Molecular Quantum-dot Cellular Automata (QCA): Beyond Transistors

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Supported by National Science Foundation

Outline of presentation

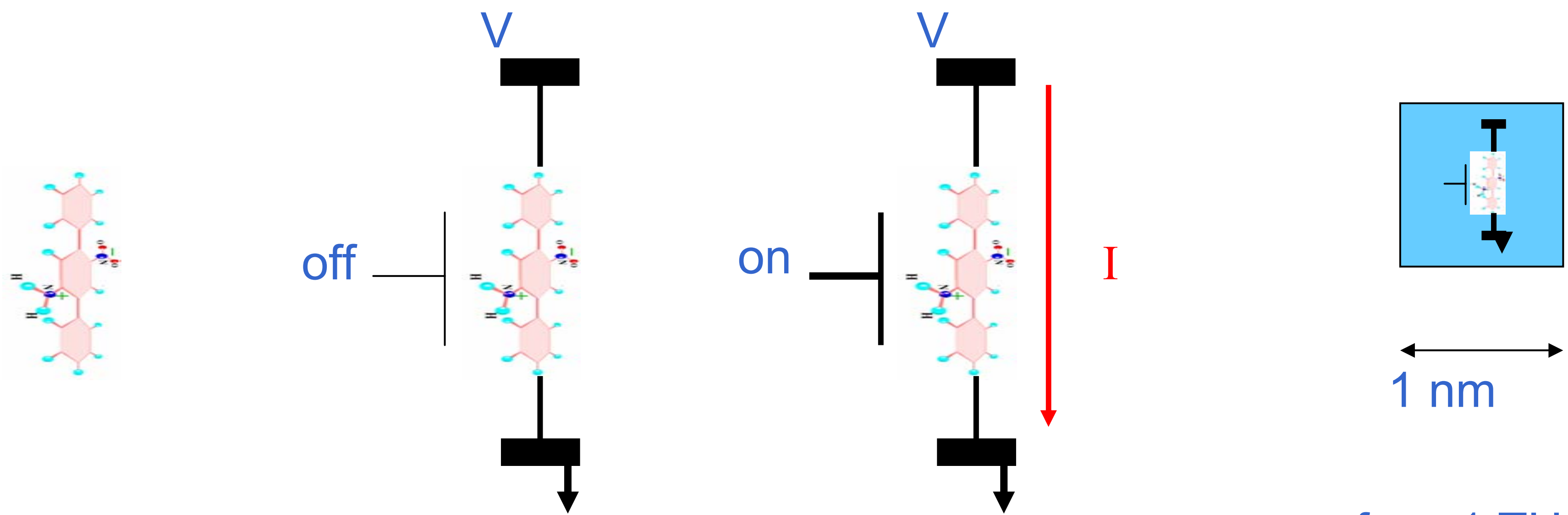
- Introduction and motivation
- QCA paradigm
- QCA implementations
  - Metal-dot
  - Semiconductor-dot
  - Magnetic
  - Molecular
- Circuit and system architecture
- Summary

Goal: Electronics at the single-molecule scale

The Dream of Molecular Transistors

Why don’t we keep on shrinking transistors until they are each a single molecule?

Dream molecular transistors



low conductance state

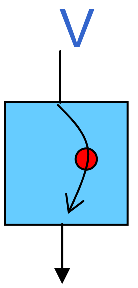
high conductance state

f_{max}=1 THz

Molecular densities: 1nm x 1nm → $10^{14}/cm^2$

Transistors at molecular densities

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



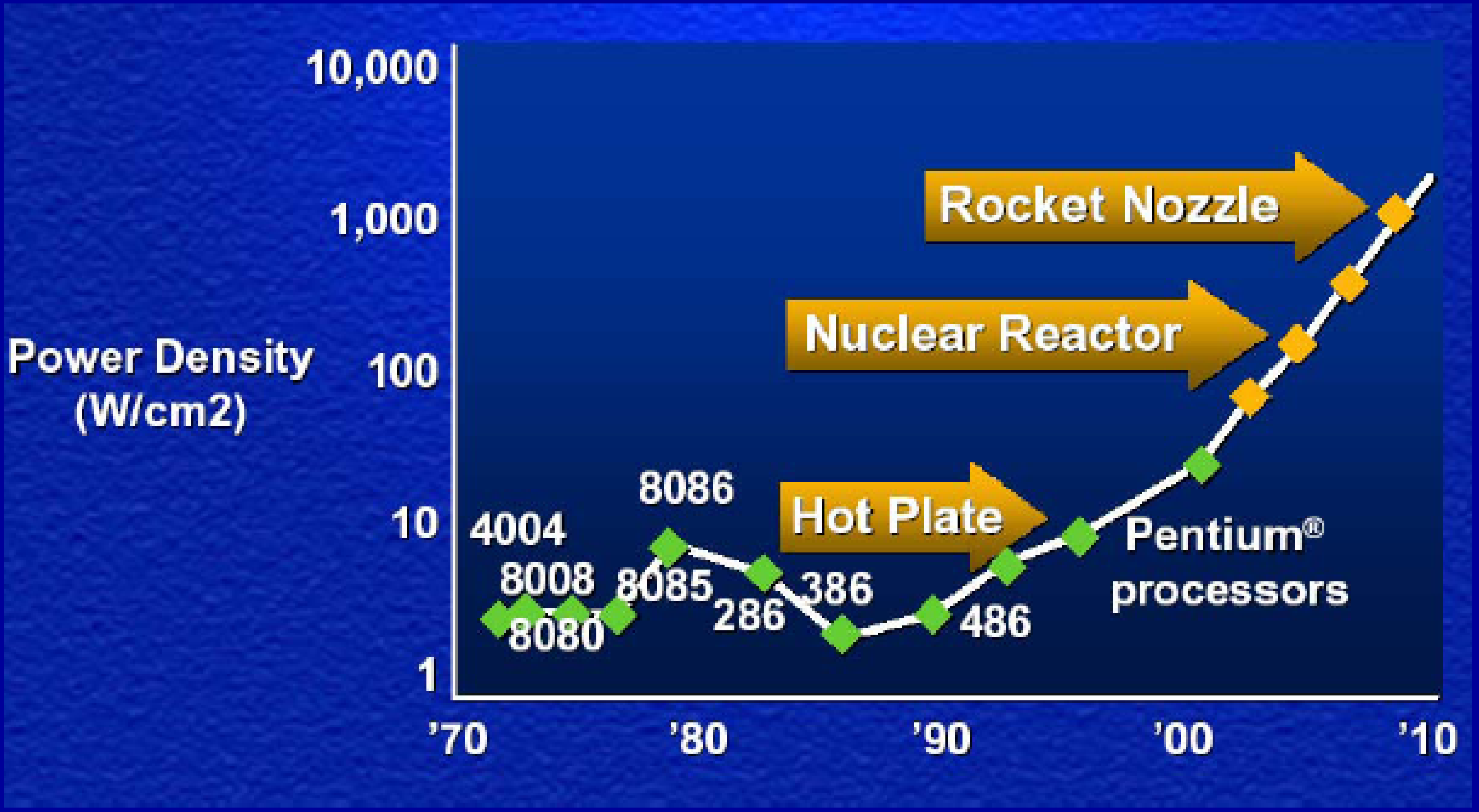
Power dissipation (Watts/cm^2)

