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Author(s)

Craig Lent	DEBENEDICTIS,ERIK P.	Greg Snider
Jerry Floro	Marco Ottavi	Mike Niemier
MURPHY,SARAH	Peter Kogge	PRAGER,AARON A.
Robert Hull		

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Agreement: Sandia Contact has agreed to incorporate above listed conditions prior to release. Comments:			

Administrator Approver	LUCERO,ARLENE M.

Quantum Dot Cellular Automata (QDCA) Strategic Partnership: Extending Moore's Law: Part 1, Physical Sciences Issues

Erik DeBenedictis[1] (PI), Jerry Floro[1,3], Robert Hull[3], Peter Kogge[2], Craig Lent[2], Sarah Murphy[1,2], Mike Niemier[2], Marco Ottavi[1], Aaron Prager[1,2], Greg Snider[2]

([1]Sandia, [2]Notre Dame, [3]U. Virginia)

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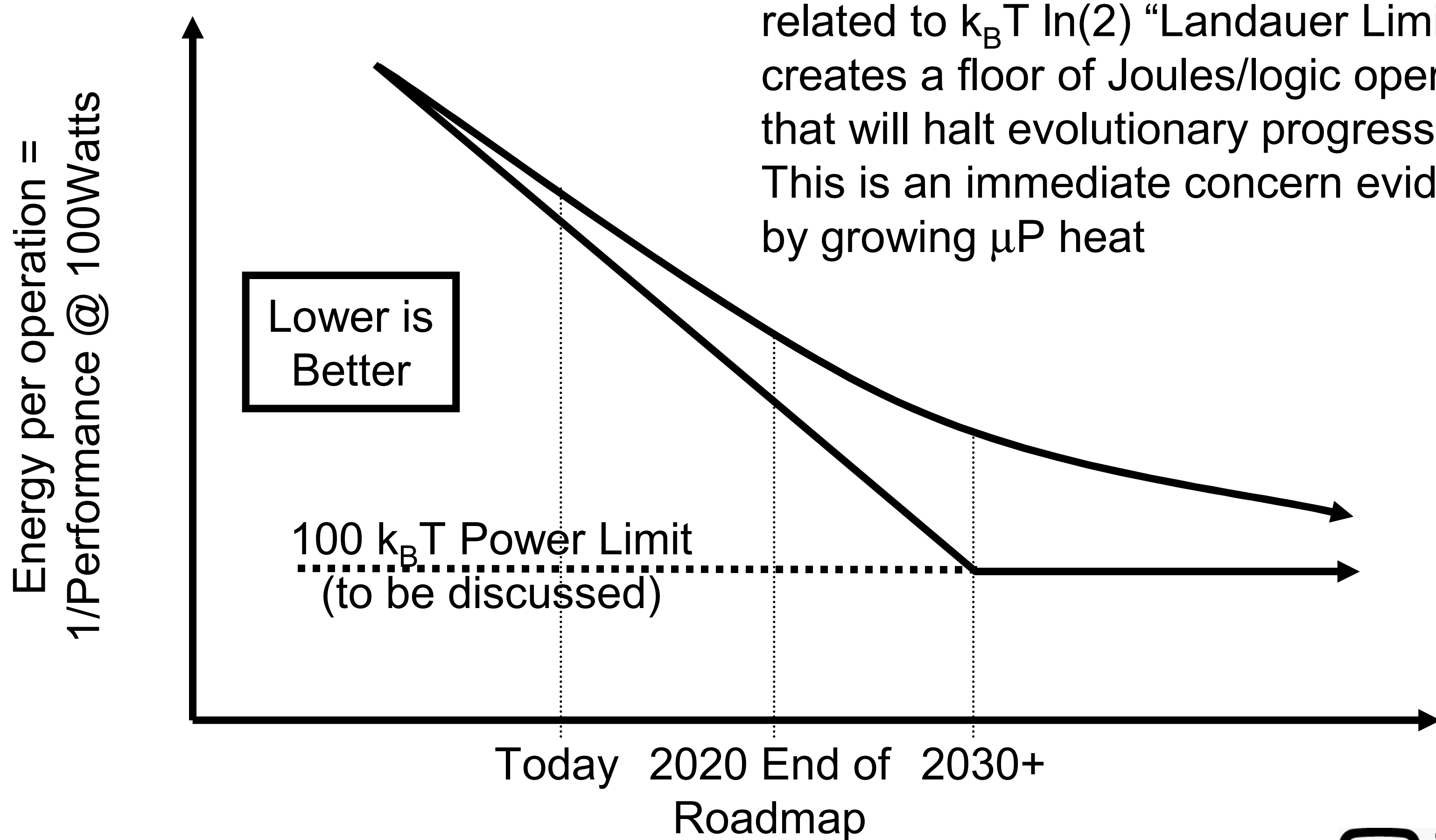
Experiments Under Discussion

- Continuation of Quantum Fortress work 1100
- Molecular QCA 1800
- Quantum Computing Tie-In
  - Architecture
  - Quantum Dot Measurements
  - Quantum Dot Manufacturing classical/quantum
- Computer Architecture beyond limits of Moore's Law
- Simulation of information+Physics

Moore's Law for Logic Switching Power

A 100 $k_B T$ "thermal device limit" closely related to $k_B T \ln(2)$ "Landauer Limit" creates a floor of Joules/logic operation that will halt evolutionary progress
This is an immediate concern evidenced by growing µP heat



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Emerging Research Devices (notes 2005)

- Table shows drop in replacements for CMOS transistors that defeat limit in previous slide
- Color code: OK, marginal, unacceptable
- CNFET on table only for political reasons

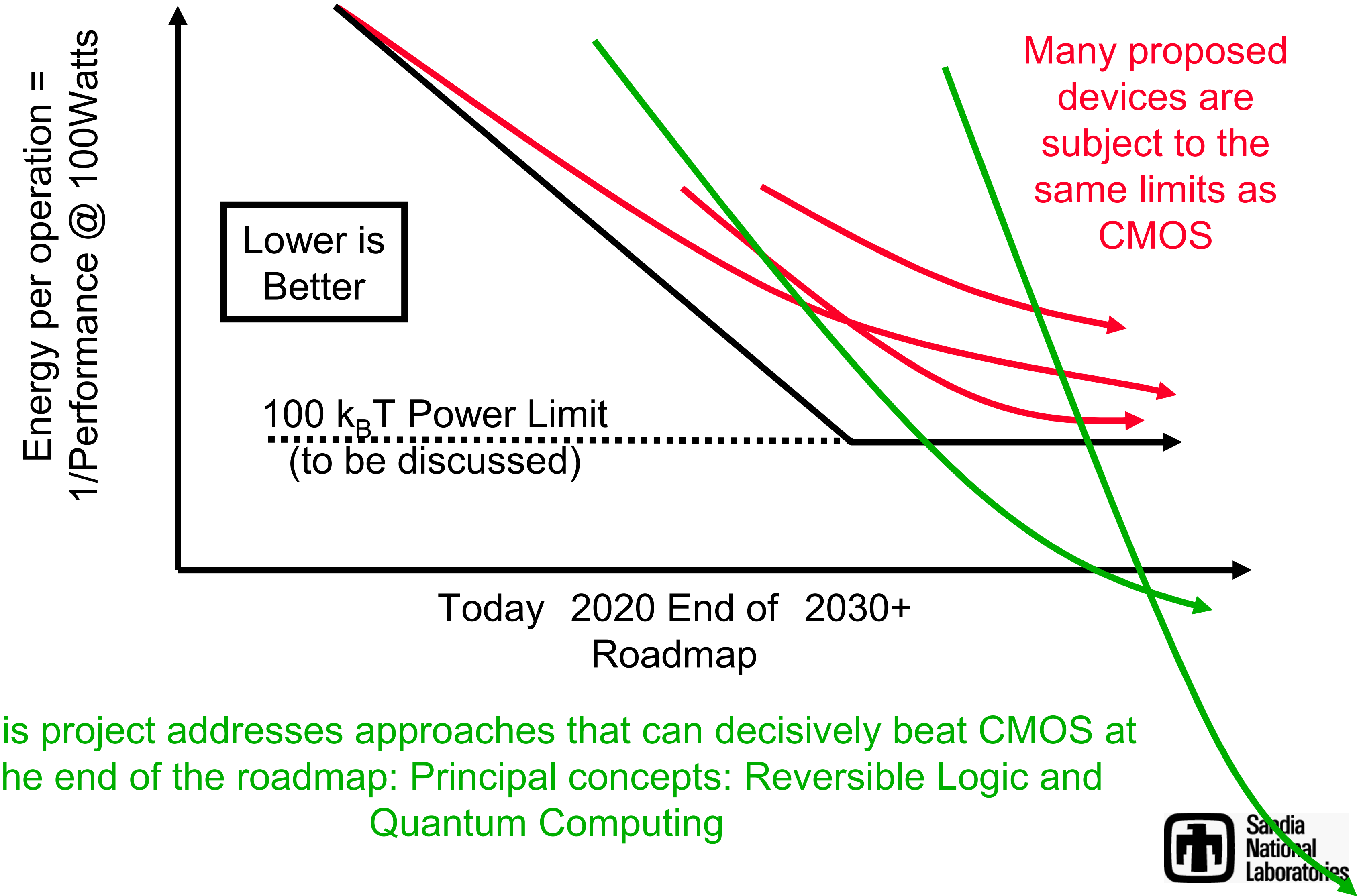
> 20	>16 - 18
>18 - 20	< 16

For each Technology Entry (e.g. 1D Structures, sum horizontally over the 8 Criteria
Max Sum = 24
Min Sum = 8

Evaluation of Emerging Research Logic Device Technologies against Technology Evaluation Criteria

Logic Device Technologies	Scalability	Perform-ance	Energy Efficiency	Gain	Operational Reliability	Room Temp. Operation ***	CMOS Compatibility **	CMOS Architectural Compatibility *
1D Structures	2.4	2.4	2.1	2.4	2.3	2.9	2.4	2.6
Resonant Tunneling Devices	1.4	2.0	1.9	1.7	1.7	2.9	2.1	2.1
SETs	1.9	1.0	2.5	1.3	1.2	1.9	2.4	2.0
Molecular Devices	1.9	1.1	2.0	1.1	1.3	2.6	1.9	1.6
Ferromagnetic Devices	1.5	1.2	1.8	1.5	1.8	2.2	1.5	1.8
Spin Transistor	1.7	1.7	2.2	1.5	2.0	2.2	1.7	1.8

Obeying Moore's Law and Beating CMOS



This project addresses approaches that can decisively beat CMOS at the end of the roadmap: Principal concepts: Reversible Logic and Quantum Computing

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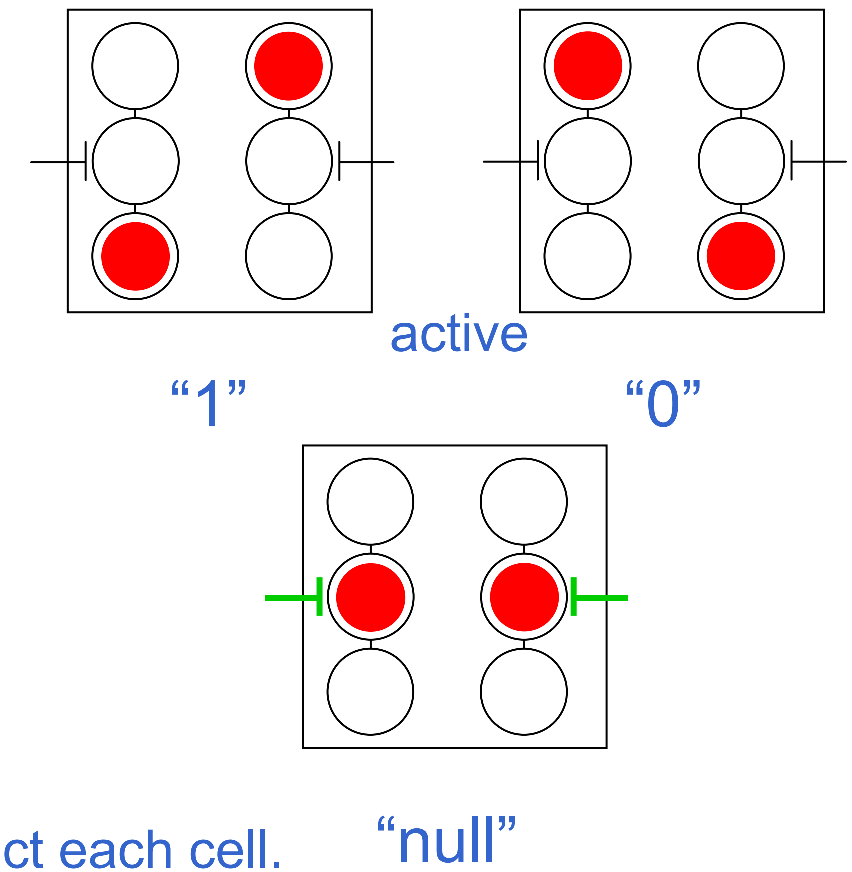
Tie Between Information and Device Physics

- We use Boolean logic today, based on AND-OR-NOT
- AND and OR gates “destroy” information, which creates heat irrespective of physical implementation (to be described later)
- This limit can be circumvented by a different form of logic that does not “destroy” information
- However, this will also require different devices…

Quantum-dot cellular automata

Represent binary information by charge configuration of cell.



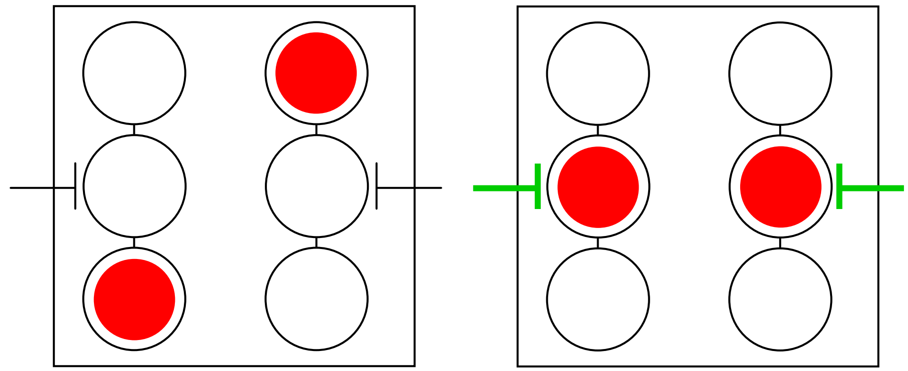
QCA cell

- Dots localize charge
- Two mobile charges
- Tunneling between dots
- Clock signal varies relative energies of “active” and “null” dots

Clock need not separately contact each cell.

Quantum-dot cellular automata

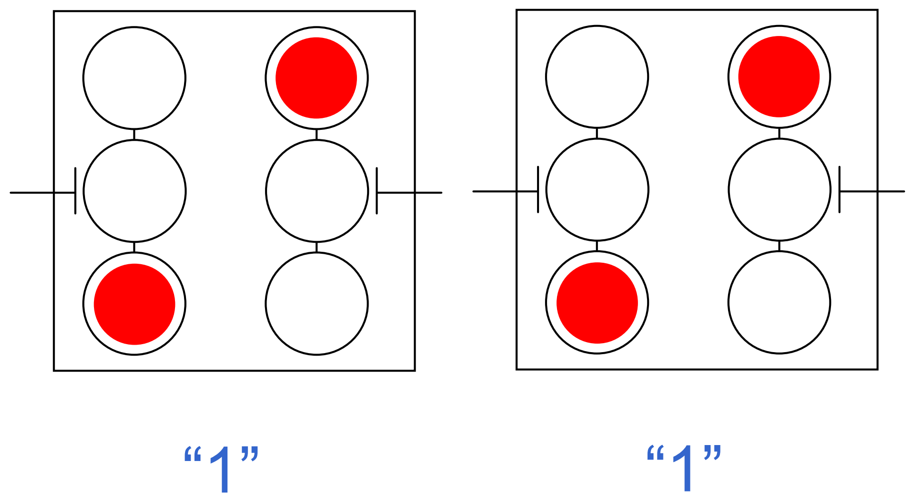
Neighboring cells tend to align in the same state.



“1” “null”

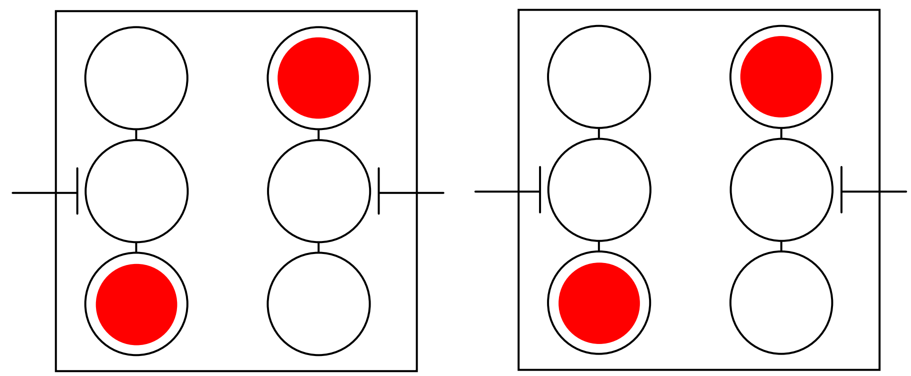
Quantum-dot cellular automata

Neighboring cells tend to align in the same state.



Quantum-dot cellular automata

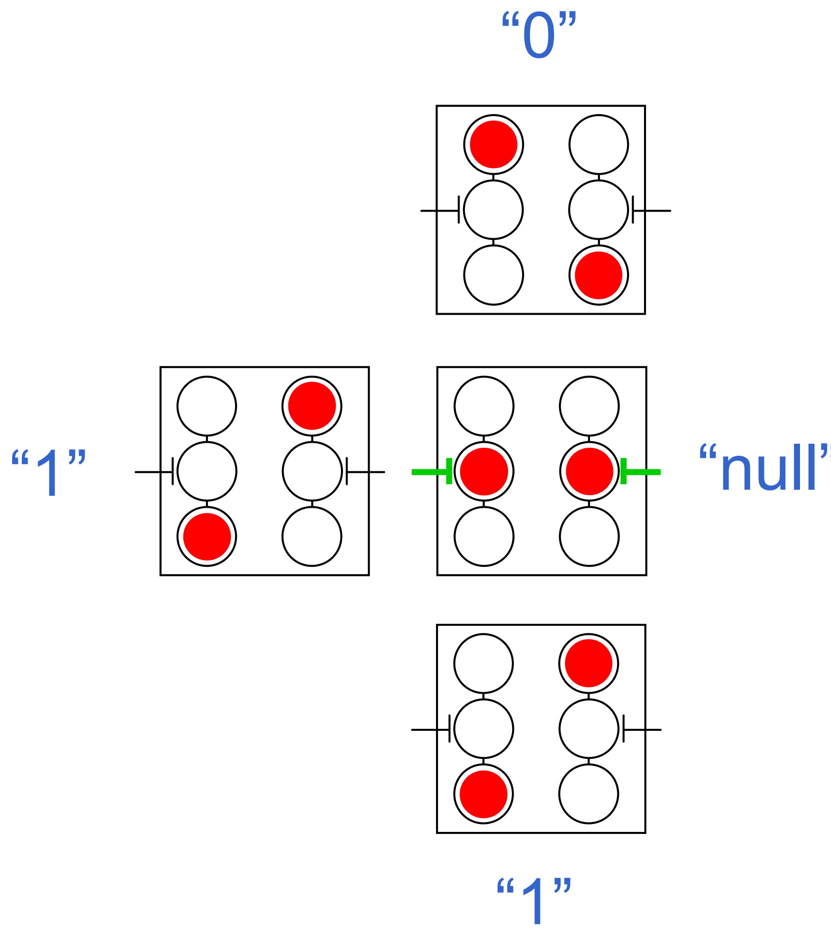
Neighboring cells tend to align in the same state.



