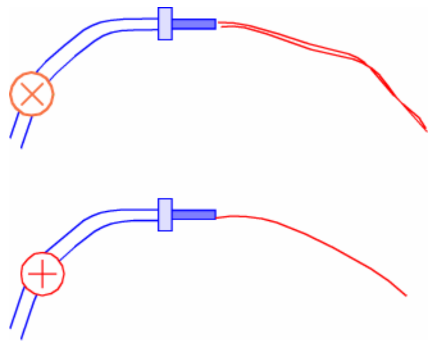
Solid-state transistors



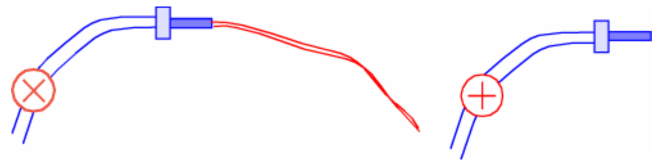
CMOS IC

Exponential down-scaling

Problems shrinking the current-switch



Valve shrinks also – hard to get good on/off



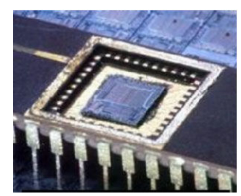
Current becomes small - resistance becomes high
Hard to turn next switch
Charge becomes quantized

Power dissipation threatens to melt the chip.

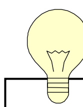
Electromechanical relay

Vacuum tubes

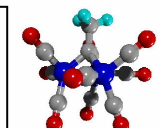
Solid-state transistors



CMOS IC



New idea



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.

Zuse's paradigm

✓ • Binary

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

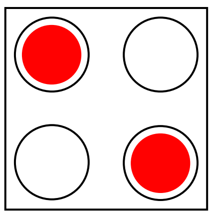
Revolutionary, not incremental, approach

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

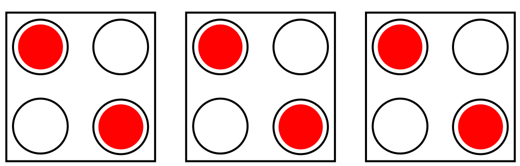


A cell with 4 dots

2 extra electrons

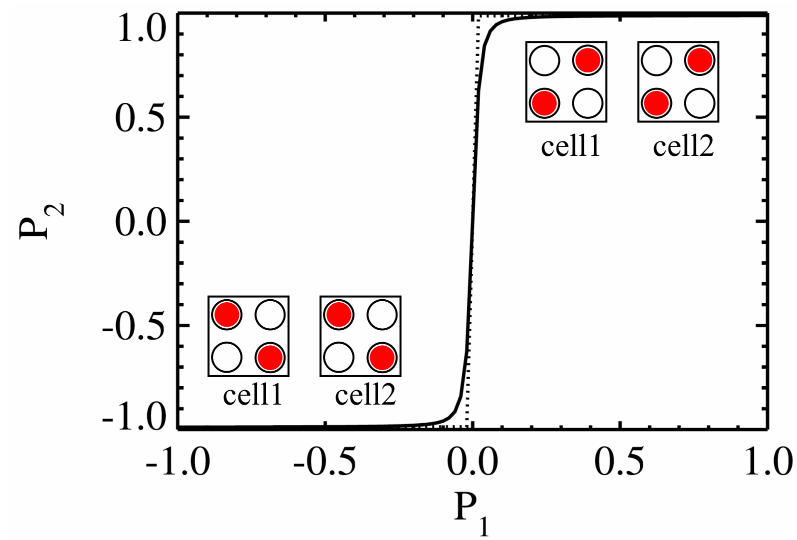
Tunneling between dots

Polarization P = -1
Bit value “0”



Neighboring cells tend to align.
Coulombic coupling

Cell-cell response function



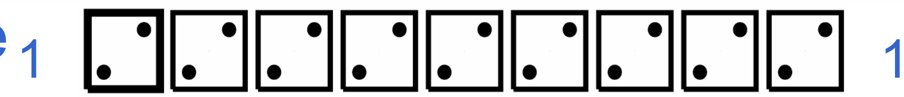
Bistable, nonlinear cell-cell response

Restoration of signal levels

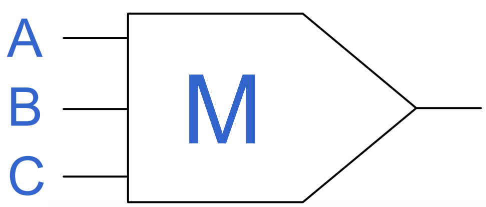
Robustness against disorder

QCA devices

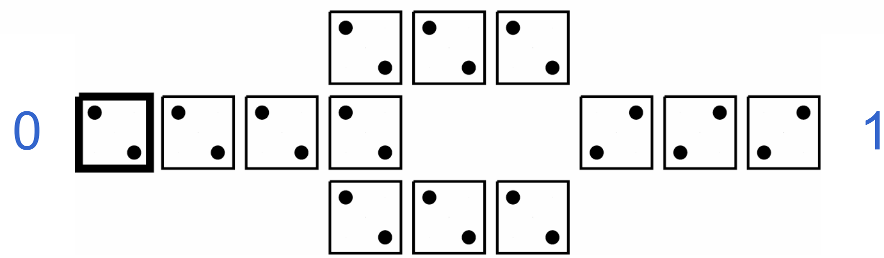
Binary wire

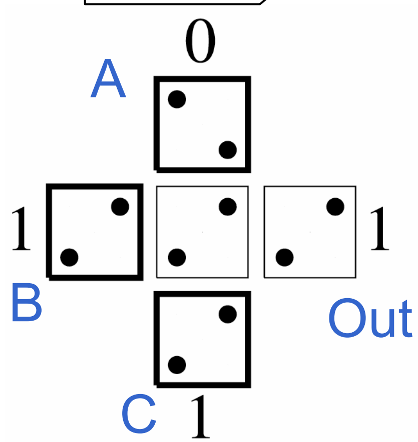


Majority gate

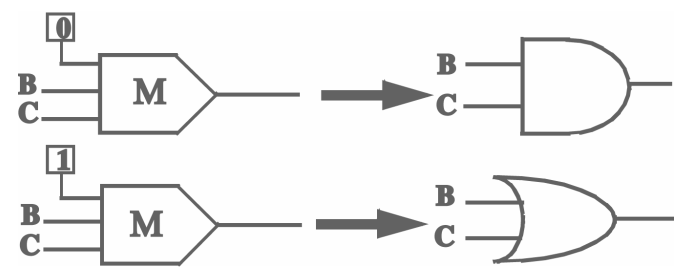


Inverter



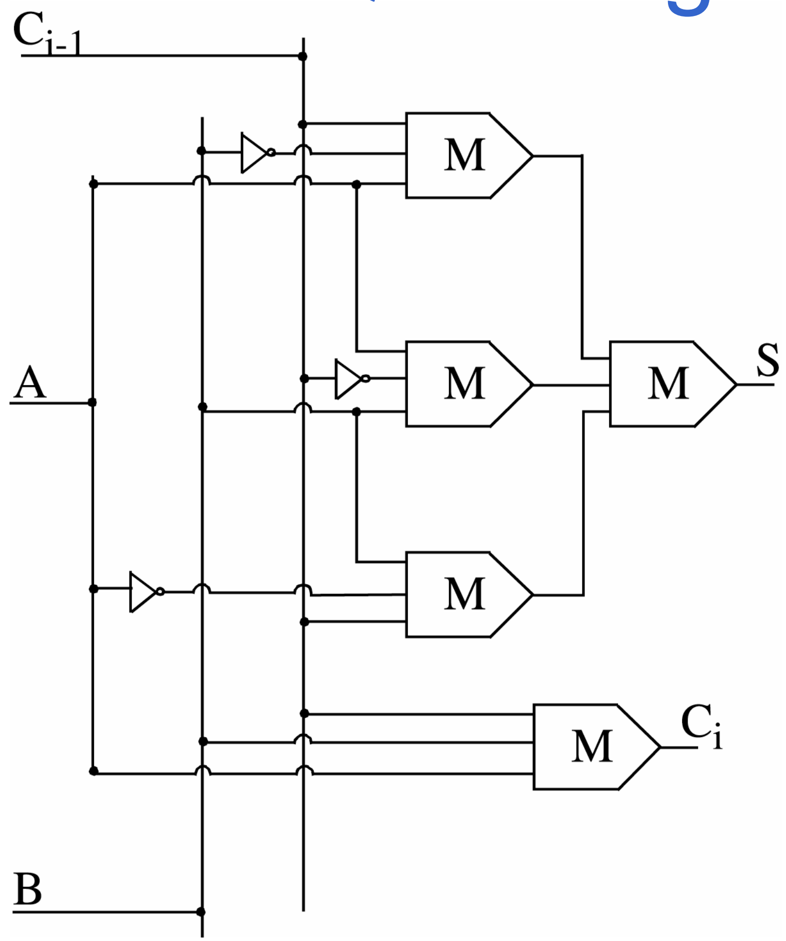


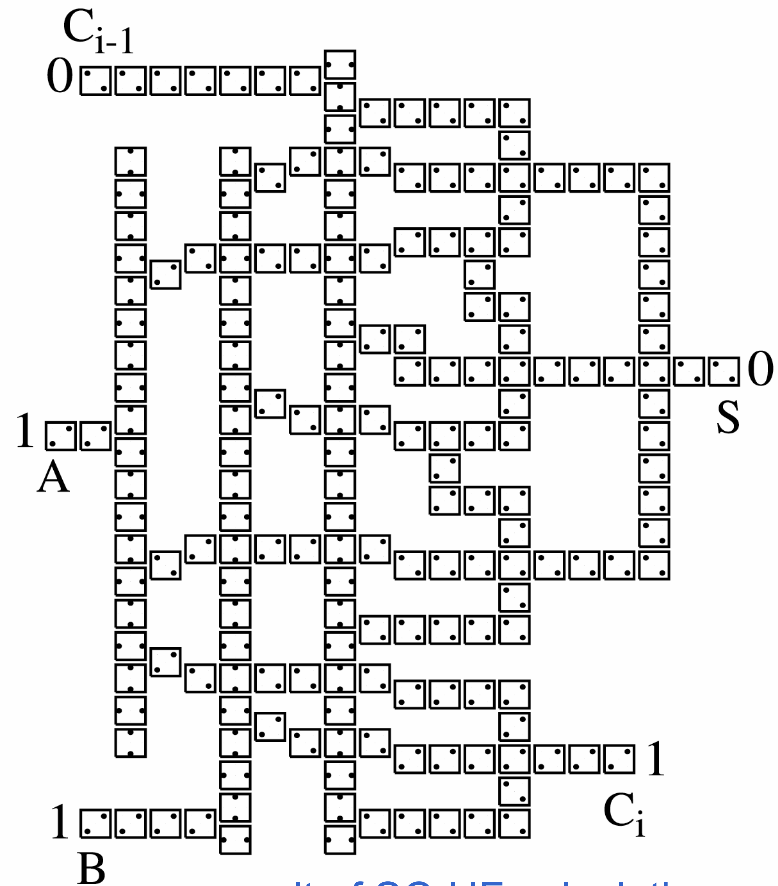
	A	B	C	Output
AND gate	0	0	0	0
	0	0	1	0
	0	1	1	1
	0	1	0	0
OR gate	1	1	0	1
	1	1	1	1
	1	0	1	1
	1	0	0	0



Programmable 2-input AND or OR gate.

QCA single-bit full adder

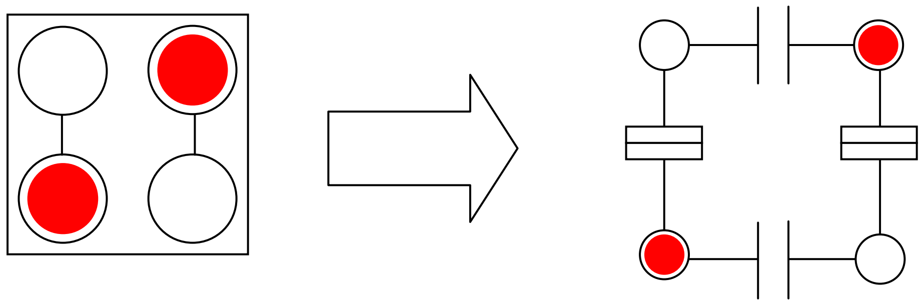




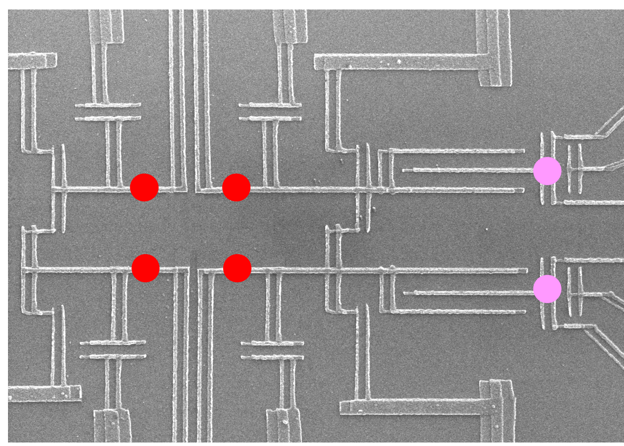
result of SC-HF calculation
with site model

Hierarchical layout and design are possible.

QCA devices exist



Metal-dot QCA implementation



Al/AlO_x on SiO_2

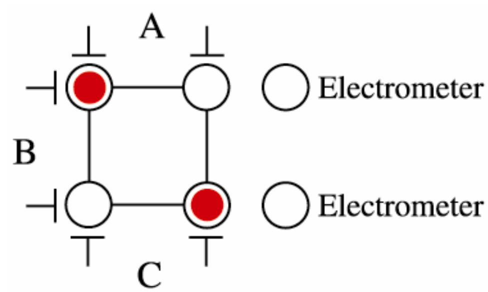
"dot" = metal island

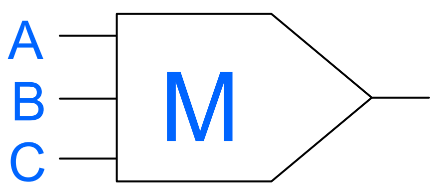
70-300 mK

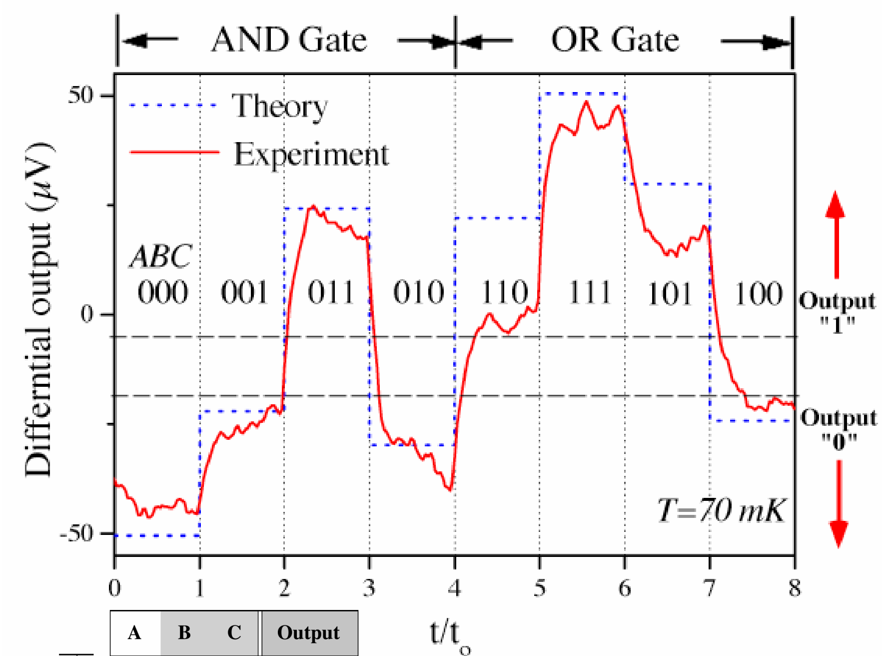
Greg Snider, Alexei Orlov, and Gary Bernstein

Metal-dot QCA cells and devices

- Majority Gate







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	0	1	0	0
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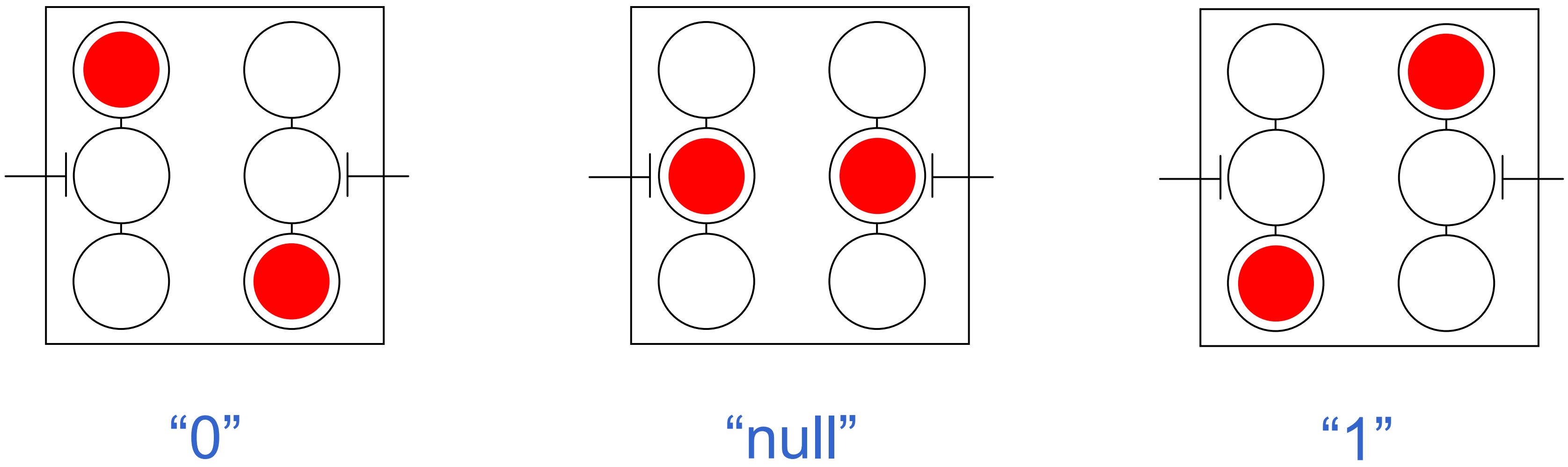
	1	1	1	1
	1	0	1	1
	1	0	0	0

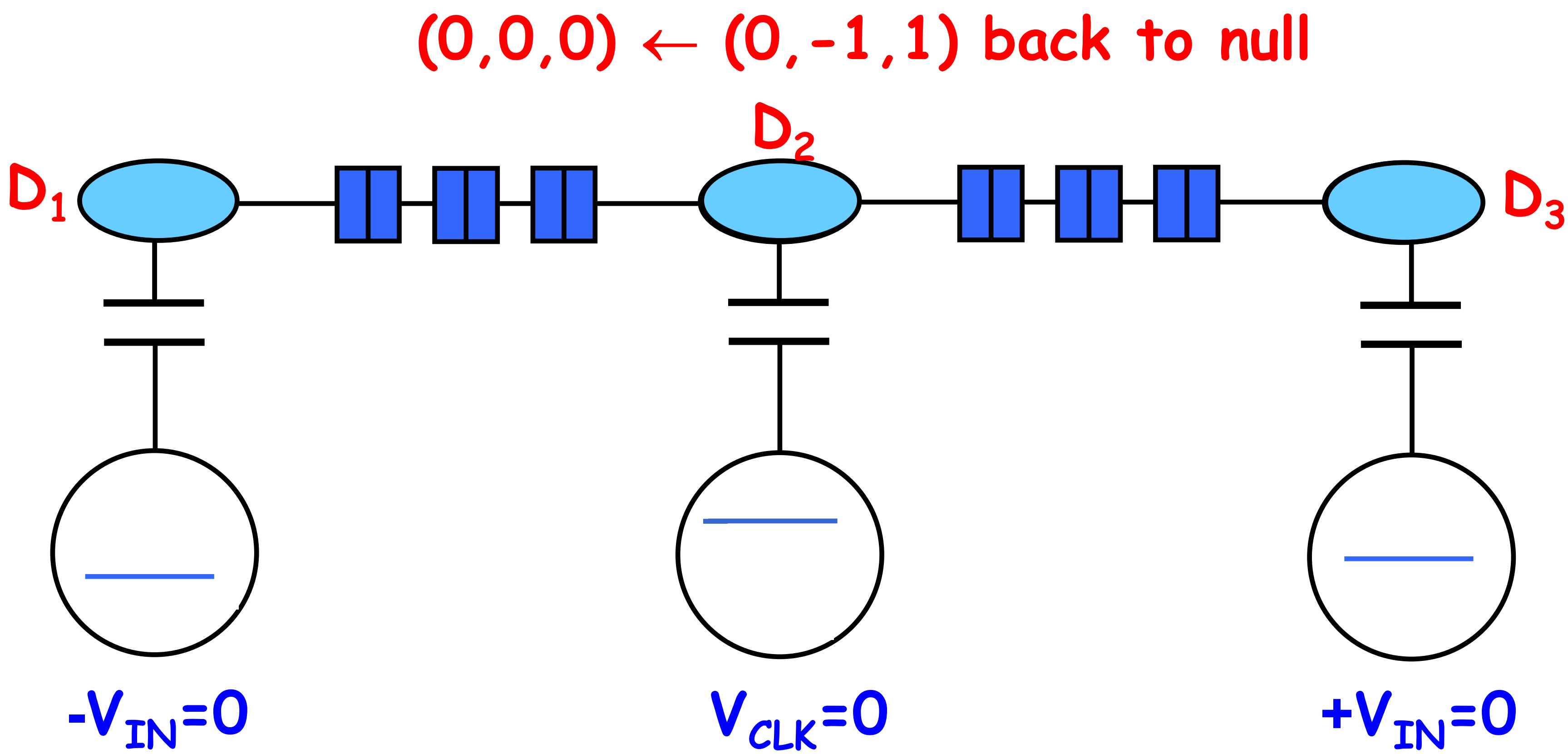
Amlani, A. Orlov, G. Toth, G. H. Bernstein, C. S. Lent, G. L. Snider, *Science* **284**, pp. 289-291 (1999).

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.

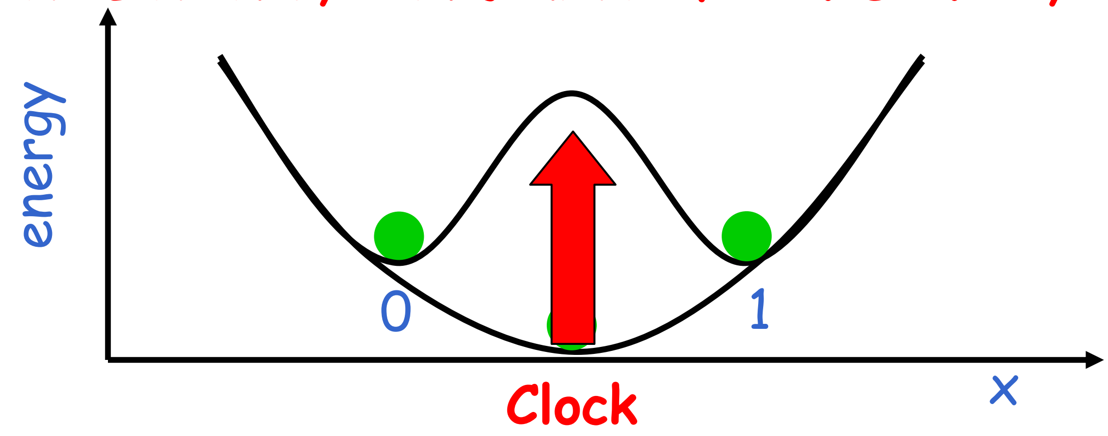
Three-dot QCA latch operation

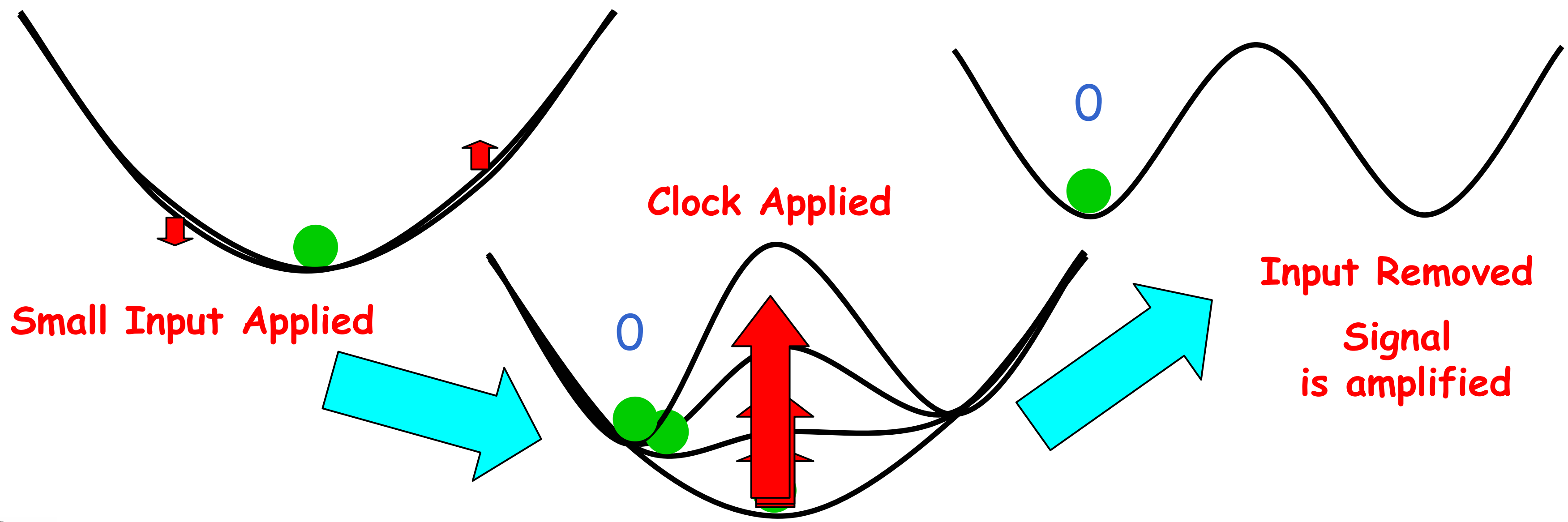


- Clock supplies energy, input defines direction of switching
- Three states of the QCA latch: "0" , "1" and "null"

Clocking in QCA

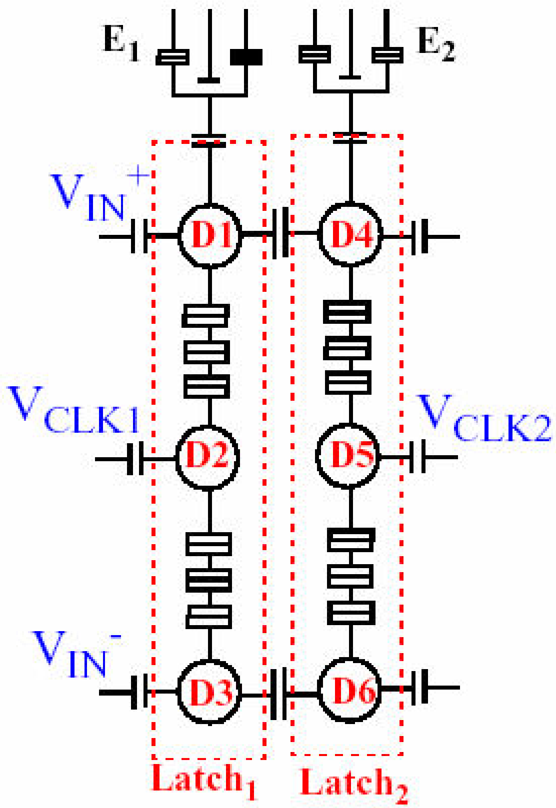
Keyes and Landauer, IBM Journal of Res. Dev. 14, 152, 1970