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:
7nm gate length, 10^9 logic transistors/cm^2 @ 3×10^{10} Hz for 2016

Power Density Will Get Even Worse

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



The Dream of Molecular Transistors

New paradigm: Quantum-dot Cellular Automata

Represent information with molecular charge configuration.

Zuse's paradigm

✓• Binary

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

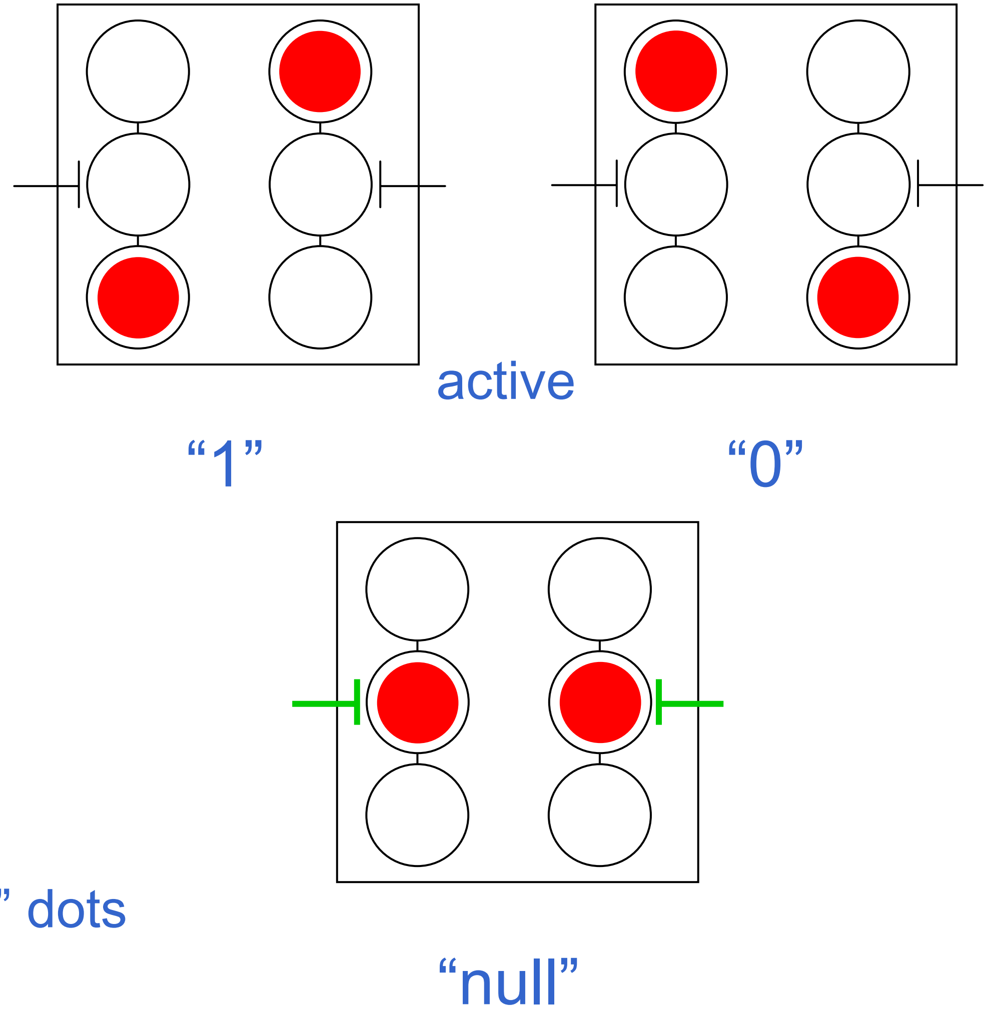
Revolutionary, not incremental, approach

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 of cell.