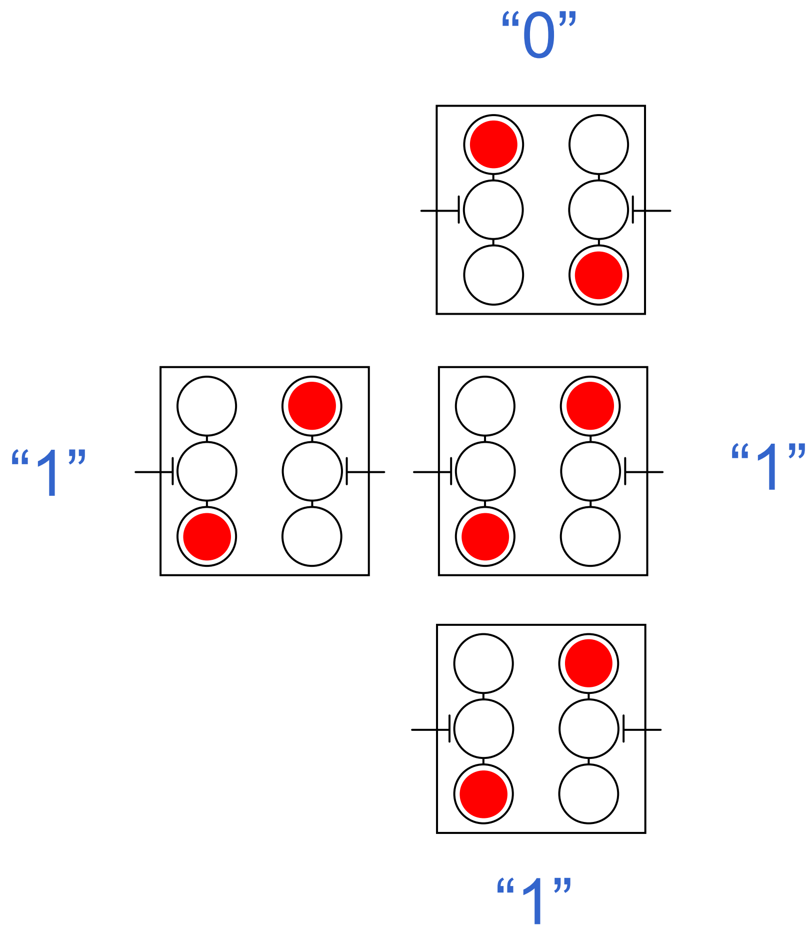
"1" "1"

This is the COPY operation.

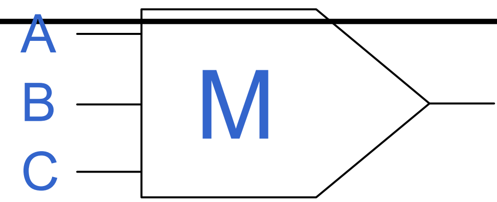
Majority Gate



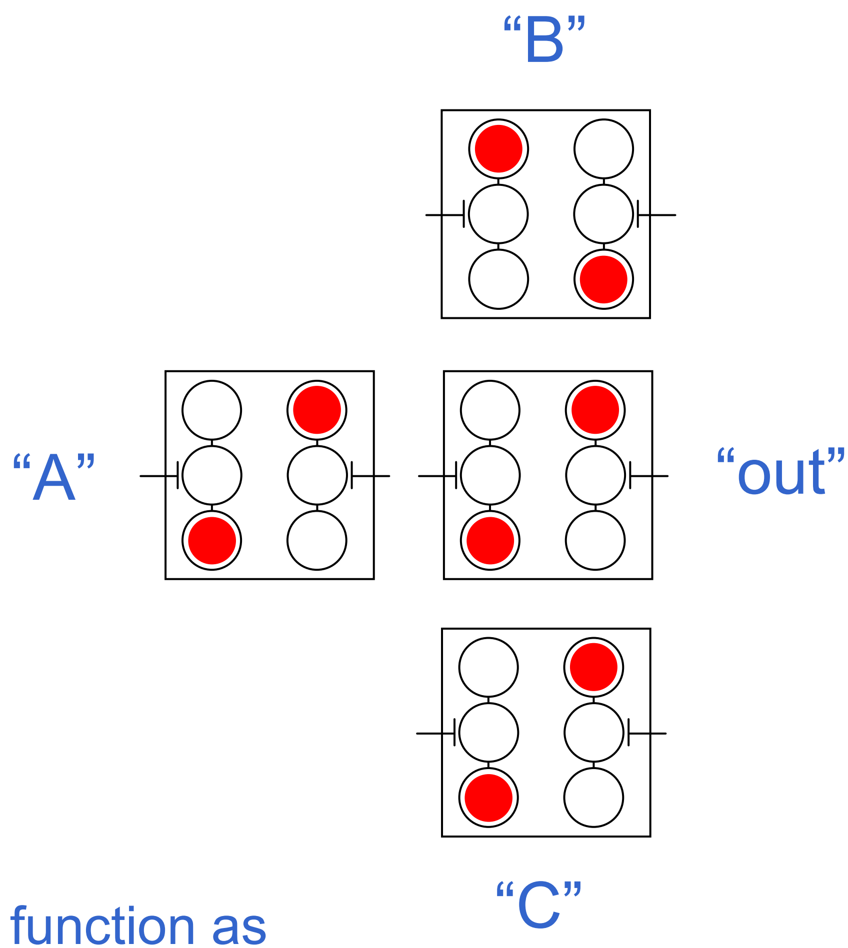
Majority Gate



Majority Gate

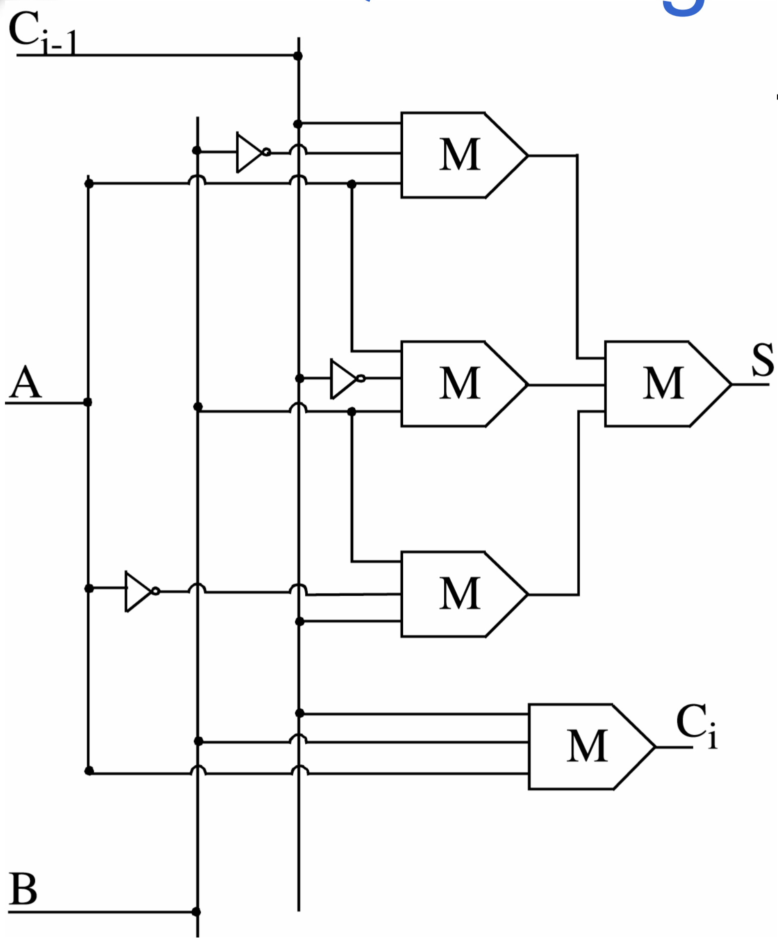


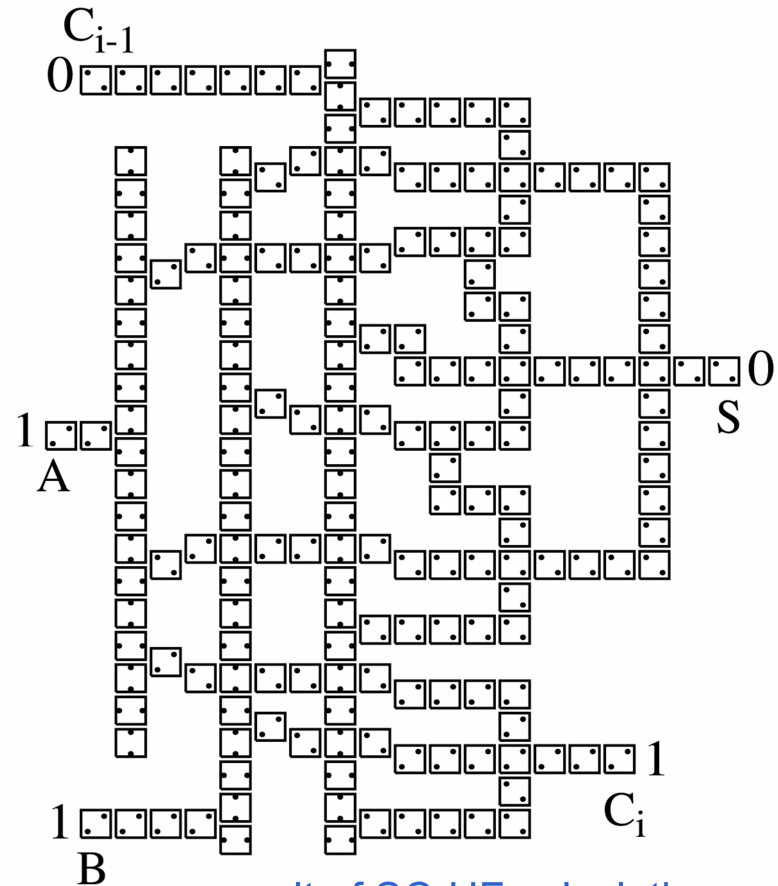
	A	B	C	Output
AND gate	0	0	0	0
	0	0	1	0
	0	1	1	1
	0	1	0	0
OR gate	1	1	0	1
	1	1	1	1
	1	0	1	1
	1	0	0	0



Three input majority gate can function as programmable 2-input AND/OR gate.

QCA single-bit full adder





result of SC-HF calculation with site model

Hierarchical layout and design are possible.

Simple-12 microprocessor (Kogge & Niemier)

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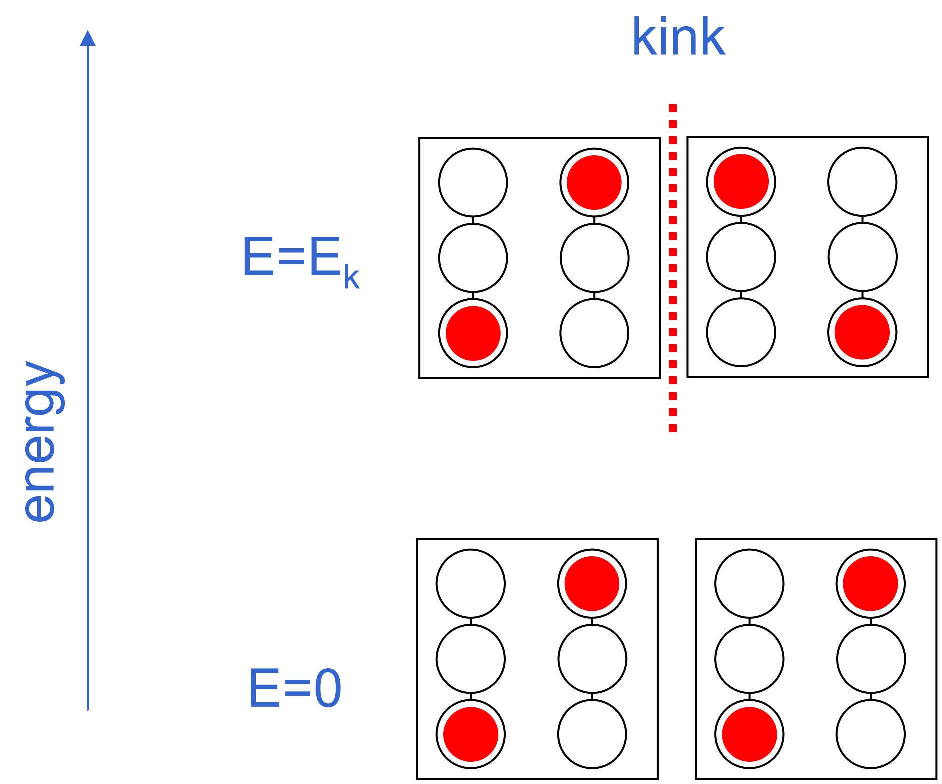
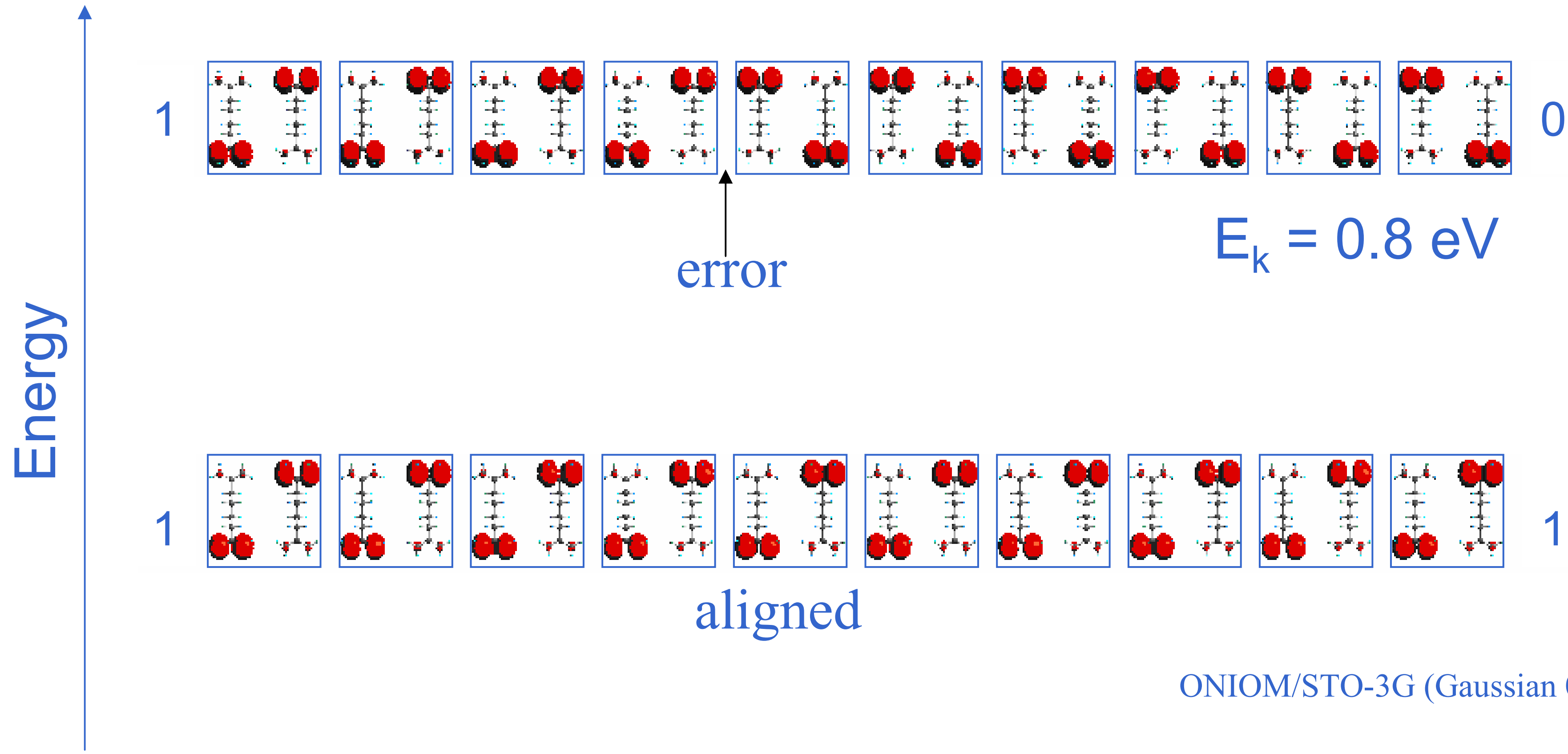
Computational wave: adder back-end

Characteristic energy



We would like "kink energy" $E_k > k_B T$.

Molecular Wire



ONIOM/STO-3G (Gaussian 03)

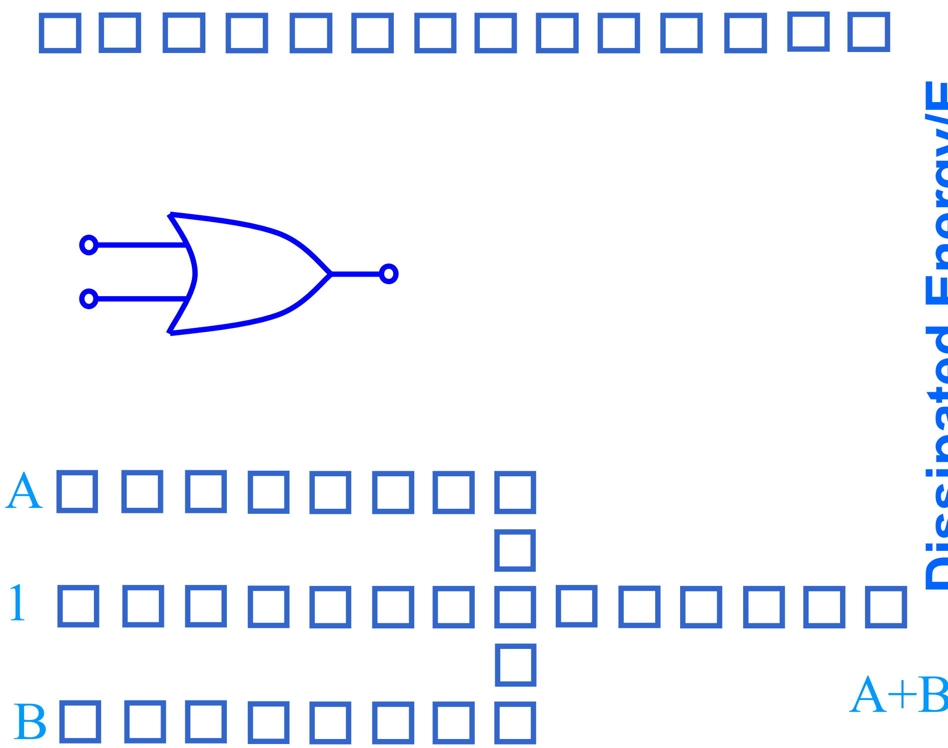
Power Gain in QCA Cells

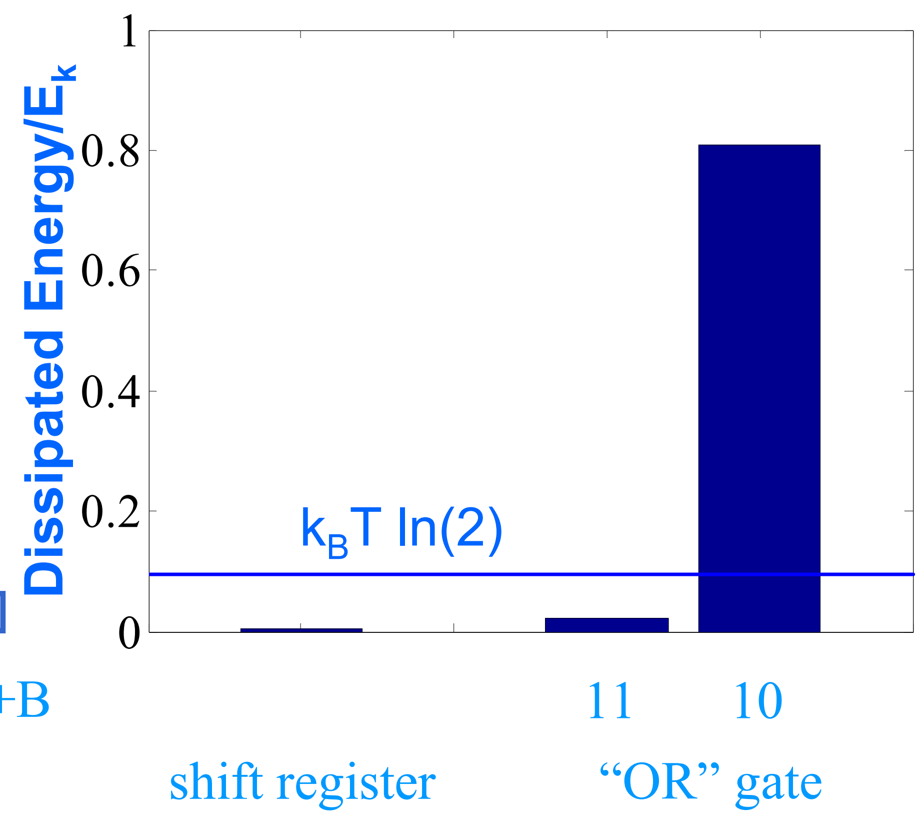
- Power gain is crucial for practical devices because some energy is always lost between stages.
- Lost energy must be replaced.
  - Conventional devices – current from power supply
  - QCA devices – from the clock
- Unity power gain means replacing exactly as much energy as is lost to environment.