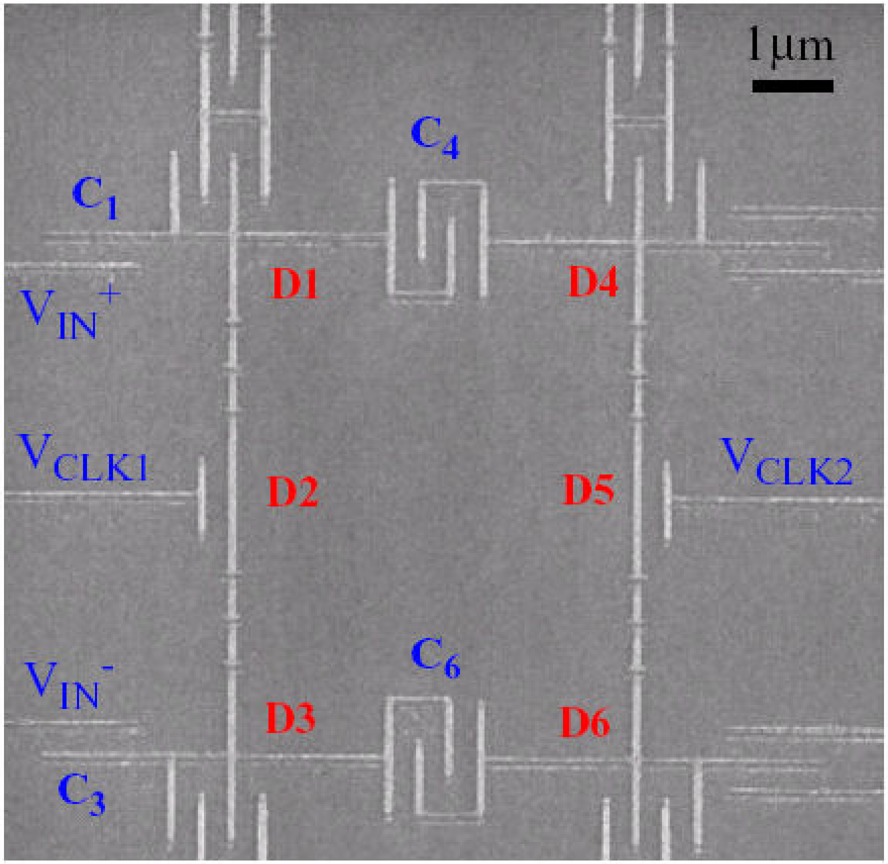


QCA Shift Register

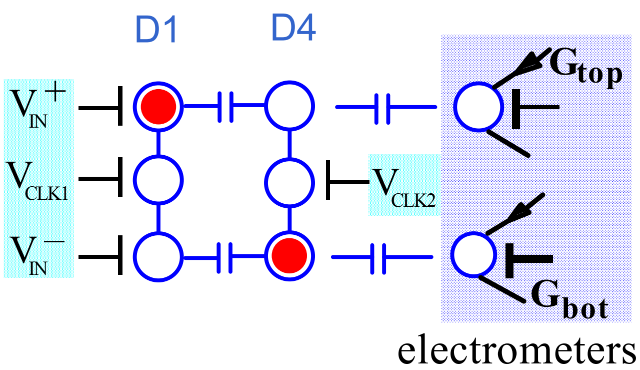
Schematic Diagram

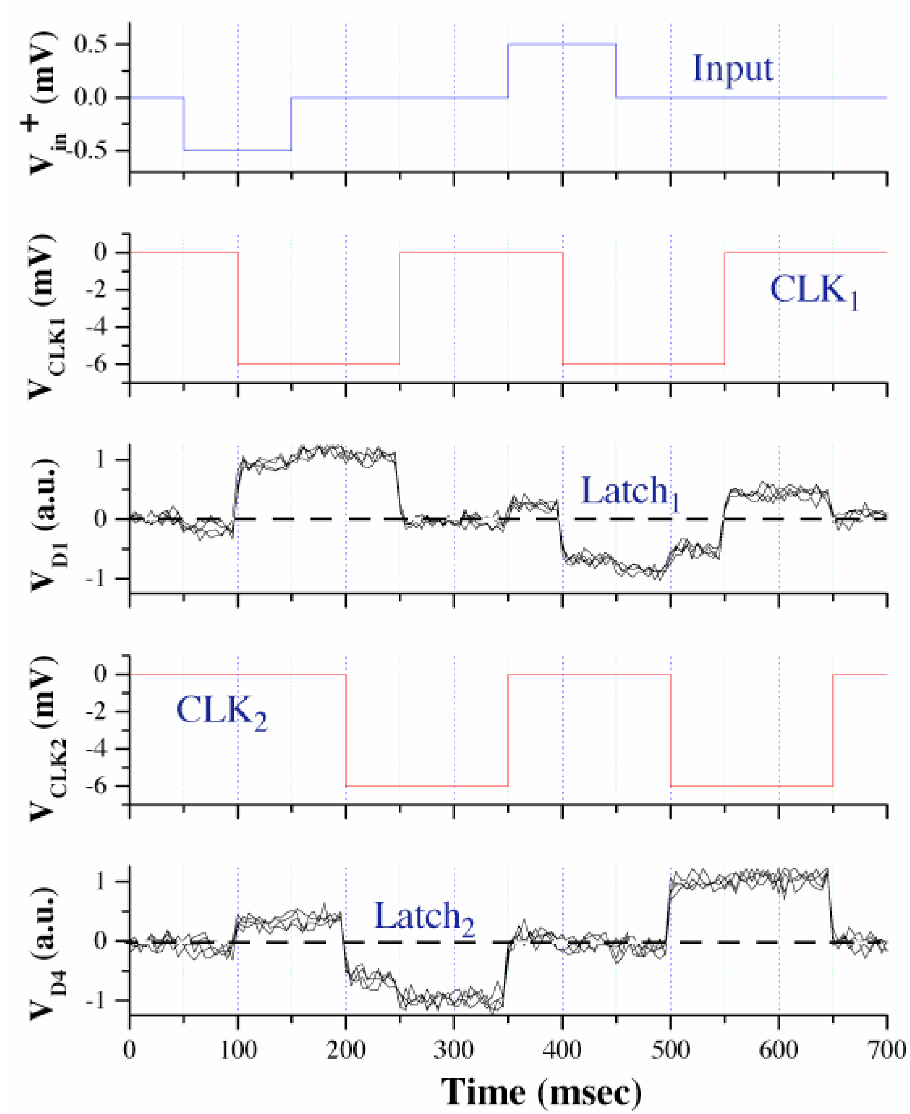


SEM Micrograph



QCA Shift Register





Interactive Demos

- link

Power gain

Power gain is essential for any practical digital technology.

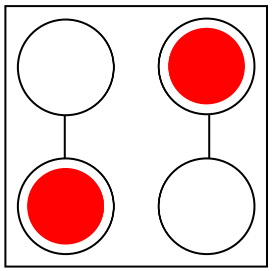
- Lacking in cross-bar and lookup-table proposals
- Lacking in randomly self-assembled circuits
- Clocked QCA has power gain.
  - Theory: Timler and Lent, J. Appl. Phys. 91, 823 (2002).
  - Experiment: Kummamuru et al., Appl. Phys. Lett. 81, 1332 (2002).

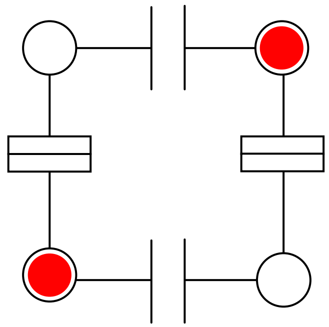
Power gain > 3 has been measured.

QCA implementations

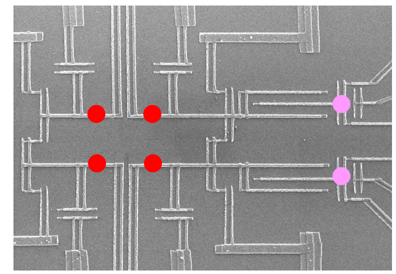
- ✓ Metal-dot QCA
  - ✓ First QCA devices
  - ✓ Clocked QCA
- Molecular QCA
  - Molecular electronics
  - Aviram molecules
  - Fe-Ru
  - 4-dot Ferrocene molecules
- Implications for architecture

From metal-dot to molecular QCA



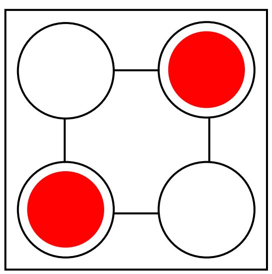


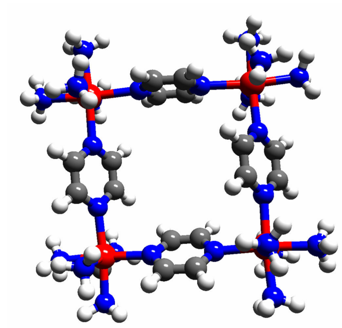
Metal tunnel junctions



“dot” = metal island

70 mK





“dot” = redox center

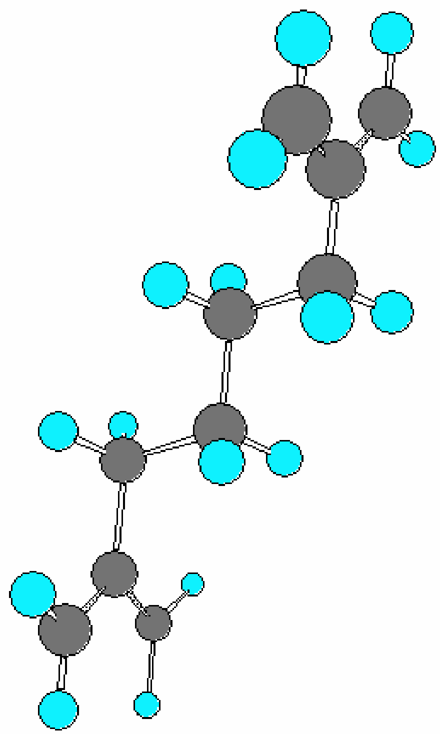
Mixed valence compounds

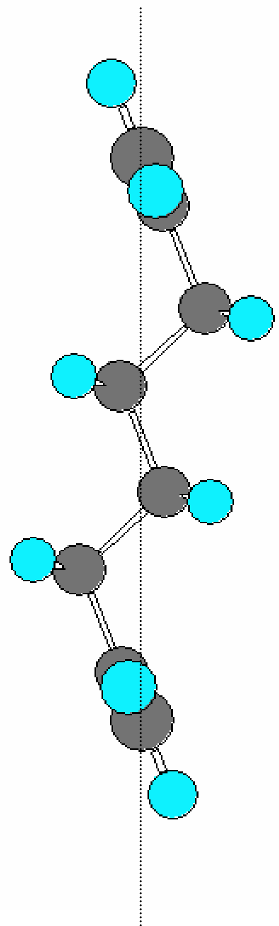
room temperature+

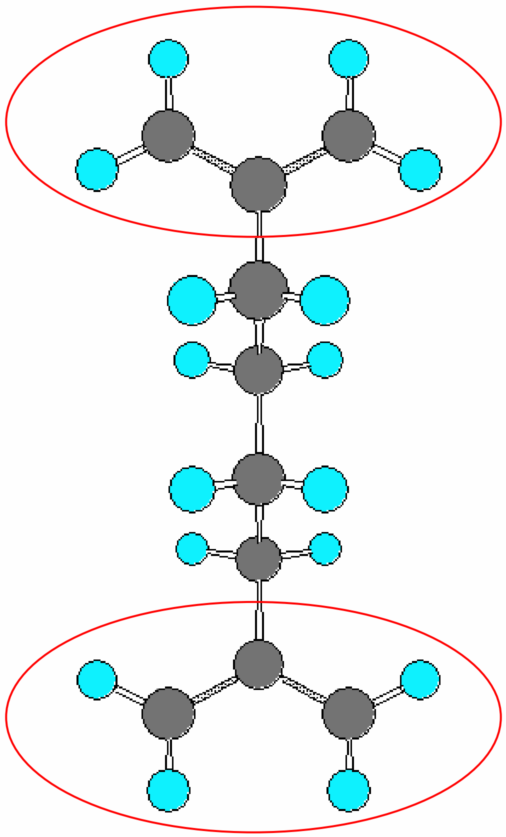
Key strategy: use *nonbonding* orbitals (π or d) to act as dots.

Aviram molecule: simple model system

1,4-diallyl butane radical cation







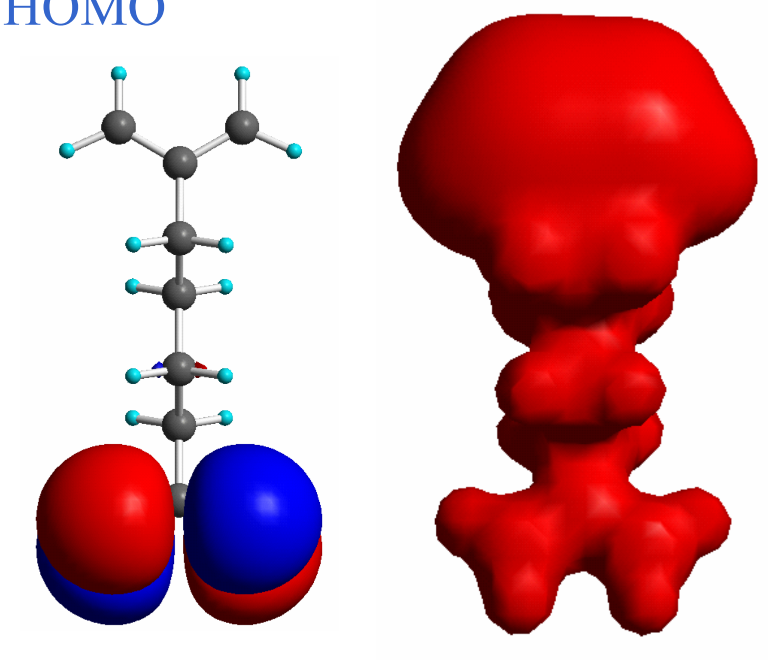
Use allyl groups as dots

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

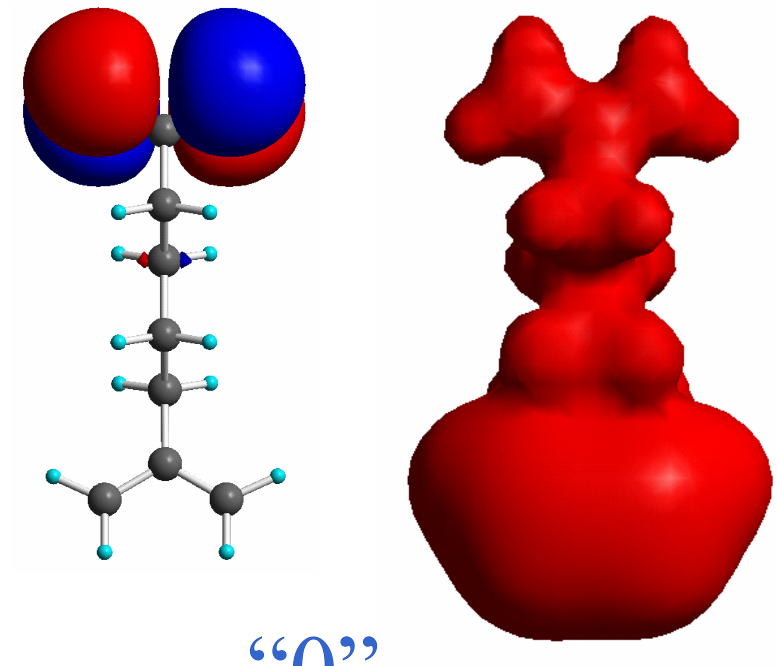
Charge configuration represents bit

HOMO

"1"



Gaussian 98 UHF/STO-3G

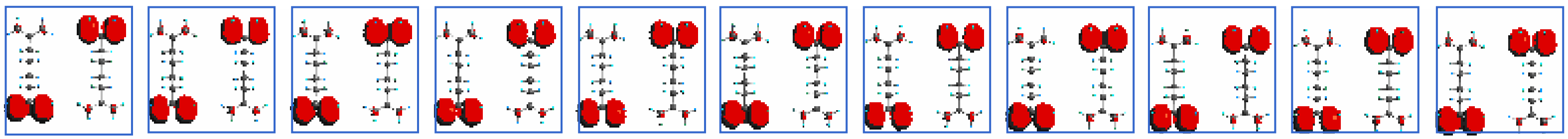


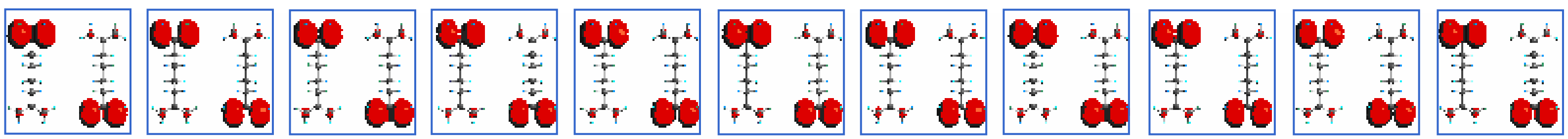
"0"

isopotential surface

Lent, Isaksen, Lieberman
Journal of American Chemical Society.
125, 1056 (2003)

Molecular wire

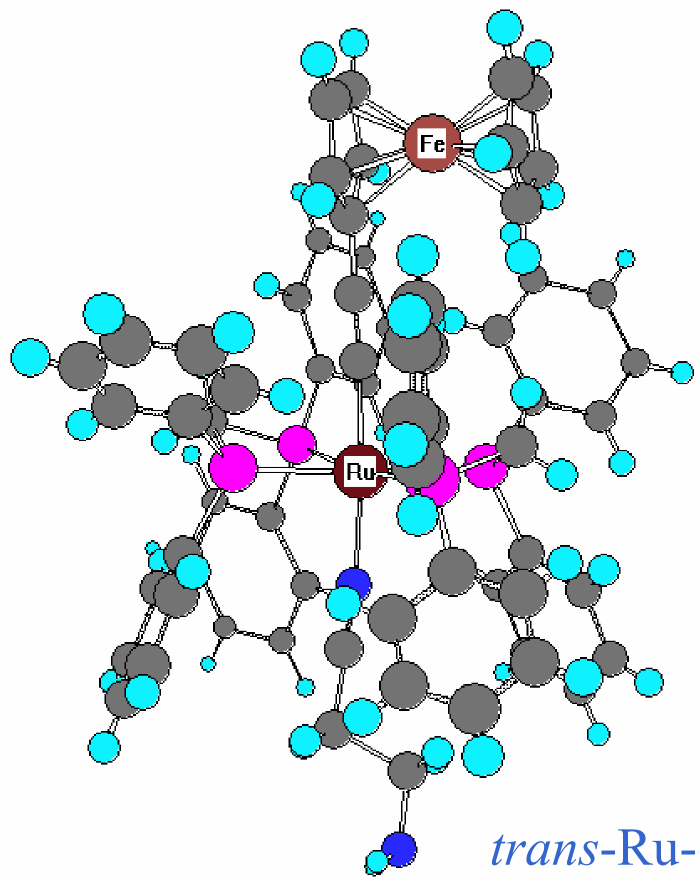
“0”  “0”

“1”  “1”

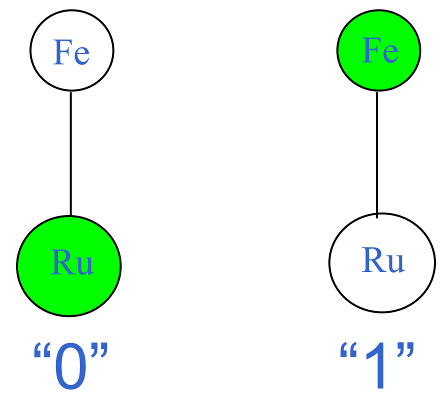
Extended Hückel (Gaussian 03)

Quantum chemistry calculation shows line acting as binary wire.

Experiments on molecular double-dot



Thomas Fehlner *et al.*
(Notre Dame chemistry group)
Journal of American Chemical Society, 125:15250, 2003



trans-Ru-$(dppm)_2(C{\equiv}CFc)(NCCH_2CH_2NH_2)$ dication

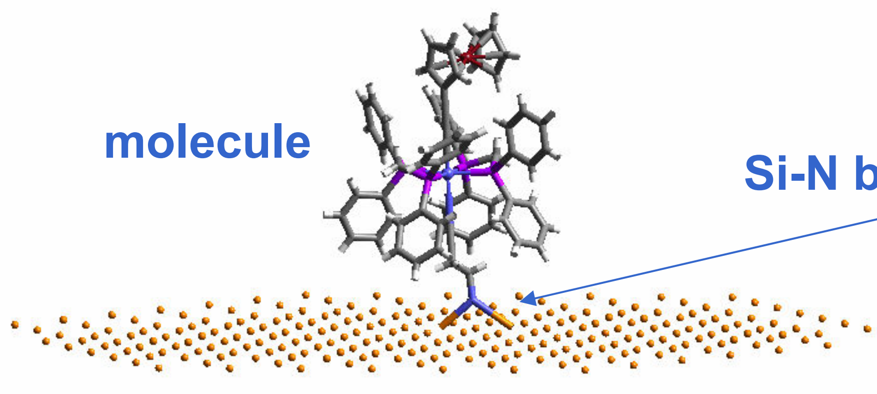
Fe group and Ru group act as two *unequal* quantum dots.

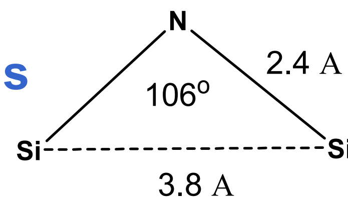
Surface attachment and orientation

molecule

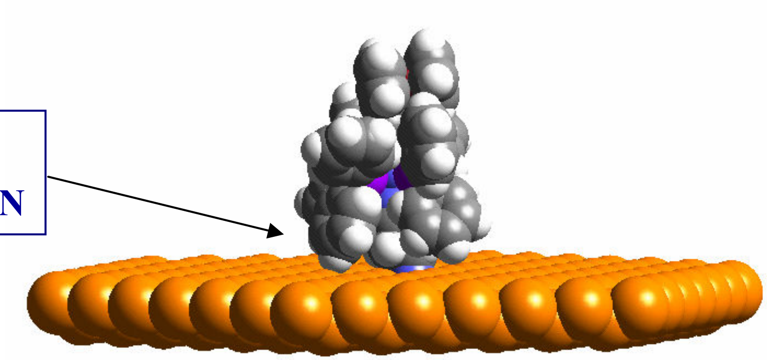
Si-N bonds

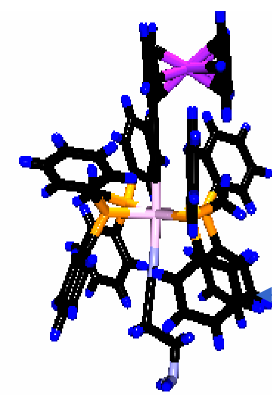
Si(111)





PHENYL GROUPS
"TOUCHING" SILICON

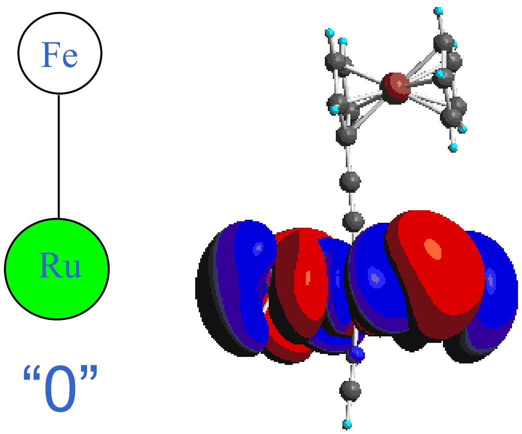


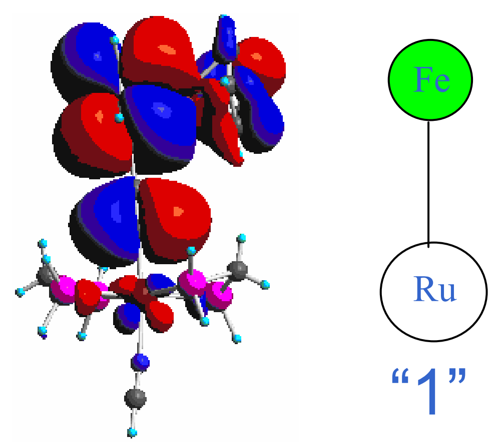


"struts"

Molecule is covalent bonded to Si and oriented vertically by "struts."

Charge configurations

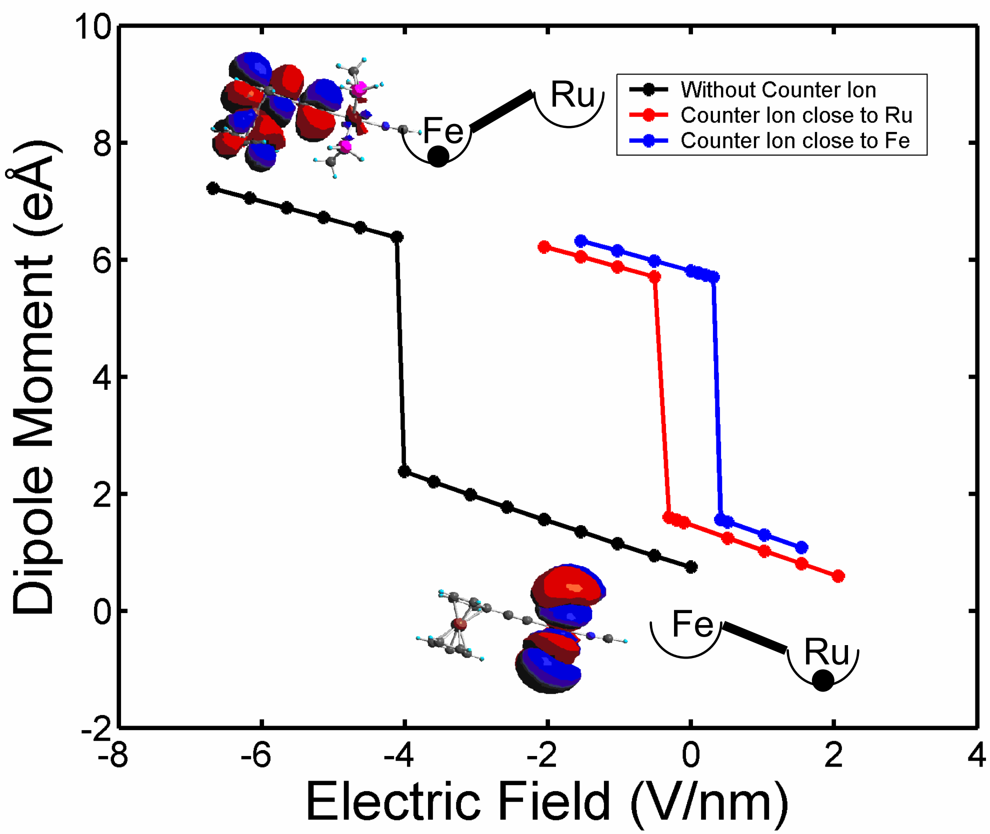




UHF/STO-3G/LANL2DZ

Bistable charge configuration.

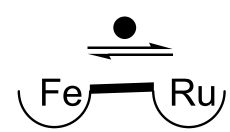
Switching by an applied field



Gaussian

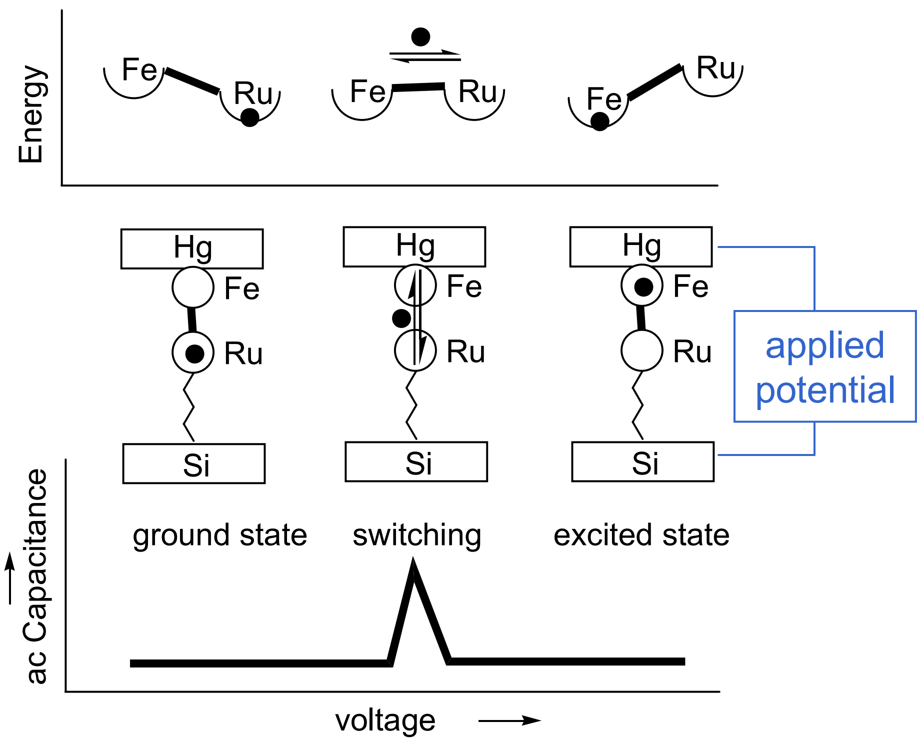
Mobile electron driven by electric field, the effect of counterions shift the response function.