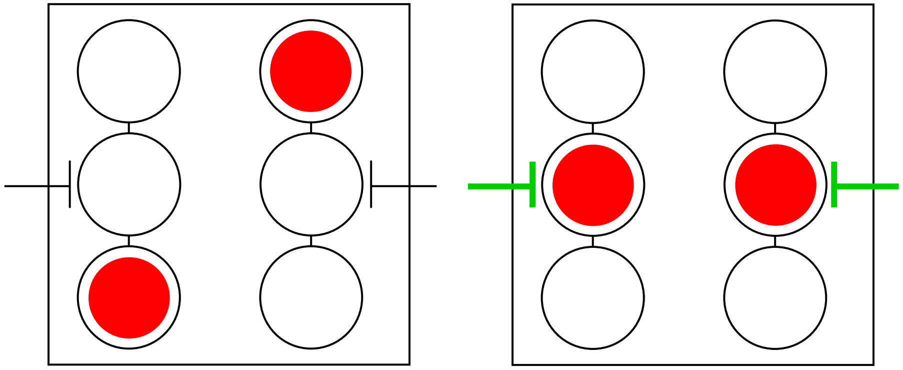
<u>QCA cell</u>

- 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

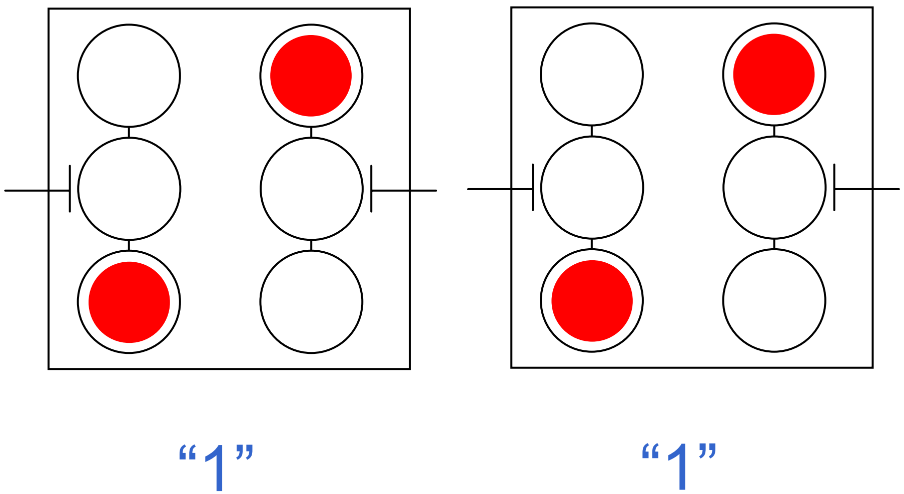
Neighboring cells tend to align in the same state.



“1” “null”

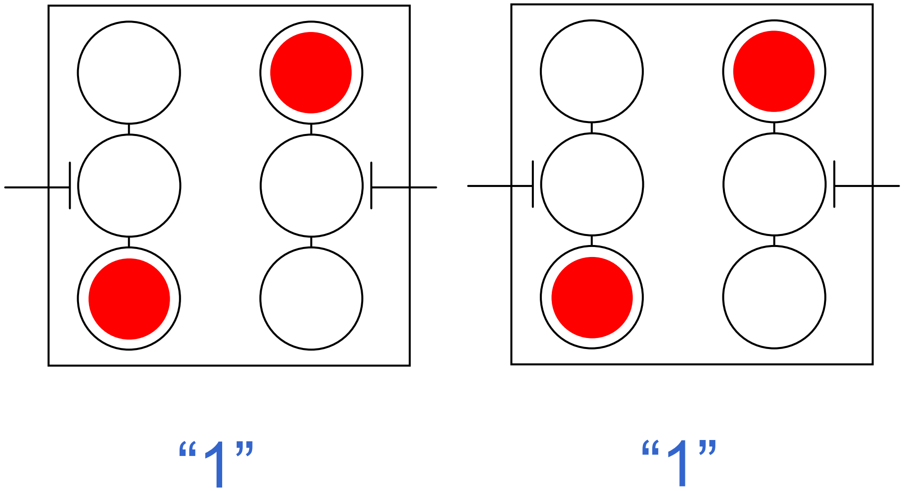
Quantum-dot cellular automata

Neighboring cells tend to align in the same state.



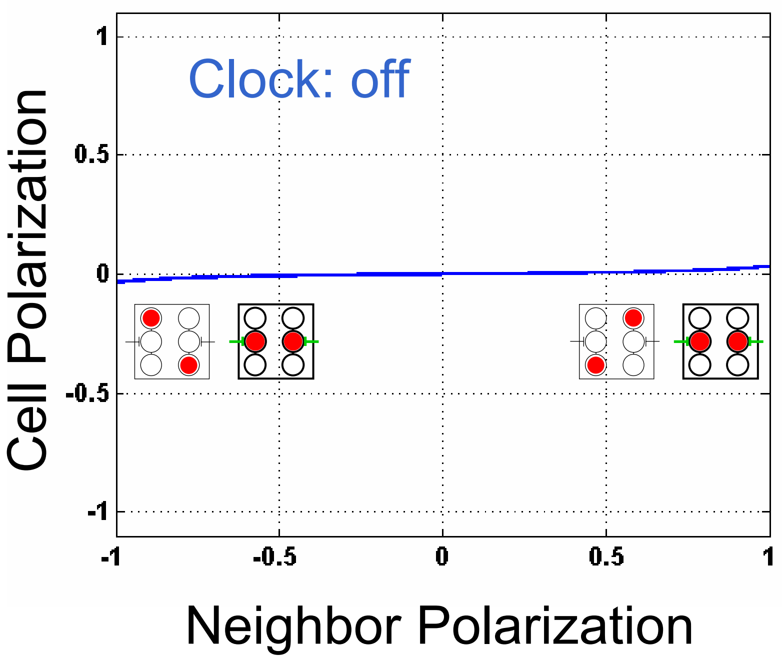
Quantum-dot cellular automata

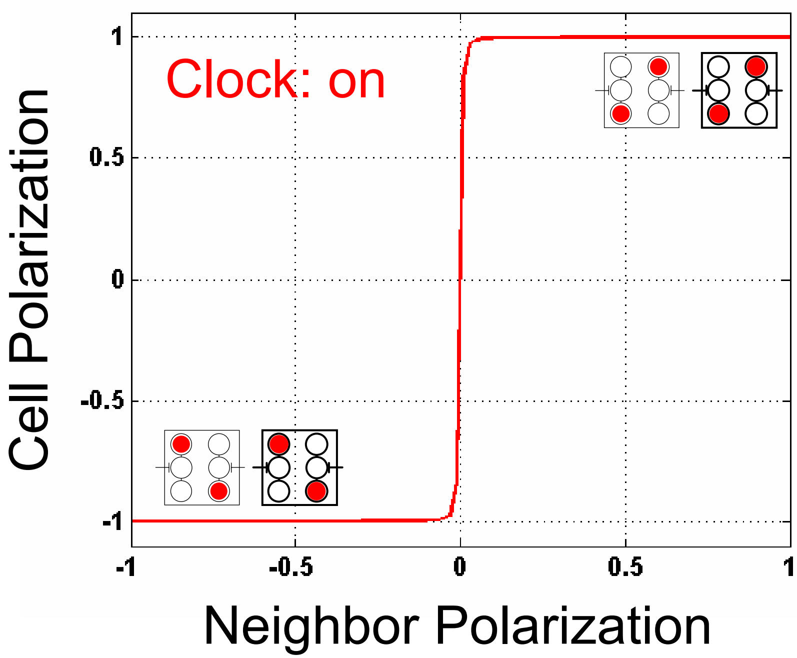
Neighboring cells tend to align in the same state.