Power gain > 3 has been measured in metal-dot QCA.

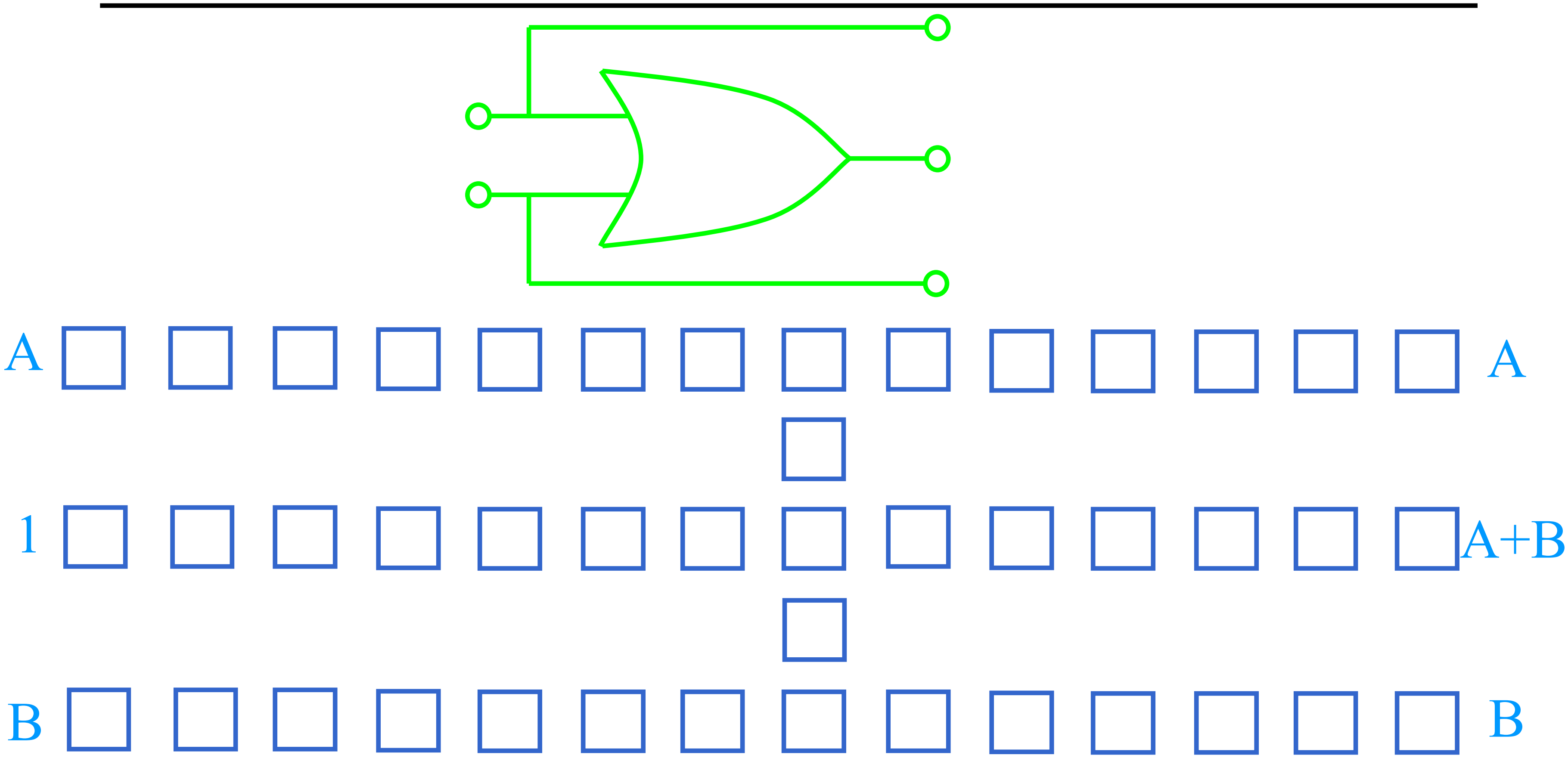
Landauer Clocking

Energy dissipation in Landauer-clocked circuit





Test circuit: OR gate



Landauer clocking with echo of inputs to outputs

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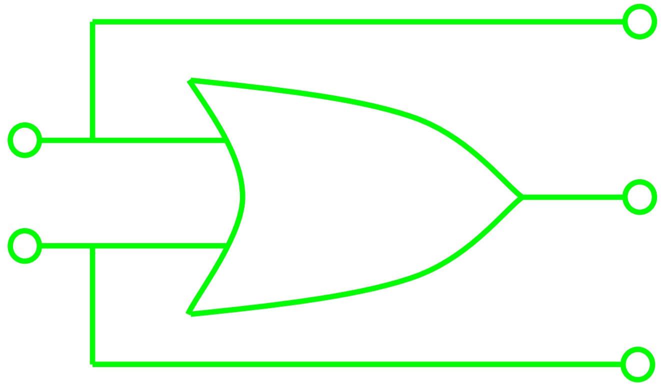
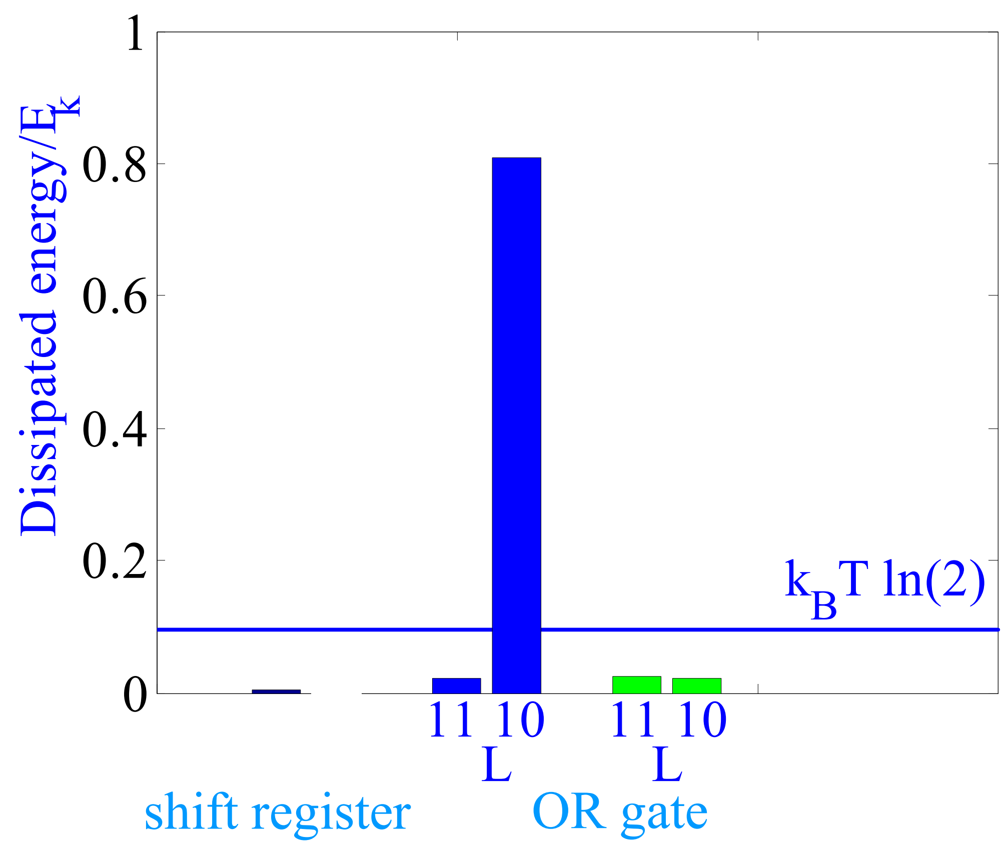
Energy dissipation in the OR gate





Energy dissipation greatly reduced with inputs echoed to outputs

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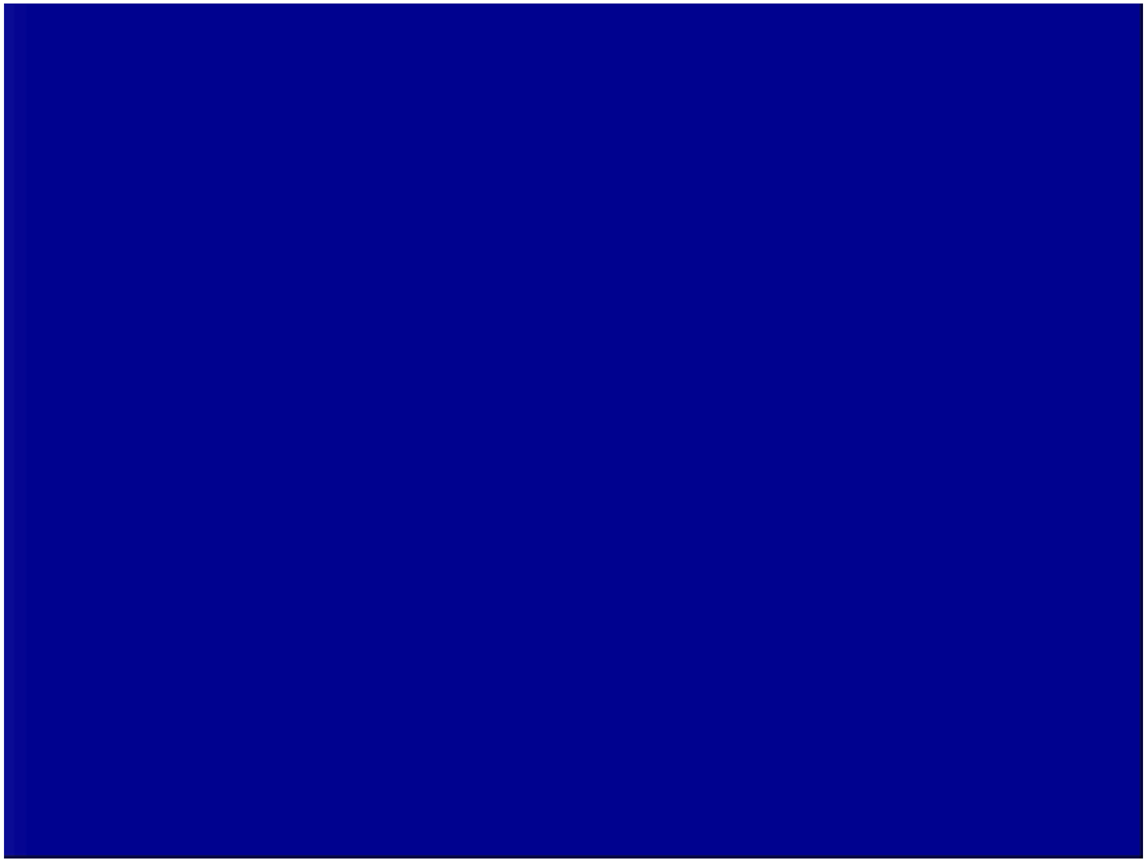
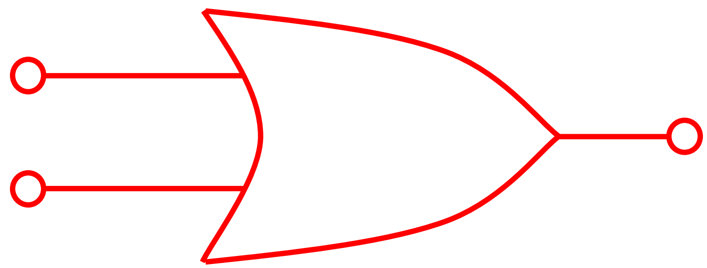
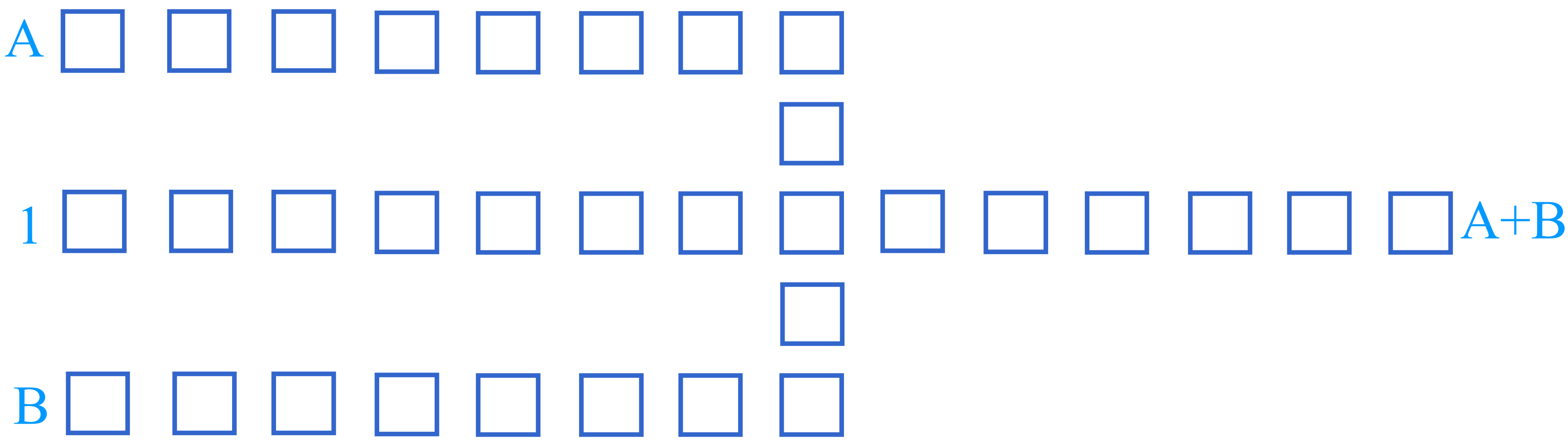
Bennett clocking of QCA



Output is used to erase intermediate results.

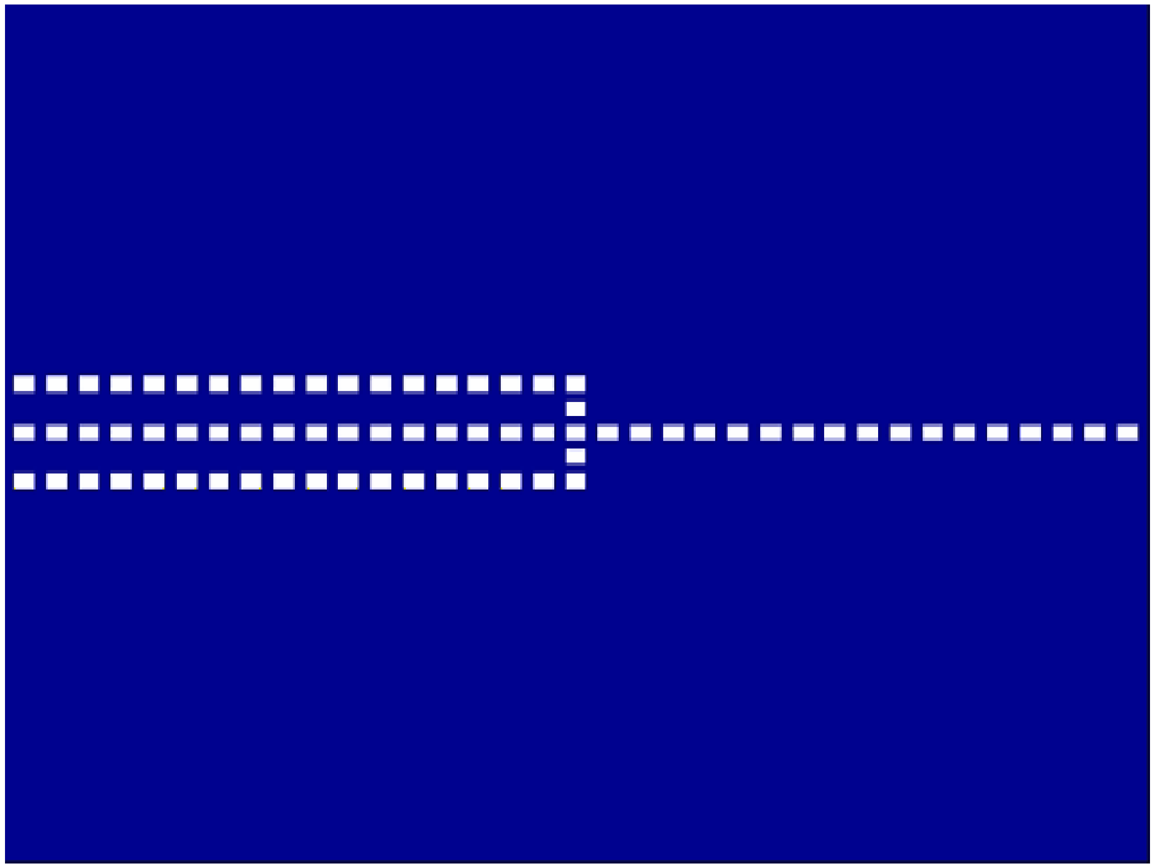
Test circuit: OR gate





Bennett clocked OR gate

Bennett clocking of QCA



For QCA no change in layout is required.