Click-clack correspond to:

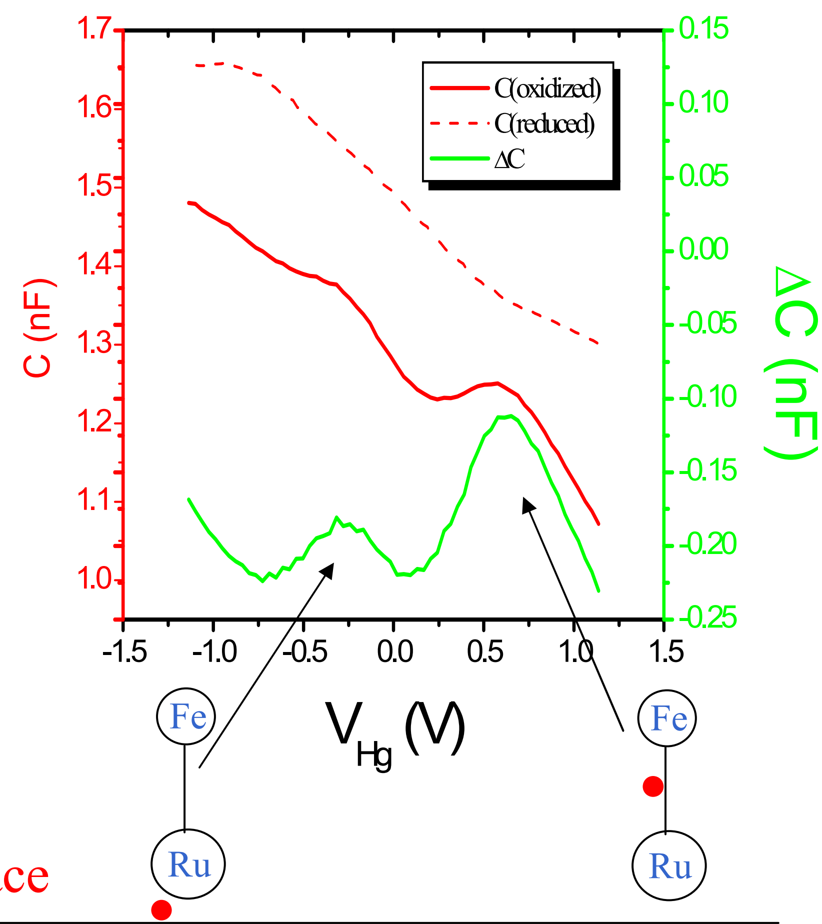


Measurement of molecular bistability

Applied field ***equalizes*** the energy of the two dots



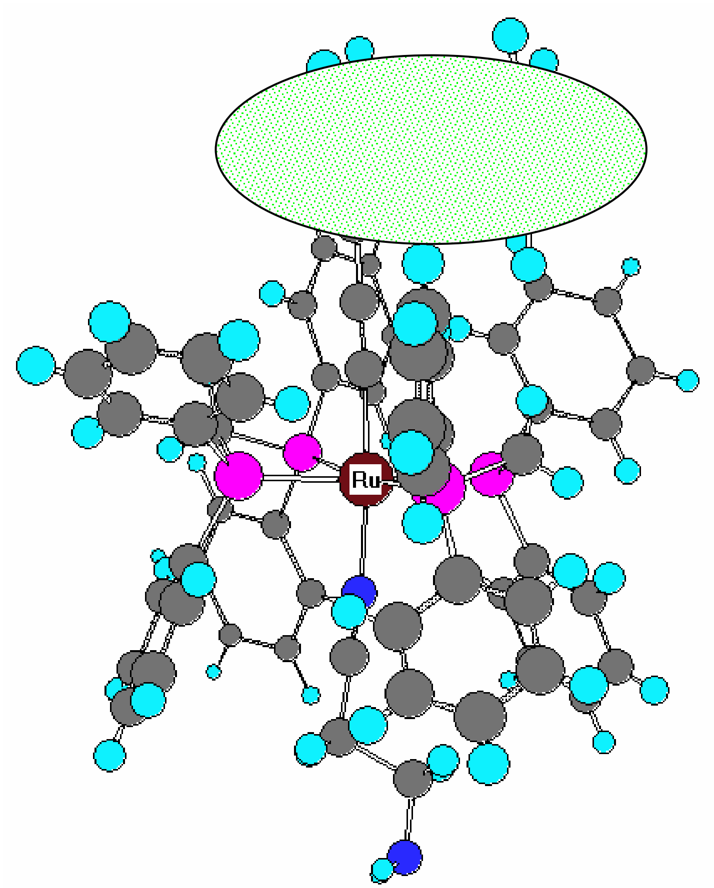
layer of molecules

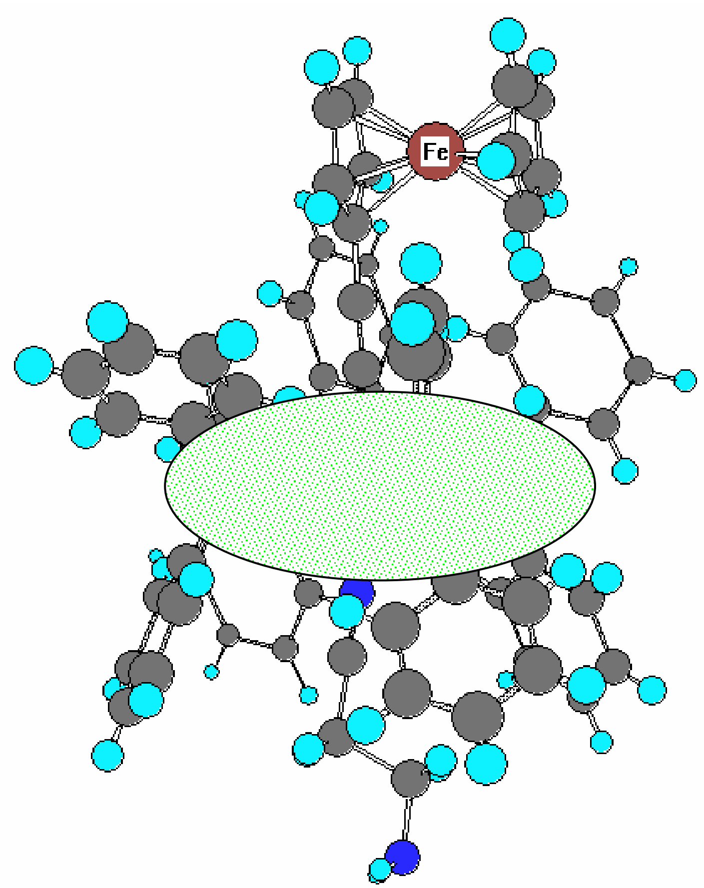


When equalized, capacitance peaks.

2 counterion charge configurations on surface

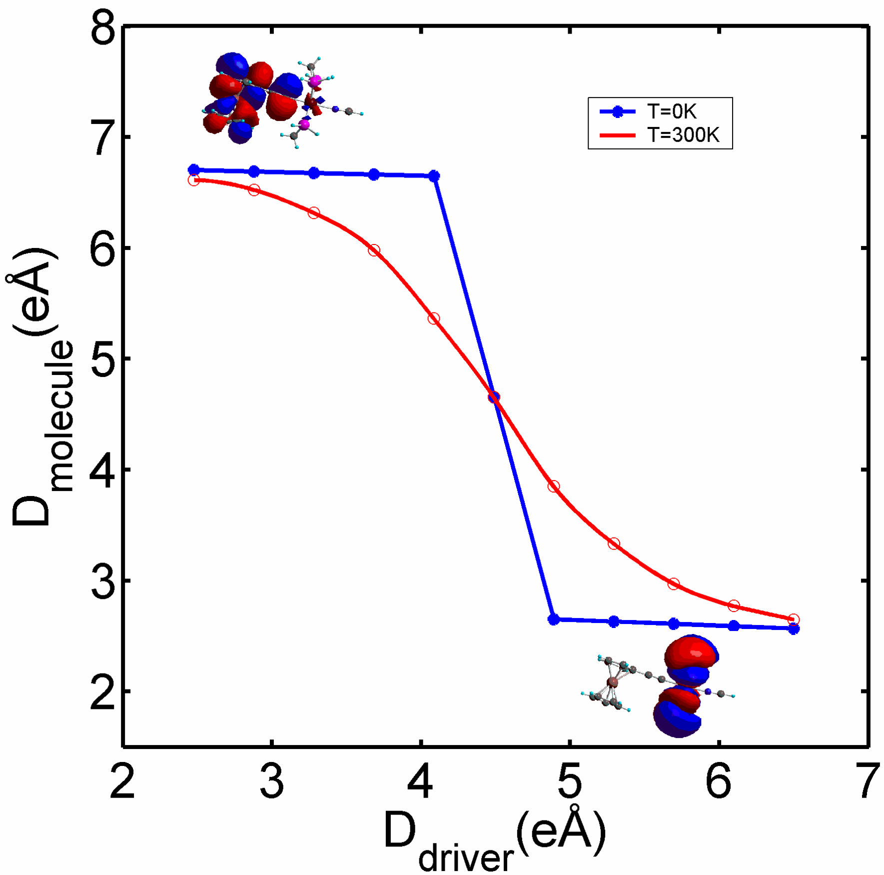
Molecule-molecule interaction





Can one molecule switch another molecule?

Switching by a neighboring molecule



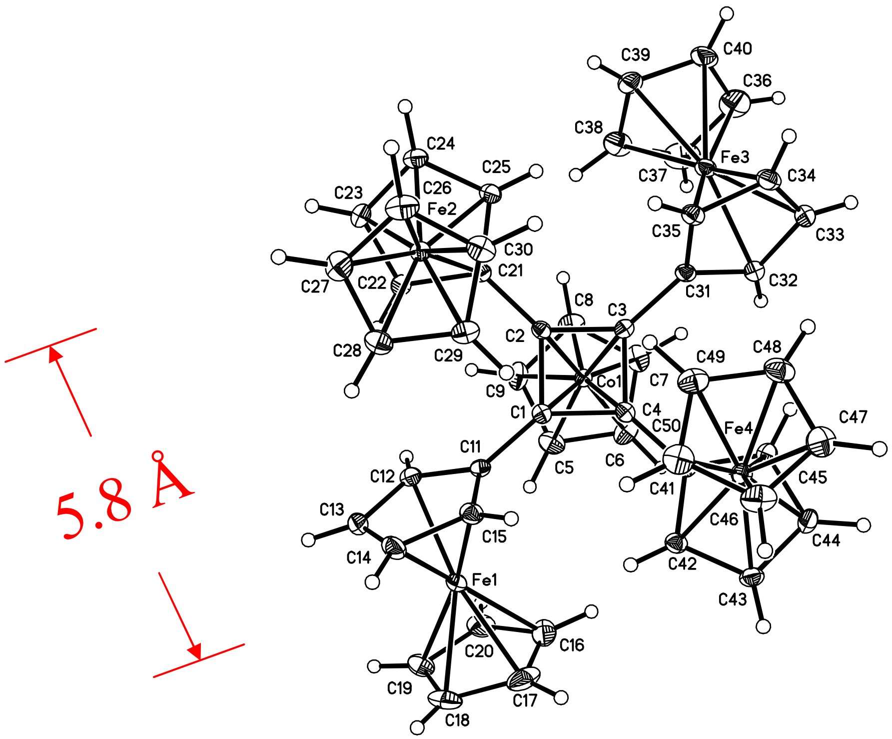
The distance between Neighboring molecules: 1 nm

External electric field: 1.2 V/nm

All counterions attach to the substrate

One molecule ***can*** switch a neighboring molecule.

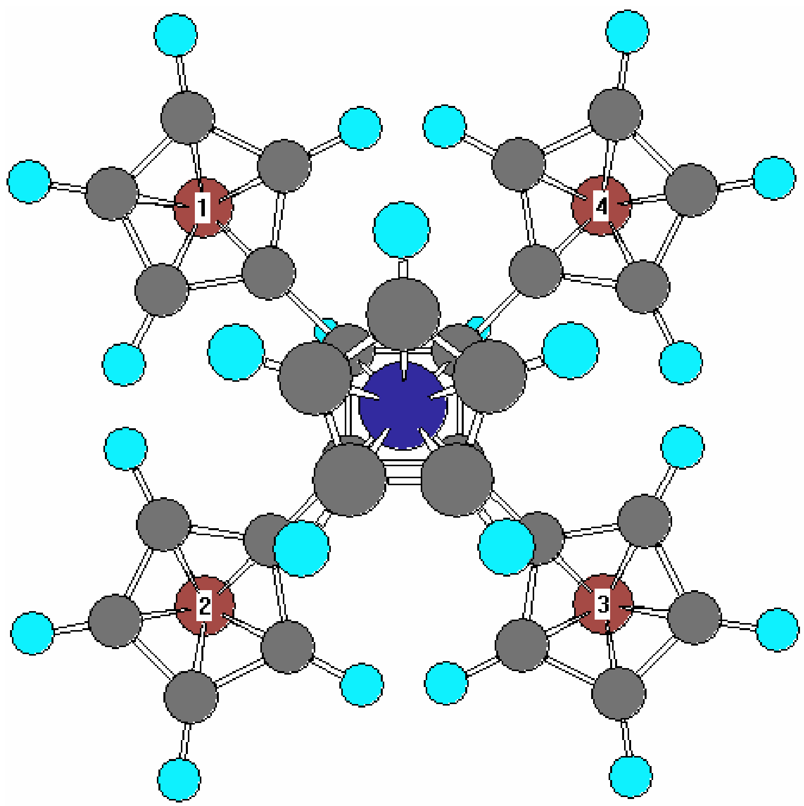
4-dot molecule

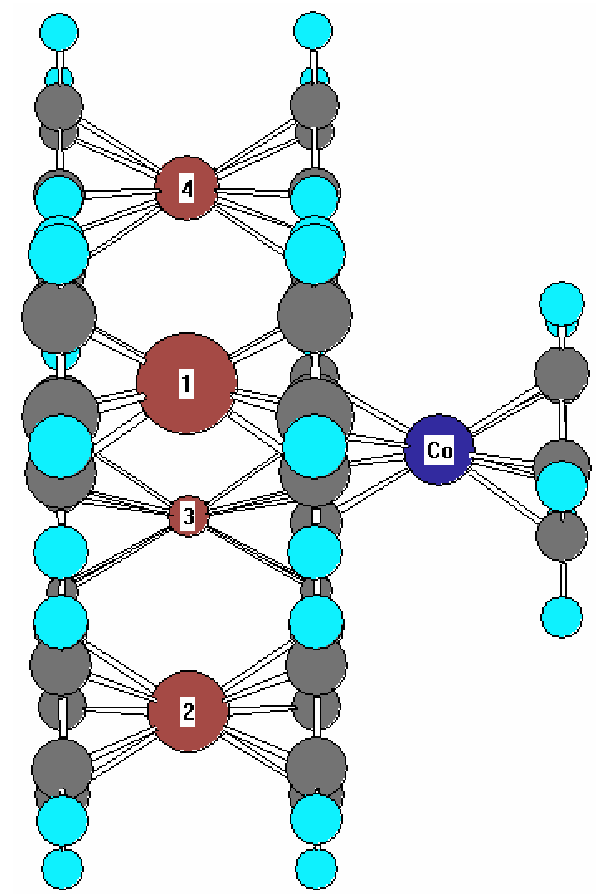


Fehlner *et al*
(Notre Dame chemistry group)
Journal of American Chemical Society
125:7522, 2003

Each ferrocene acts as a quantum dot, the Co group connects 4 dots.

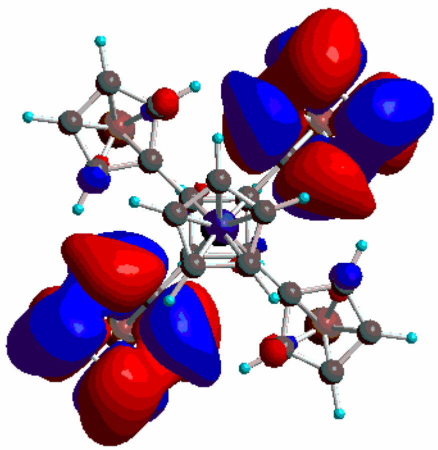
4-dot molecule



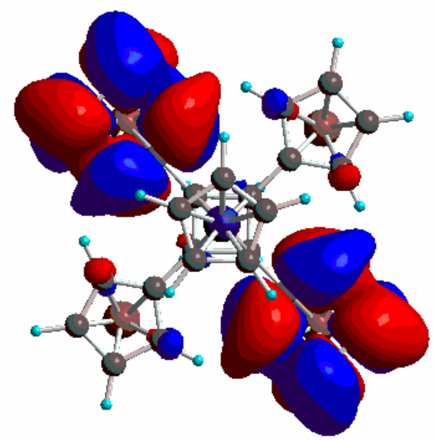


Self-assembly of 4-dot cell—no legs or struts.

Bistable configurations



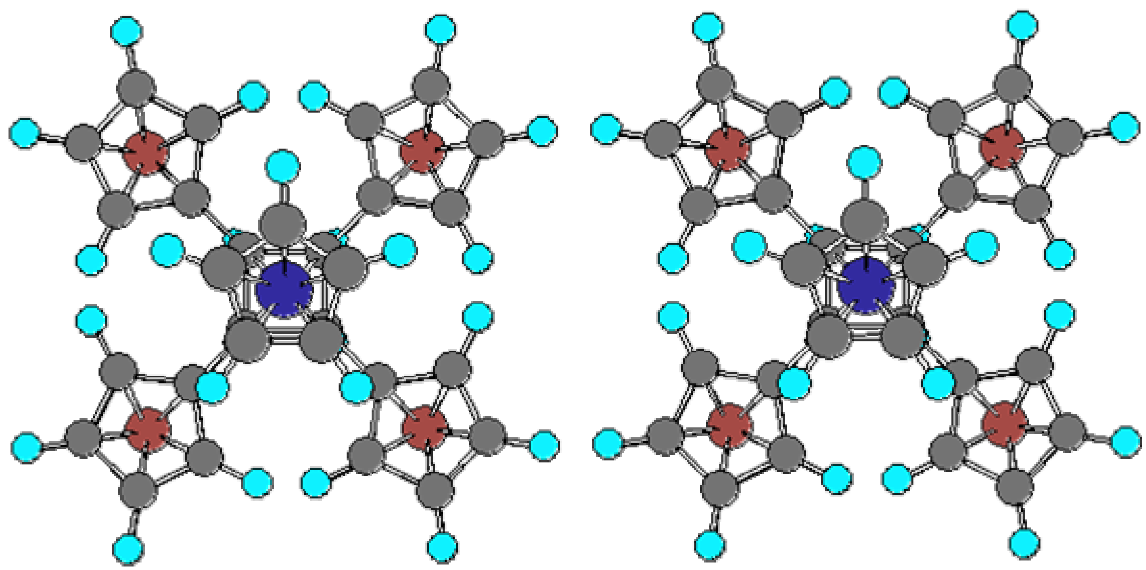
“0”



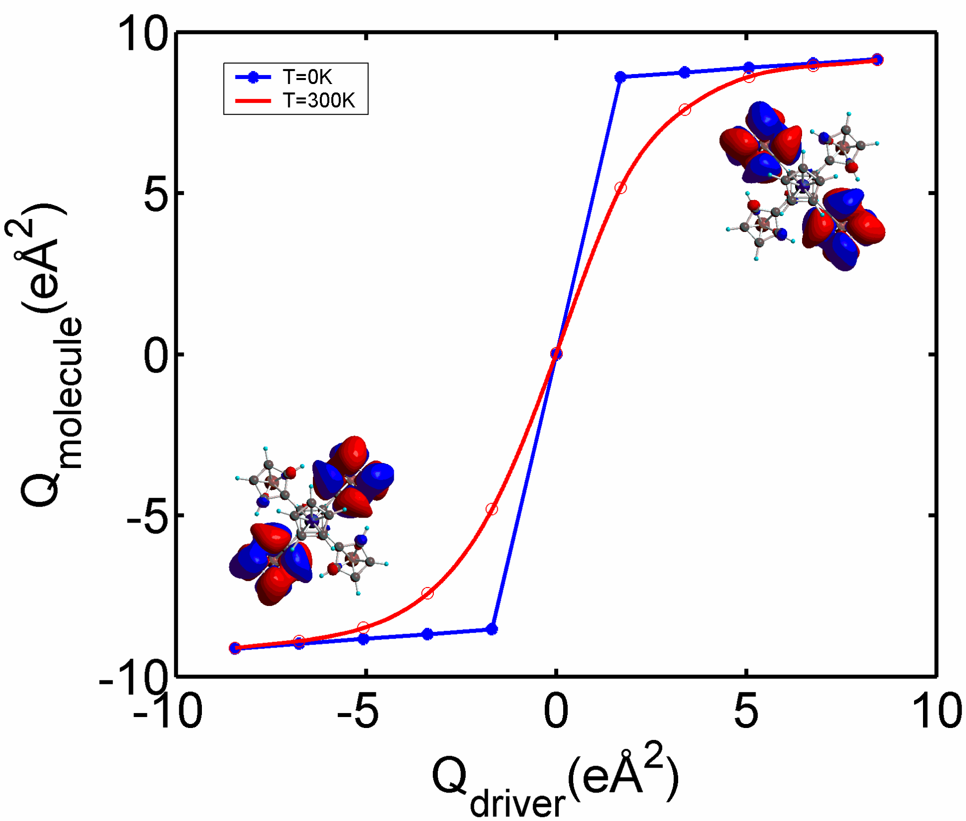
“1”

Guassian-98 UHF/STO-3G/LANL2DZ

Can one molecule switch the other ?

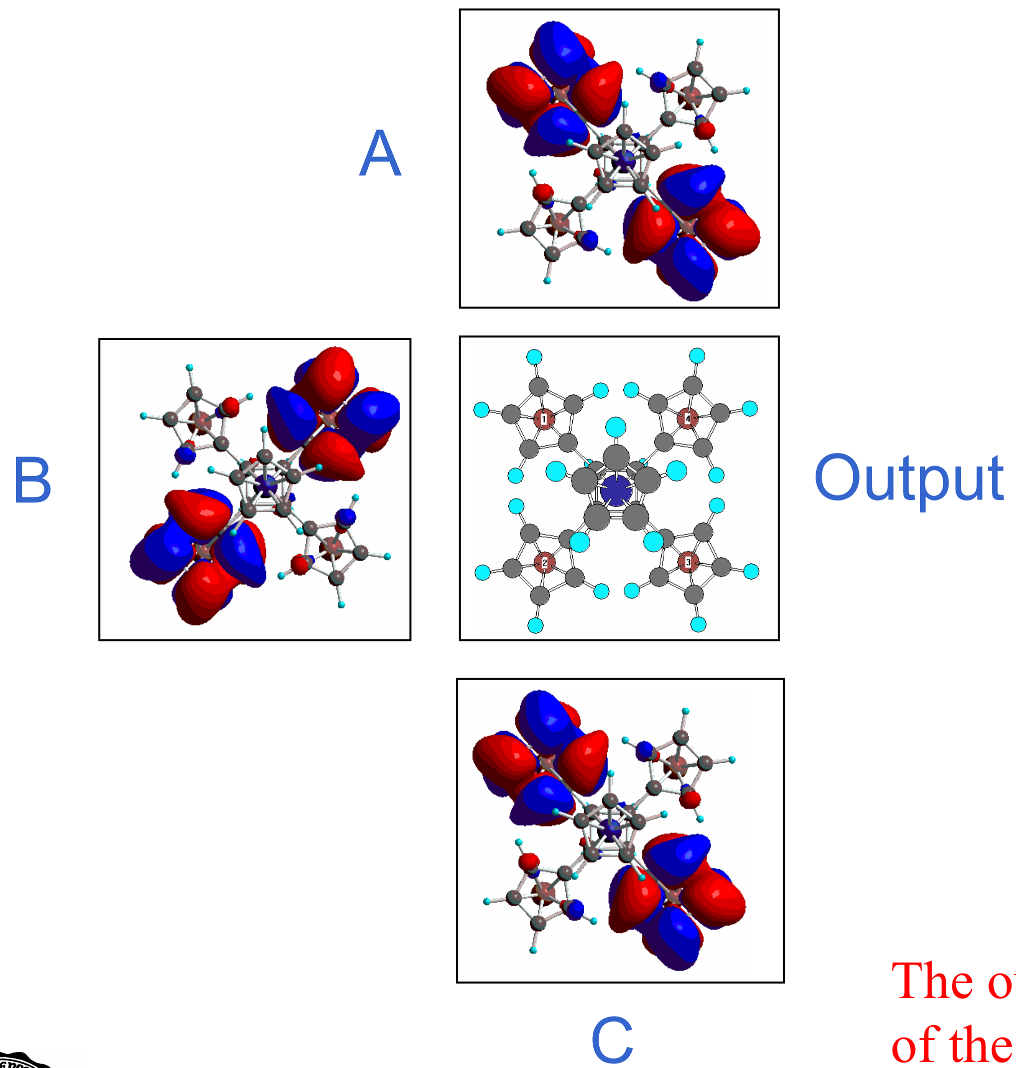


Switching molecule by a neighboring molecule



Coulomb interaction is sufficient to couple molecular states.

Majority gate



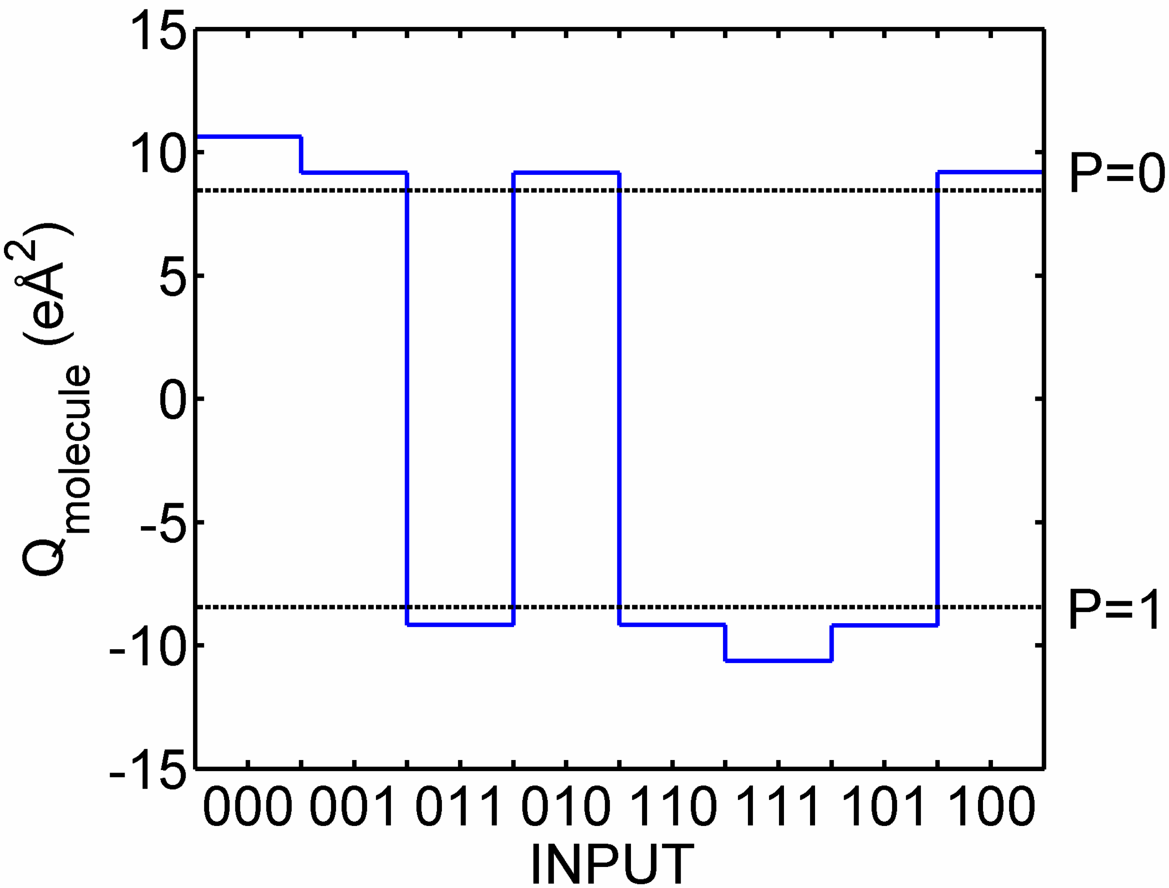
A	B	C	Output
0	0	0	0
0	0	1	0
0	1	1	1
0	1	0	0
1	1	0	1
1	1	1	1
1	0	1	1
1	0	0	0

AND gate (rows with A = 0)

OR gate (rows with A = 1)

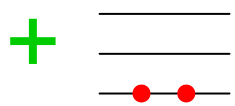
The output cell assumes the value of the majority of the input cells.