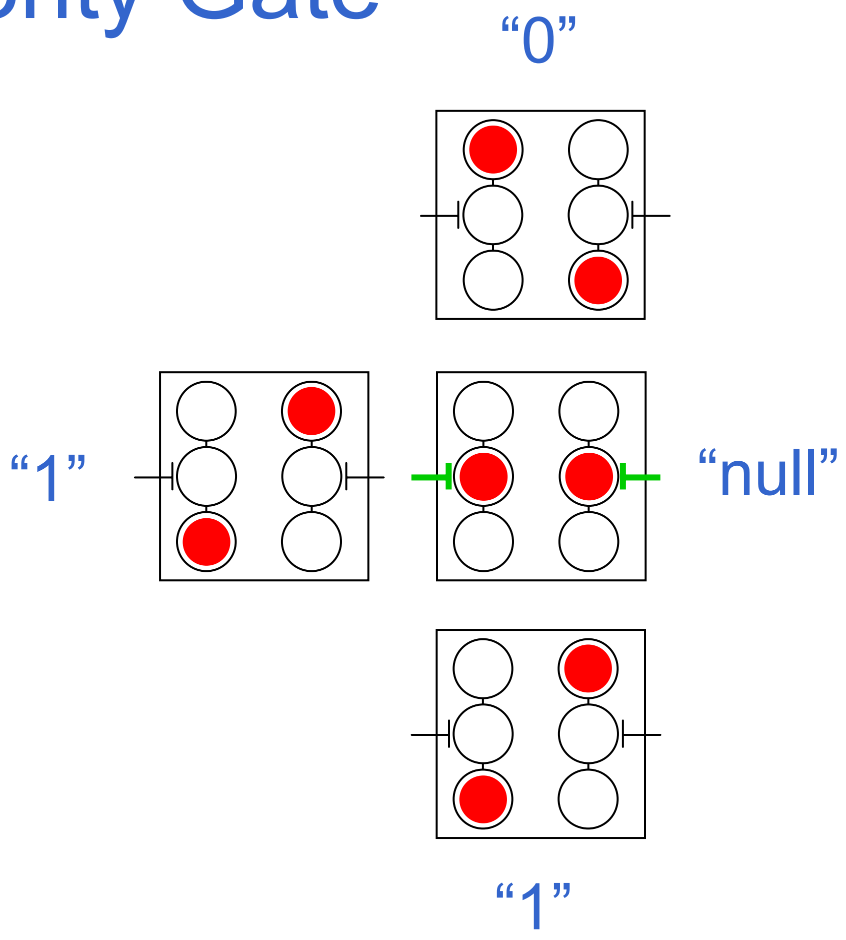
This is the COPY operation.