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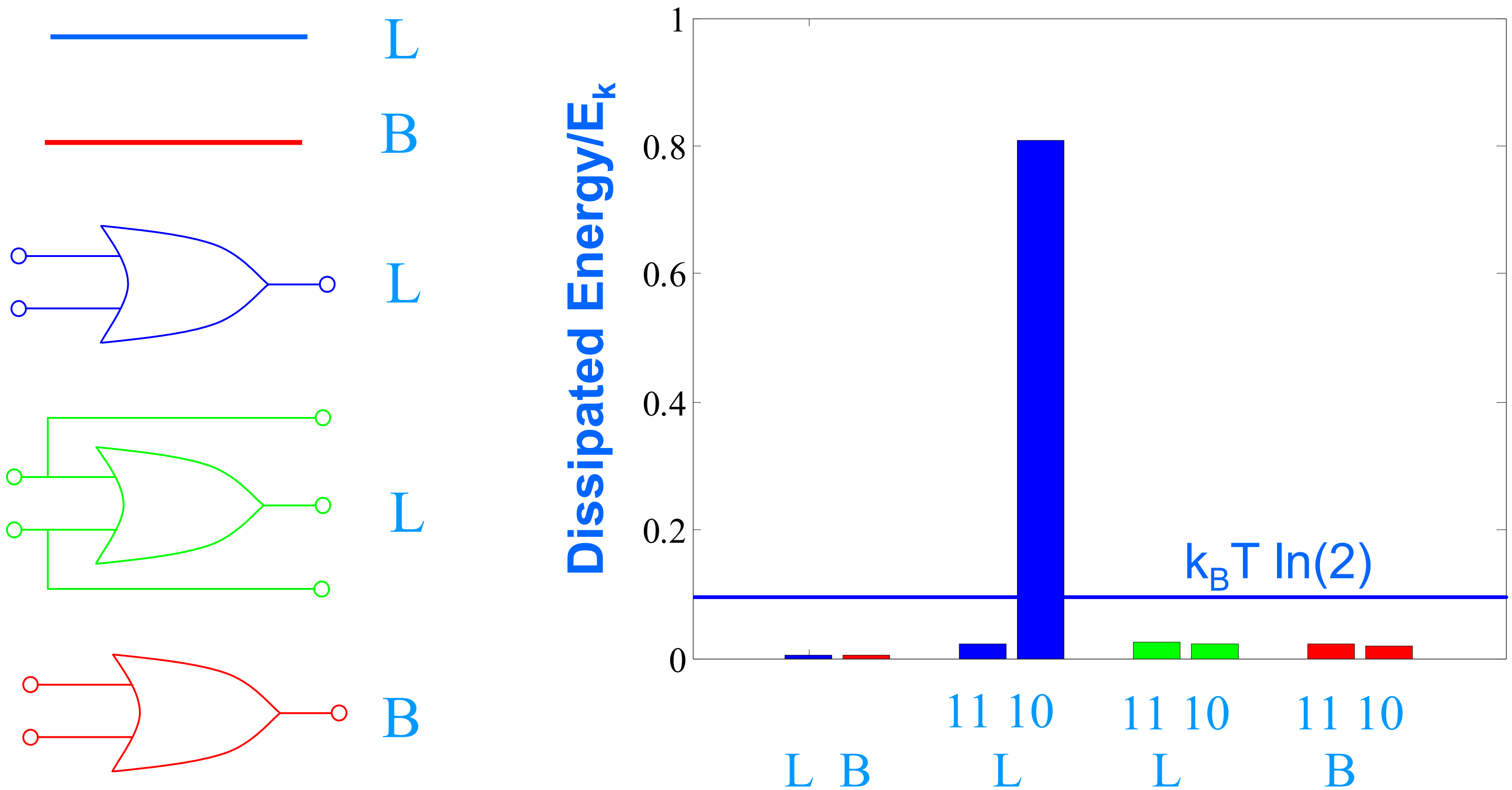
Bennett-style computation may be practical in QCA



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

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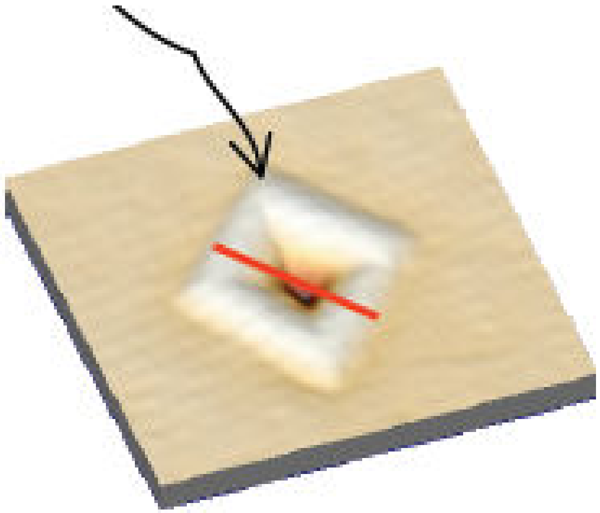
QCA implementations

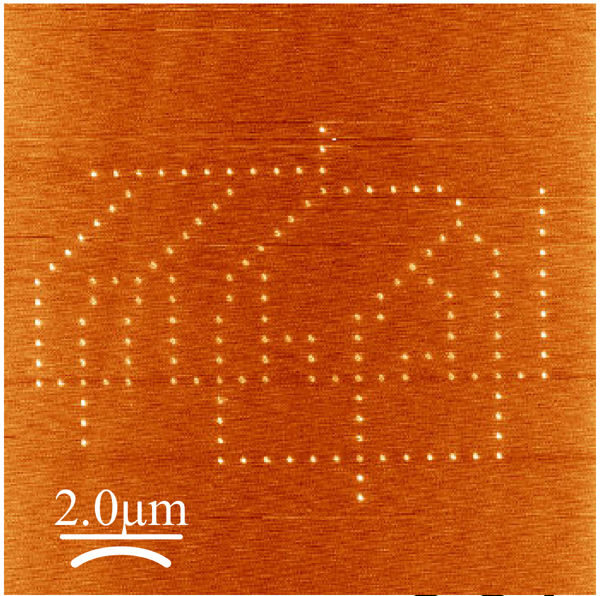
- Semiconductor-dot QCA
  - SiGe quantum fortresses
  - Silicon P-doping
  - GaAs
  - Silicon dot SET’s
- Magnetic QCA
- Metal-dot QCA
- Molecular QCA
- CMOS analogue

LDRD Status

- Current work underway at Sandia to find novel ways to create QCA cells
- SiGe identified as potential material system
- MBE growth of SiGe Quantum Fortresses underway
- FIB pattern designed and fabricated to allow electrical testing of Quantum Fortresses
- Electrical contact and testing will be undertaken this fall at University of Notre Dame

SiGe Quantum Fortresses

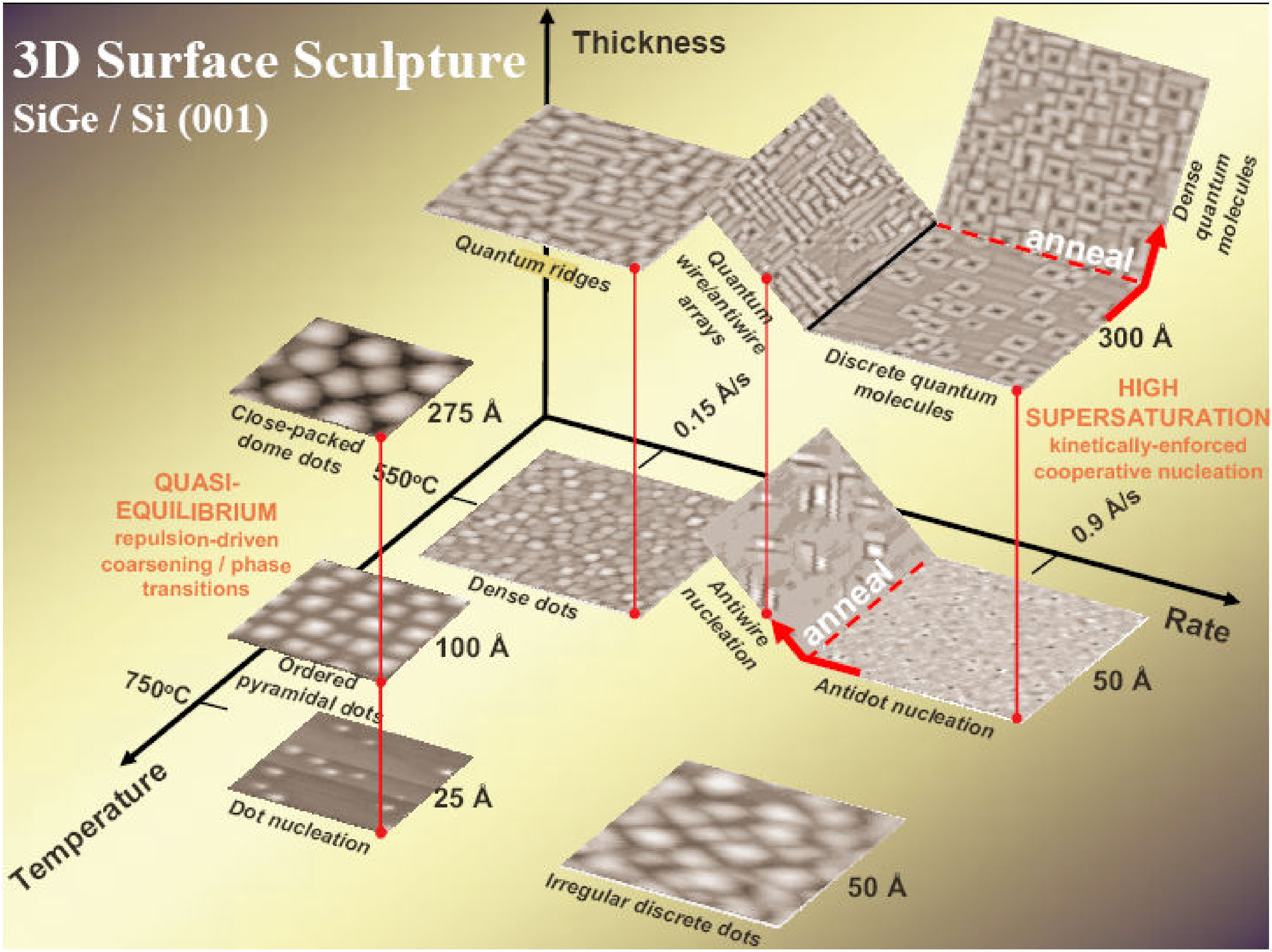




- Potential new way to create QCA cells
- Self-Assembled with 4 fold symmetry
- Fortress growth can be directed

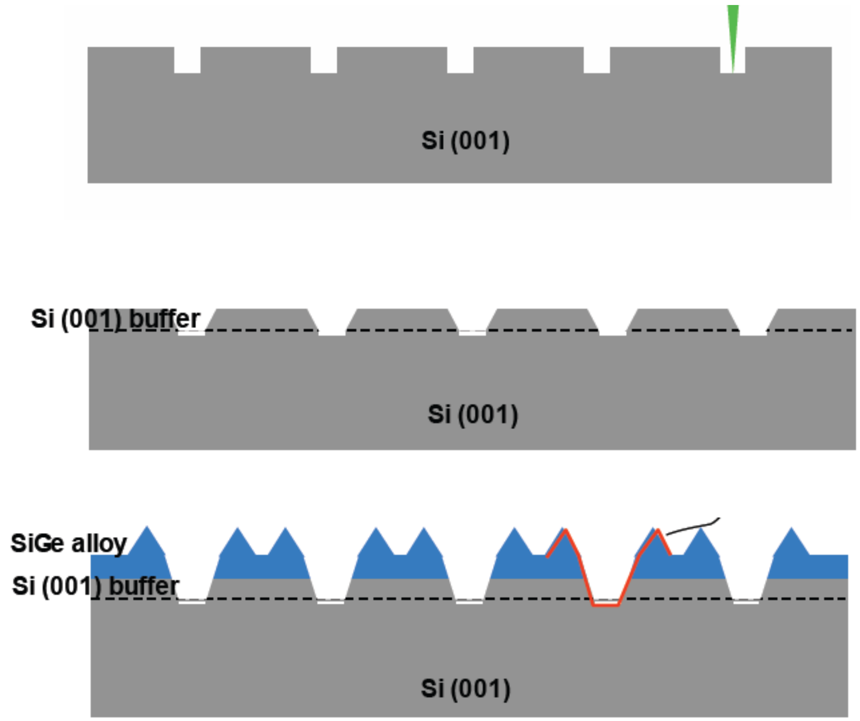
SiGe Quantum Fortresses

- When grown at optimum conditions, Silicon Germanium alloys form "fortress-like" structure
- 4-fold symmetry of structure may allow it to be used as a QCA cell
- Growth can be directed by introducing defects to the crystal surface

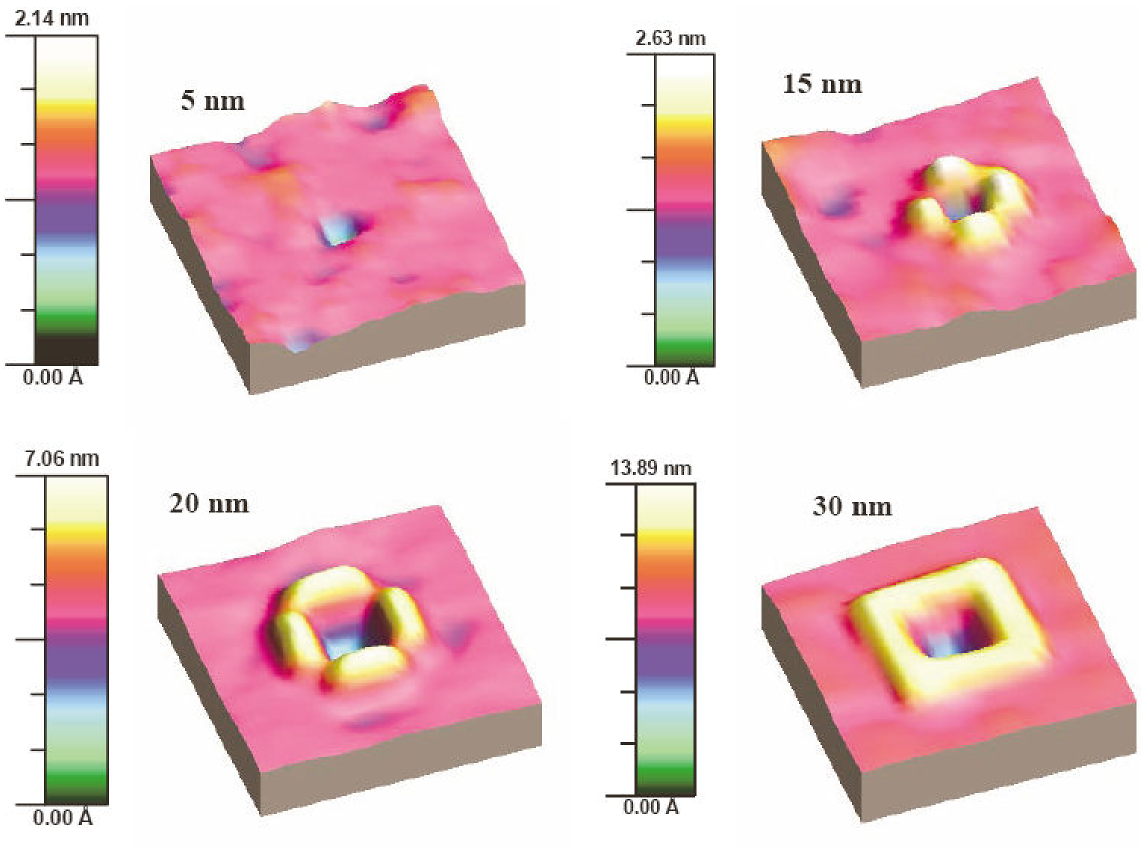

3D Surface Sculpture
SiGe / Si (001)
Thickness
Rate
Temperature
Quantum ridges
Quantum wire/antiwire arrays
Dense quantum molecules
anneal
300 Å
Discrete quantum molecules
HIGH SUPERSATURATION
kinetically-enforced cooperative nucleation
0.15 Å/s
0.9 Å/s
Close-packed dome dots
275 Å
550°C
QUASI-EQUILIBRIUM
repulsion-driven coarsening / phase transitions
Dense dots
Antiwire nucleation
anneal
50 Å
Antidot nucleation
Ordered pyramidal dots
100 Å
750°C
25 Å
Dot nucleation
Irregular discrete dots
50 Å

SiGe Quantum Fortresses

- Silicon is patterned using a gallium FIB
- 7nm Si buffer is grown
- .6Å/s Si and .3Å/s Ge are grown, to a total thickness of 200Å.



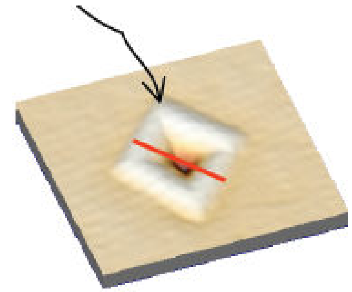
Quantum Fortress Growth

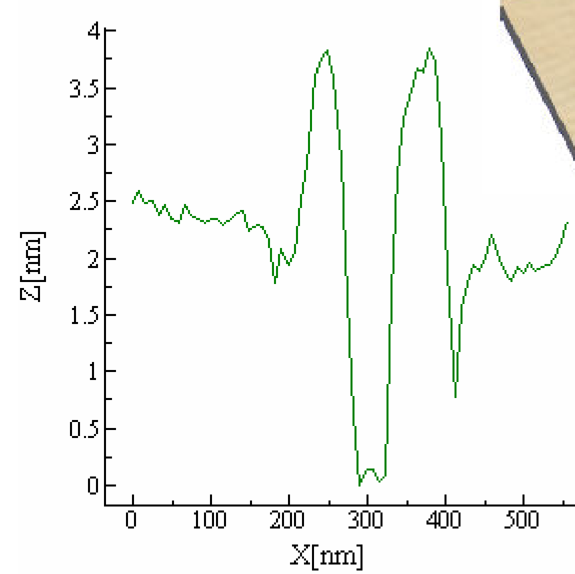


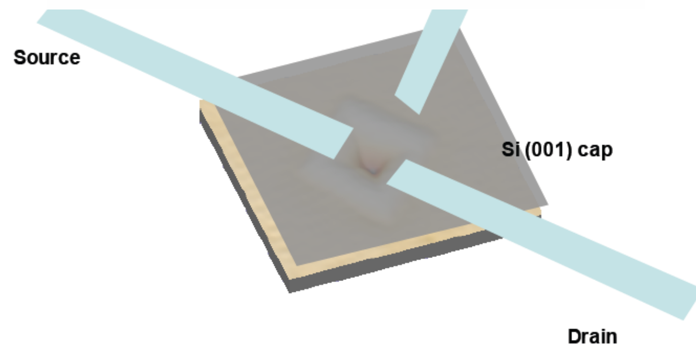
h nm $Ge_{0.3}Si_{0.7}$/Si(100), 550° C, 0.09 nm/s

SiGe Quantum Fortresses

- Quantum fortresses form around the gallium damage sites, roughly 220nm x 220nm.
- X-Ray Diffraction indicates that significant germanium enrichment occurs, allowing carrier confinement
- These may be used as electrical devices such as SETs or Quantum Cellular Automata cells