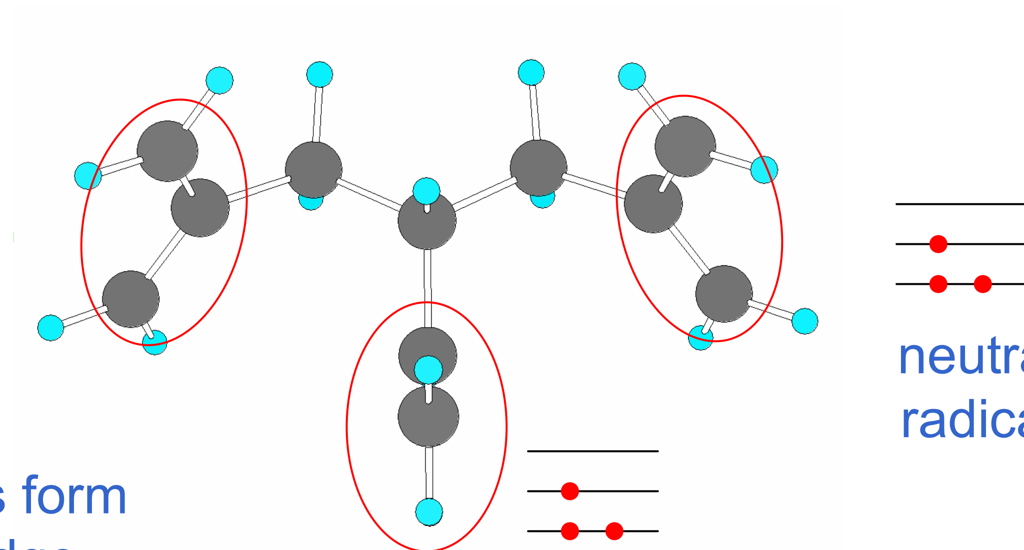
Calculated response



Majority gate operation confirmed (in theory).

Molecular 3-dot cell

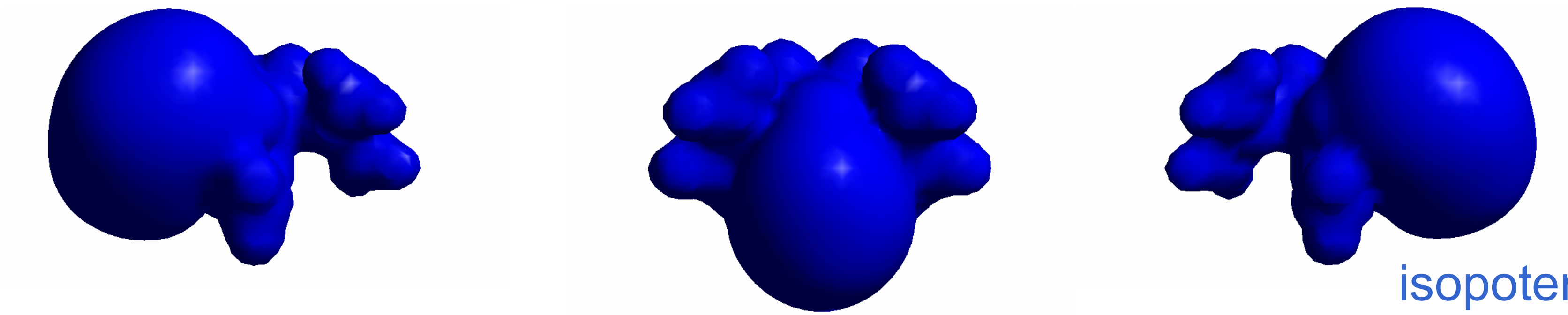




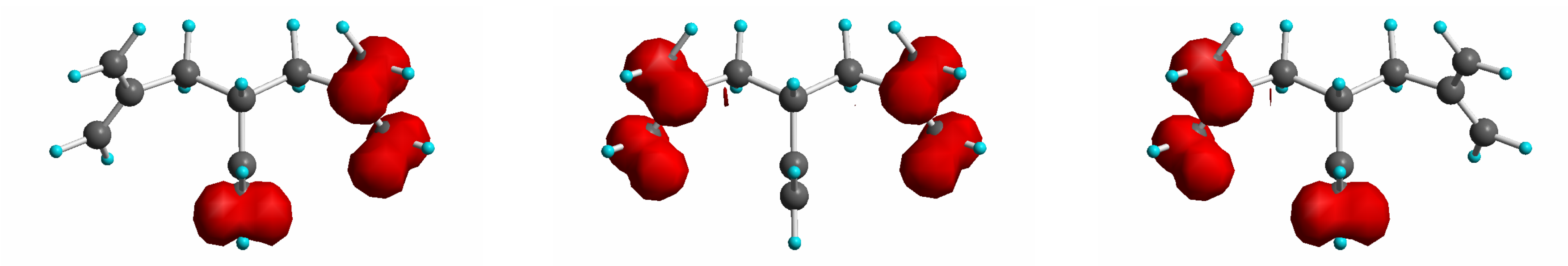
Three allyl groups form “dots” on alkyl bridge.

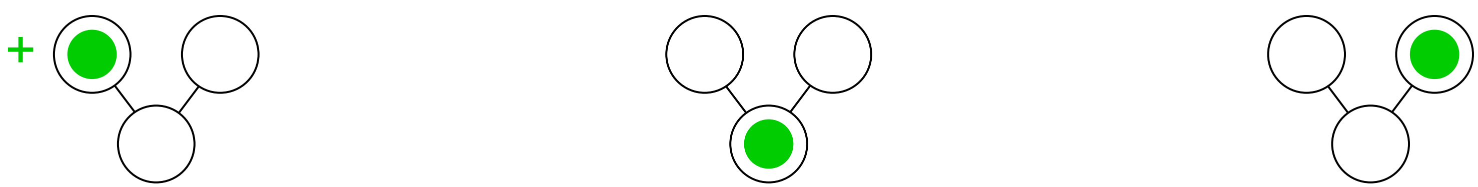
For the molecular cation, a hole occupies one of three dots.

Charge configuration represents bit



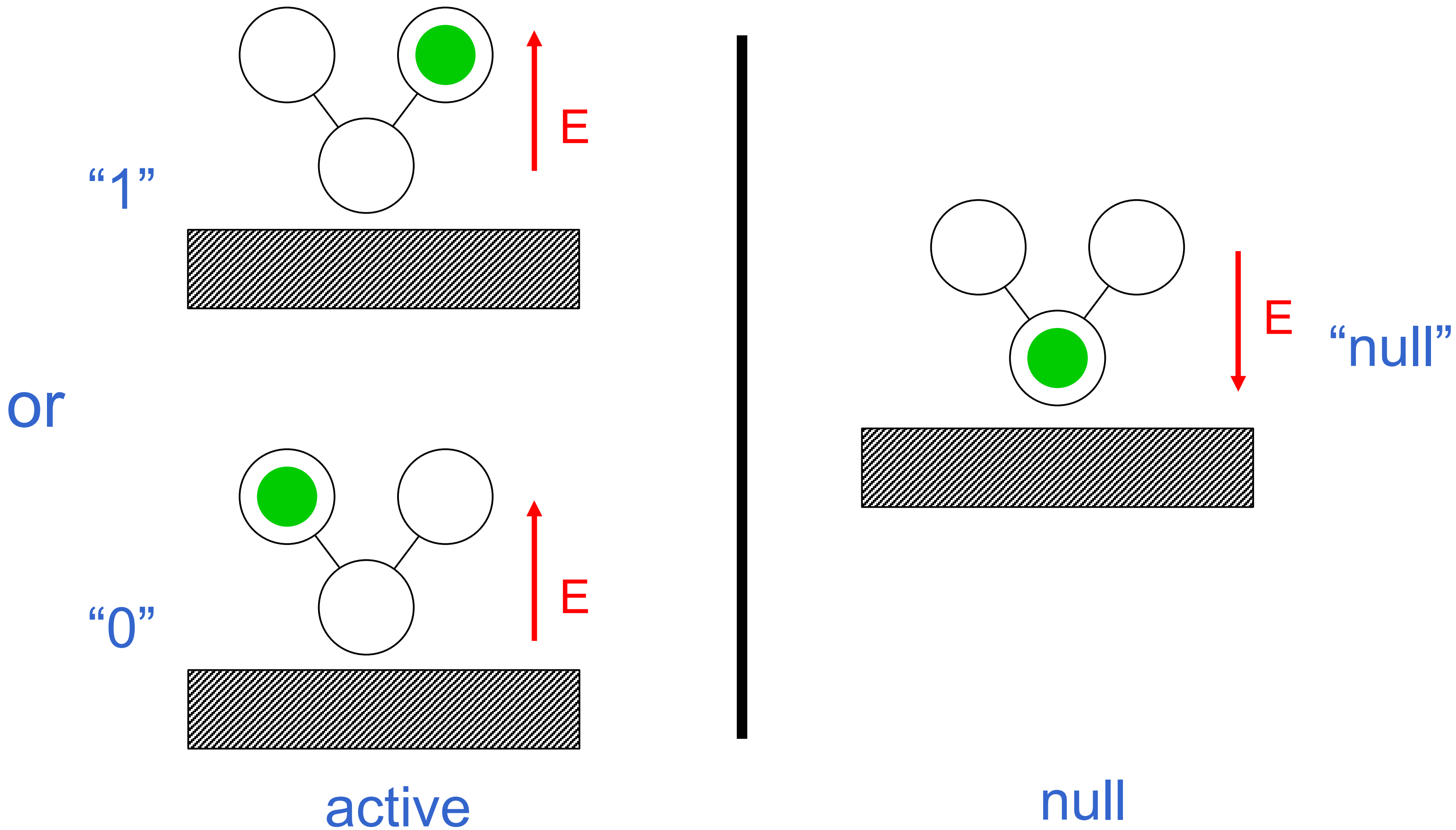
isopotential surfaces





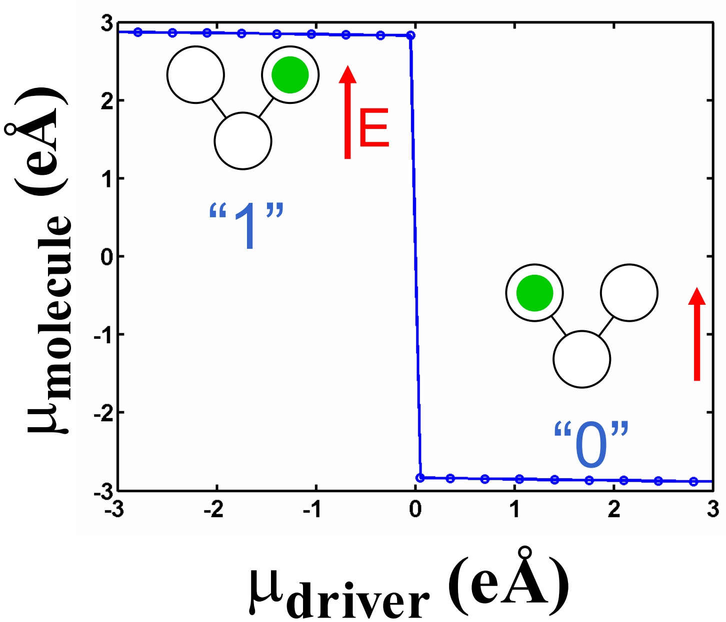
"0"   "null"   "1"

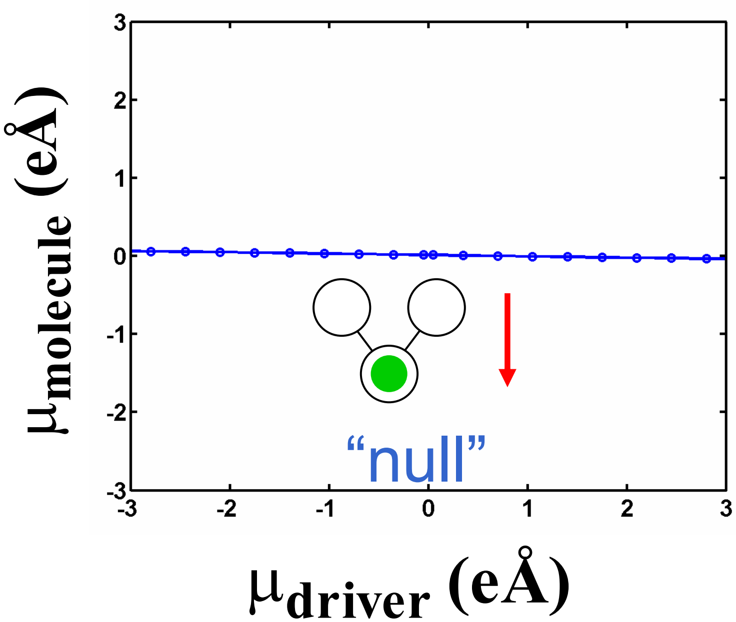
Clocking field



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

Clocking field alters response function

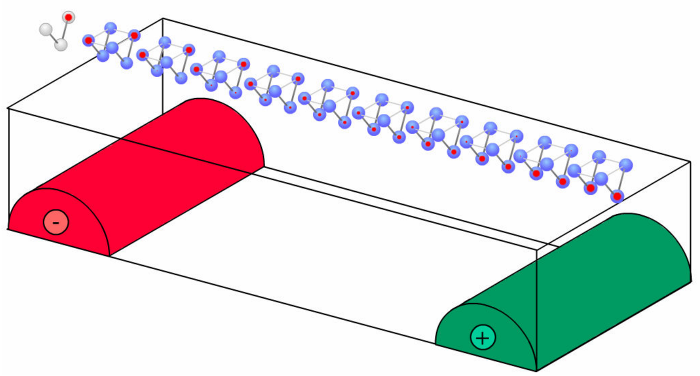


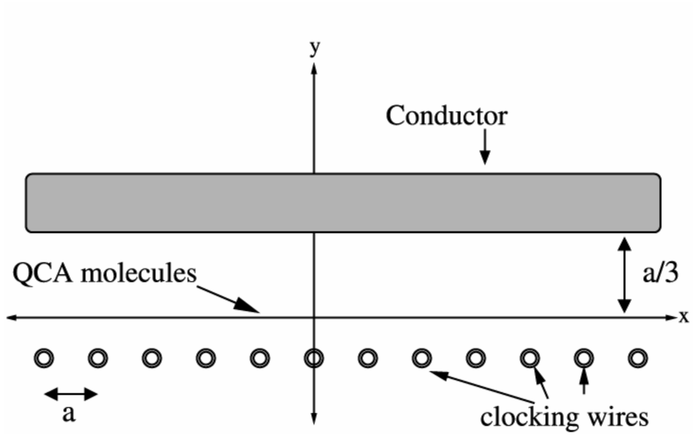


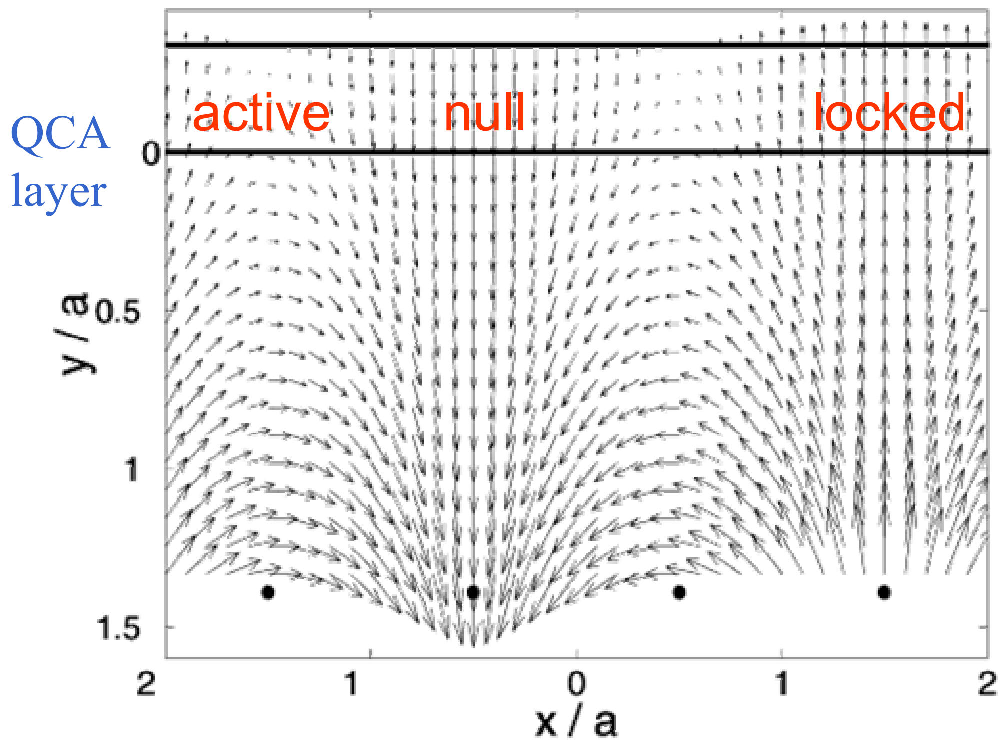
- Clocking field positive (or zero)
- Positive charge in top dots
- Cell is active – nonlinear response to input

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

Clocked Molecular QCA



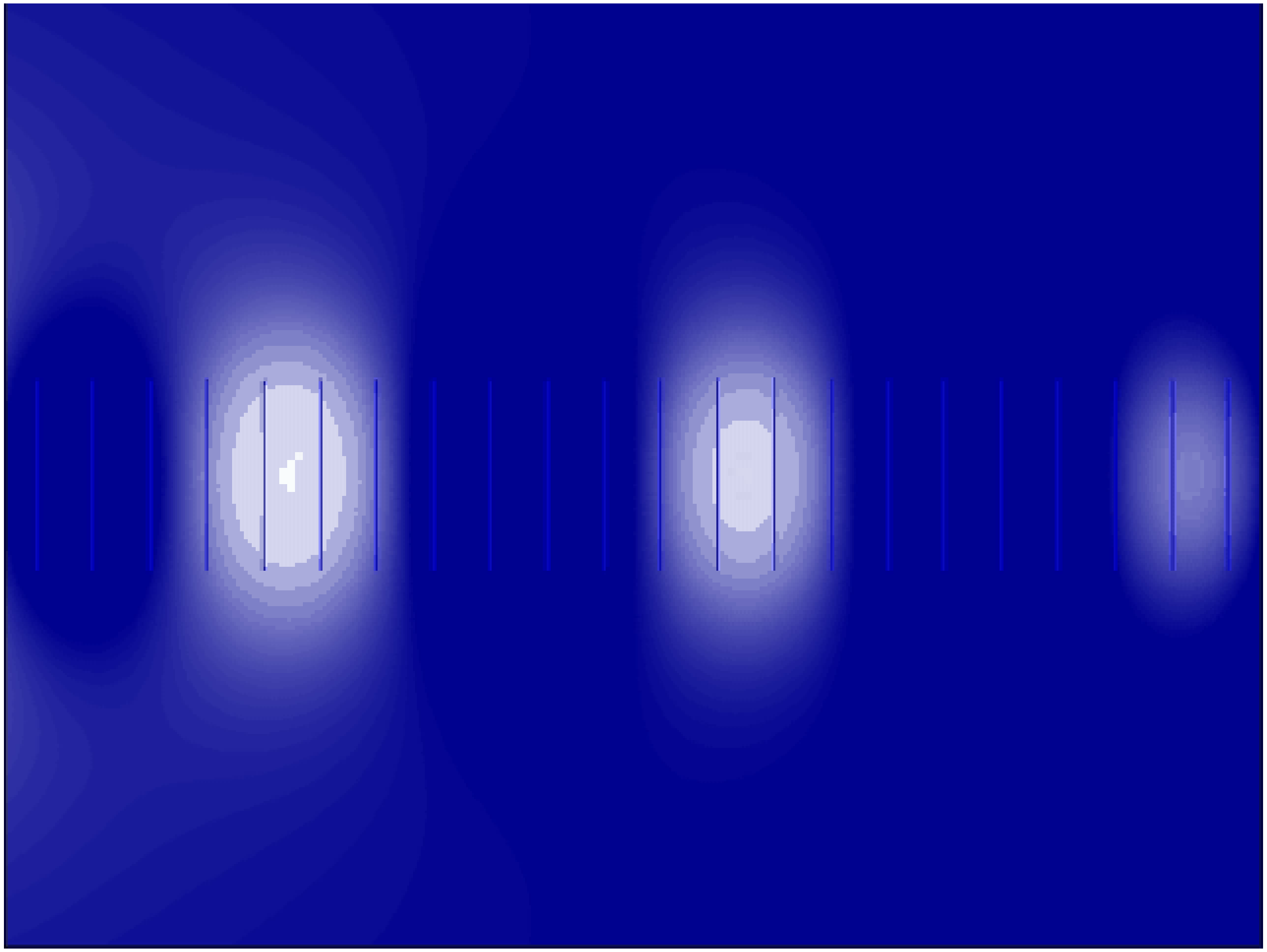




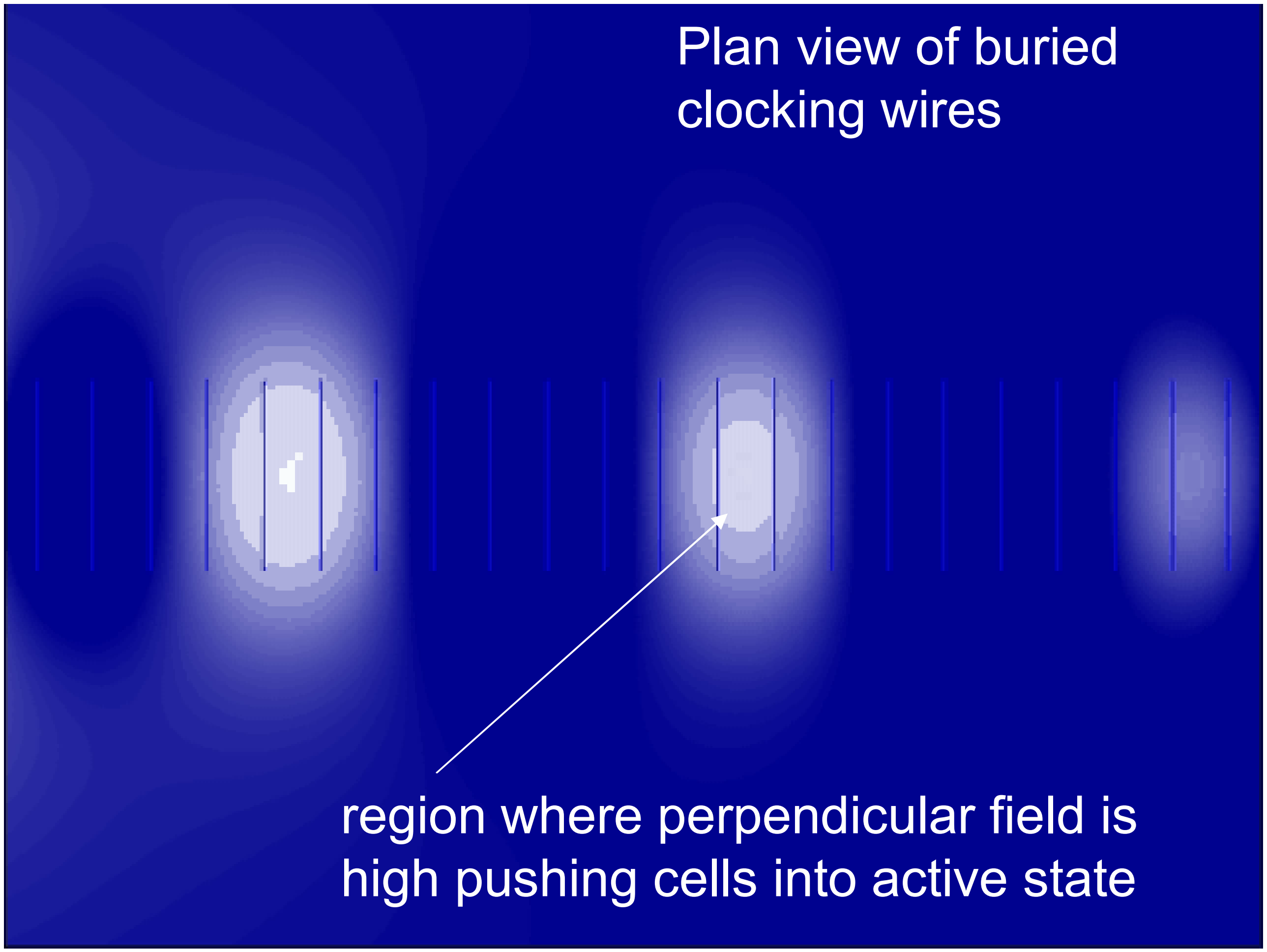
Hennessey and Lent, JVST (2001)

Active domains can be moved across surface by applying a time-varying voltage to the clocking wires.