QCA cell-cell response function

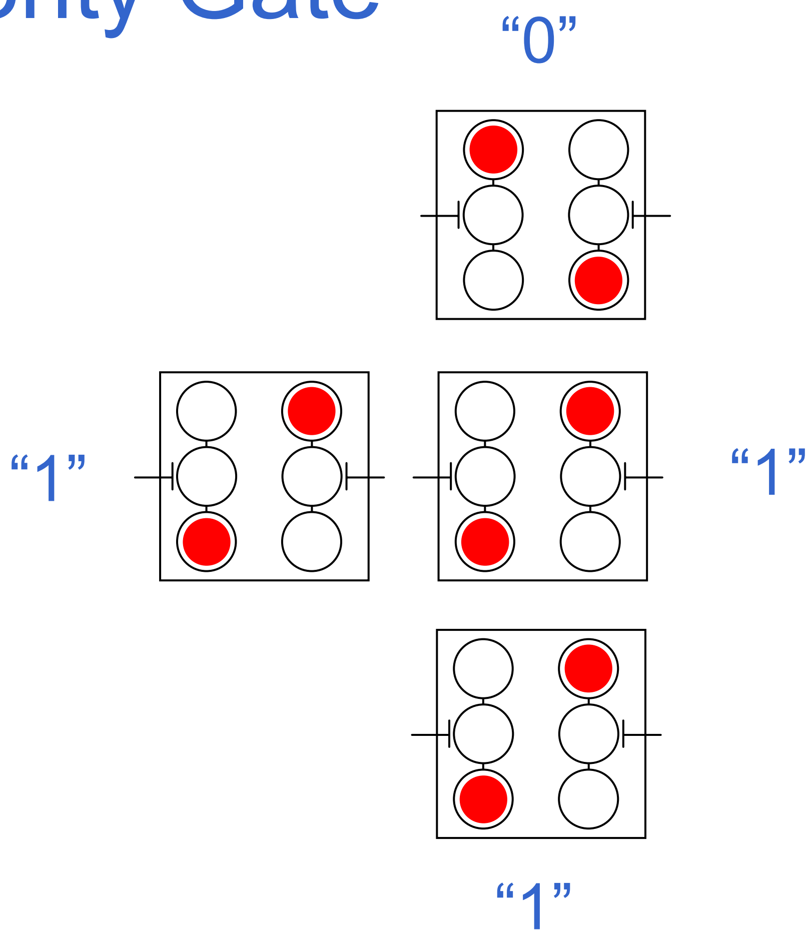




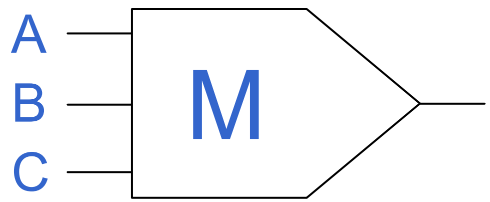
Majority Gate



Majority Gate



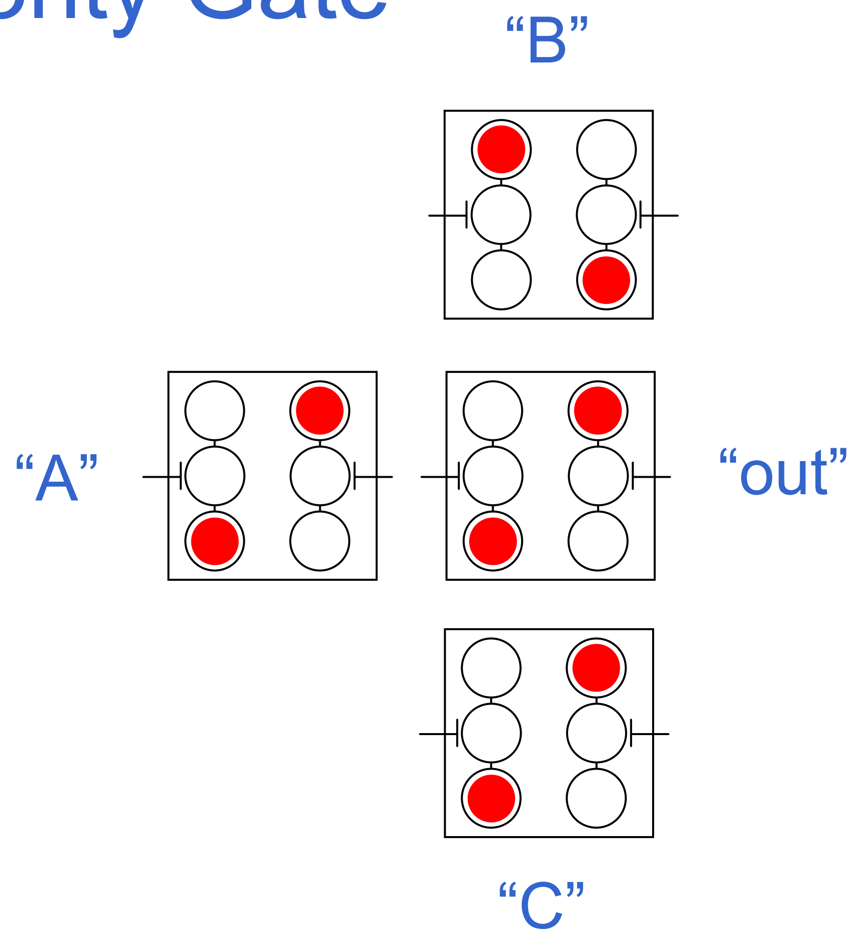
Majority Gate



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

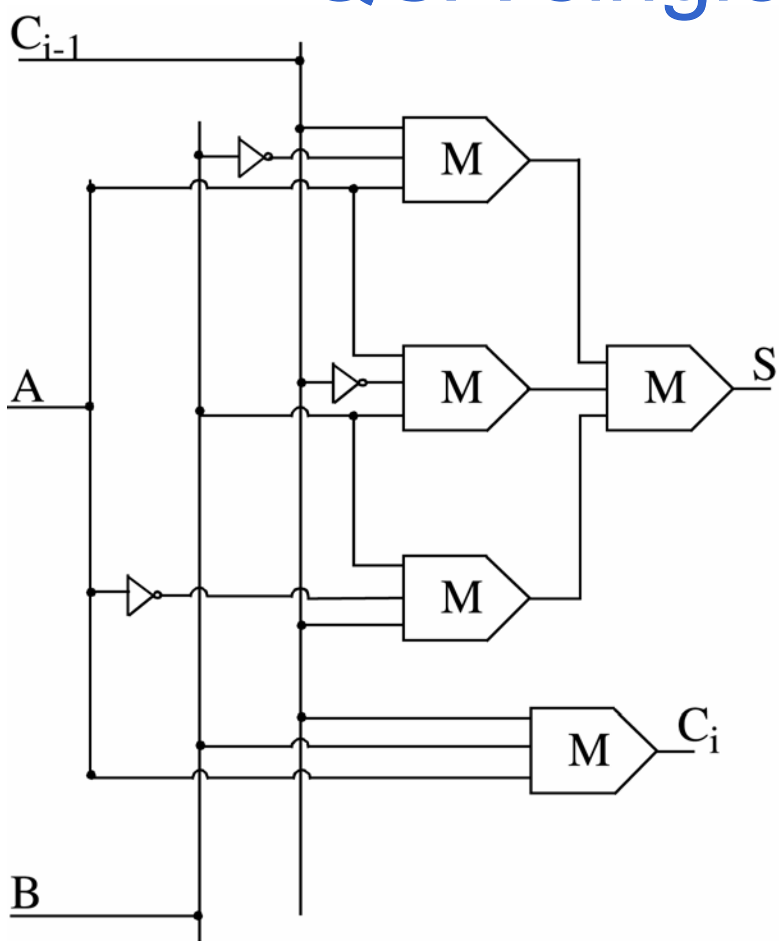
AND gate (rows with A = 0)

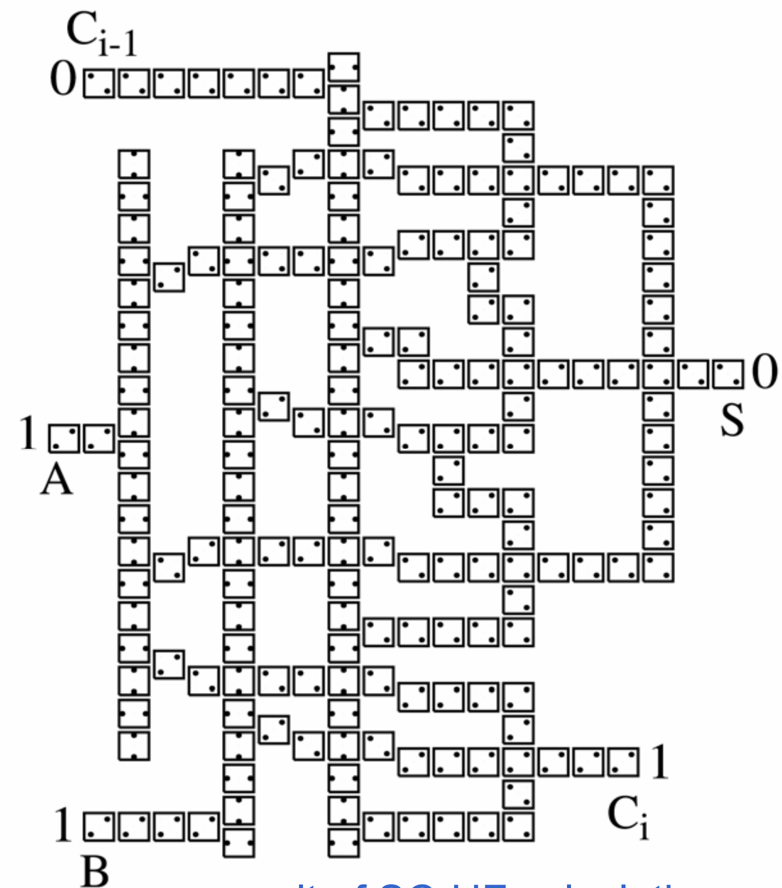
OR gate (rows with A = 1)