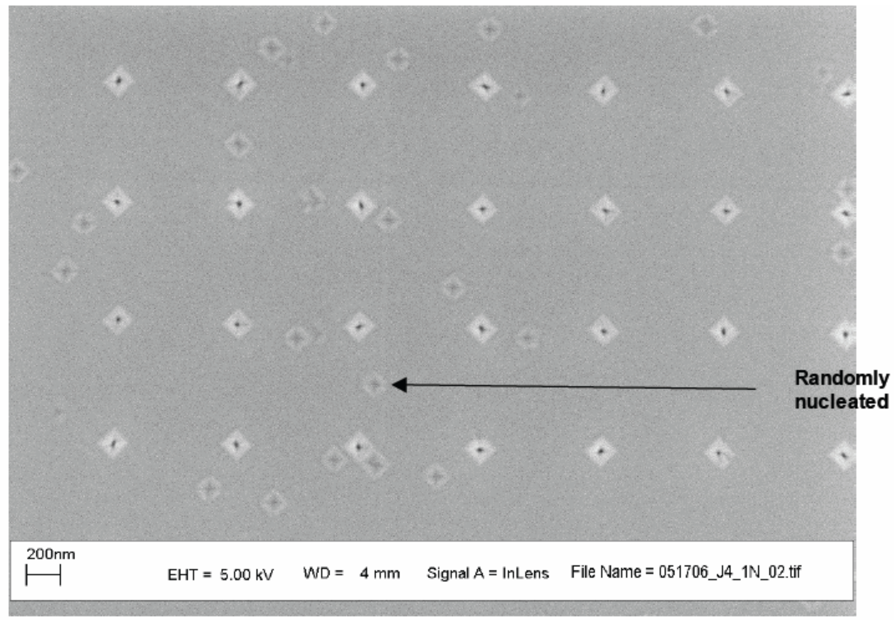






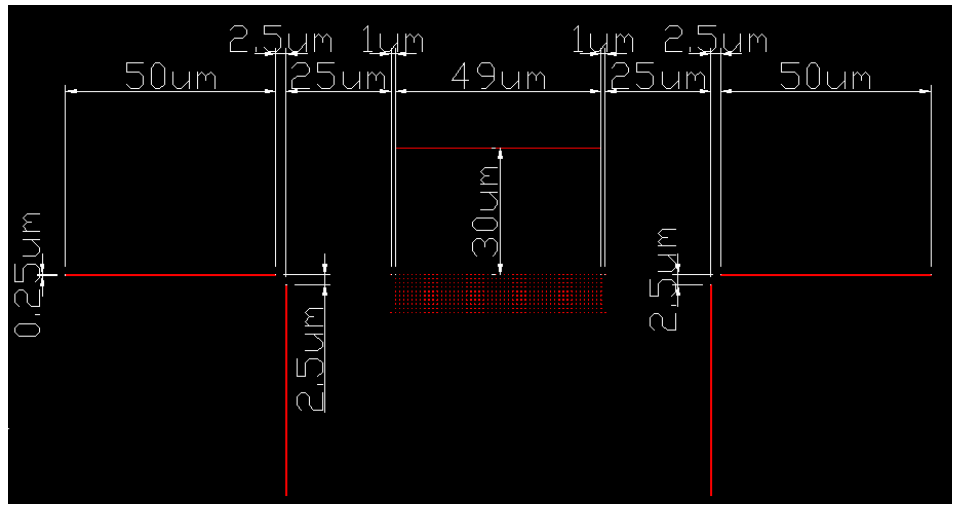
SiGe Quantum Fortresses

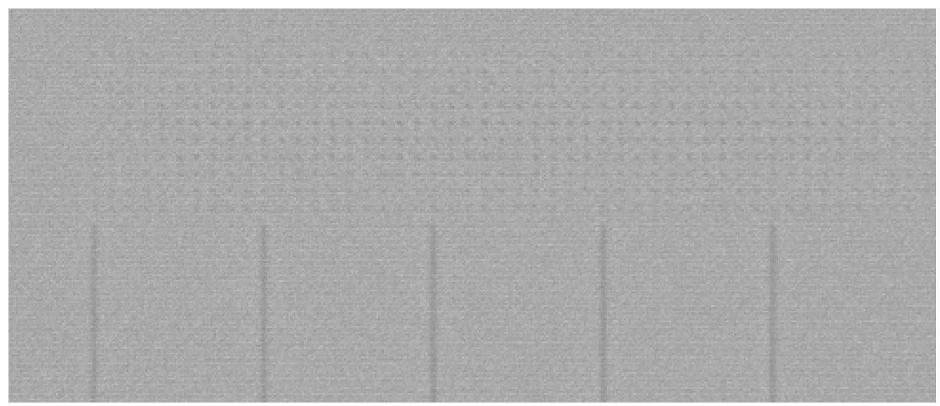
- Undirected nucleation also occurs, increasing the quantum dot density beyond the original pattern



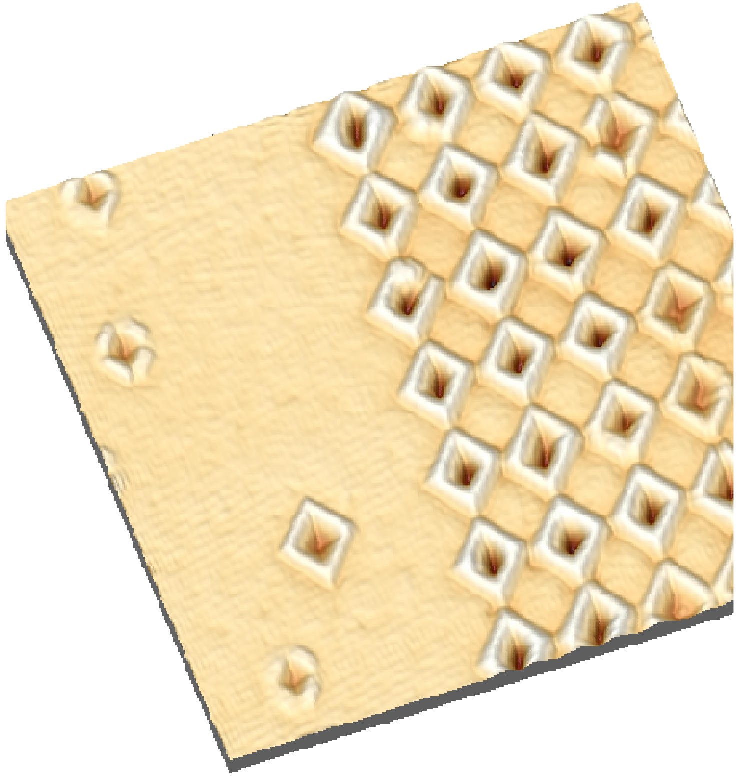
Quantum Fortress Patterning

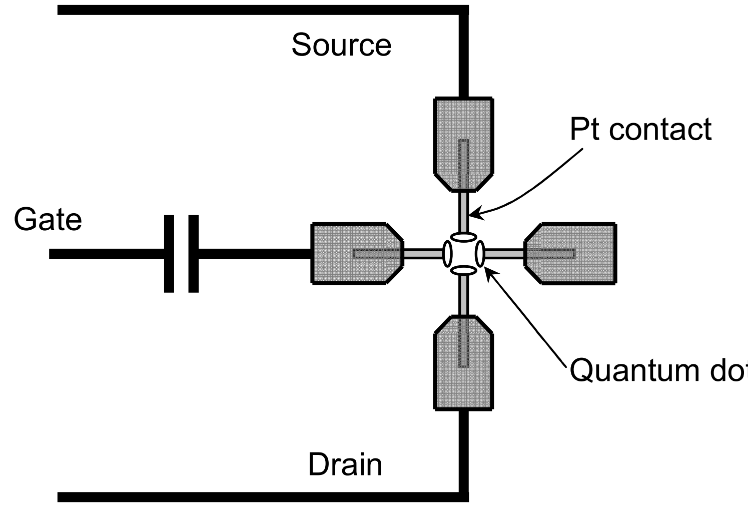
- Current experiments are attempting to grow capped, aligned samples which can be contacted using e-beam lithography and metal deposition
- Grid of Dots with fiducial marks created to facilitate electrical testing



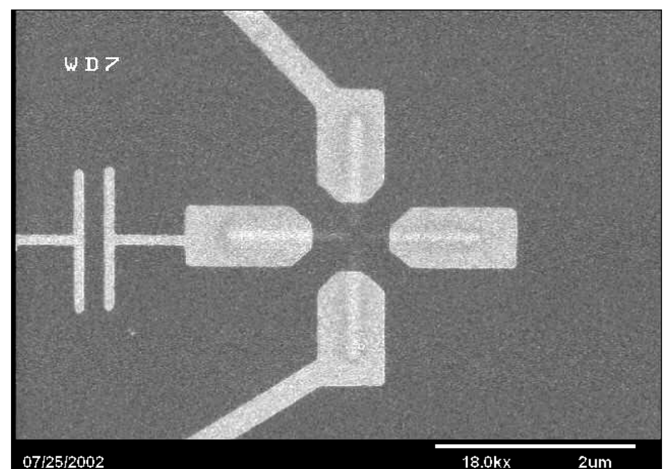


Quantum Fortress QCA

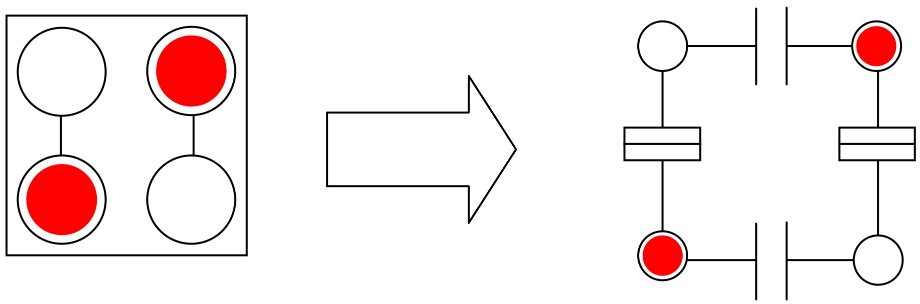




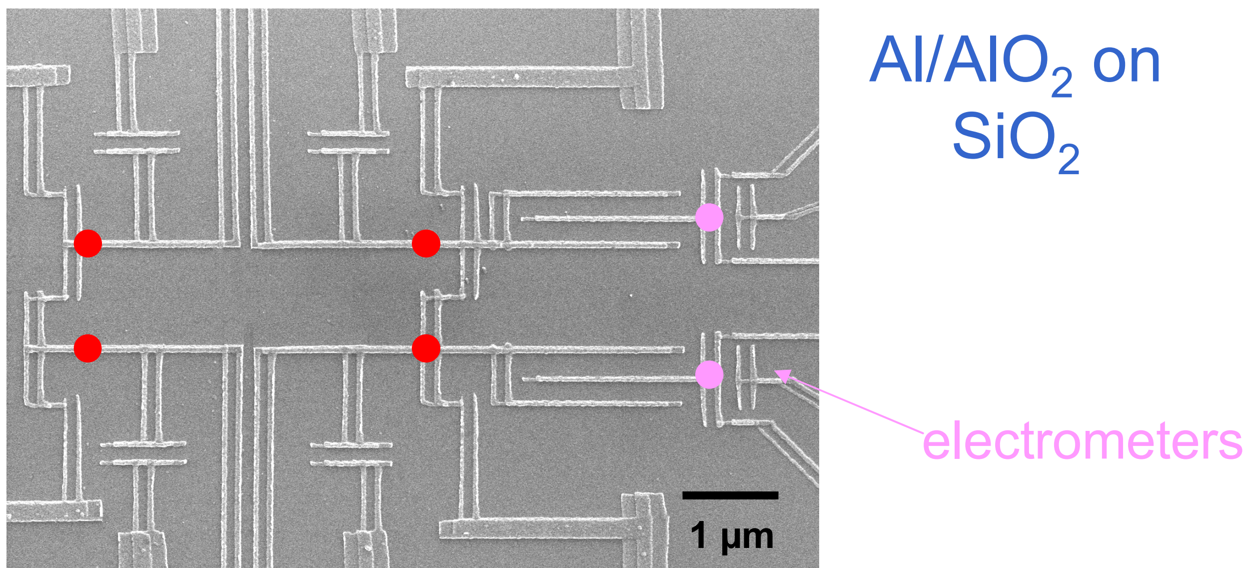
FIB are used to deposit Pt contacts to ease the alignment requirements of the E-beam lithography.



Metal-dot QCA implementation



Metal tunnel junctions



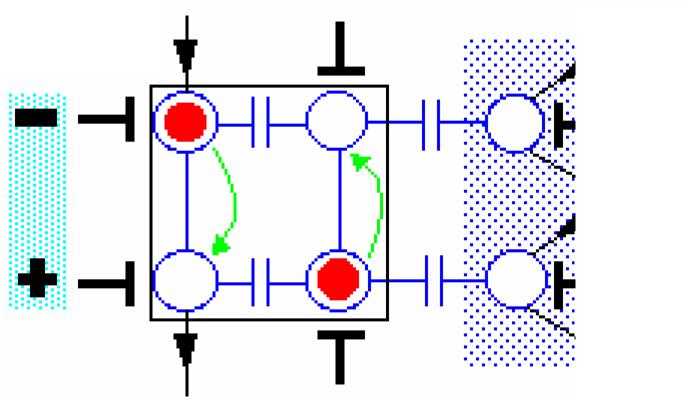
Al/AlO_2 on SiO_2

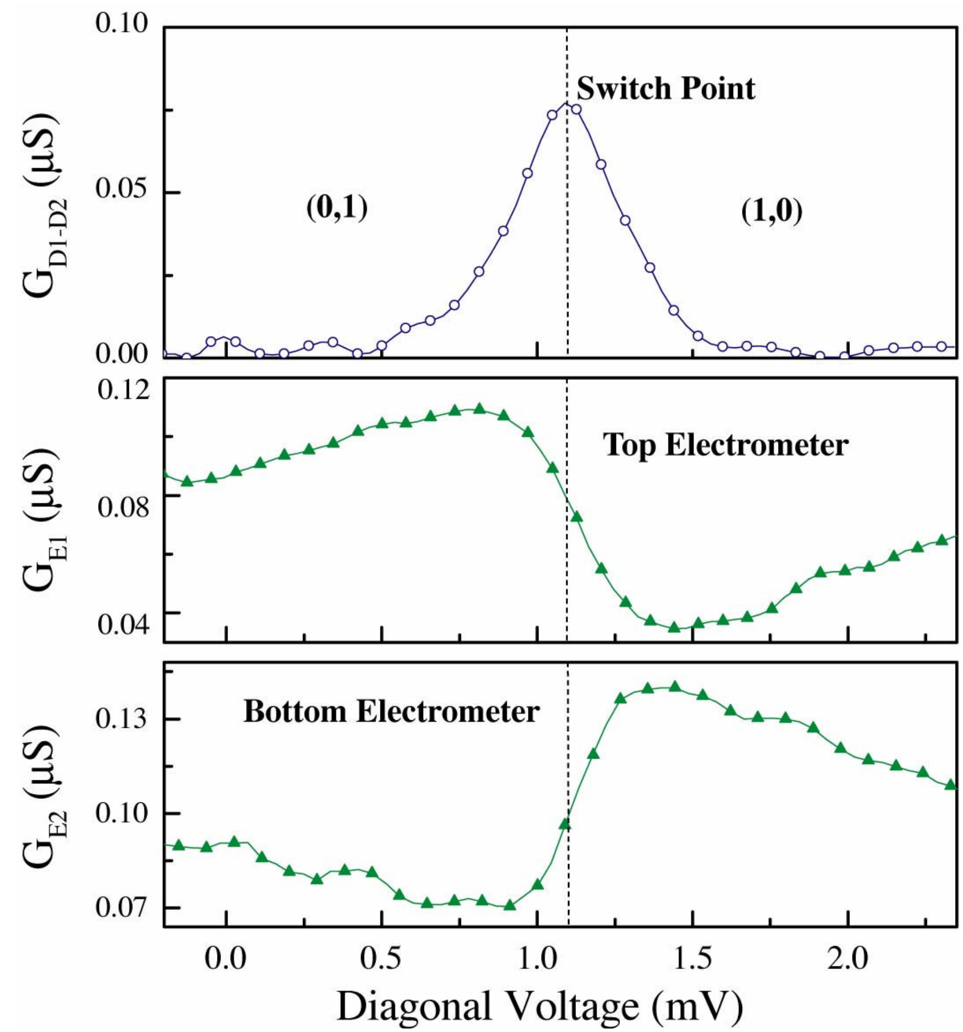
70 mK

“dot” = metal island

Metal-dot QCA cells and devices

- Demonstrated 4-dot cell

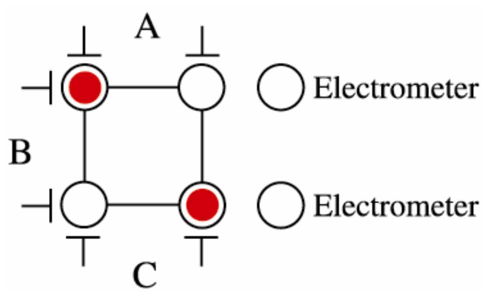


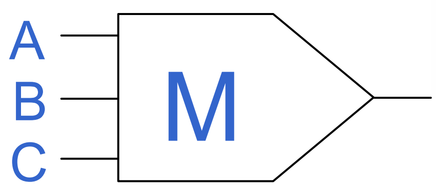


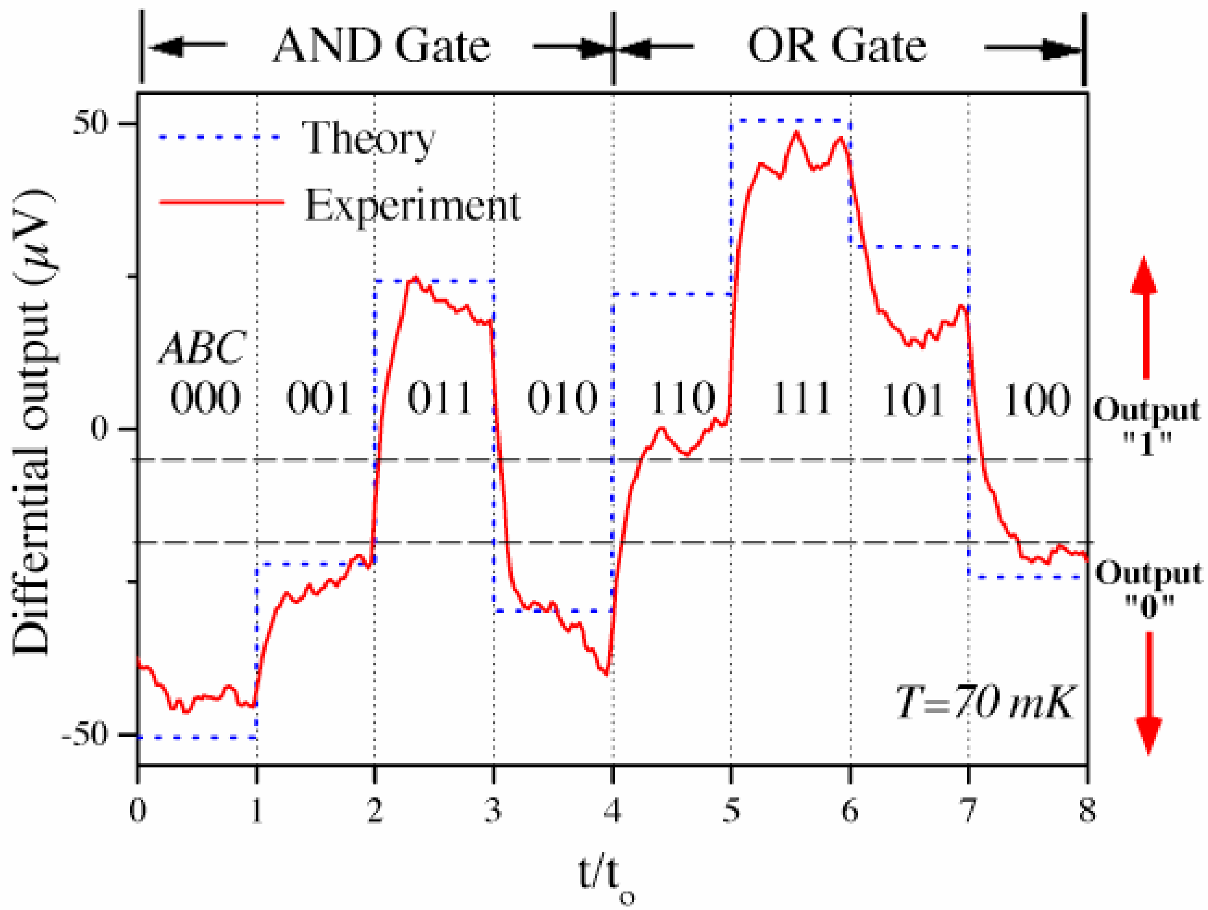
A.O. Orlov, I. Amlani, G.H. Bernstein, C.S. Lent, and G.L. Snider, *Science*, **277,** pp. 928-930, (1997).