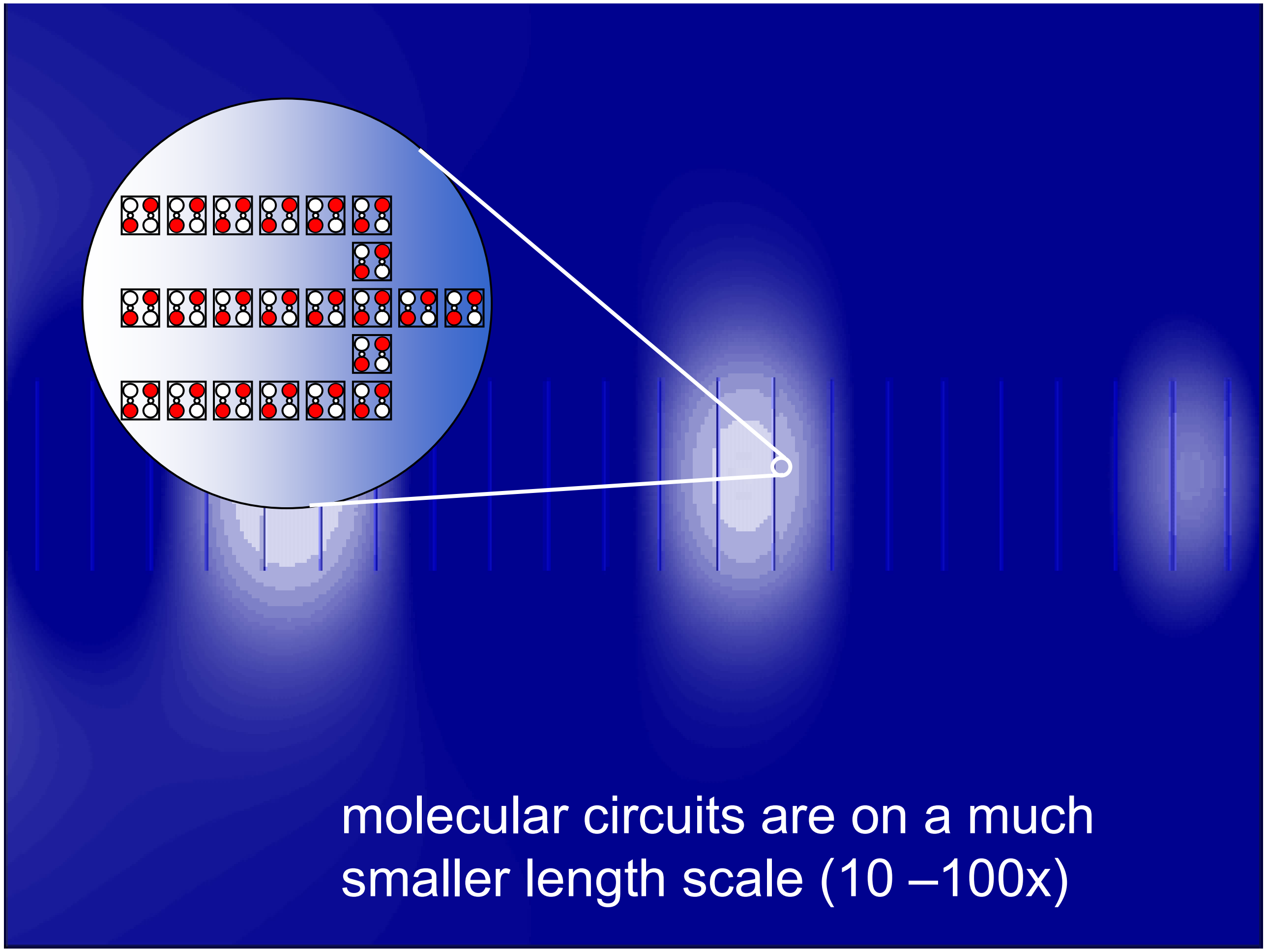
Clocking field: linear motion



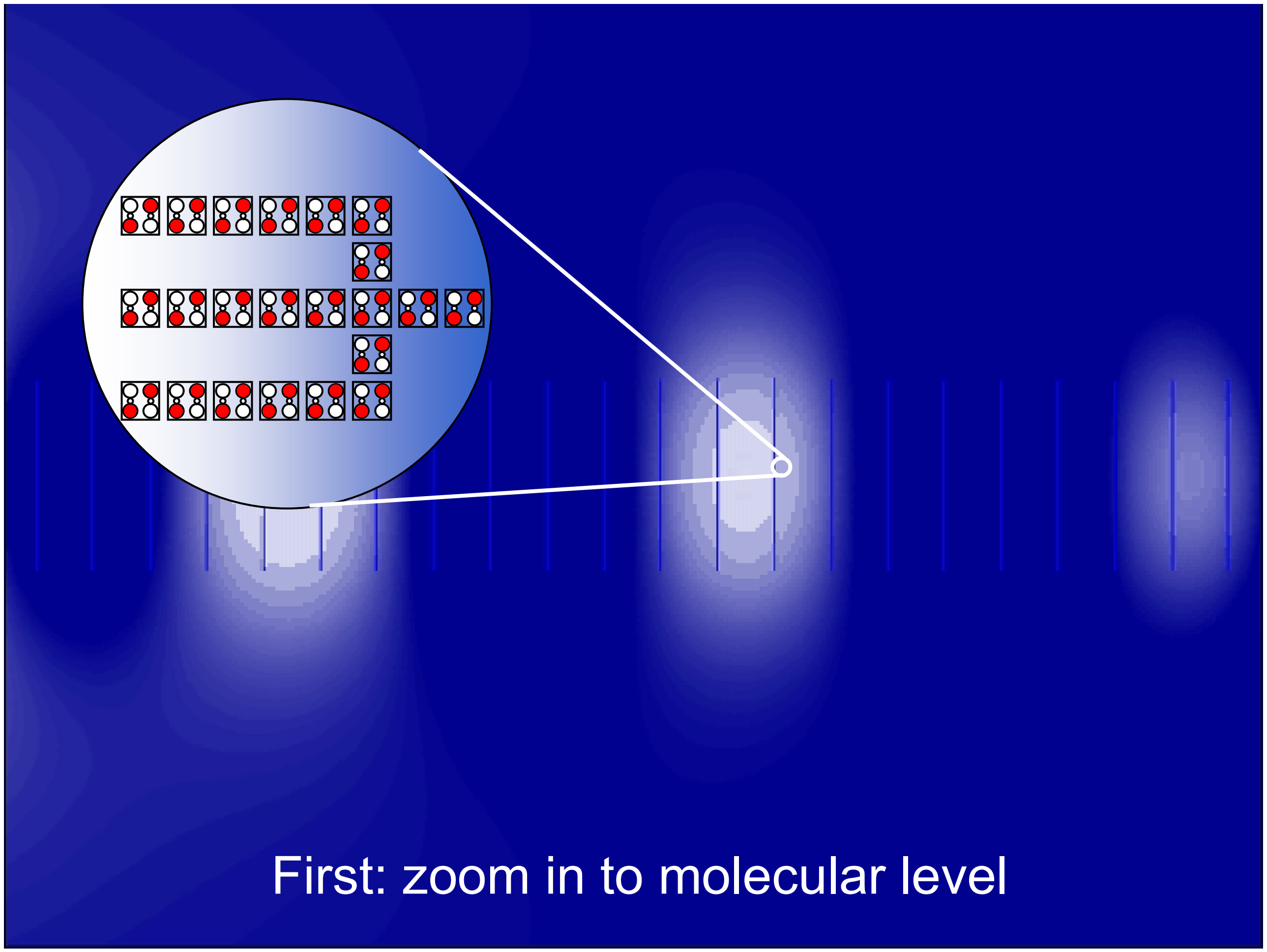
Molecular circuits and clocking wires



Molecular circuits and clocking wires



Molecular circuits and clocking wires



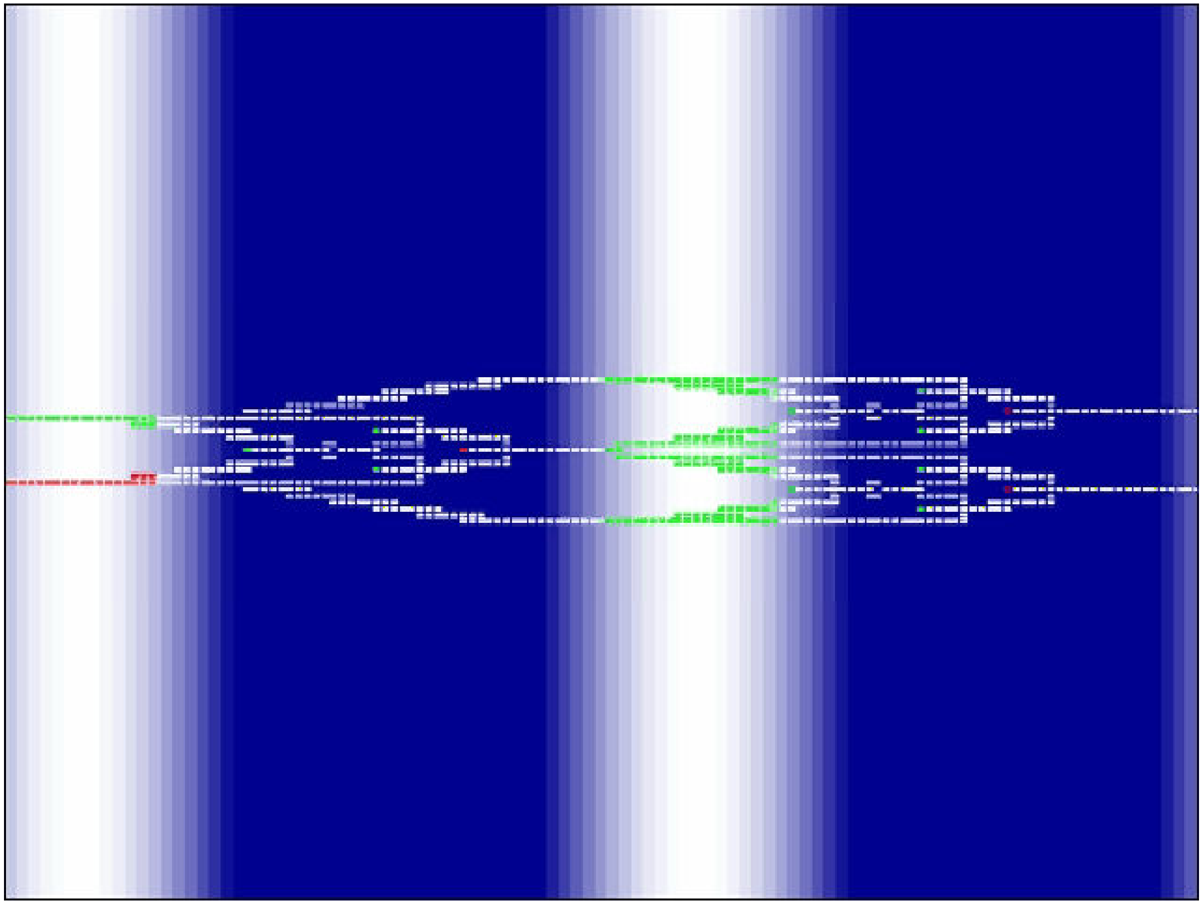
Field-clocking of QCA wire: shift-register

Computational wave: majority gate

Computational wave: adder back-end

XOR Gate

Permuter



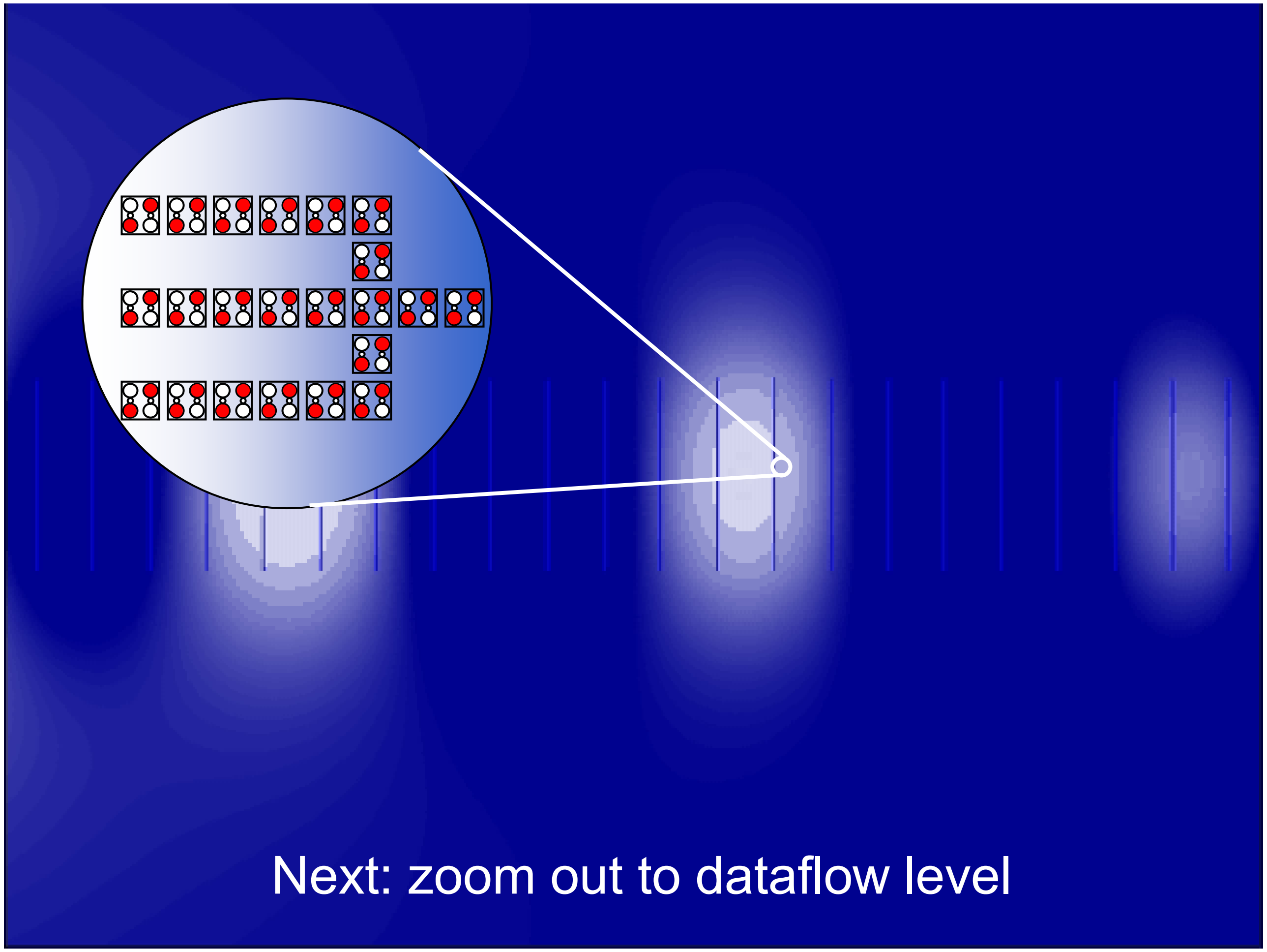
Triple-Wide Wire

Advantages: easier fabrication, works at higher temperatures

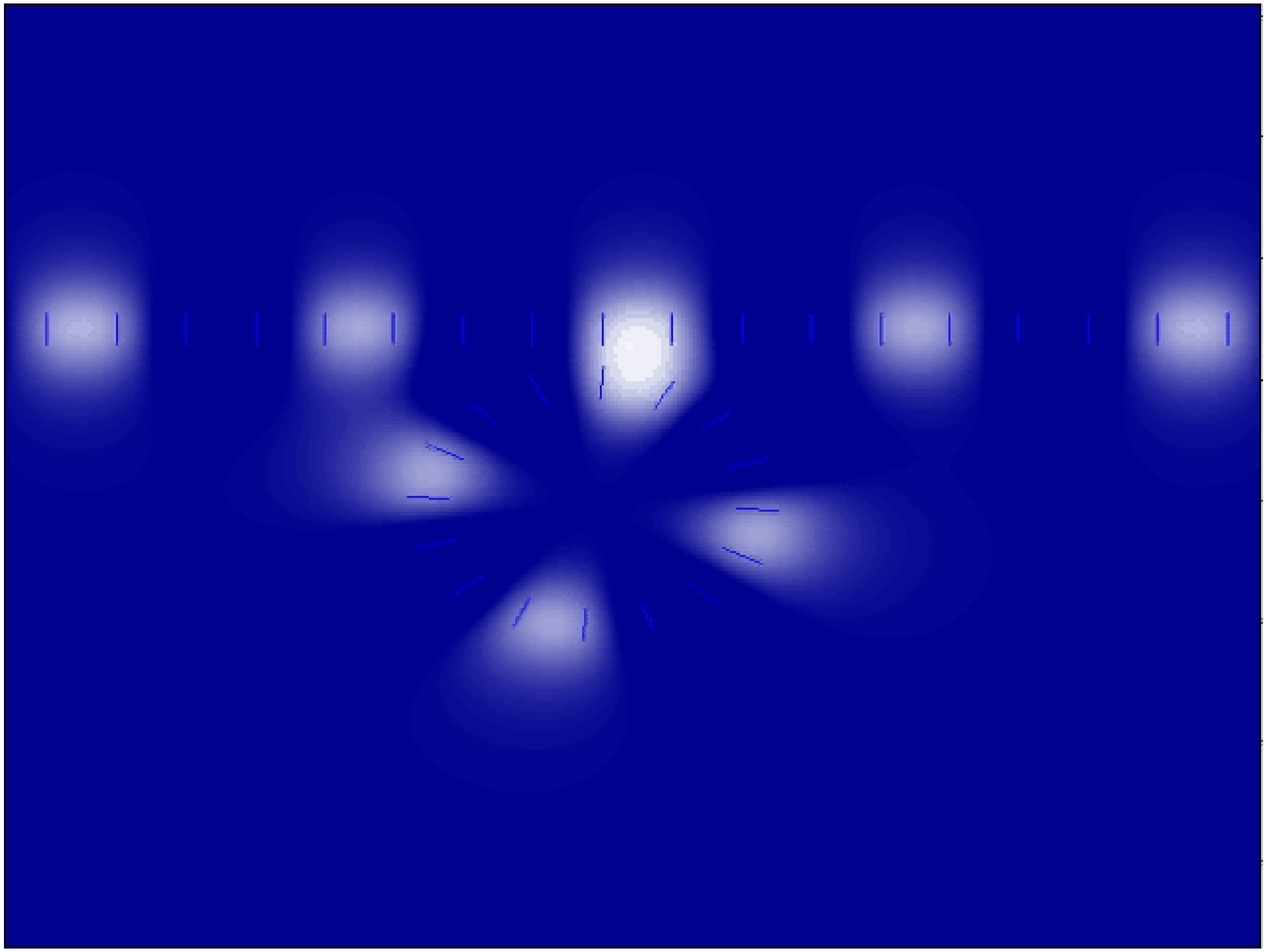
Wider QCA wires

Redundancy results in defect tolerance.