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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  - Molecular
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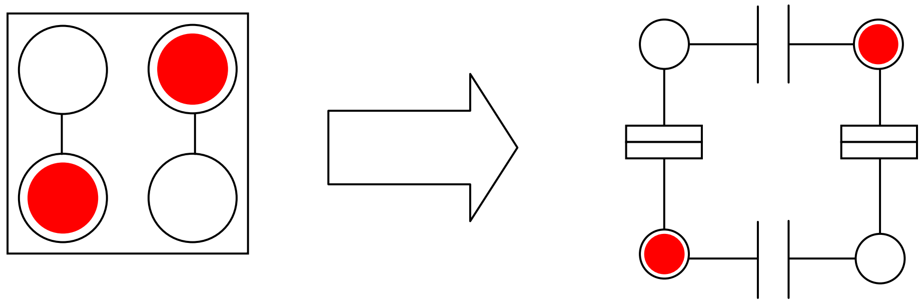
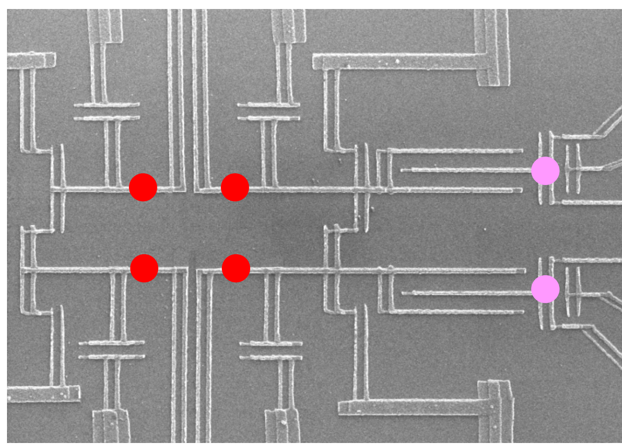
QCA devices exist



Metal-dot QCA implementation



Al/AlO_x on SiO_2

electrometers

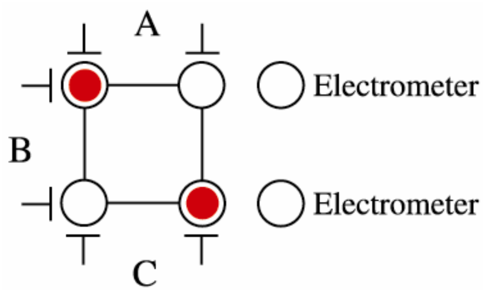
“dot” = metal island

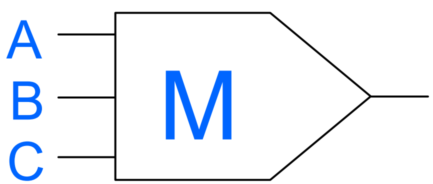
70-300 mK

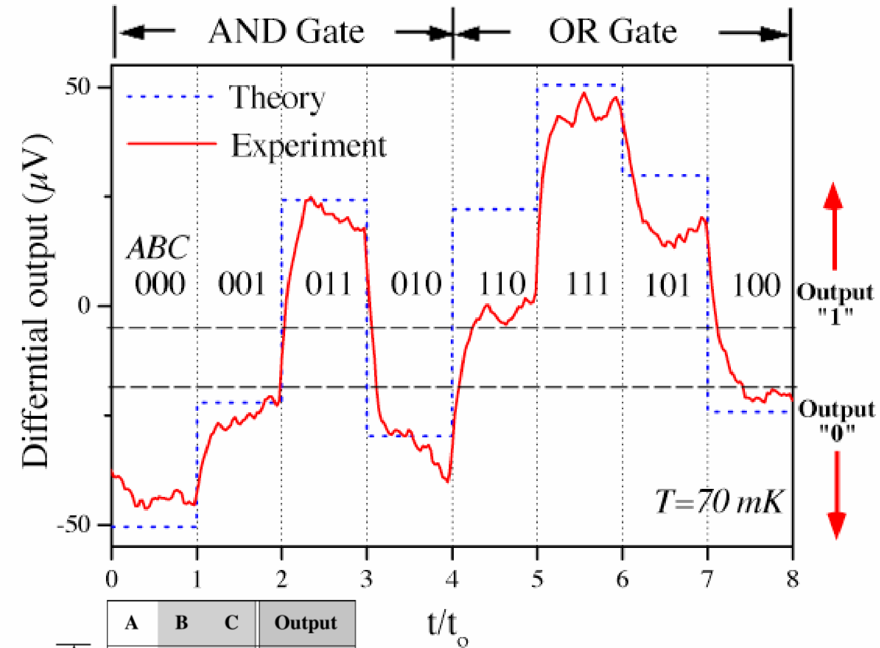
Greg Snider, Alexei Orlov, and Gary Bernstein

Metal-dot QCA cells and devices

- Majority Gate





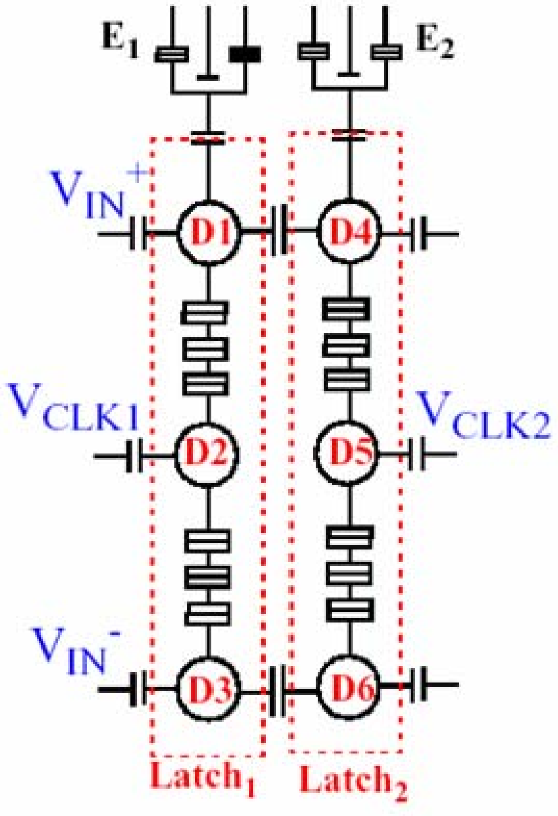


	A	B	C	Output
AND gate	0	0	0	0
AND gate	0	0	1	0
AND gate	0	1	1	1
AND gate	0	1	0	0
OR gate	1	1	0	1
OR gate	1	1	1	1
OR gate	1	0	1	1
OR gate	1	0	0	0