Majority Gate

	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

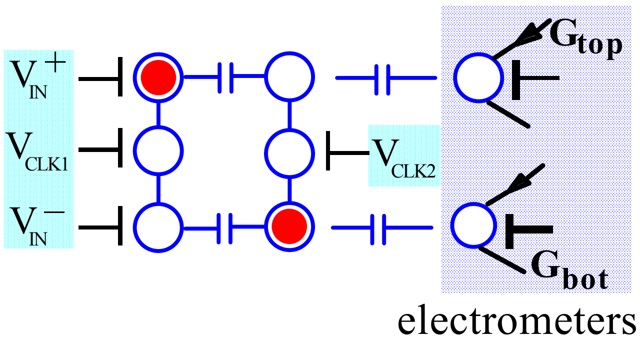


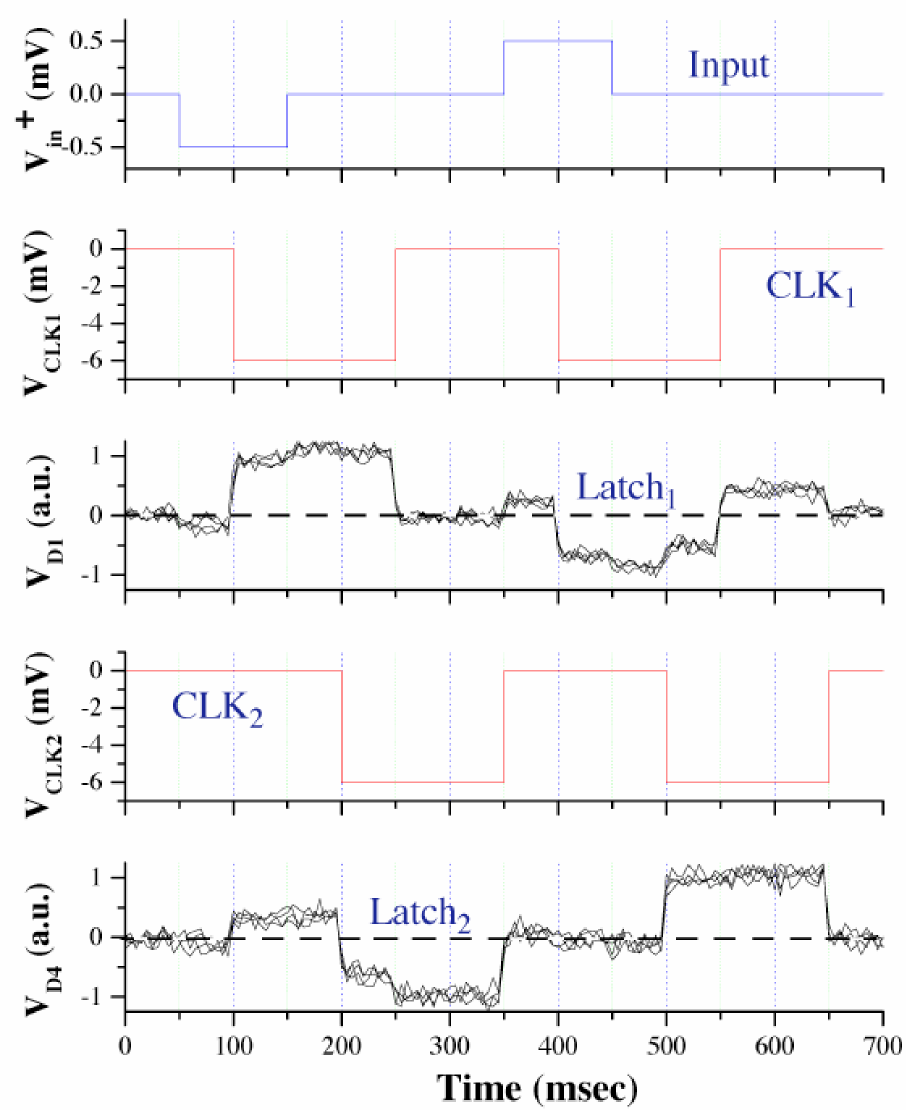




Amlani, A. Orlov, G. Toth, G. H. Bernstein, C. S. Lent, G. L. Snider, *Science* **284**, pp. 289-291 (1999).

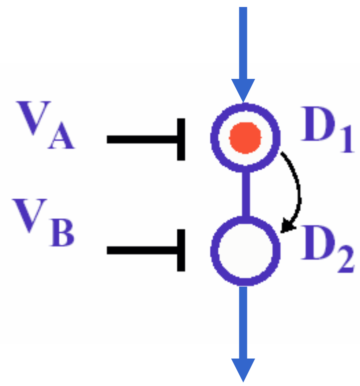
QCA Shift Register



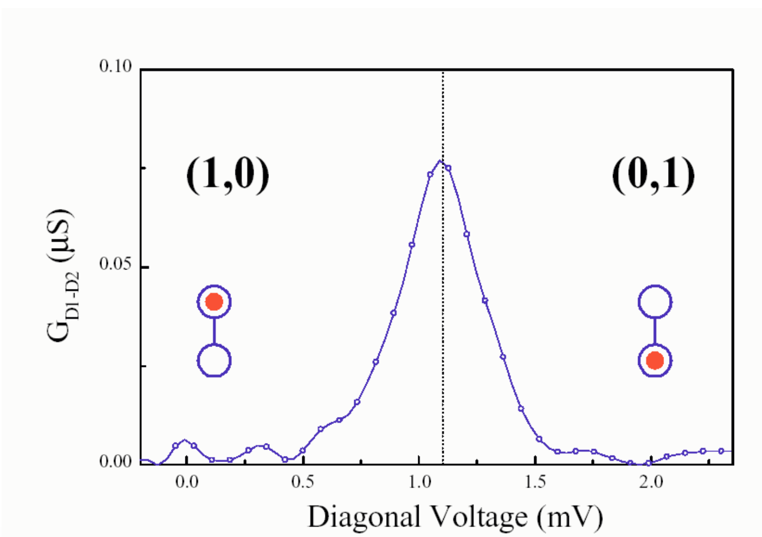


Electron Switching in QCA

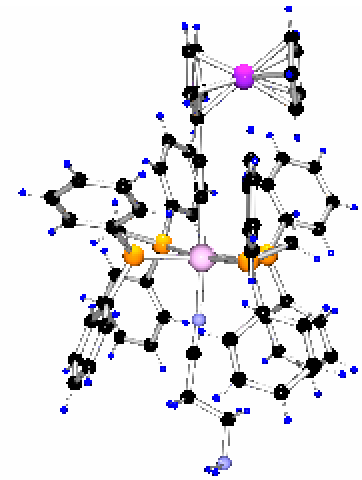
Metal Dots



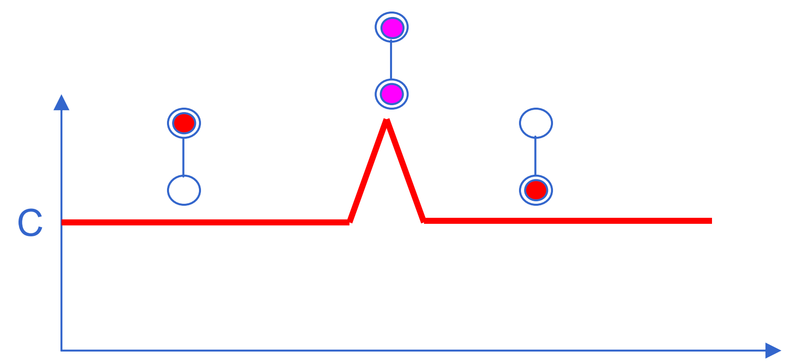
Measure conductance



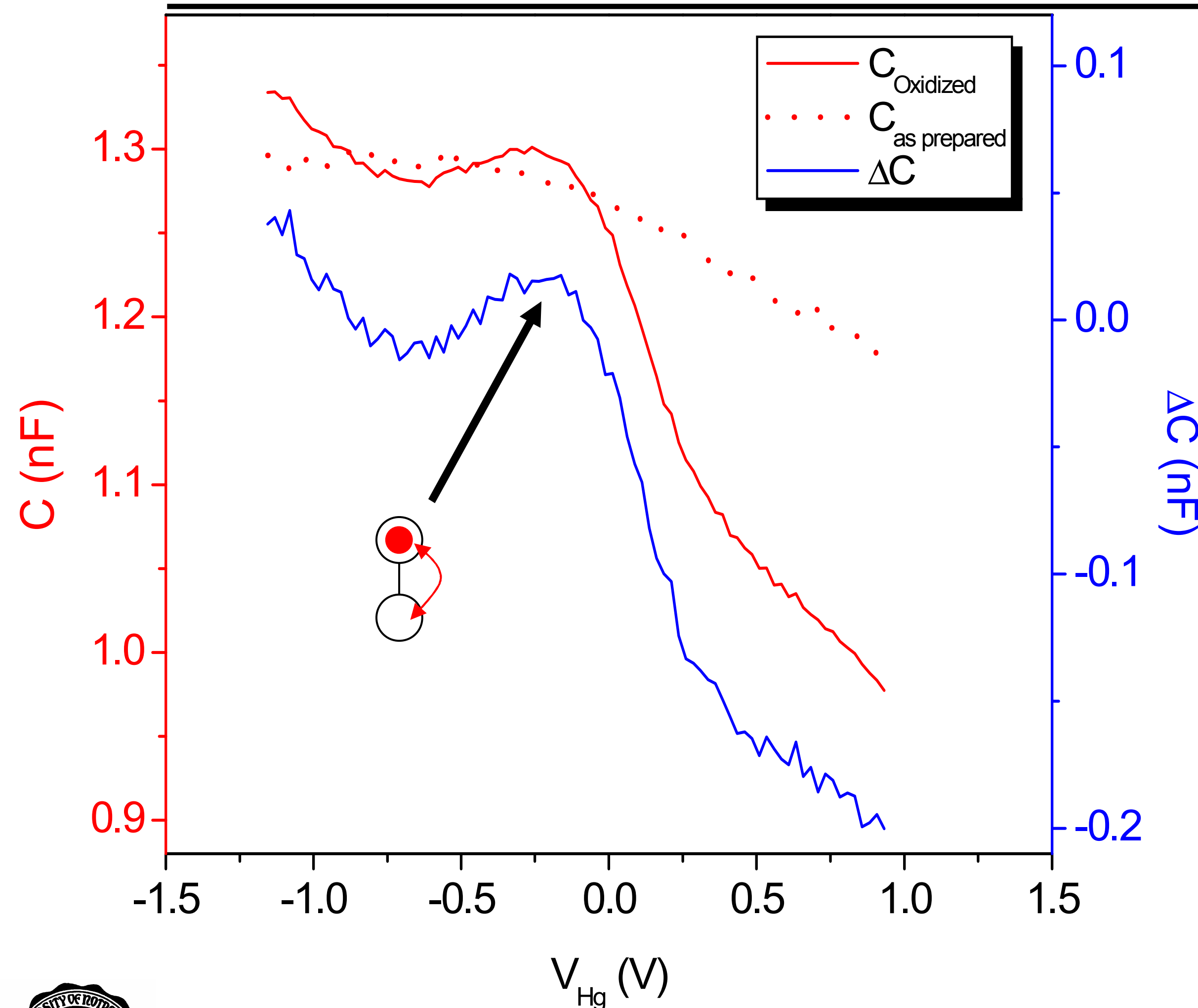
Molecular Dots



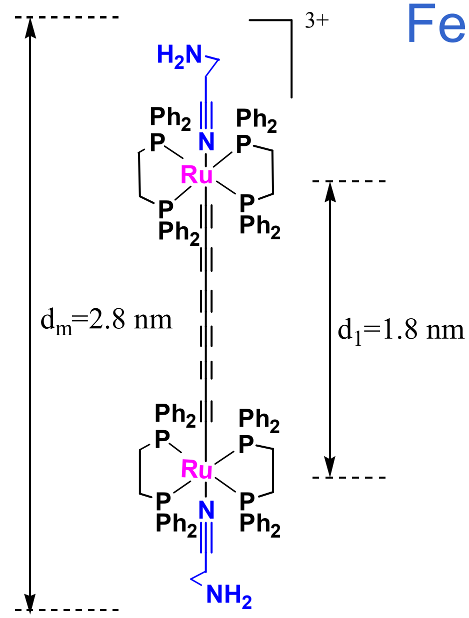
Measure capacitance



Double-dot click-clack



Hua & Fehlner



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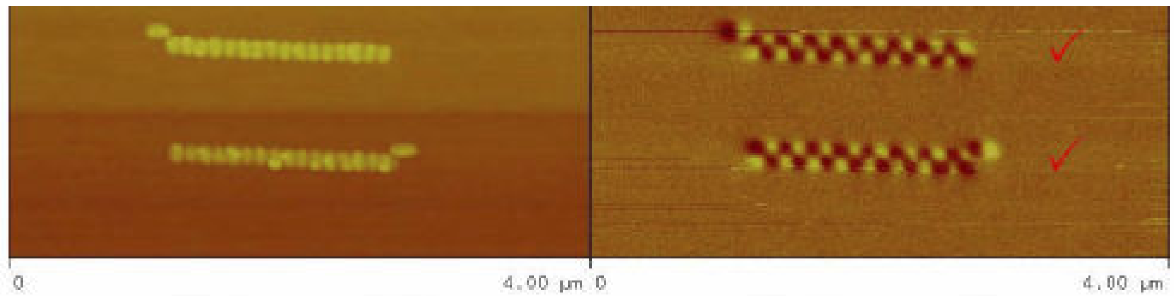
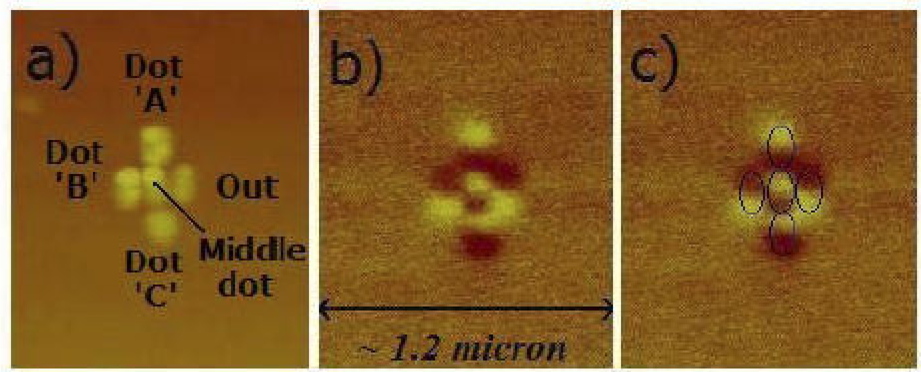
Magnetic QCA cell



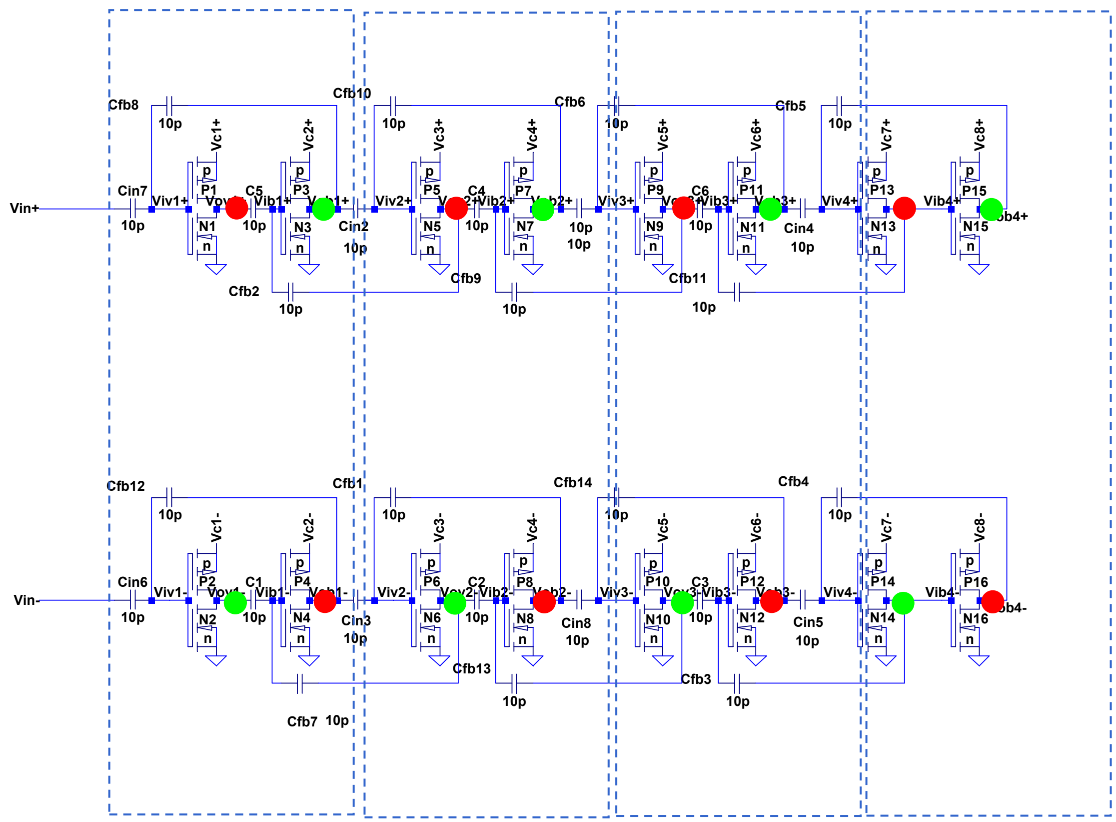
Bernstein, Imrae, Metlushko, Orlova, Zhou, Csaba, Porod, Magnetic QCA Systems, Microelectronics Journal, 36, 619 (2005).



- Dots are permalloy islands
- Limited to > ~20 nm sizes

CMOS analogue of QCA

- “Dots” are CMOS nodes
- Instead of charge quantization use transistor action
- Room temperature
- Slow performance
- Test-bed for architecture and power dissipation ideals



Silicon P-dot QCA cell

APPLIED PHYSICS LETTERS **89**, 013503 (2006)

Demonstration of a silicon-based quantum cellular automata cell

M. Mitic,[a] M. C. Cassidy, K. D. Petersson,[b] R. P. Starrett, E. Gauja, R. Brenner, R. G. Clark, and A. S. Dzurak
Centre for Quantum Computer Technology, School of Electrical Engineering and School of Physics, The University of New South Wales, Sydney, New South Wales 2052, Australia

C. Yang and D. N. Jamieson
Centre for Quantum Computer Technology, School of Physics, University of Melbourne, Victoria 3010, Australia

(Received 8 March 2006; accepted 18 May 2006; published online 5 July 2006)

We report on the demonstration of a silicon-based quantum cellular automata (QCA) unit cell incorporating two pairs of metallically doped (n^+) phosphorus-implanted nanoscale dots, separated from source and drain reservoirs by nominally undoped tunnel barriers. Metallic cell control gates, together with Al–AlO$_x$ single electron transistors for noninvasive cell-state readout, are located on the device surface and capacitively coupled to the buried QCA cell. Operation at subkelvin temperatures was demonstrated by switching of a single electron between output dots, induced by a driven single electron transfer in the input dots. The stability limits of the QCA cell operation were also determined. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2219128]