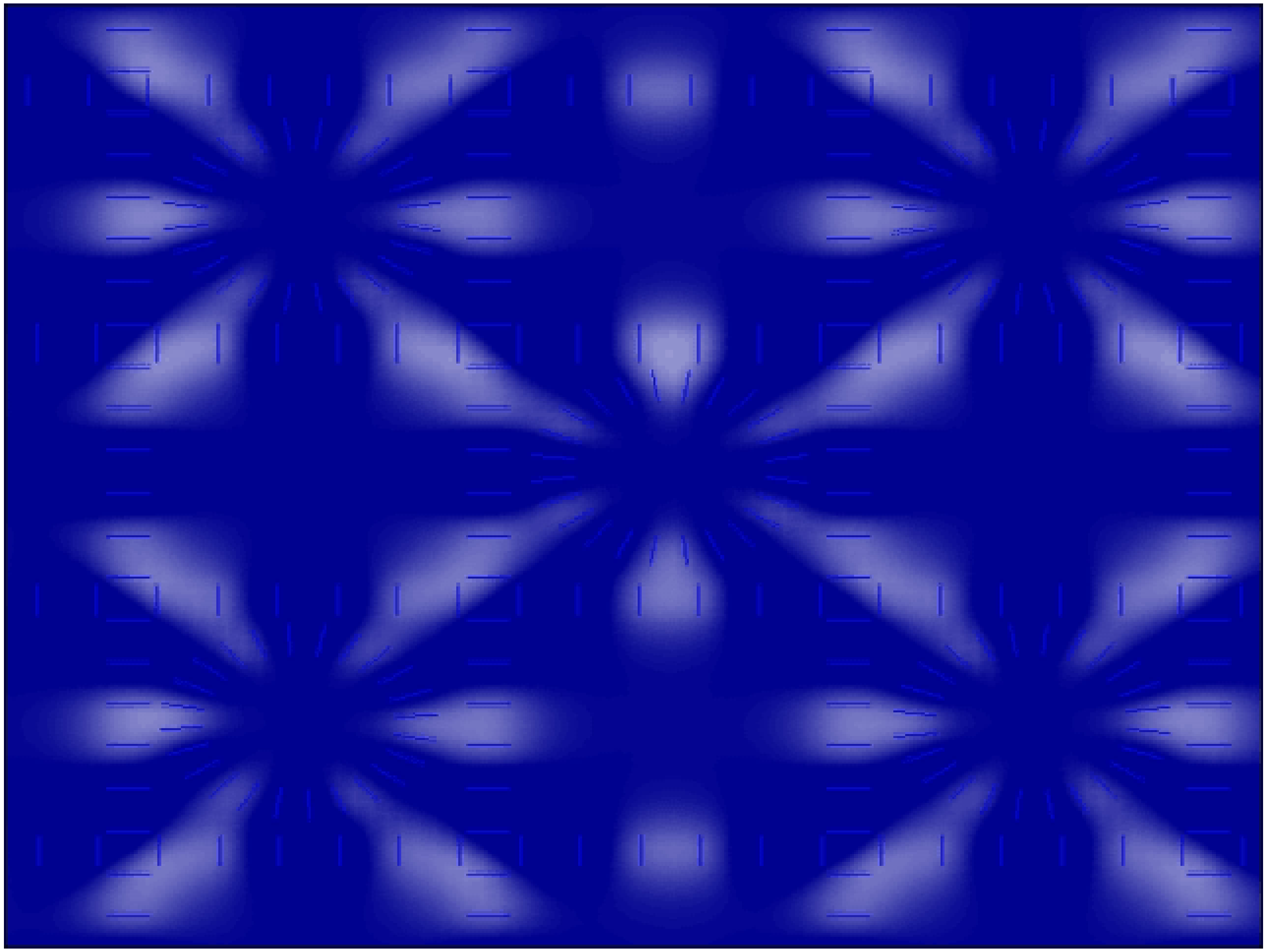
Molecular circuits and clocking wires



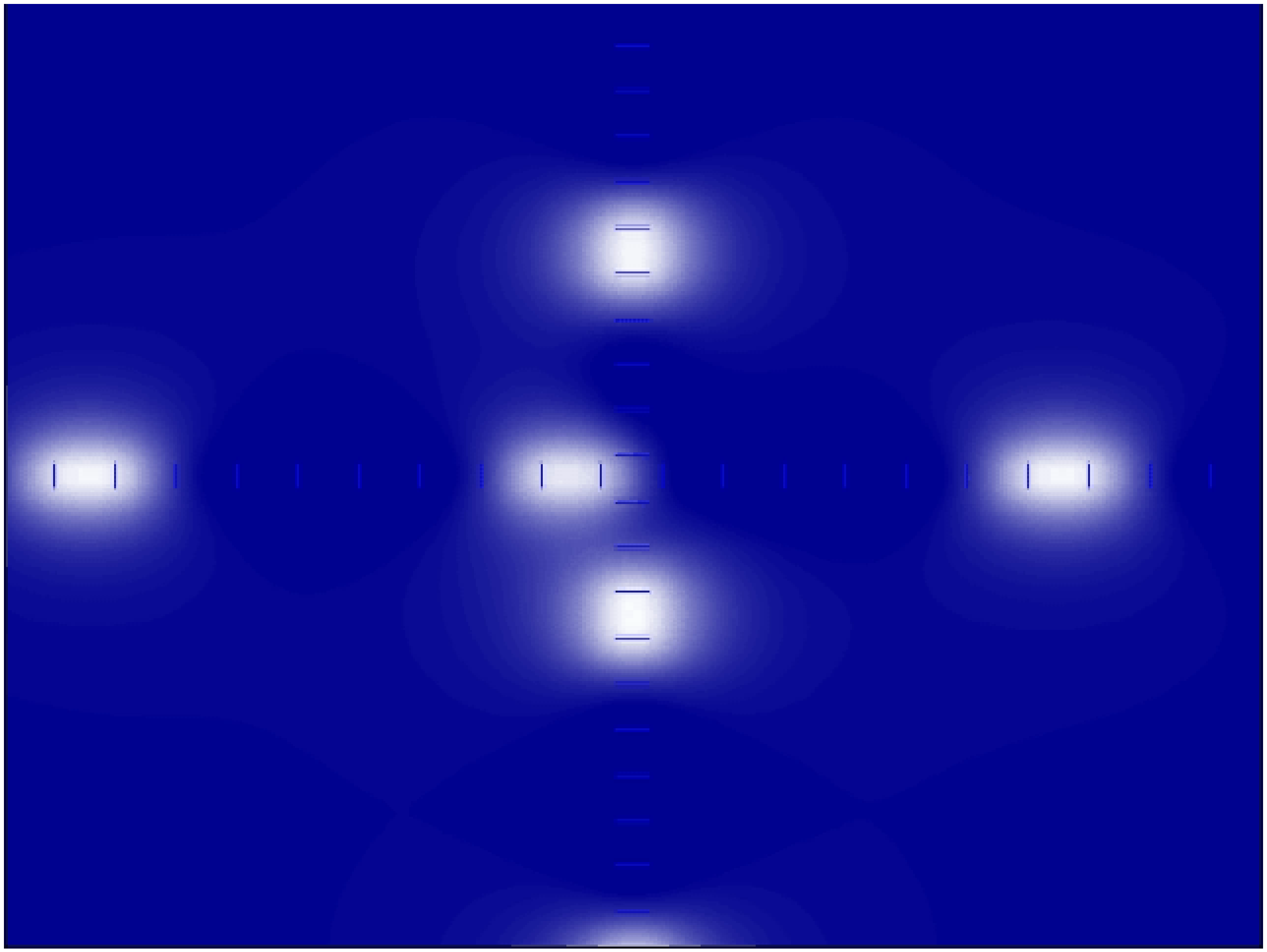
Clocking field: propagation + loop



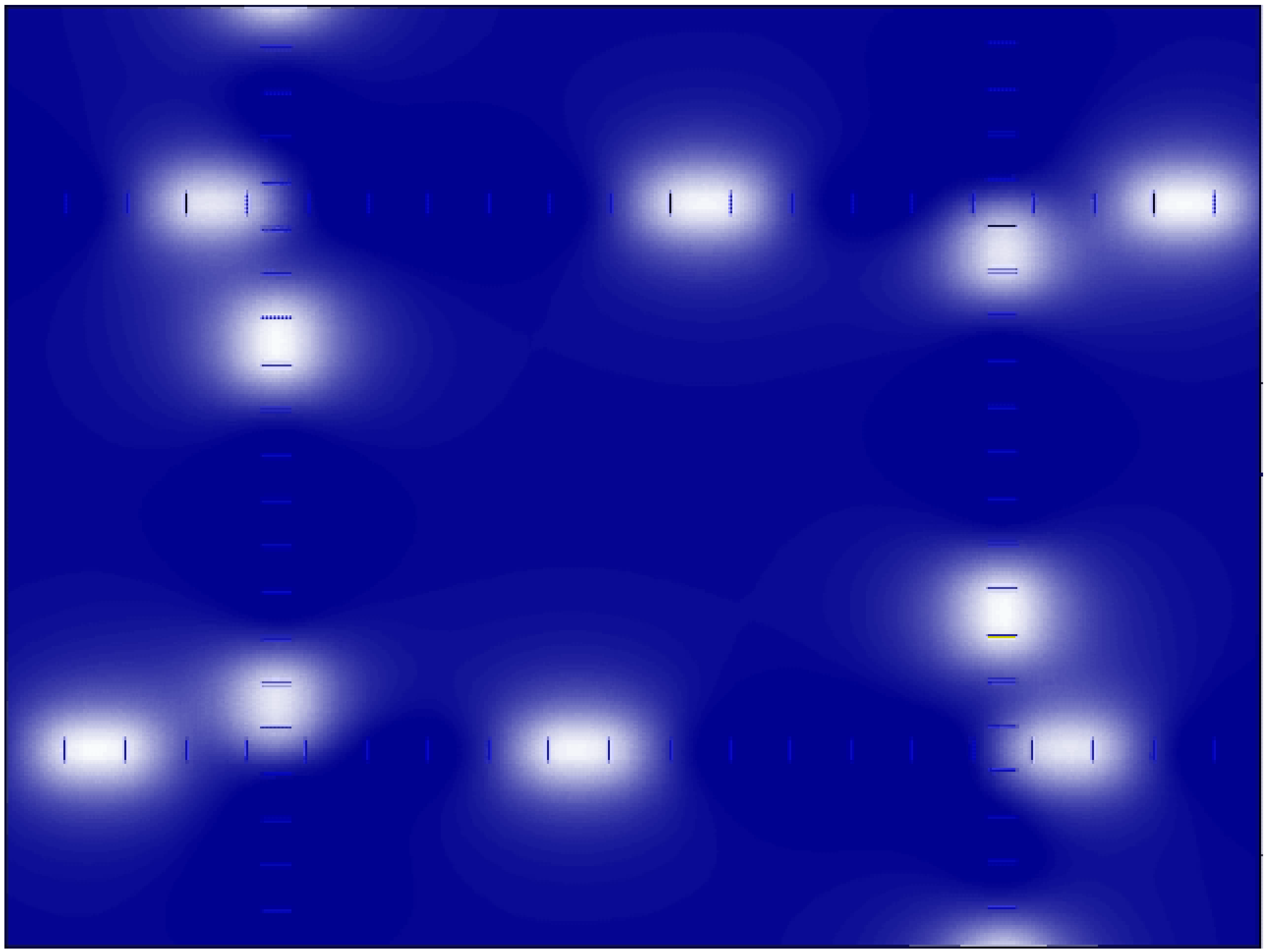
Universal floorplan



Crossing signals in the plane



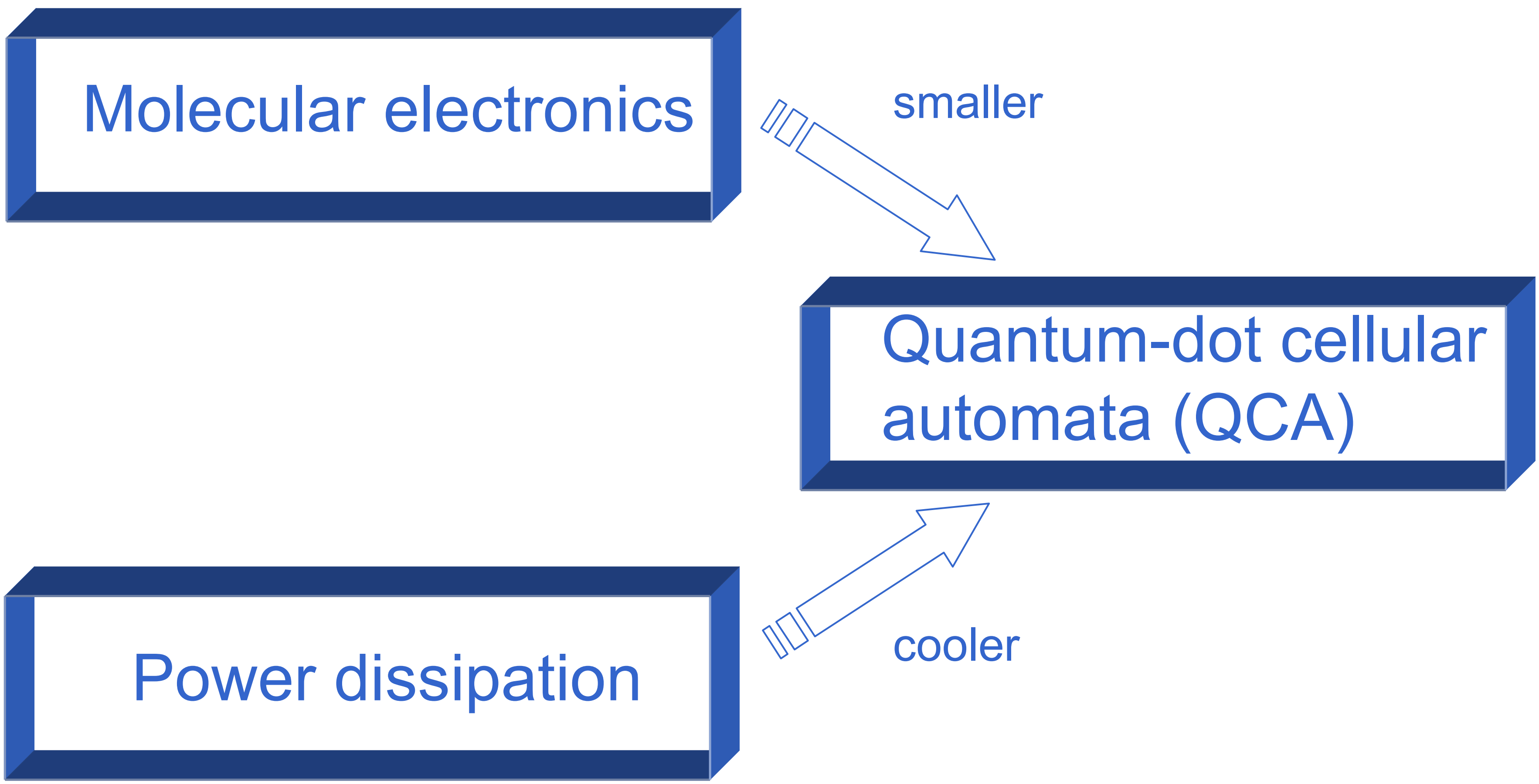
Multiple crossovers



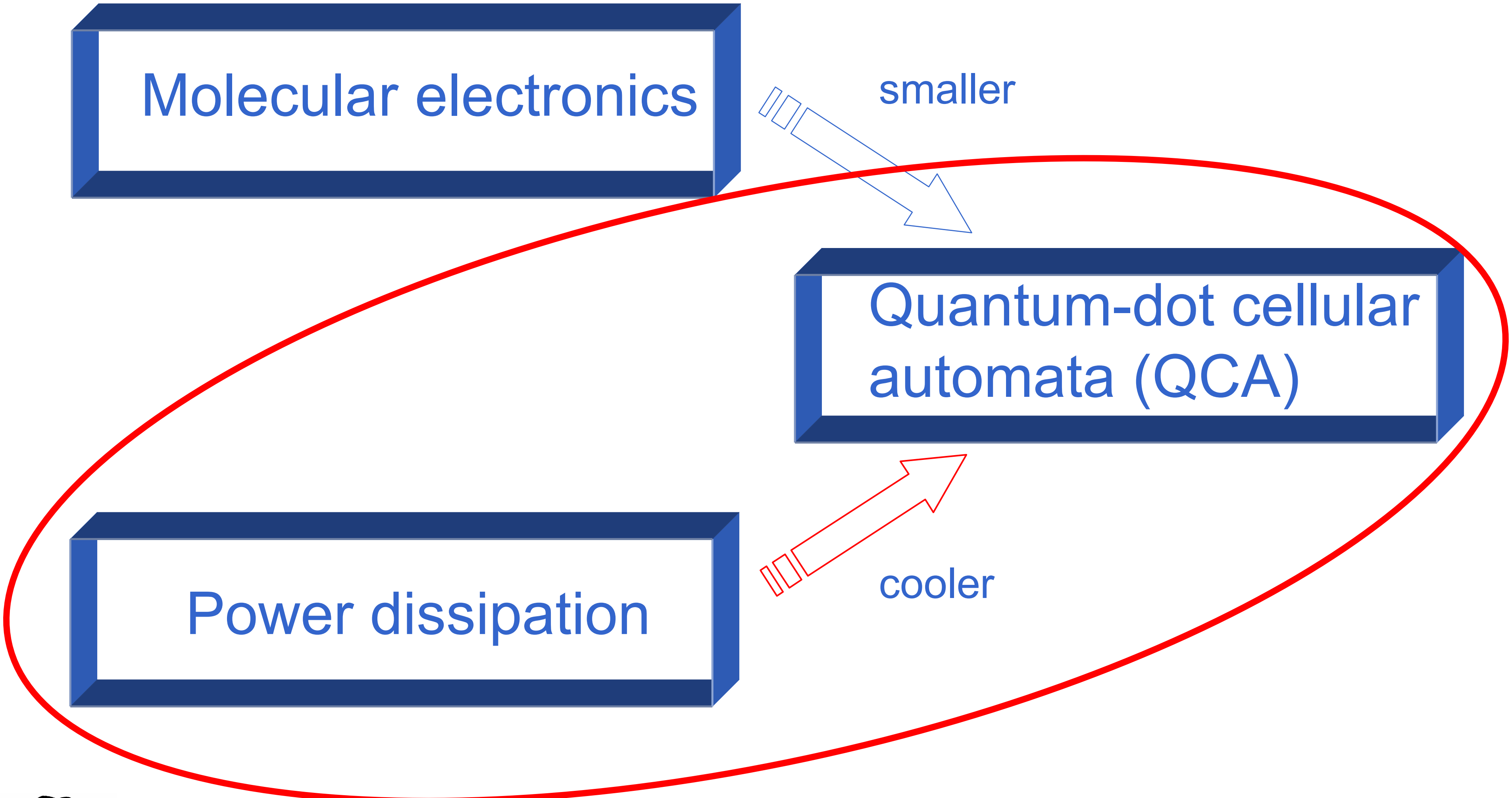
Interdisciplinary challenge

- Electrical Engineering
- Computer Science
- Chemistry
- Physics

Convergence

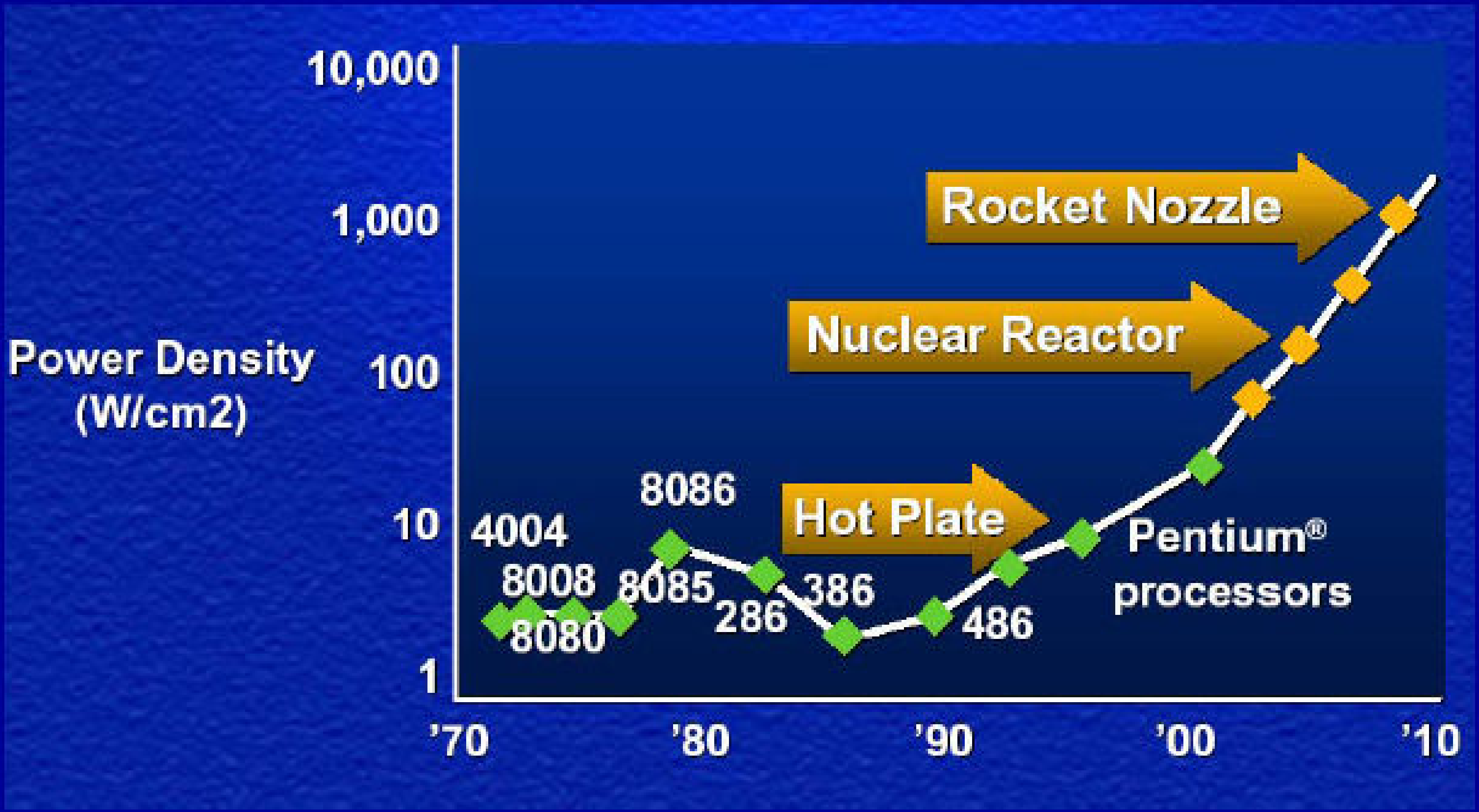


Convergence



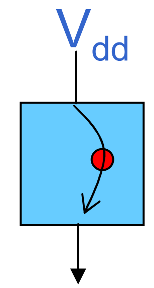
Power Density Will Get Even Worse

(Andrew S. Grove, Luncheon Talk in IEDM'02)



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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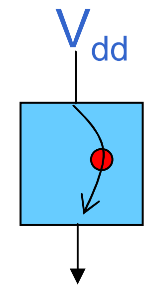


Power dissipation (Watts/cm^2)

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

Physics of computation

- Is there a fundamental lower limit on energy dissipation per bit?
- What is the distinguishability criterion in thermal environment?

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 $k_B T \log(2)$?

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)

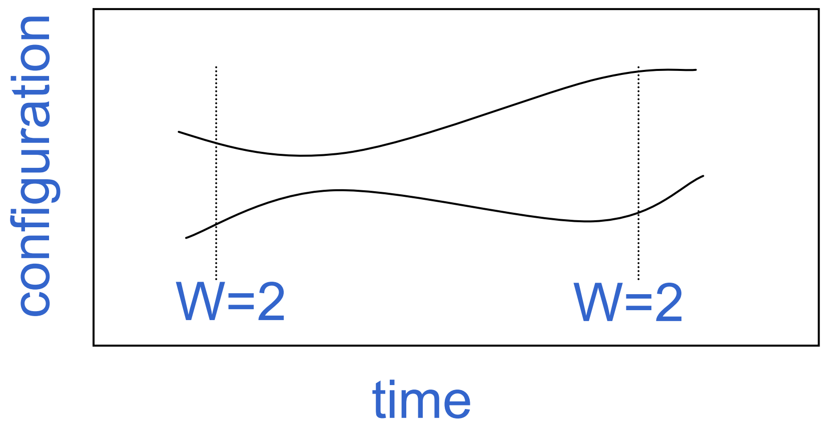
Minimum energy for computation

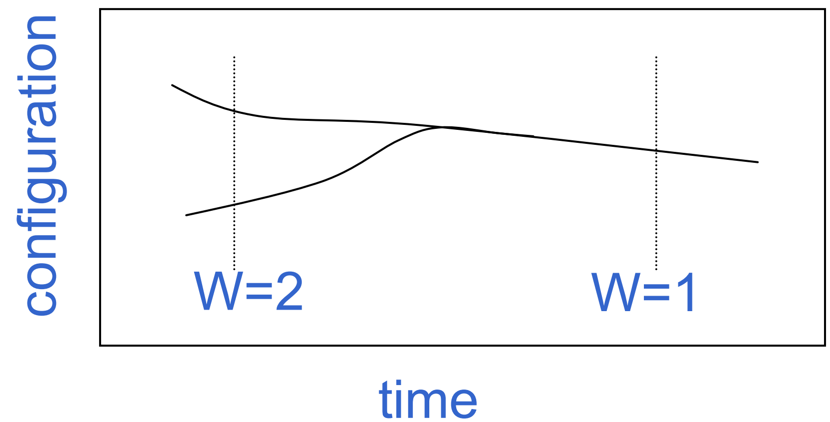
- Maxwell's demon (1875) – by first measuring states, could perform reversible processes to lower entropy
- Szilard (1929), Brillouin (1962): *measurement* causes $k_B T$ log(2) dissipation per bit.
- Landauer (1961,1970): only *erasure* of information must cause dissipation of $k_B T$ log(2) per bit.
- 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

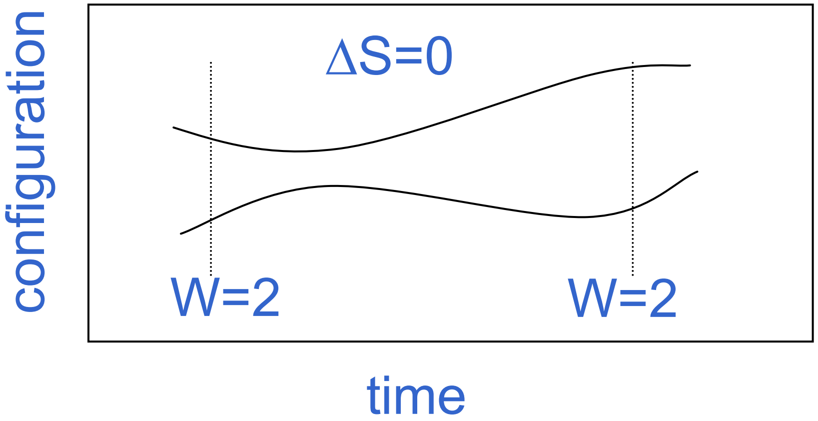


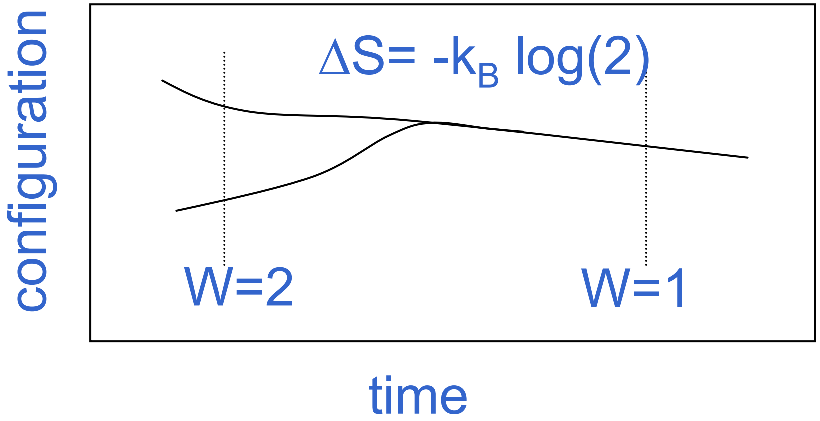


Entropy $S=k_B \log(W)$

Boltzmann’s tombstone

Physical reversibility ⇔ logical reversibility





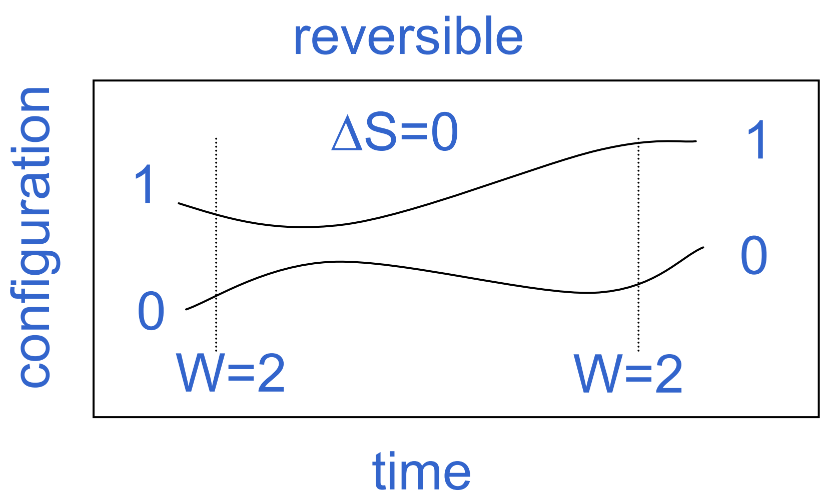
Entropy $S=k_B \log(W)$
Total $\Delta S > 0$. (2nd Law of Thermodynamics)

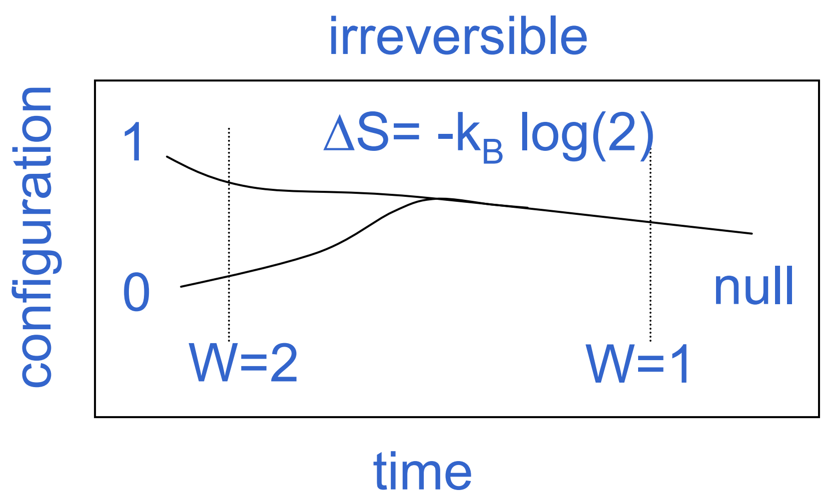
Reduction of entropy in system must be accompanied by transfer of entropy elsewhere.

Either:

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

Physical reversibility ⇔ logical reversibility



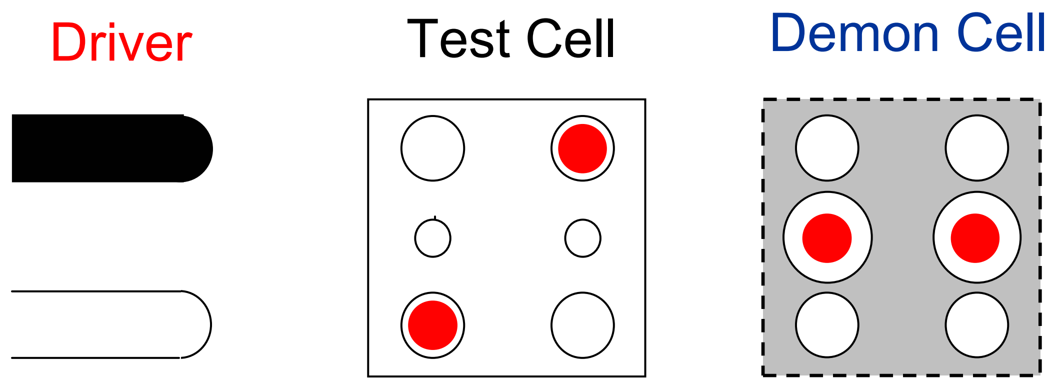


Logical reversibility means that inputs are logically determined by outputs.

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

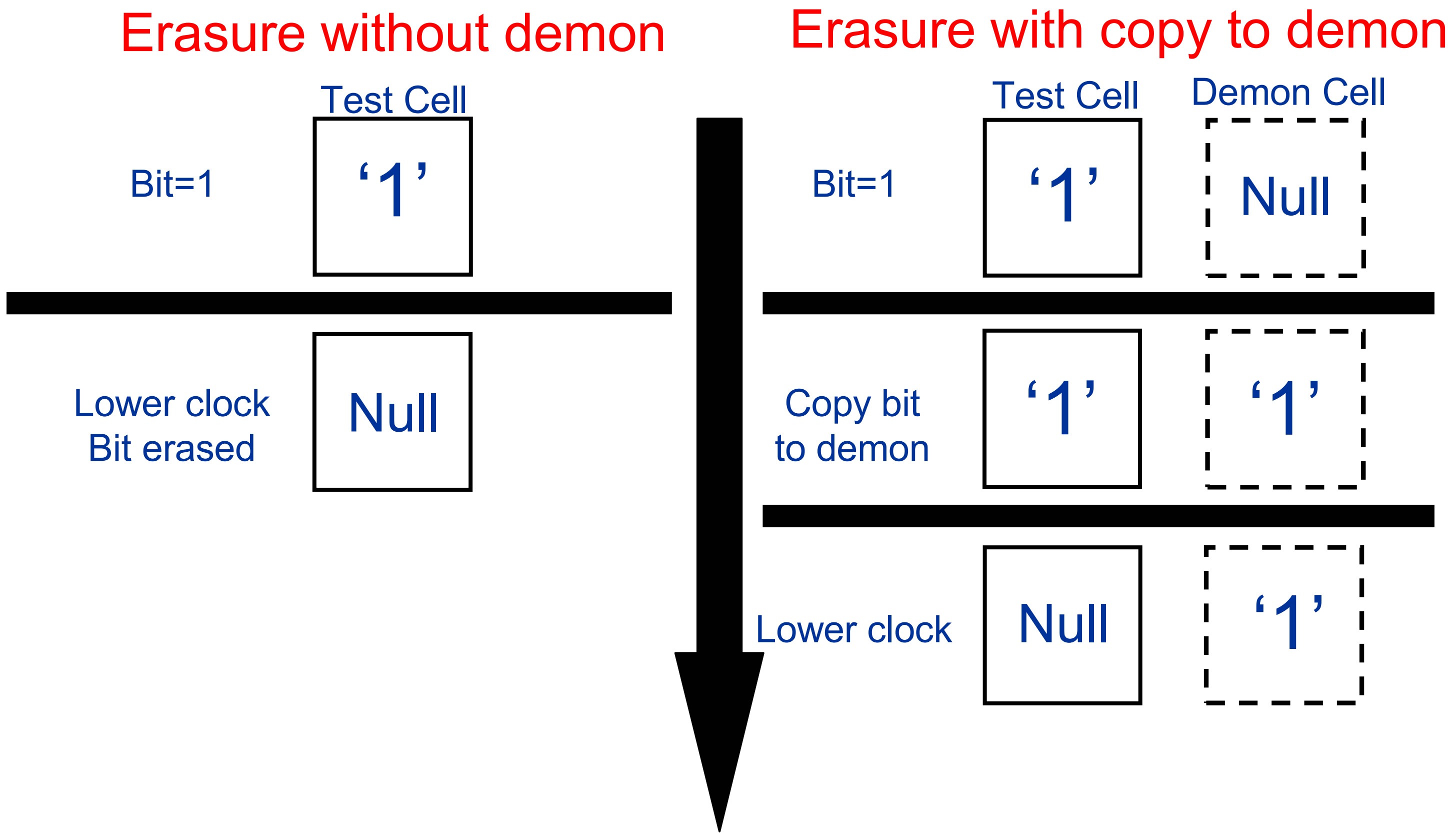
Logically irreversible computation *cannot* be implemented by physically reversible process. Example: erasure.

QCA system considered



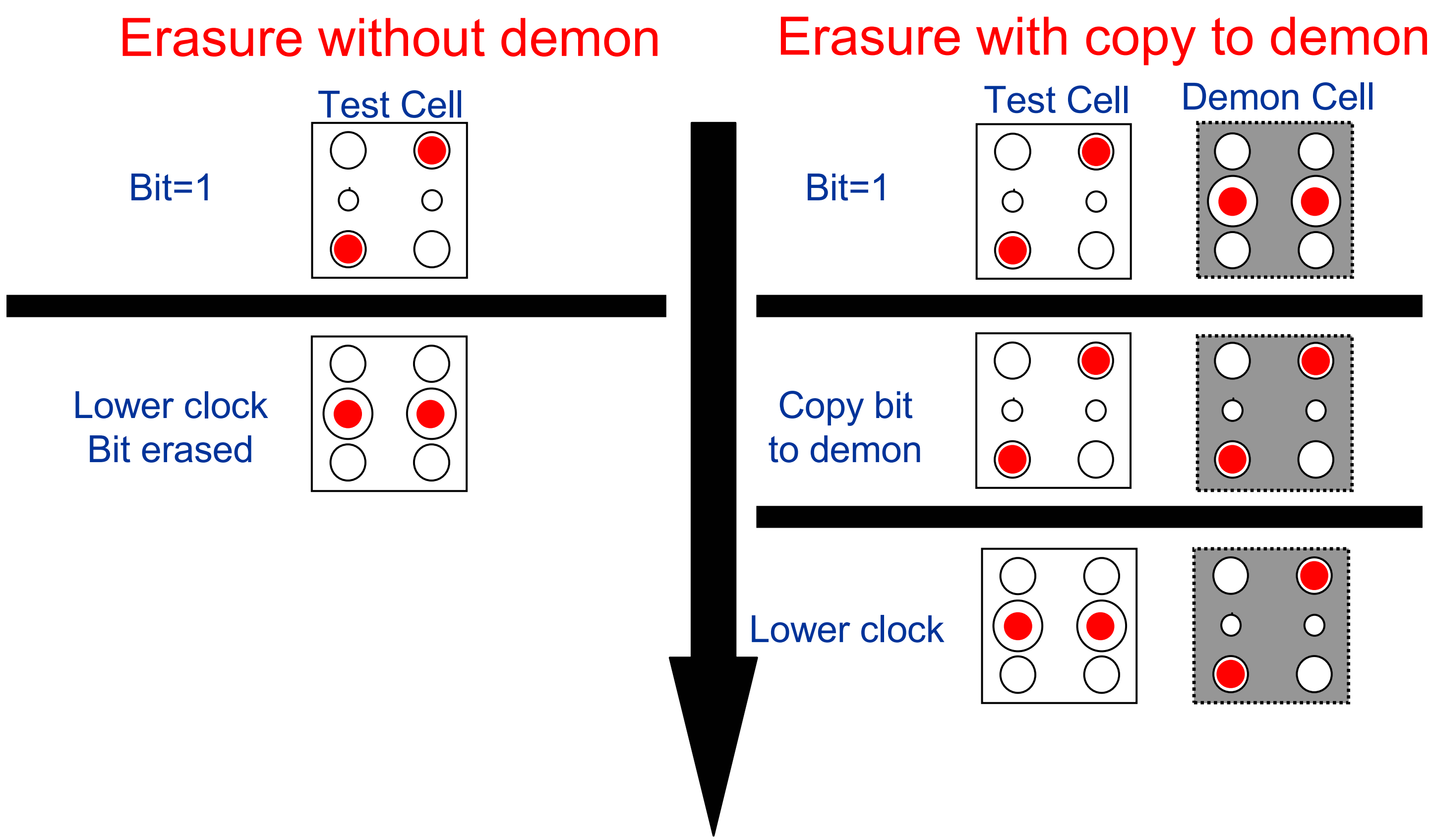
- Driver- provides input bit
- Demon cell (after Maxwell's Demon)- measures and copies the polarization of the test cell

Bit erasure

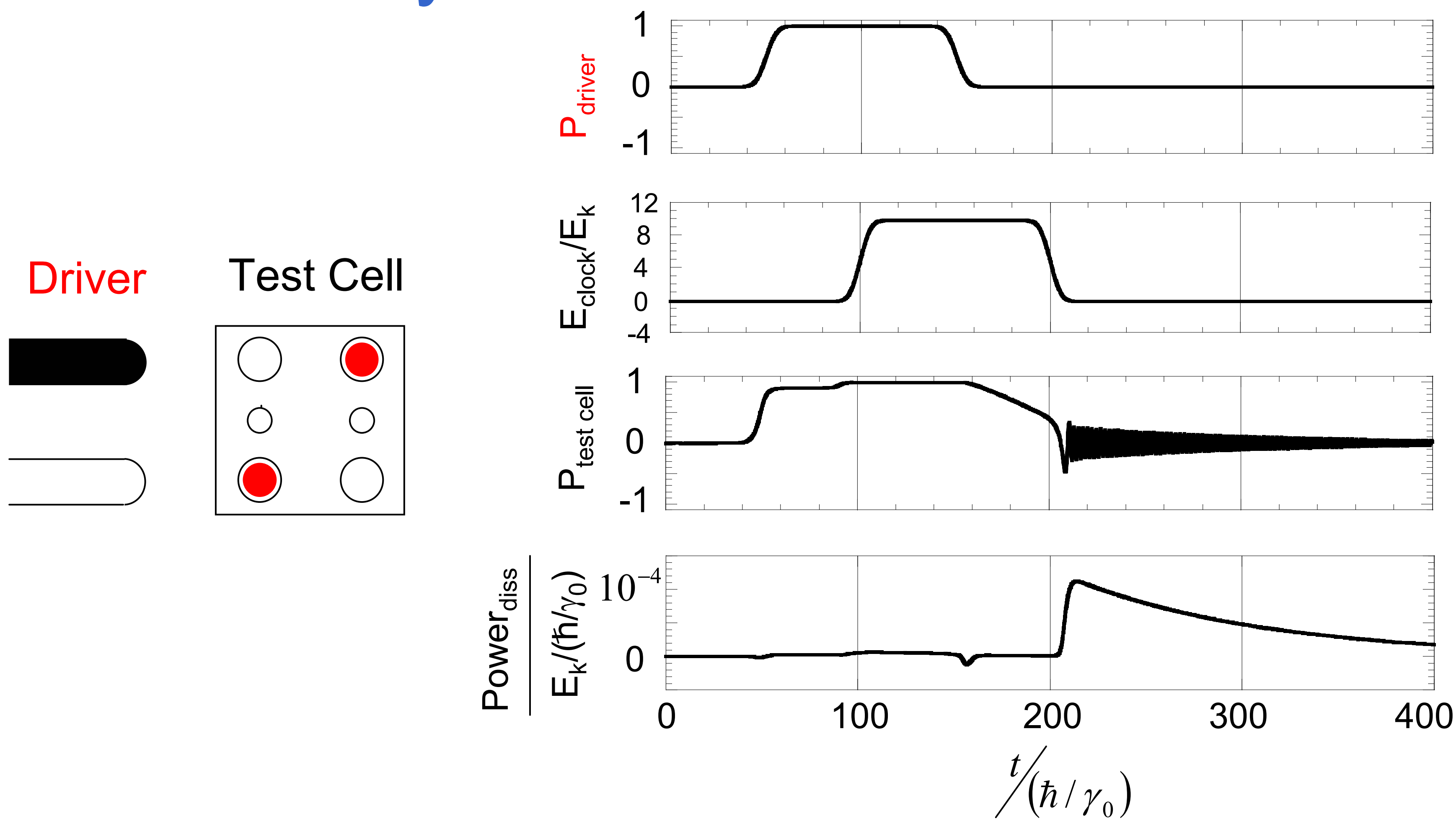


Erasure without demon
Test Cell
Bit=1
'1'
Lower clock
Bit erased
Null
Erasure with copy to demon
Test Cell
Demon Cell
Bit=1
'1'
Null
Copy bit
to demon
'1'
'1'
Lower clock
Null
'1'