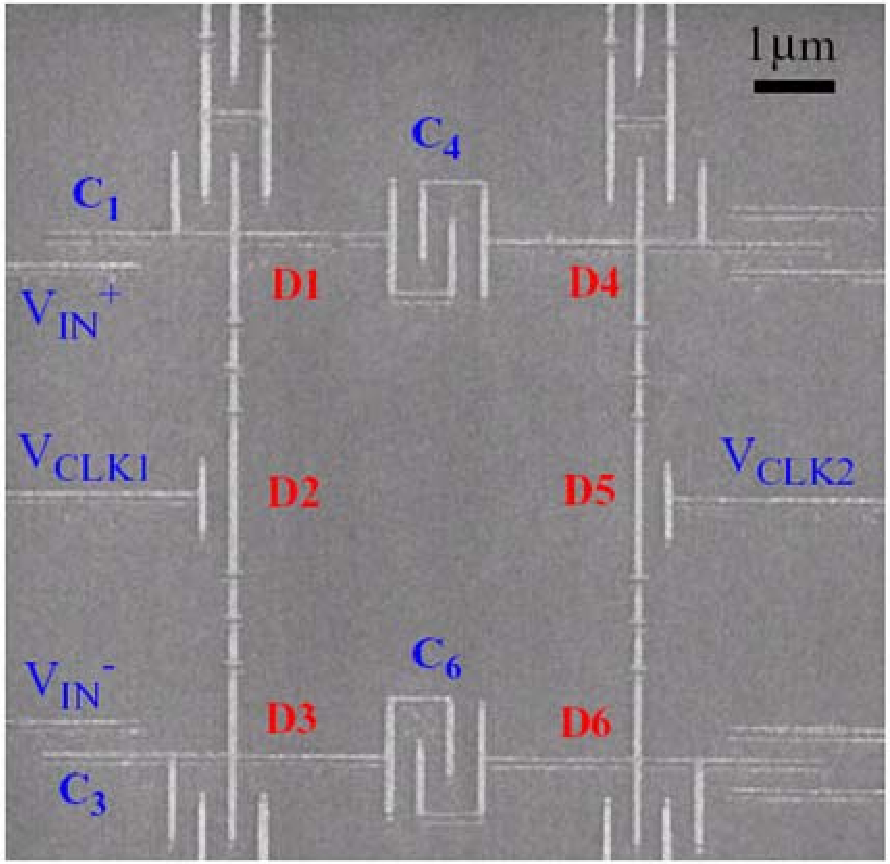
Amlani, A. Orlov, G. Toth, G. H. Bernstein, C. S. Lent, G. L. Snider, *Science* **284**, pp. 289-291 (1999).