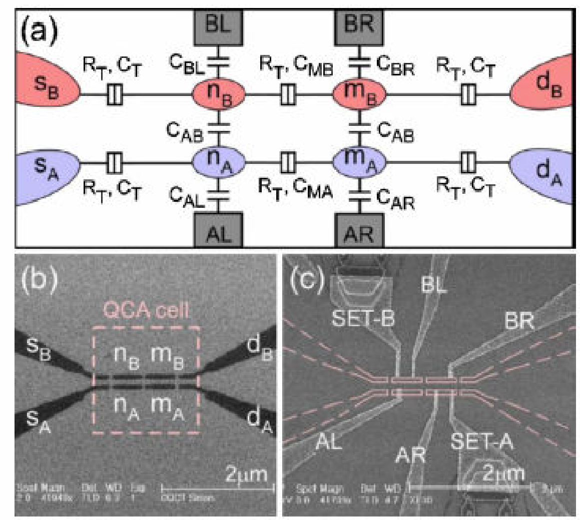
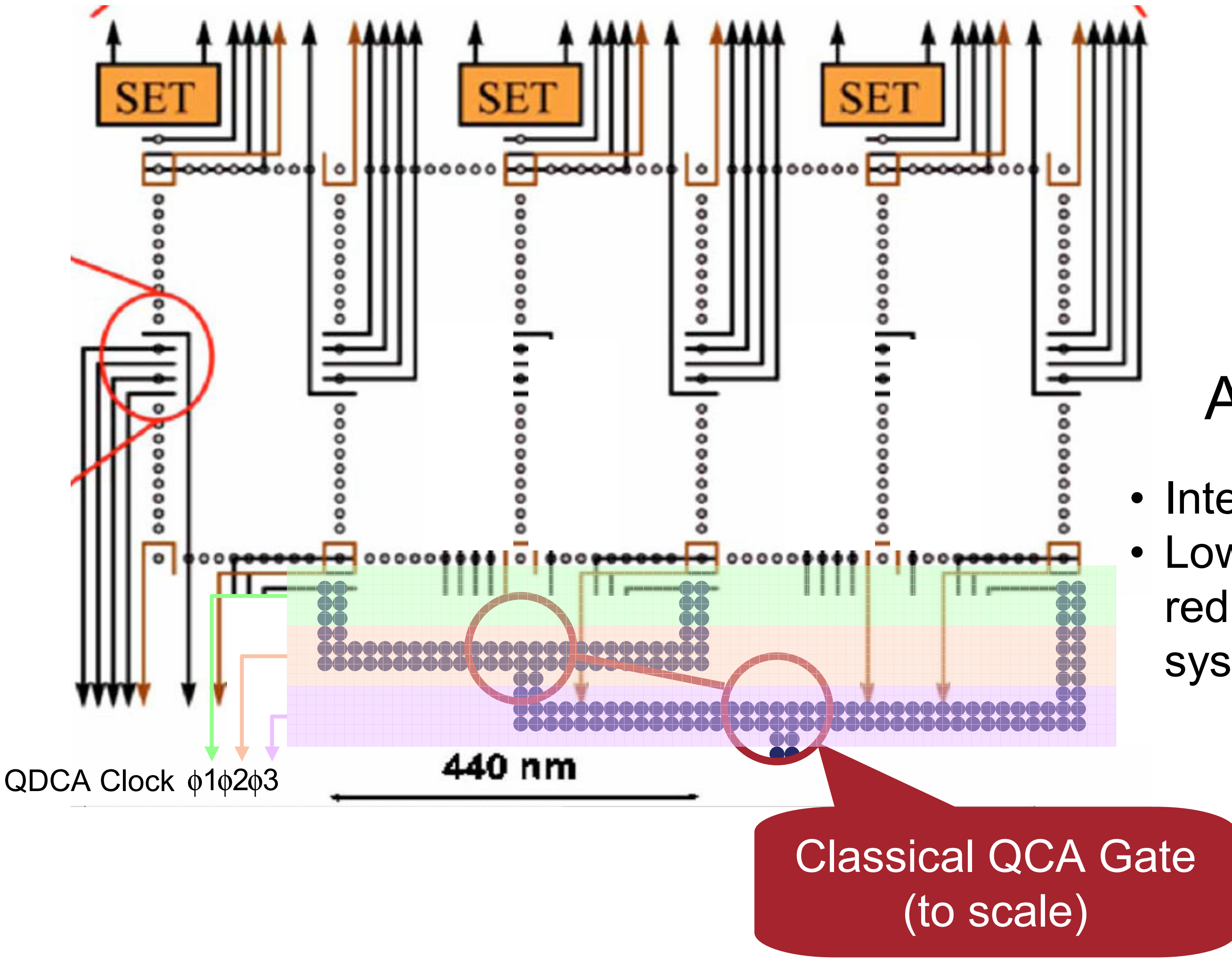


FIG. 1. (Color online) (a) Simplified circuit equivalent of the QCA cell, (b) SEM image of phosphorus-implanted n^+ regions (dark in image), and (c) SEM image of completed device. The buried n^+ dots and leads are marked using dashed lines.

- Dots defined by implanted phosphorus
- Single-donor creation foreseen
- Direct measurement of cell switching

QDCA Logic Directly Attached to QC



Advantages:

- Integration on one substrate
- Low power dissipation reduces load on cooling system

Base diagram from Physical Review B 74, 045311 2006,
Two-dimensional architectures for donor-based quantum computing

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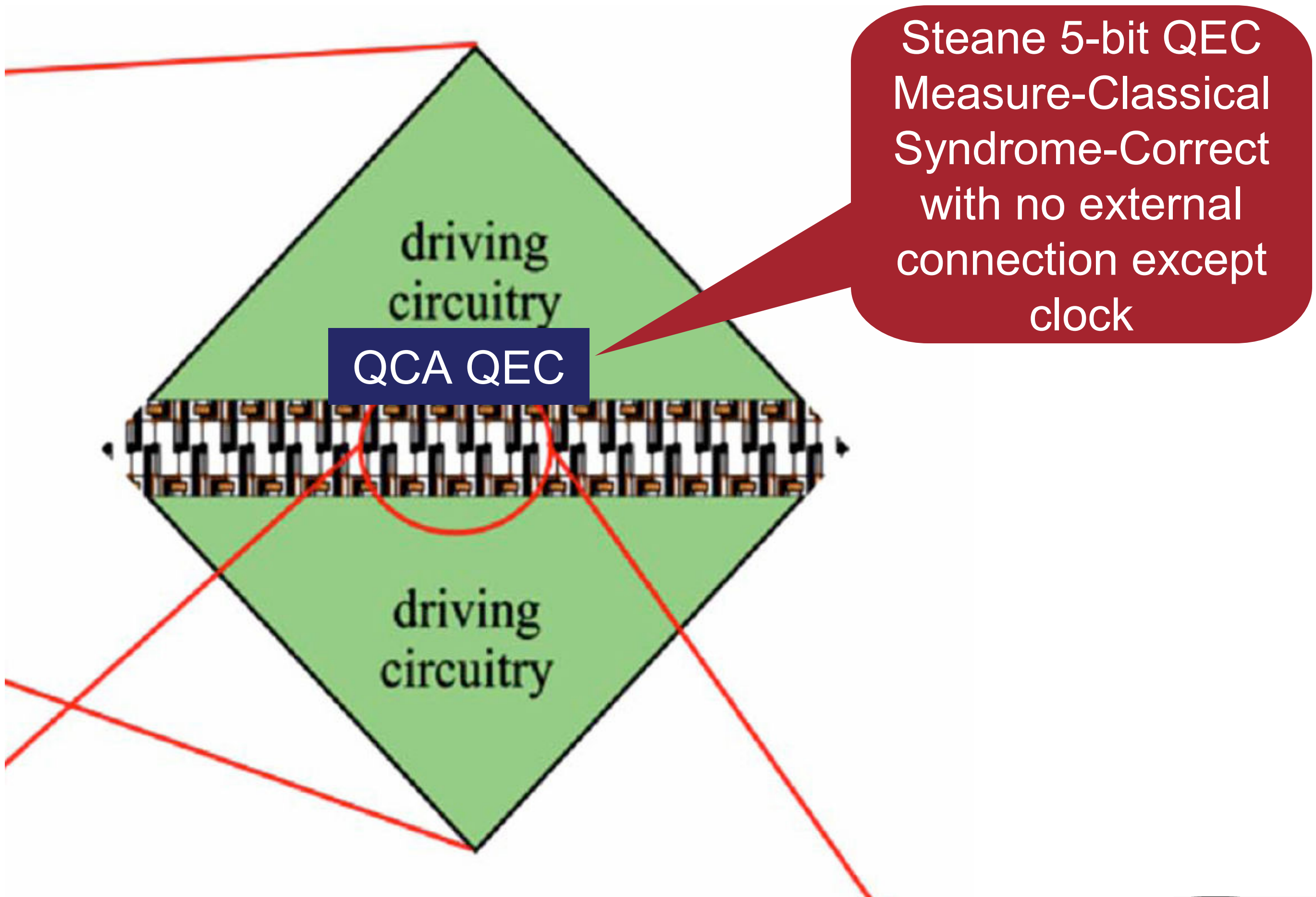
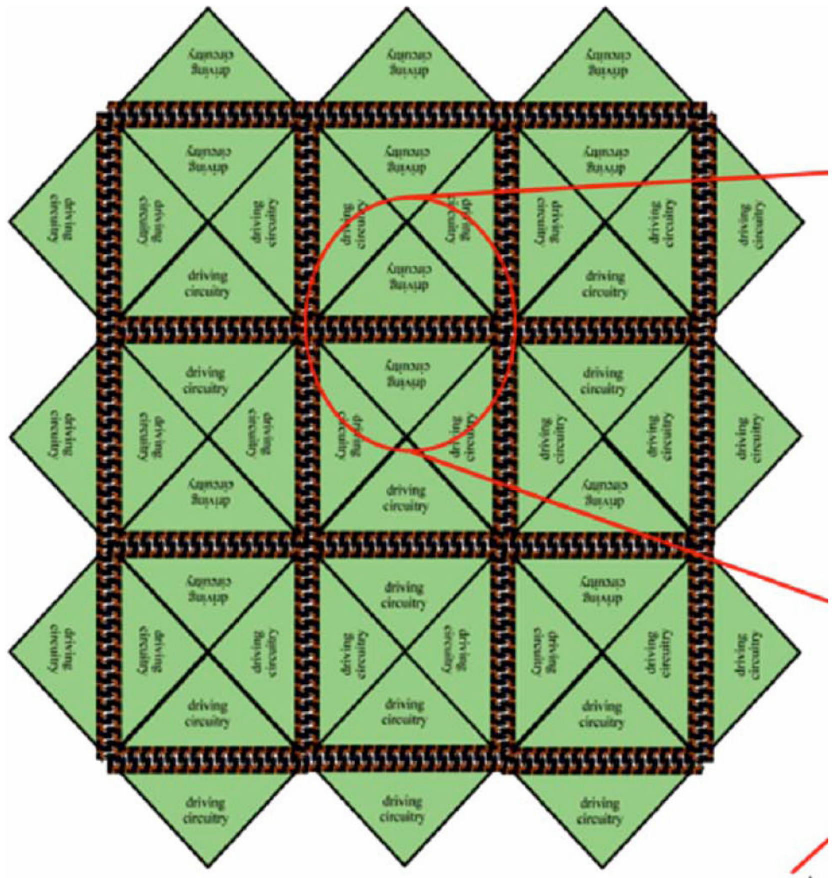
Self-Contained Classical+Quantum Logic



Base diagram from Physical Review B 74, 045311 2006,
Two-dimensional architectures for donor-based quantum computing

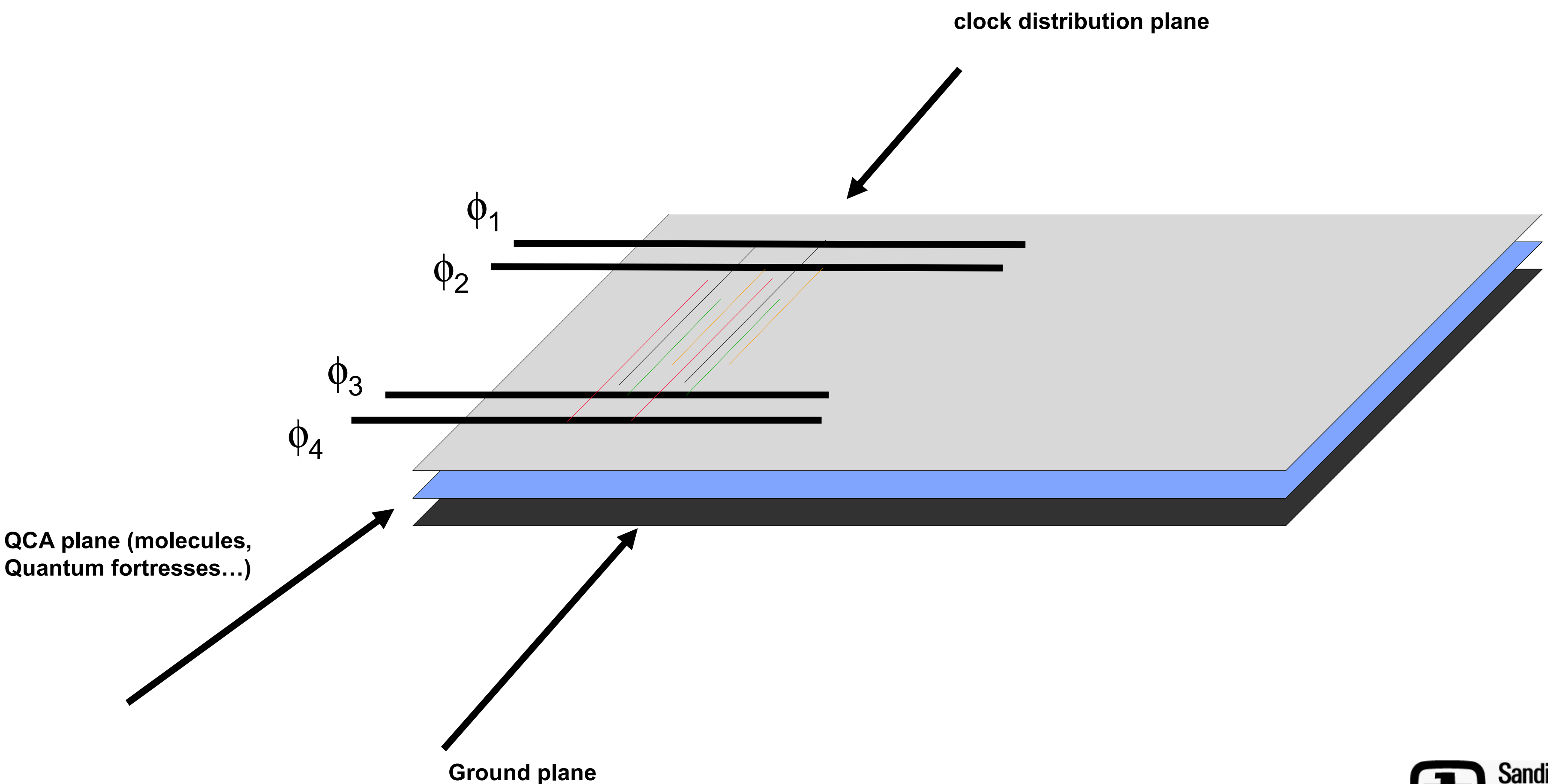
Large QC and QCA Arrays



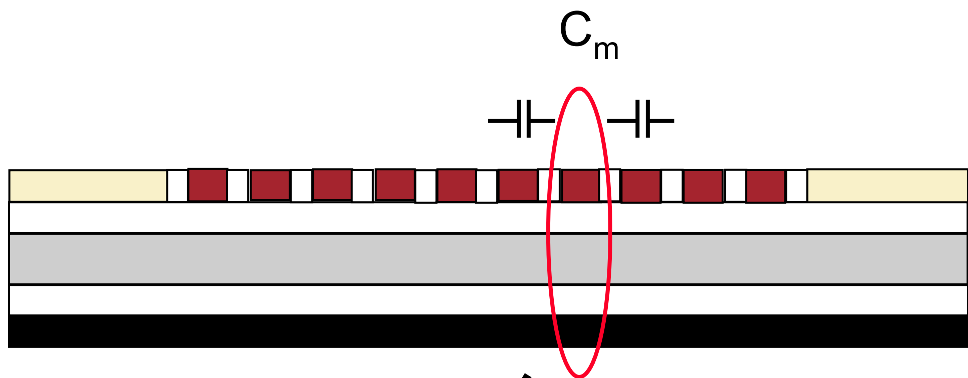
Advantages

- QCA logic "lives" in the single electron world, thus avoiding the need to amplify single electron signals to CMOS levels
- QCA logic would be used to execute the classical part of QEC recovery mechanisms, which is most (e. g. 99%) of the activity in a projected QC
- Each QCA "island" would consume less resources than SET, amplifier, bonding pad, and cable to controller through cryostat it replaces
- QCA would allow the classical circuitry to be implemented on-chip without over-heating the dilution refrigerator.

QCA chip isometric view



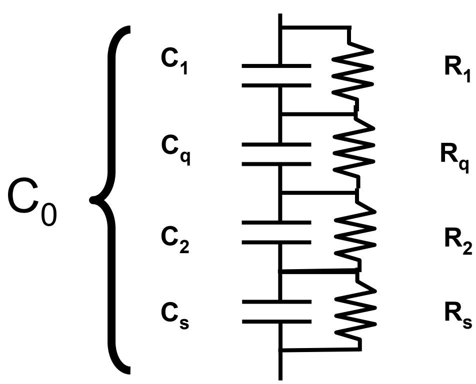
Implementations



Molecular QCA

Quantum fortress

…



Four layers:

1. Upper insulating;
2. QCA
3. Lower insulating
4. Substrate

$$C=\varepsilon_0\varepsilon_r A/d$$

$$R=\rho d/A$$

$$C_{tot}= C_L+kC_m$$

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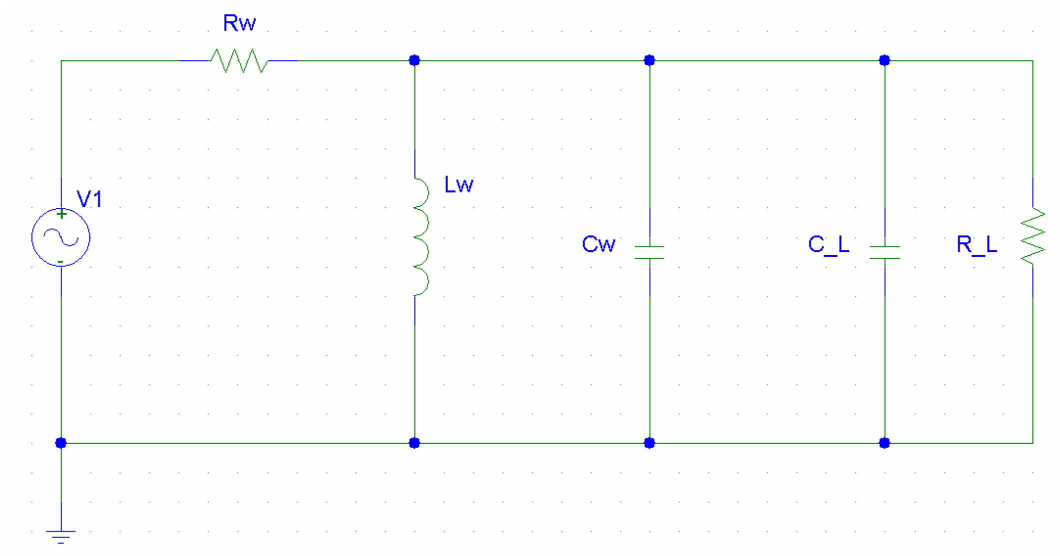
Clock with RLC resonant circuit



- Parallel RLC circuit
- Ideally at resonating frequency no current is drained from the voltage supply
- The dissipation is related to the parasitic resistance in through the layers of the clocked circuit and the resistance of the clock wires
- To achieve a resonating frequency of 1 THz the LC product should be ~10^{-24}
- Consequently L~ pH and C~ pF

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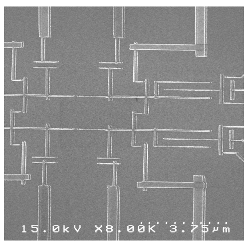
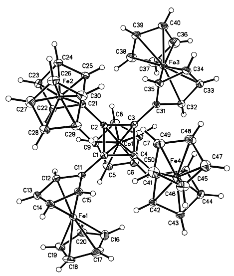
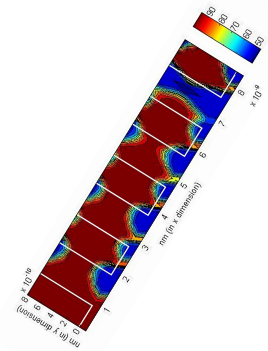
System + Application Architectures

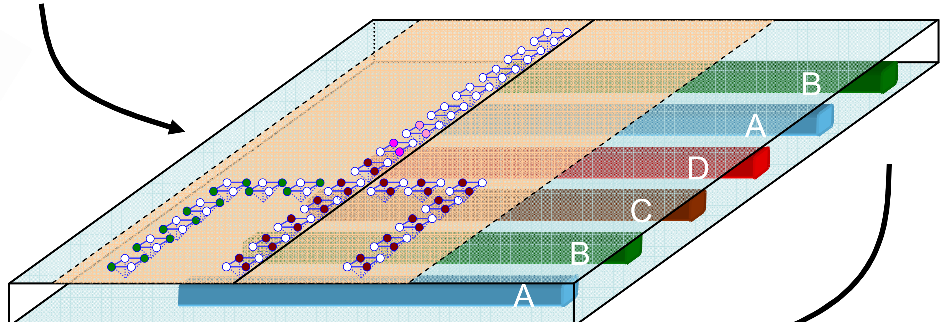
Grounded in device physics & simulation





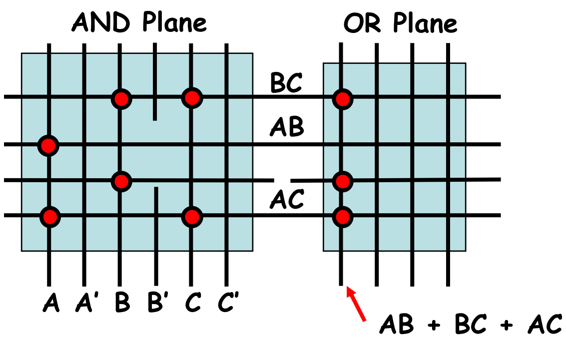


Incorporate clock driven dataflow

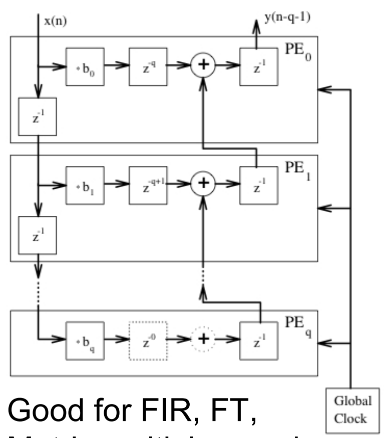


Device architecture maps well to many system architectures…

Reconfigurable

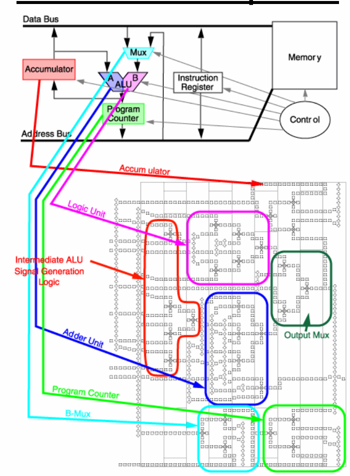


Systolic



Good for FIR, FT, Matrix multiply, graph algorithms, etc.