Bit erasure in a QCA cell

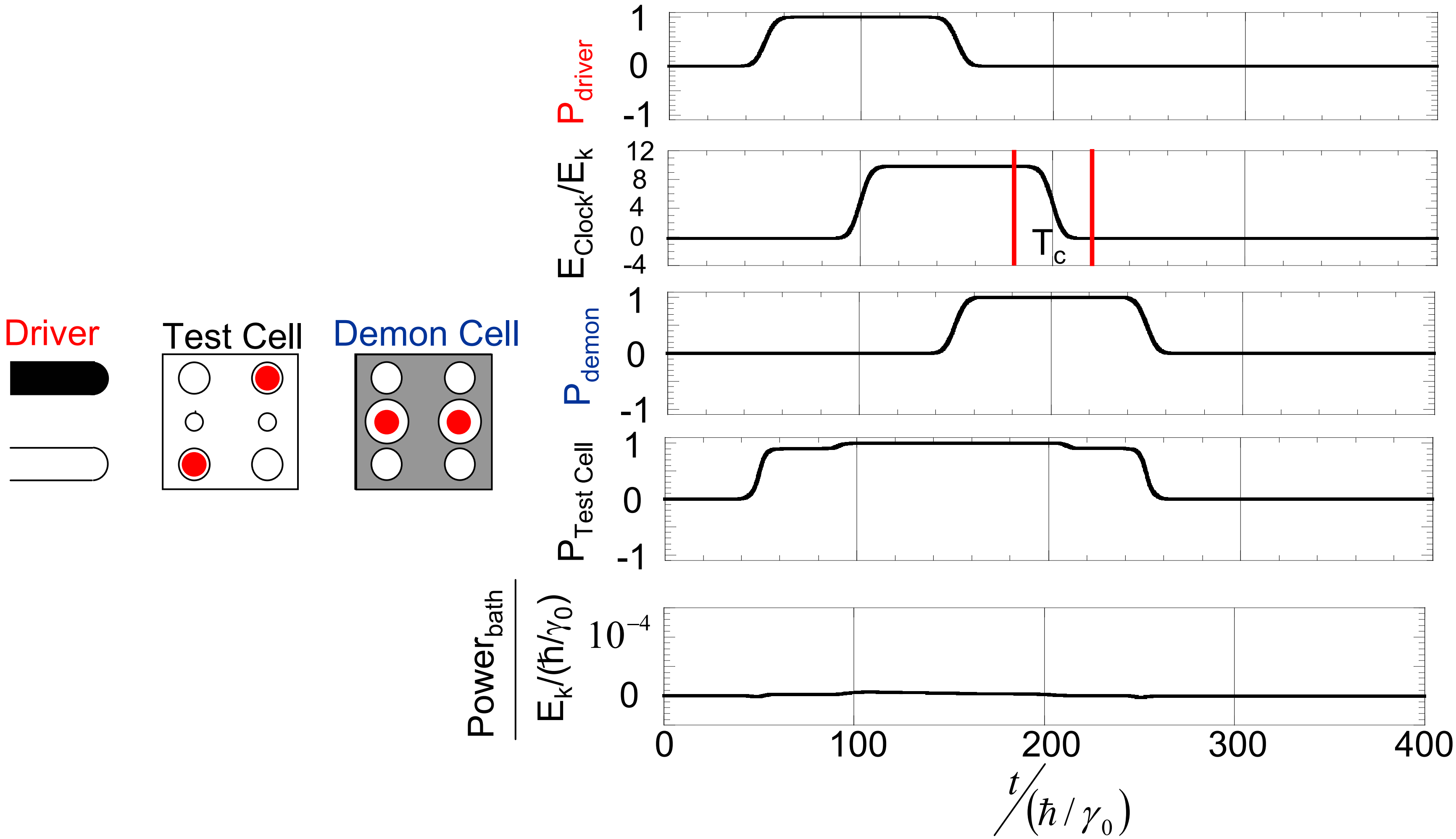


Erasure dynamics without demon cell



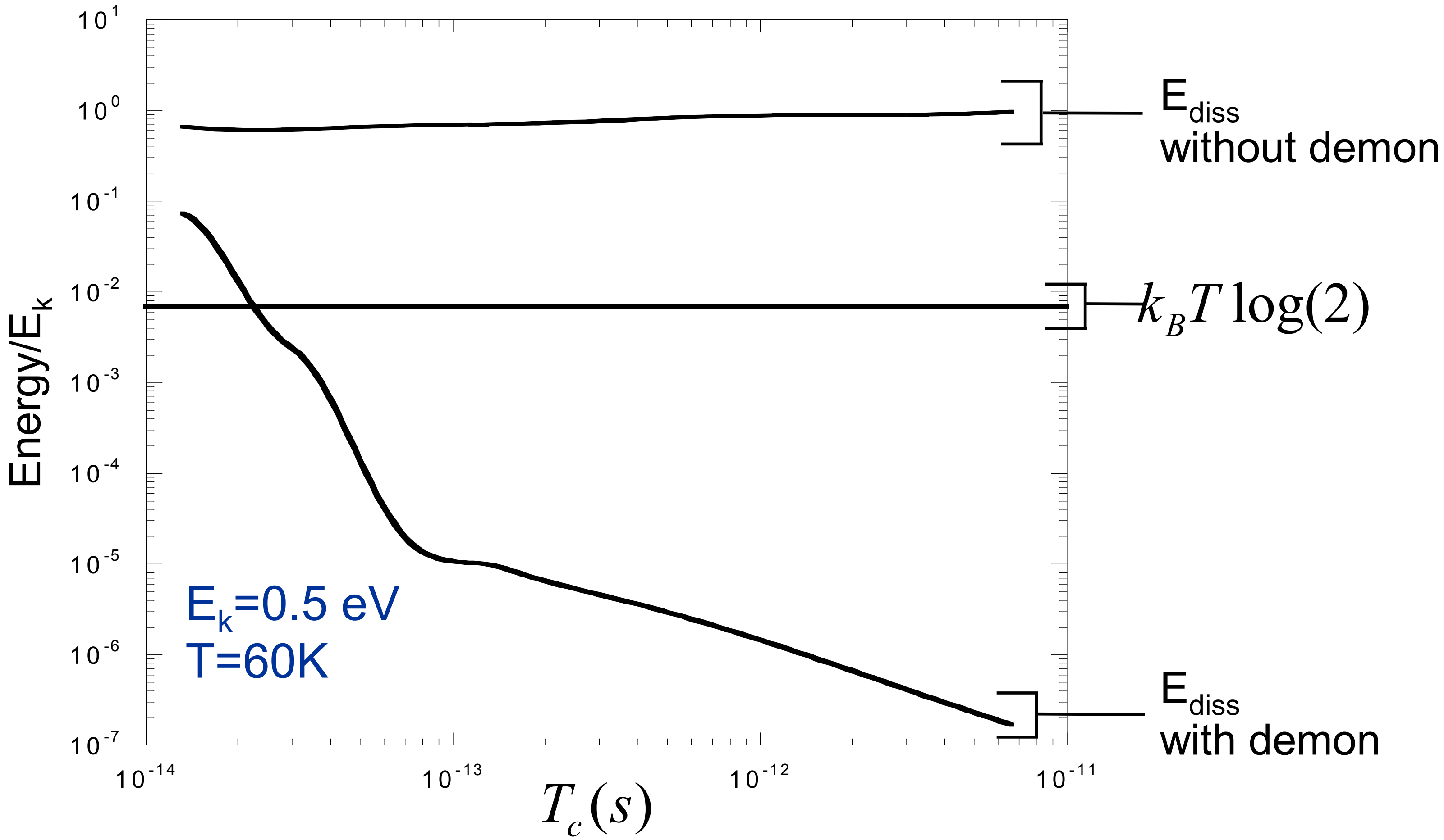
Without a demon cell, erasing the bit results in considerable energy dissipation.

Erasure dynamics with copy to the demon cell



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

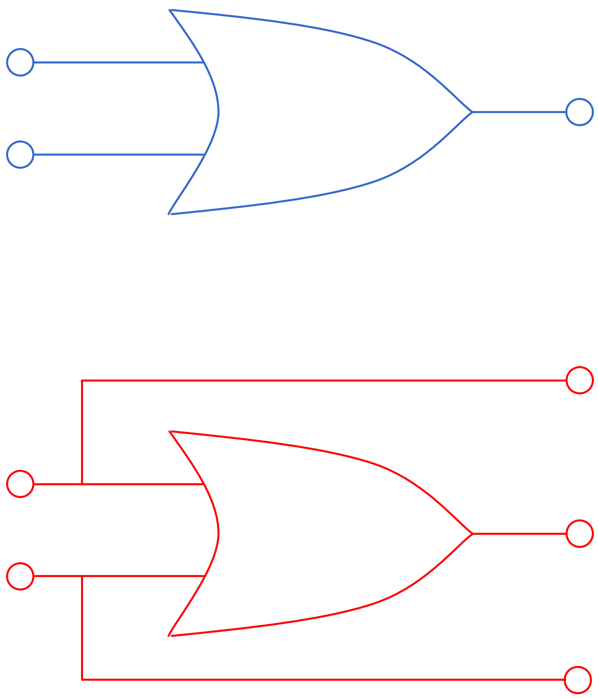
Energy loss for erasing a single bit

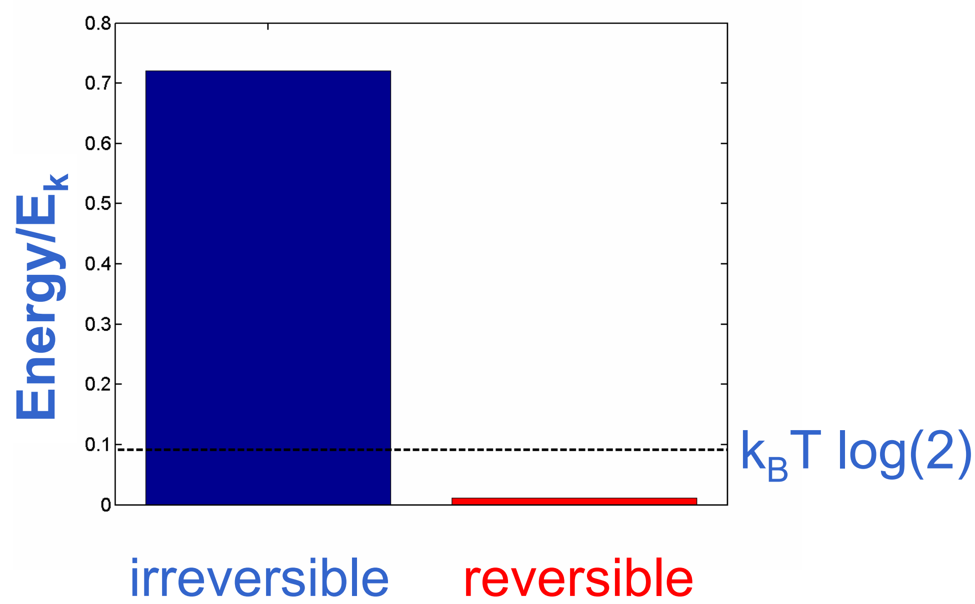


The demon cell makes the erasure reversible, so energy loss can be much less than $k_B T$ log(2).

Demon to the right: a shift register

QCA gate: reversible/irreversible



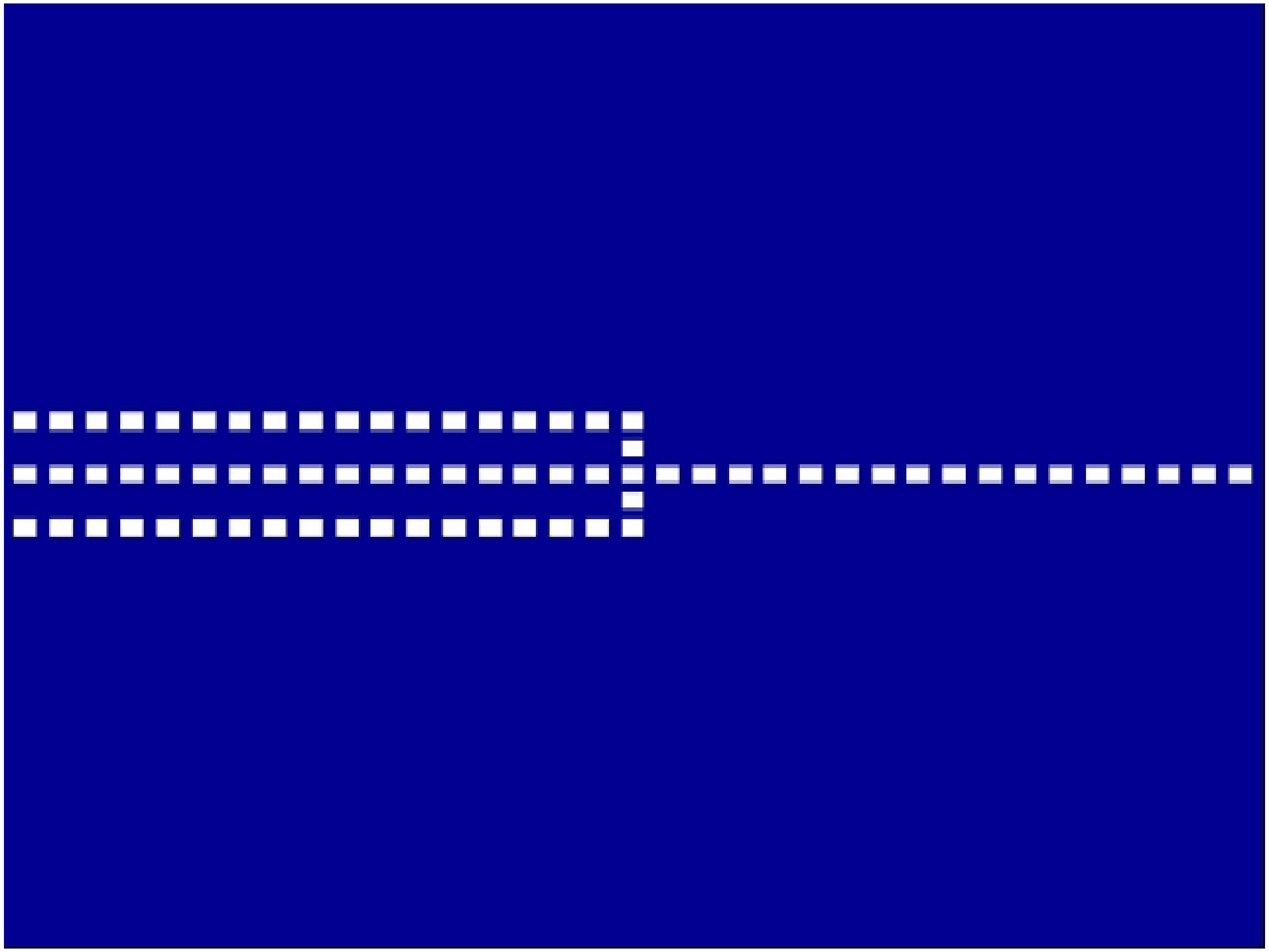


Direct time-dependent calculations shows: Logically reversible circuit can dissipate much less than $k_B T \log(2)$.

Bennett clocking of QCA

Output is used to erase intermediate results.

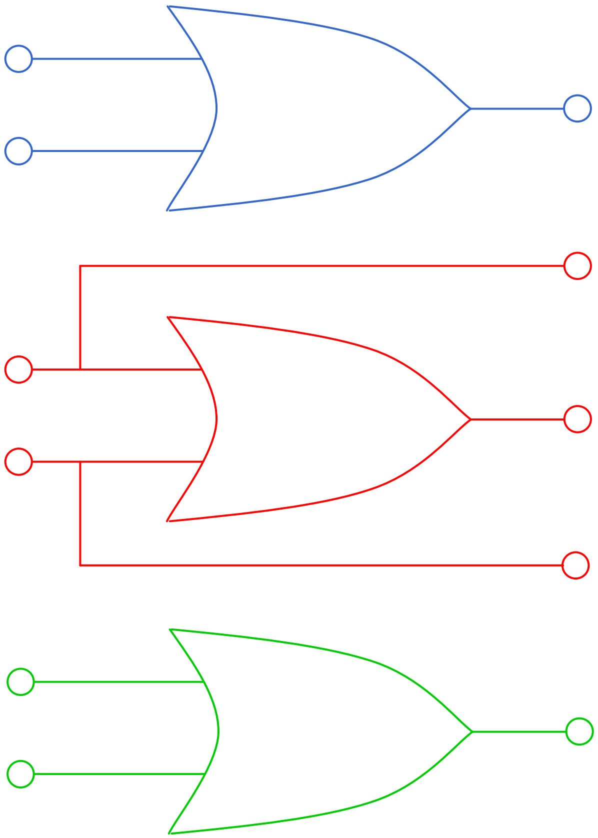
Bennett clocking of QCA

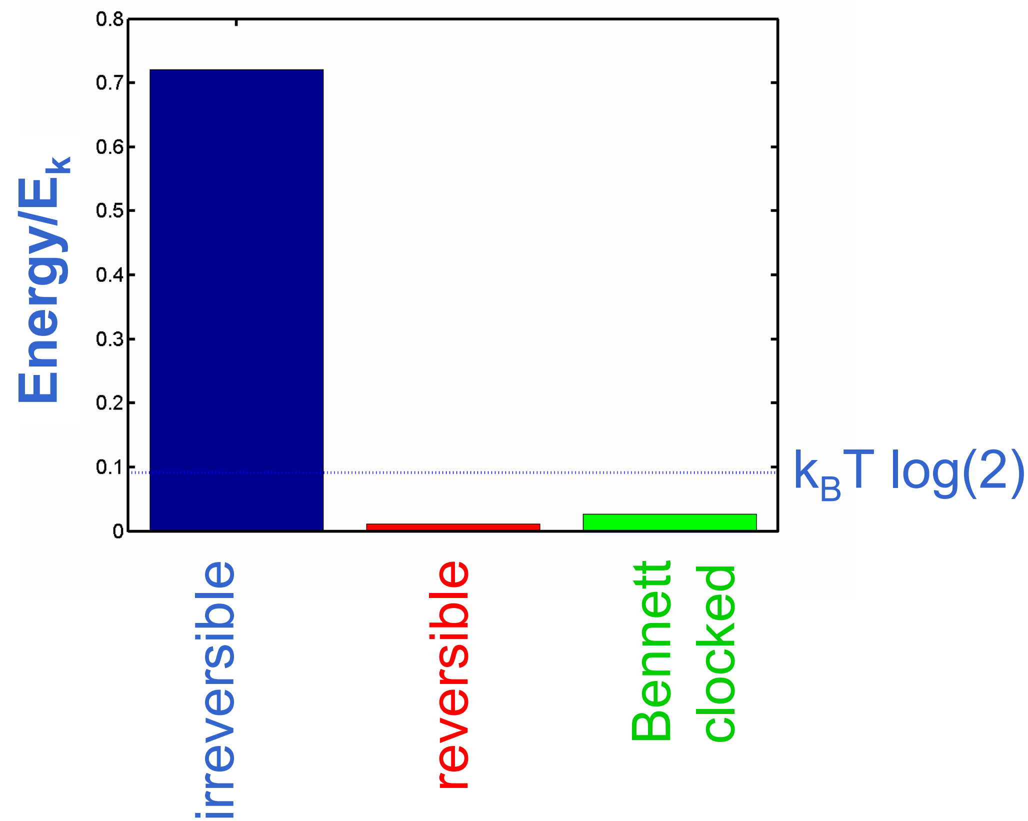


For QCA no change in layout is required.

Landauer clocking of QCA

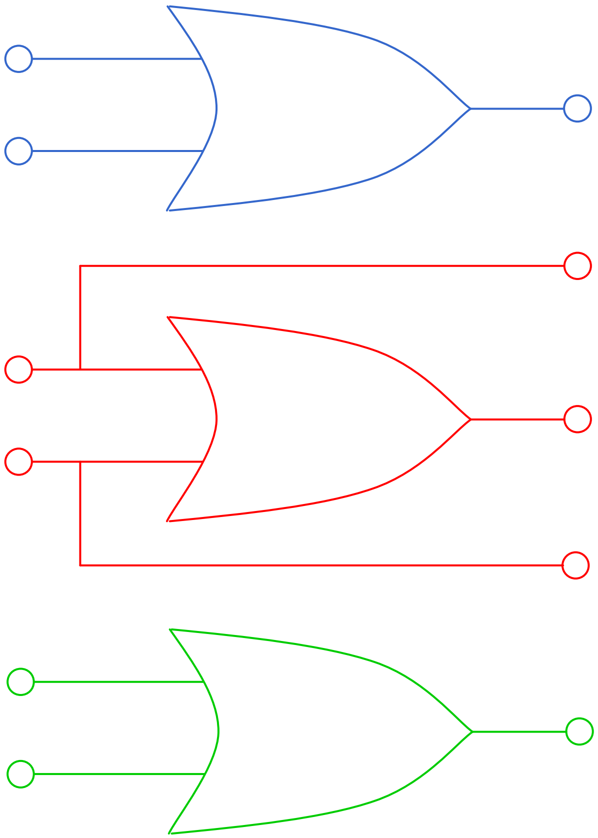
QCA gate: reversible/irreversible

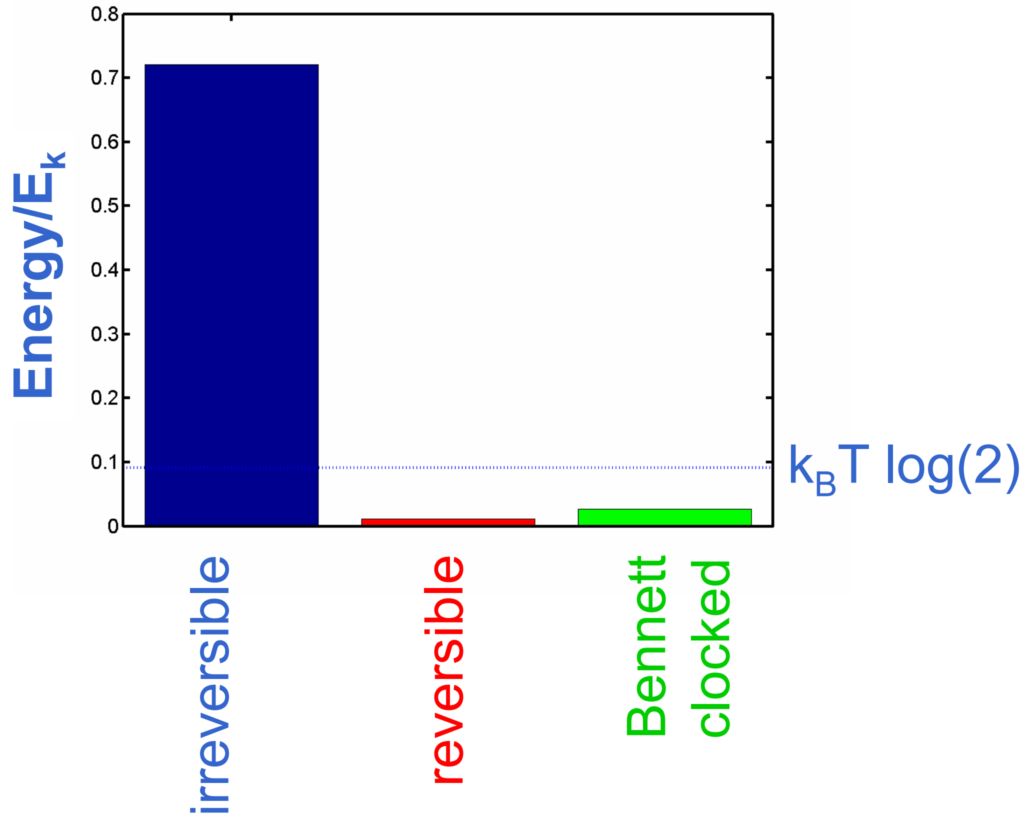




Direct time-dependent calculations shows: Logically reversible circuit can dissipate much less than $k_BT\log(2)$.

QCA gate: reversible/irreversible





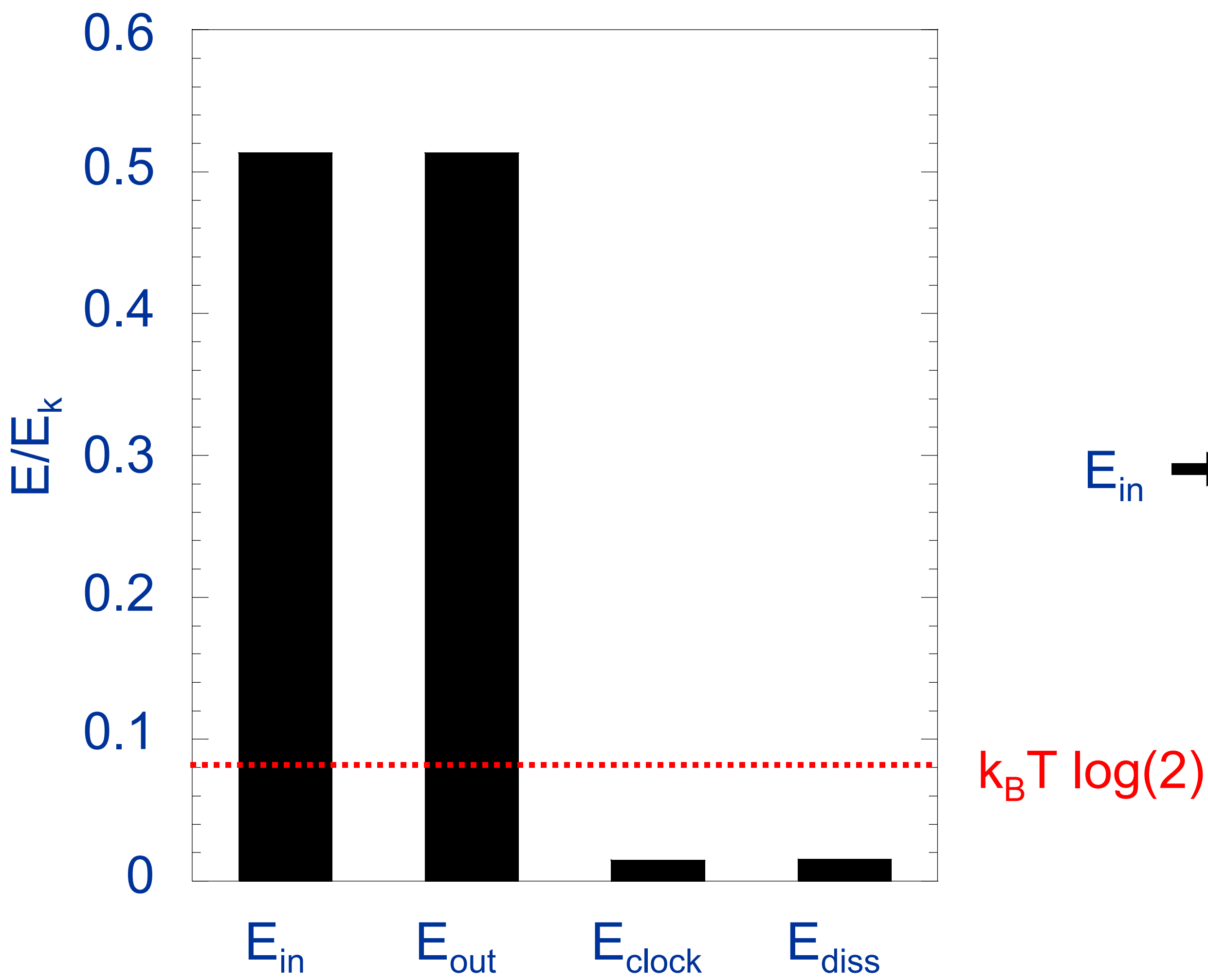
With QCA, reversible computation adds no circuit complexity. Simply redo clock timing where desired.