General Purpose



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Simulations

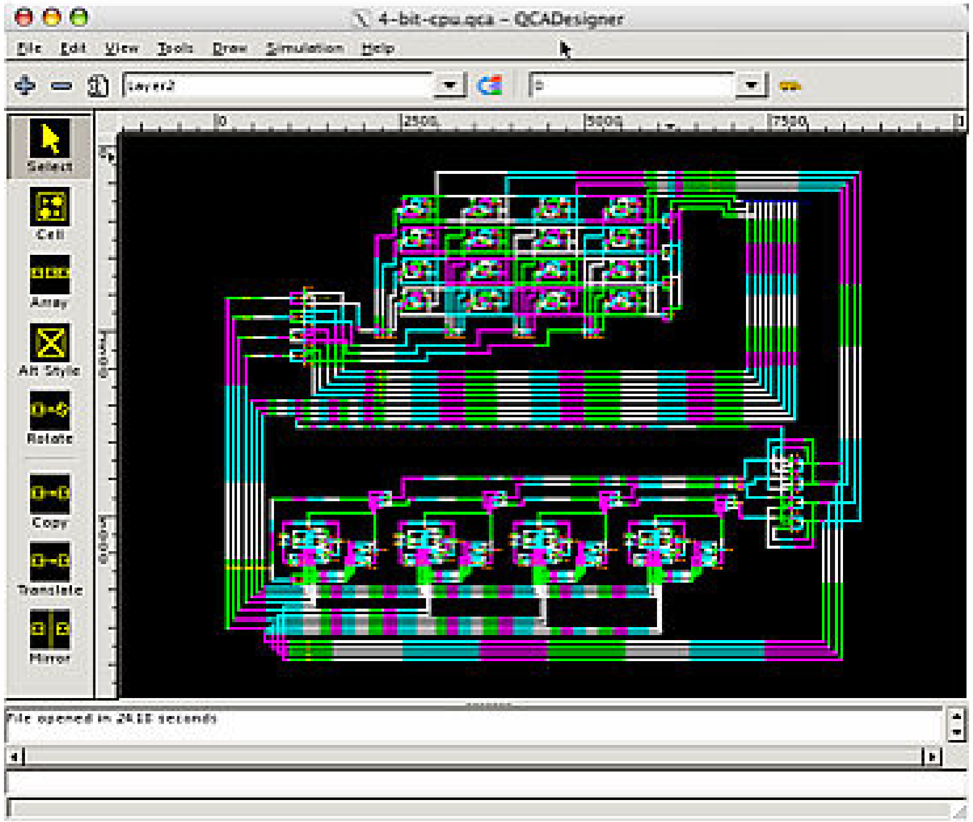
New devices **New circuits** **New architectures**	⇔	**New simulators**

Simulation levels

1) Quantum chemistry
   Ab initio, all-electron, and approx.
2) Density matrix (coherence vector)
   Quantum, dynamic, thermal effects, dissipation
3) Time-independent Schrod. Eq.
4) Semiclassical thermodynamic
5) Logic level
6) Architecture level

slow ↕ fast

QCA design tools



QCADesigner screenshot showing a simple 4-bit processor layout.

QCADesigner

Konrad Walus
U. British Columbia

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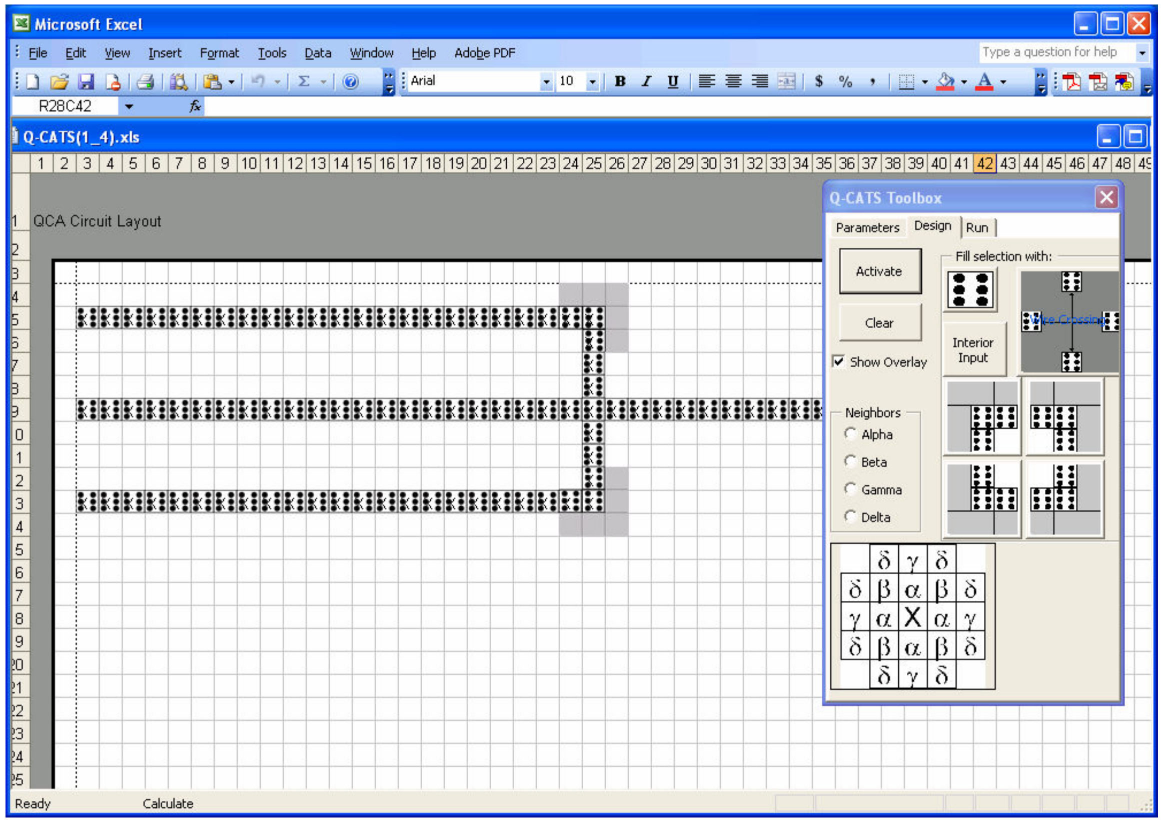
QCA design tools

QCATS

QCA
Thermodynamic
Simulator

Semiclassical



Under development

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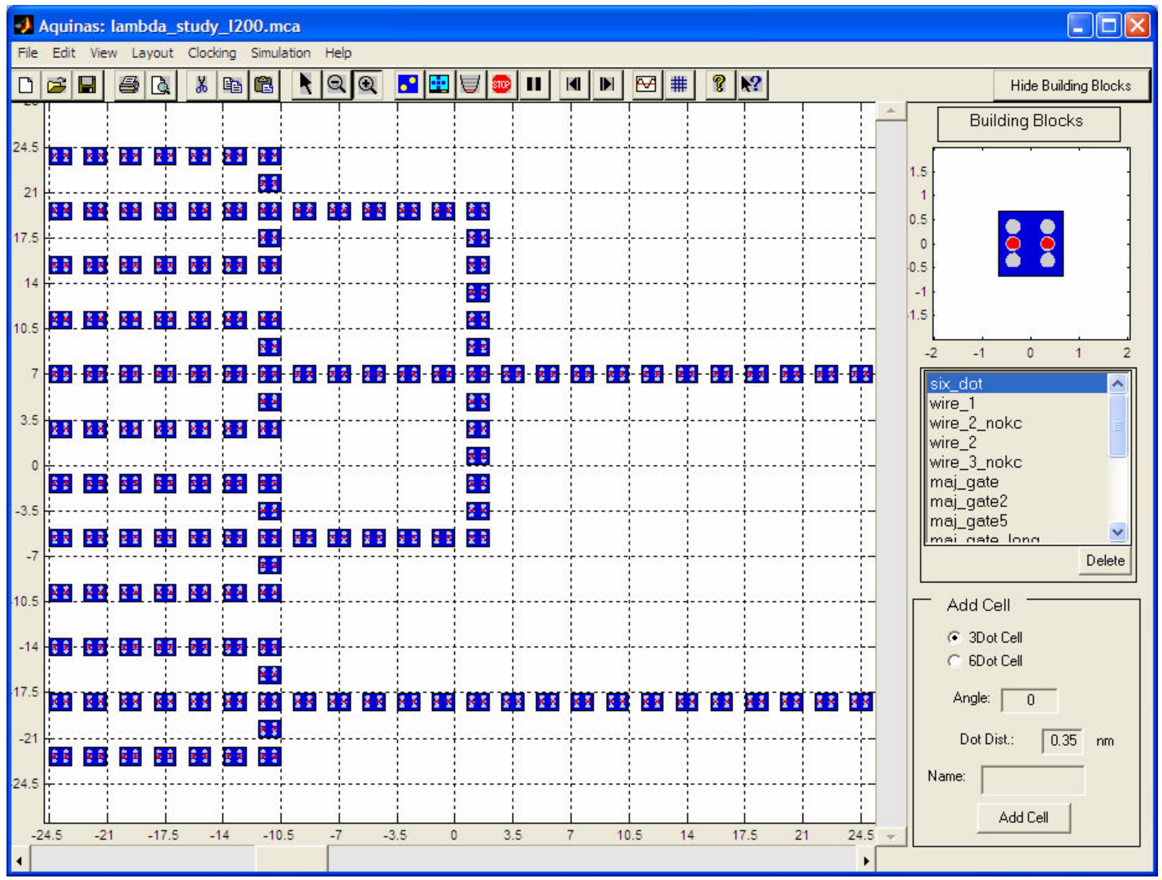
M-AQUINAS

Molecular version of A QUantum Interconnected Network Array Simulator

- GUI allows point-and-click and drag-and-drop editing of QCA circuits.
- Schrödinger solver coupled to local clocking field.



Authors: Enrique Blair
Amy DeCelles

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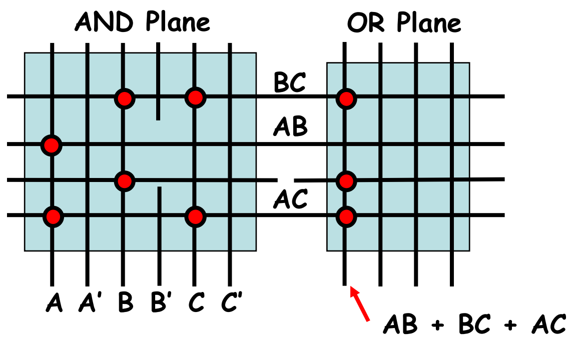
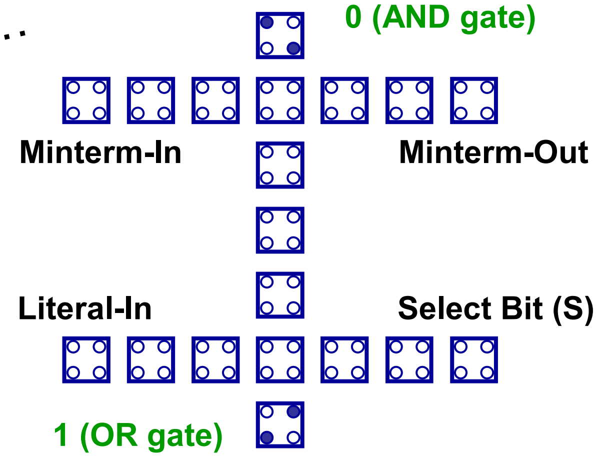
Simulation hierarchies

Architectural-level



+ Logic-level…

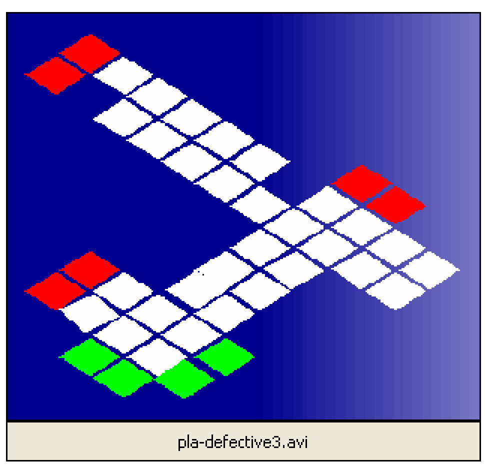


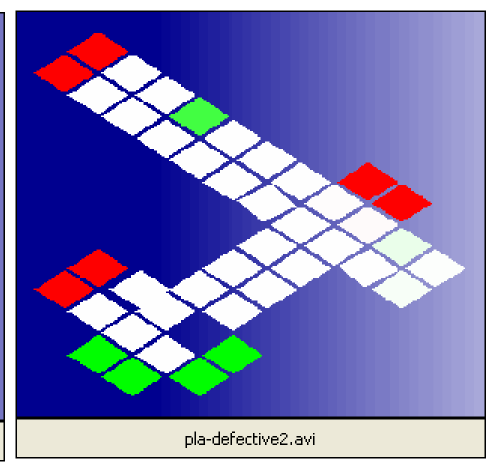
+ device-level…

Minterm-In

Literal-In

Select Bit (S)





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Application-level performance metrics

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Conclusions

- Power is a problem for logic today, and it is related to an approach to thermodynamic limits on computing
- However, these limits are due in part to historical choices that can be circumvented
  - Requires new basis for logic
  - Requires new devices, notably devices that handle information and heat differently
- Also: A tie in to coherent quantum computing

Partnership Opportunity

- This is a project under NINE and SBET
  - We are advocating research in
    - Computing beyond the limits of CMOS
    - Physics of information processing
  - The overall project's deliverables to Sandia are to bootstrap multiple projects in
    - Physical science
    - Information science
    - Simulation
  - We've tried to outline opportunity and expose Sandia to willing partners

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Experiments Under Discussion

- Continuation of Quantum Fortress work 1100
- Molecular QCA 1800
- Quantum Computing Tie-In
  - Architecture
  - Quantum Dot Measurements
  - Quantum Dot Manufacturing classical/quantum
- Computer Architecture beyond limits of Moore's Law
- Simulation of information+Physics

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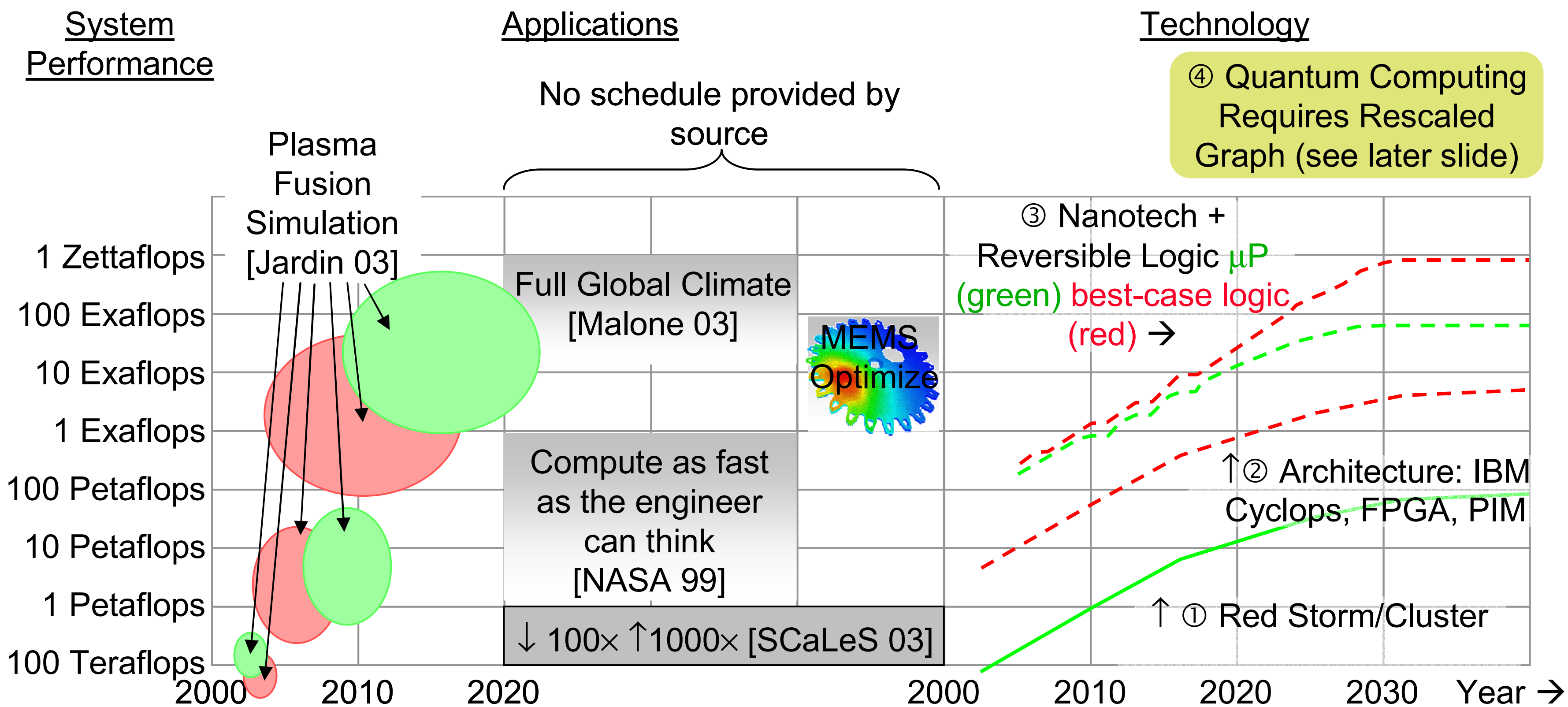
Applications and $100M Supercomputers



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[DeBenedictis 04], Erik P. DeBenedictis, "Matching Supercomputing to Progress in Science," July 2004. Presentation at Lawrence Berkeley National Laboratory, also published as Sandia National Laboratories SAND report SAND2004-3333P. Sandia technical reports are available by going to http://www.sandia.gov and accessing the technical library.

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