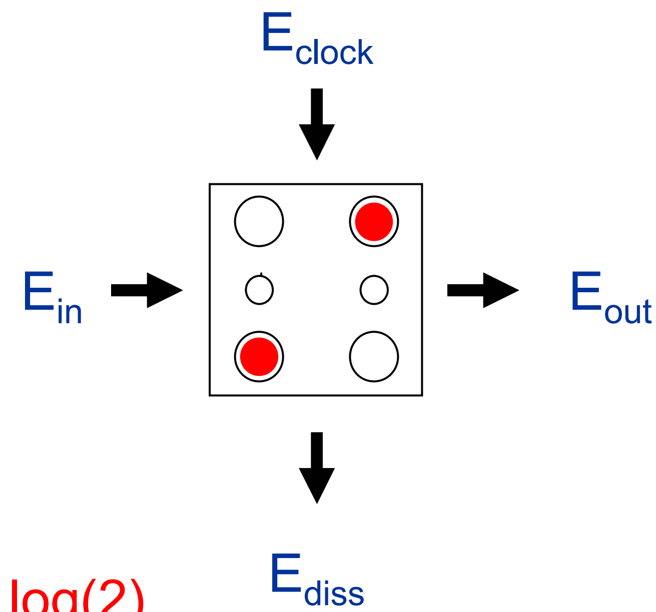
Distinguishability

Don't you need to dissipate more than $k_B T \log(2)$ to be able to distinguish a bit in a thermal environment?

Energy flow in QCA cells

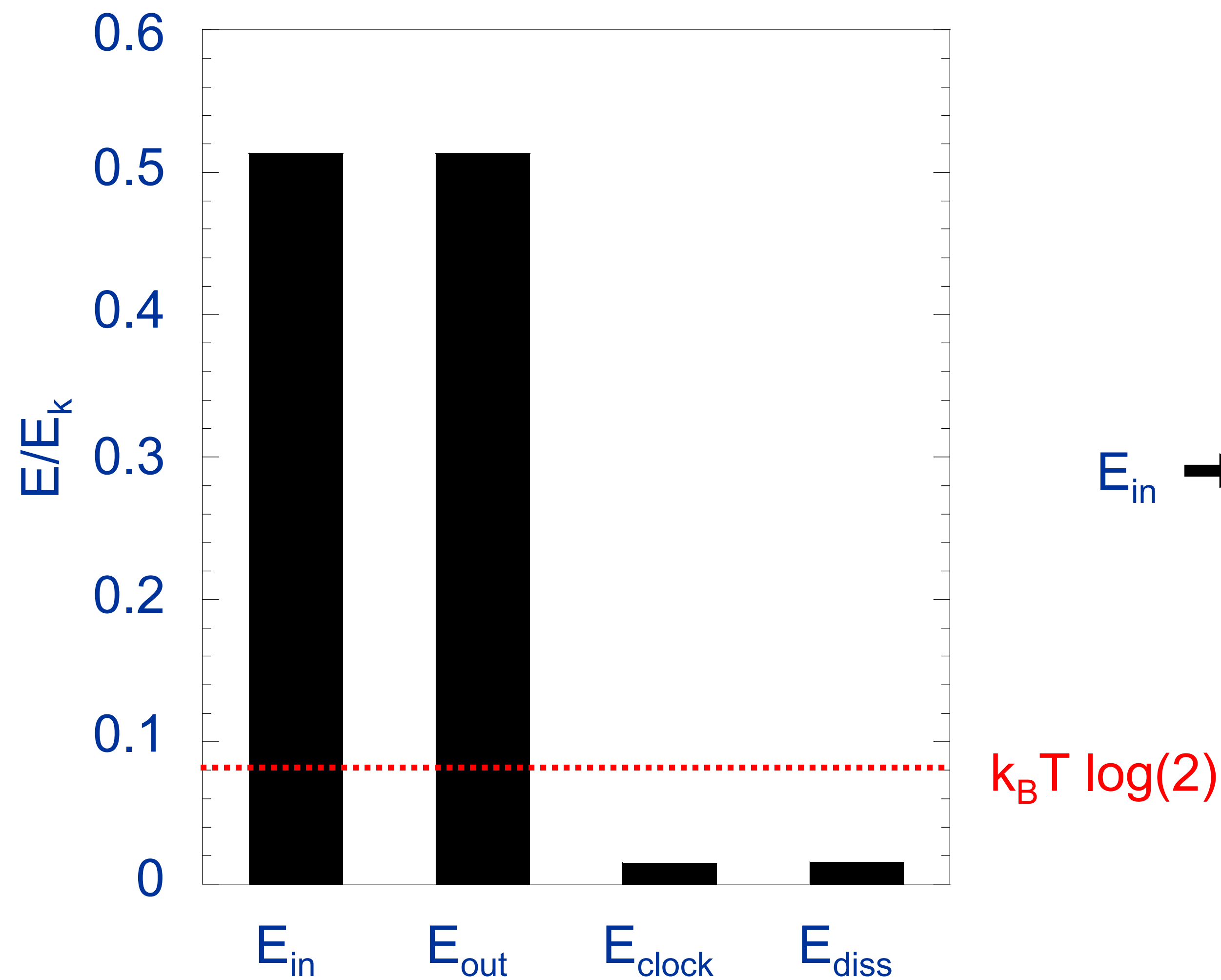
Energy flow in QCA cells

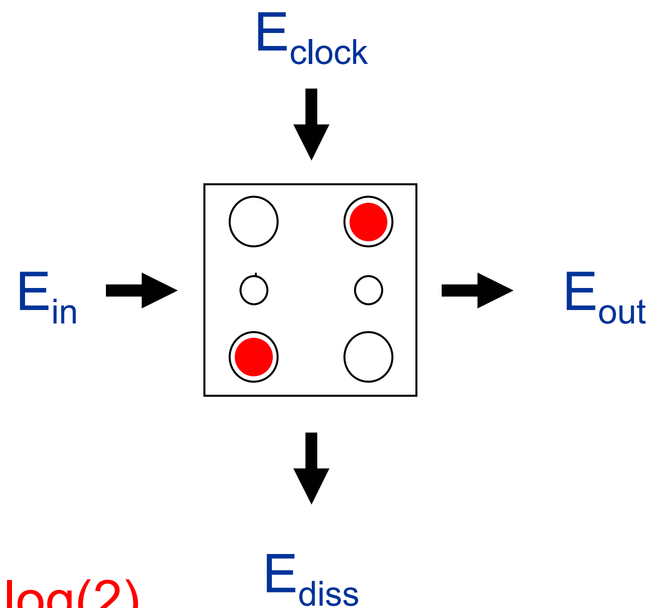




Switching events in QCA cells can dissipate much less than k_BT log(2)

Energy flow in QCA cells



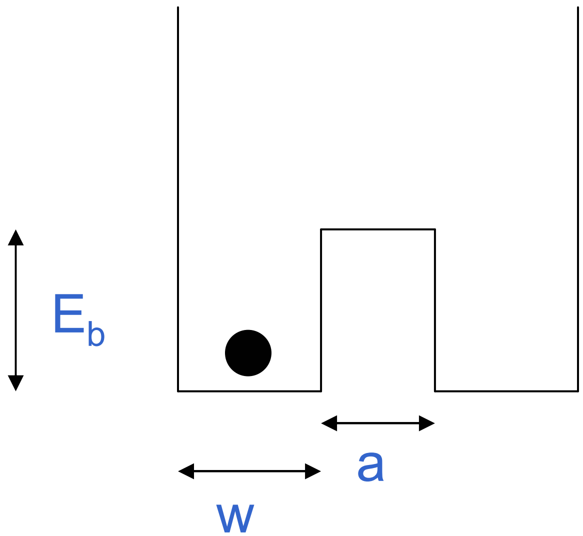


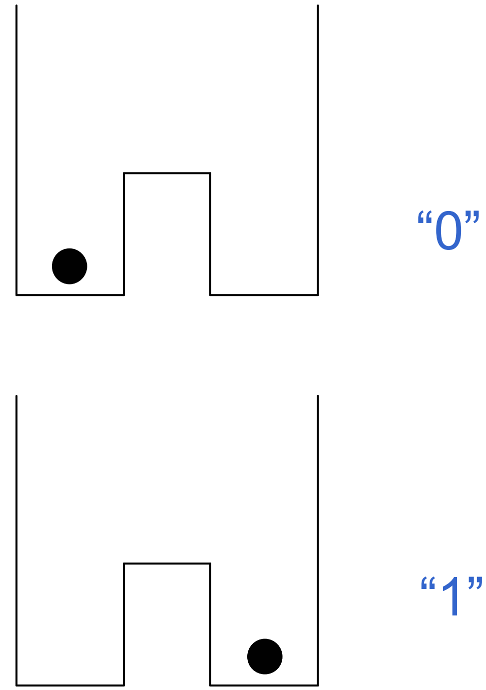
Distinguishability requires $E_{in} > k_BT\log(2)$. E_{diss} can be much less.

Distinguishability

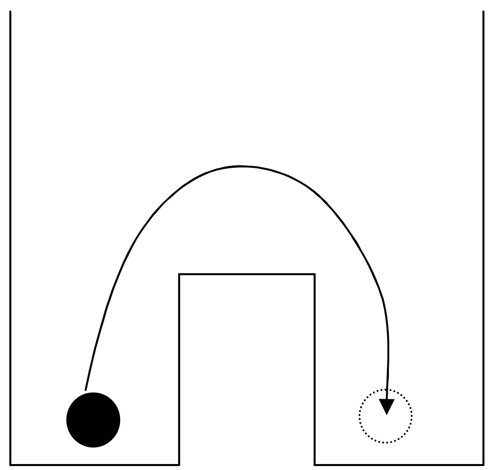
- Information is physical
- *Signal energy* must be greater than $k_B T \log(2)$ for next stage to be able to distinguish it from thermal fluctuation. (a “read” criterion)
- The signal energy need not be dissipated.
- What to do with it?
  - Bennett: Never throw away information. Reverse computation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

Double well represents bit

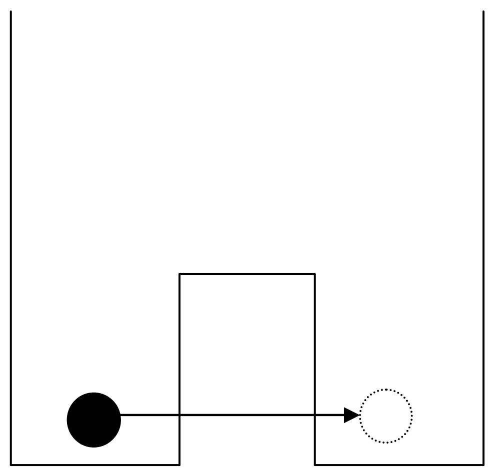




Bit switching



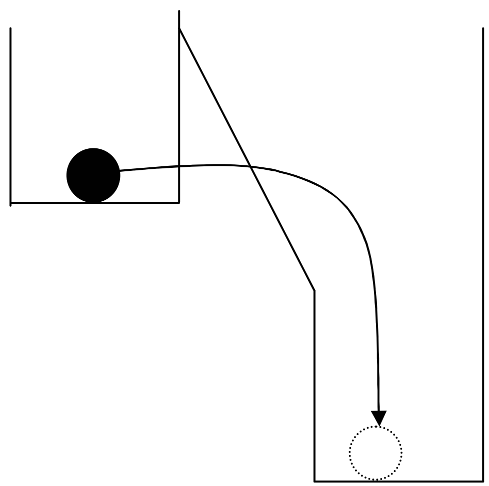
Thermal hop over barrier dissipates no energy.



Tunneling through barrier dissipates no energy.

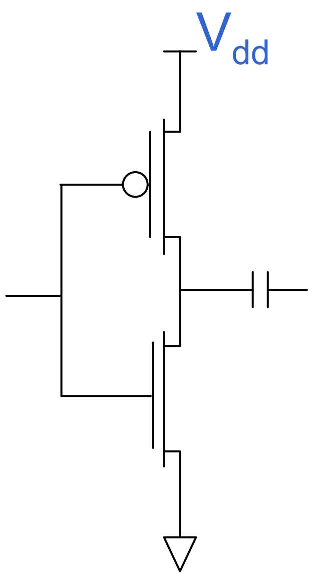
Note: Traversing an energy barrier dissipates no energy.

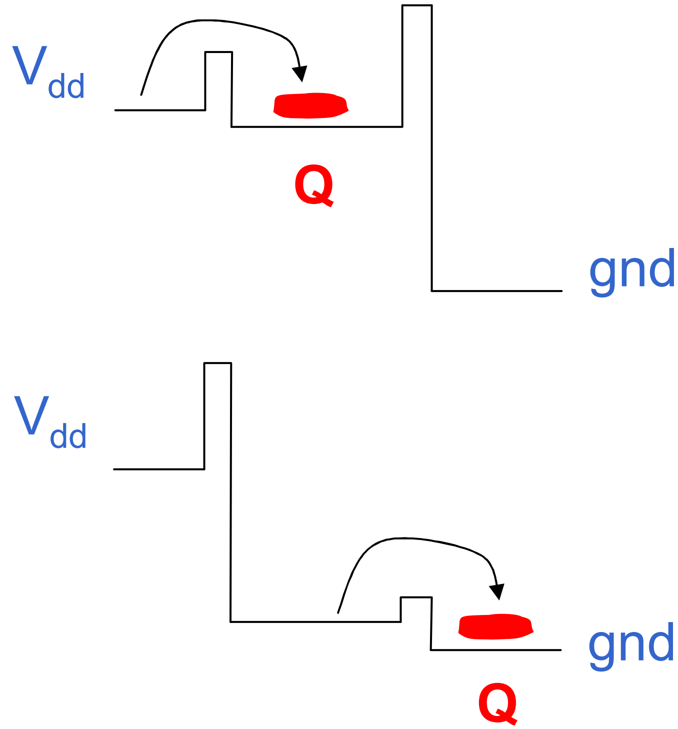
Dissipation: falling down hill



Energy dissipation is determined by energy difference between initial and final state – not barrier height.

What's wrong with transistors?



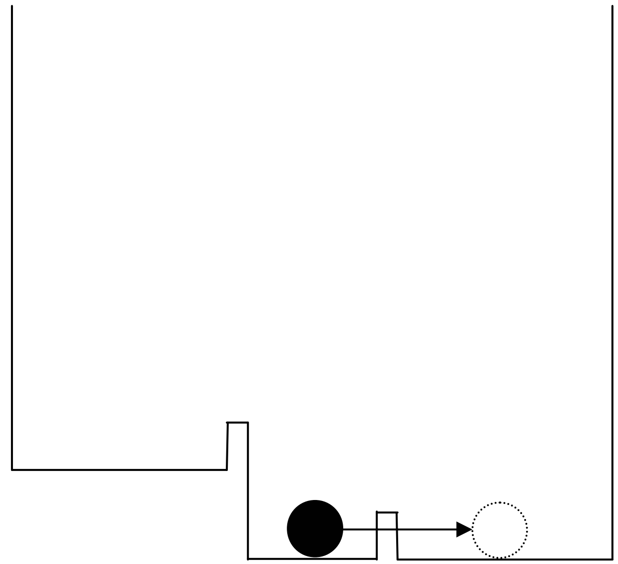


Net transport of charge from V_{dd} to ground (*falling downhill*).

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

Energy is dissipated even for logically reversible operations.

QCA adiabatic switching

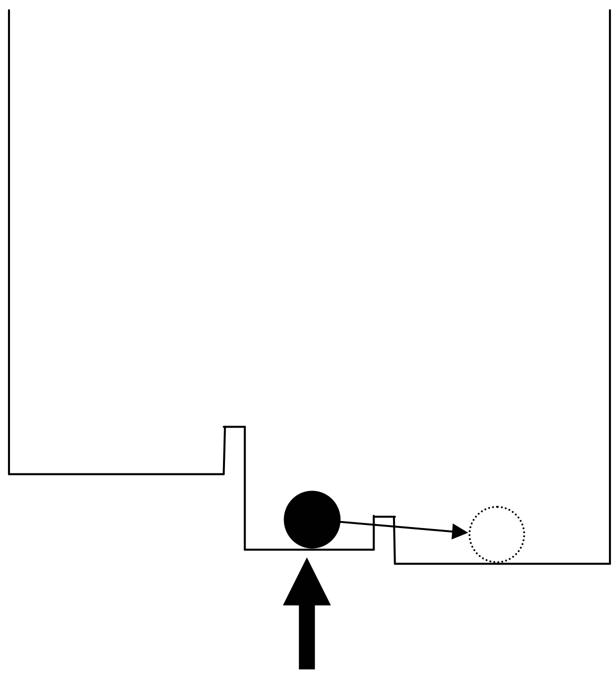


Remove input bias

Raise clocking potential

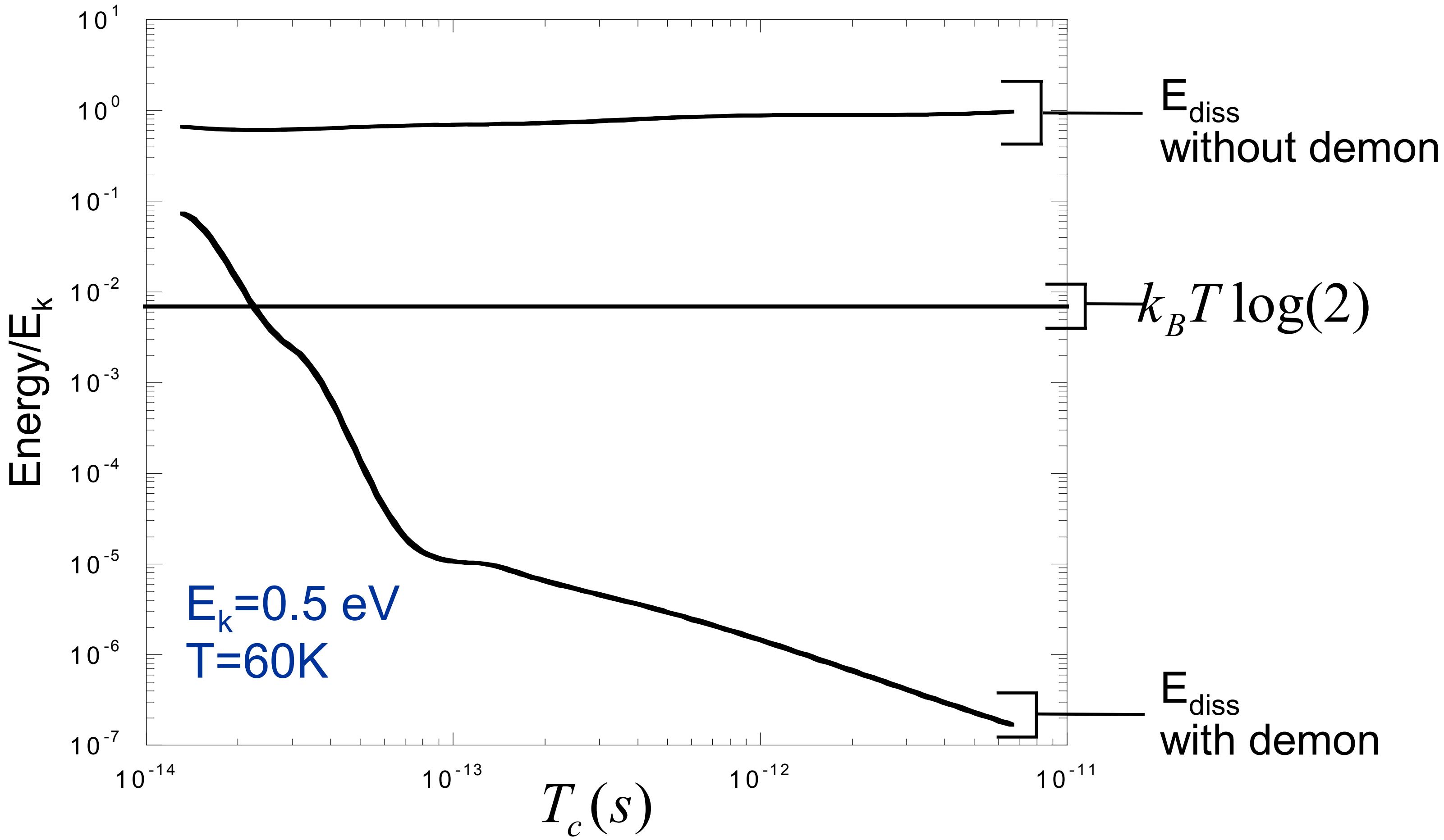
Keep system always very close to ground state.
Don't let it fall downhill.

Breakdown of adiabaticity



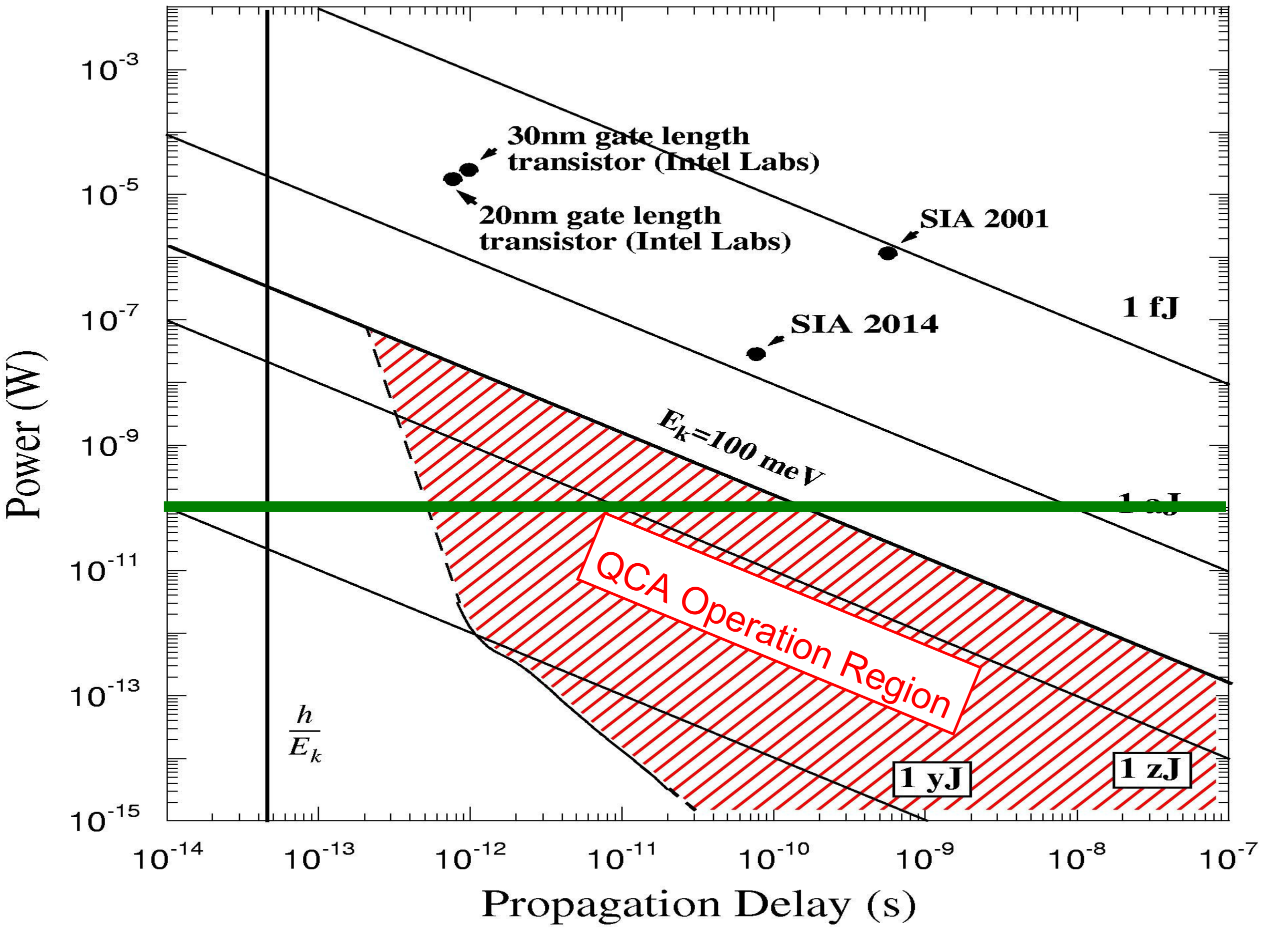
If clock moves up too fast, system cannot get to ground state without some dissipation.

Energy loss for erasing a single bit



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

QCA Power Dissipation



100 W/cm^2 @10^{12} devices/cm^2

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

Doesn't adiabatic mean slow?

Slow compared to what?

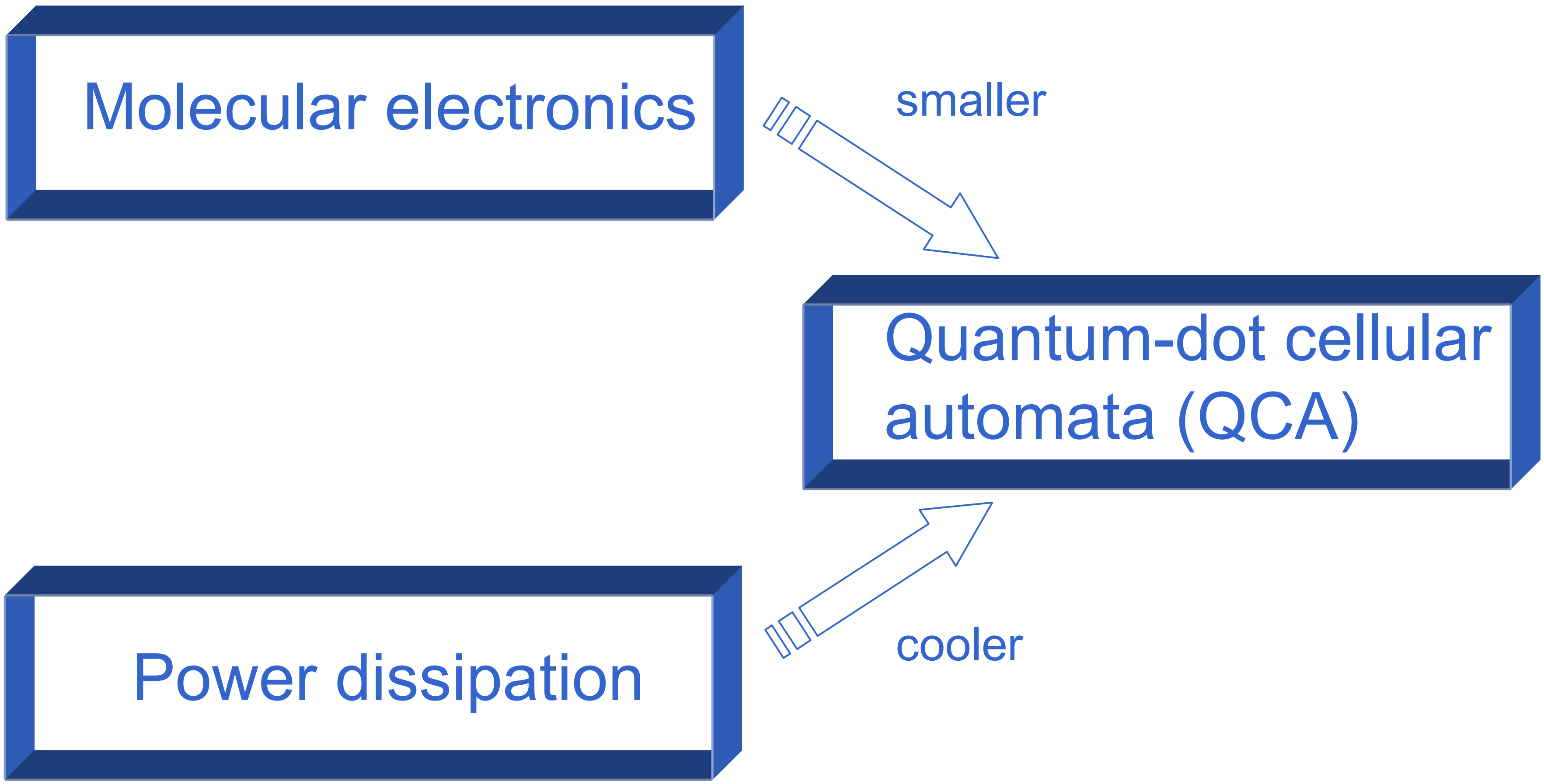
- For conventional circuits, RC
- For molecular QCA, slow compared to electron switching from one side of a molecule to the other

  ~ $\omega_B = 4 \times 10^{16}$ Hz $\rightarrow$ THz operation is feasible

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 $k_B T \log(2)$ for each erasure.
    - Moderate approach: erase as needed, manage power budget. “Landauer clocking”
    - More radical approach: partition into blocks and only erase inputs to each block. “Bennett clocking”

Convergence



Zettaflops

10^{21} flops→ 10^{25} ops

1 nm^2 devices (includes surrounding groups)

10^{14} devices/cm^2 derate for power & redundancy

10^{12} bits on the move/cm^2

10^{12} bits on the move/cm^2 * 10^{12} Hz= 10^{24} ops/cm^2

10 cm^2 chip → 10^{25} ops

Conclusions

- QCA offers path to limits of downscaling – molecular computing.
- Clocked QCA can operate at lower limits of power dissipation.
  - Only dissipate when information is erased
  - Tuned Bennett clocking: hold intermediate results in place when absolute lowest power dissipation is required
- A clear path, but much research remains to be done.
  - Chemistry, physics, electrical engineering, computer science

Thanks for your attention.