QCA Shift Register

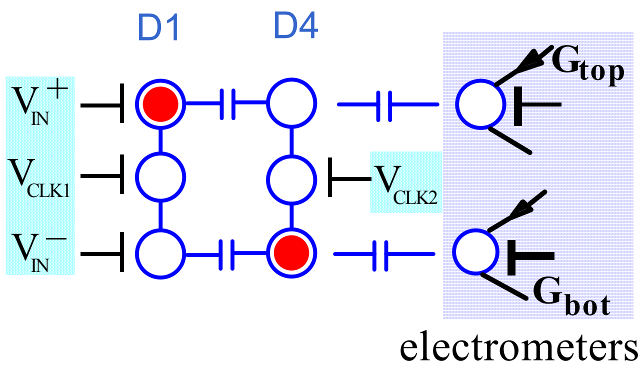
Schematic Diagram

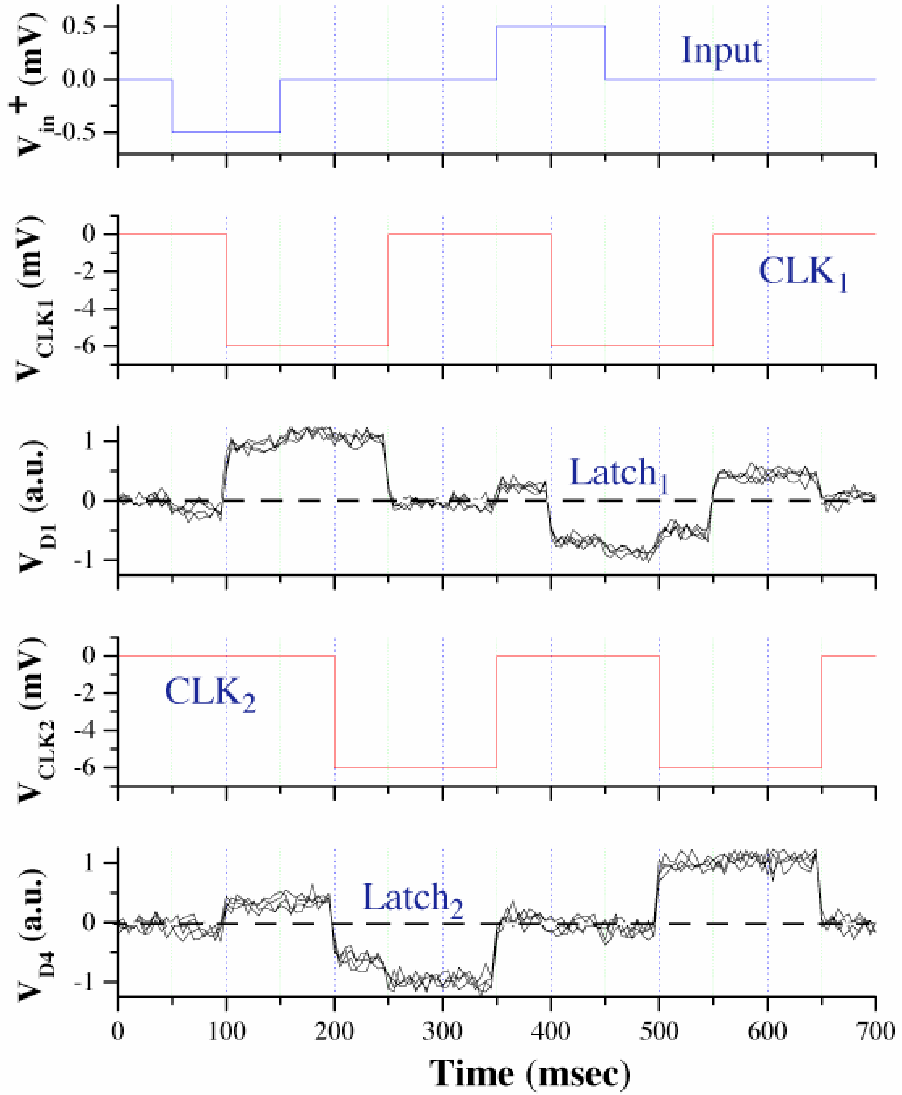


SEM Micrograph



QCA Shift Register





Metal-dot QCA devices exist

- Single electron analogue of molecular QCA
- Gates and circuits:
  - Wires
  - Shift registers
  - Fan-out
  - Power gain demonstrated
  - AND, OR, Majority gates

- Work underway to raise operating temperatures

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.

GaAs-AlGaAs QCA cell

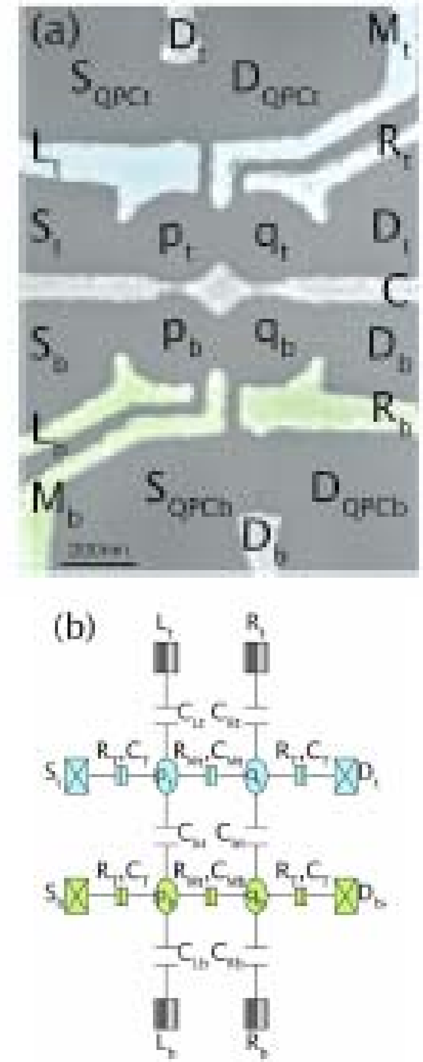
APPLIED PHYSICS LETTERS 91, 032102 (2007)

Demonstration of a quantum cellular automata cell in a GaAs/AlGaAs heterostructure

F. Perez-Martinez,[a] I. Farrer, D. Anderson, G. A. C. Jones, D. A. Ritchie, S. J. Chorley, and C. G. Smith
Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom

(Received 24 April 2007; accepted 21 June 2007; published online 17 July 2007)

The authors report on the experimental demonstration of a GaAs/AlGaAs-based quantum cellular automata cell fabricated using electron beam lithographically defined gates. These surface metallic gates form a pair of double quantum dots, as well as a pair of quantum point contacts (QPCs) that act as noninvasive voltage probes. Measurements at cryogenic temperatures show that an electron transfer in the input dots induces the relocation of a single electron in the output dots. Using the QPCs they were able to determine the operating limits of the cell. © 2007 *American Institute of Physics*. [DOI: 10.1063/1.2759257]



- Dots defined by top gates depleting 2DEG
- Direct measurement of cell switching

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]

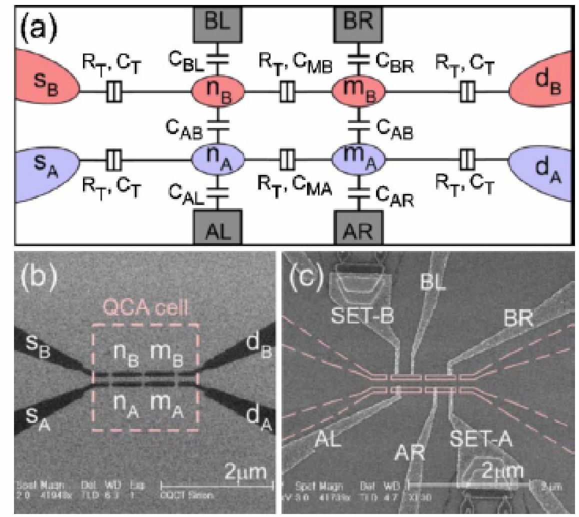


FIG. 1. (Color online) (a) Simplified circuit equivalent of the QCA cell, (b) SEM image of phosphorus-implanted n^+ regions (dark in image), and (c) SEM image of completed device. The buried n^+ dots and leads are marked using dashed lines.

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

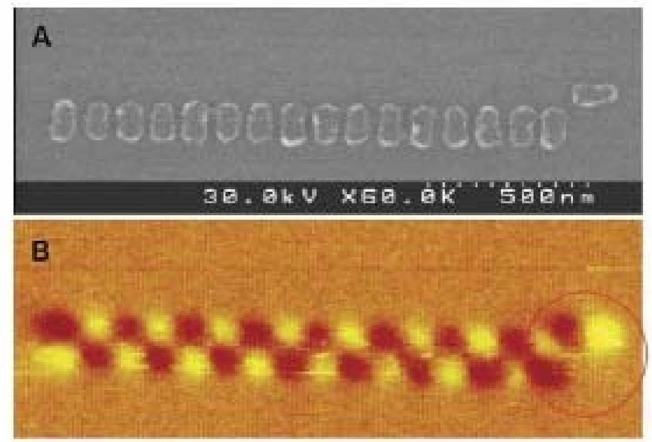
Magnetic QCA

SCIENCE VOL 311 13 JANUARY 2006

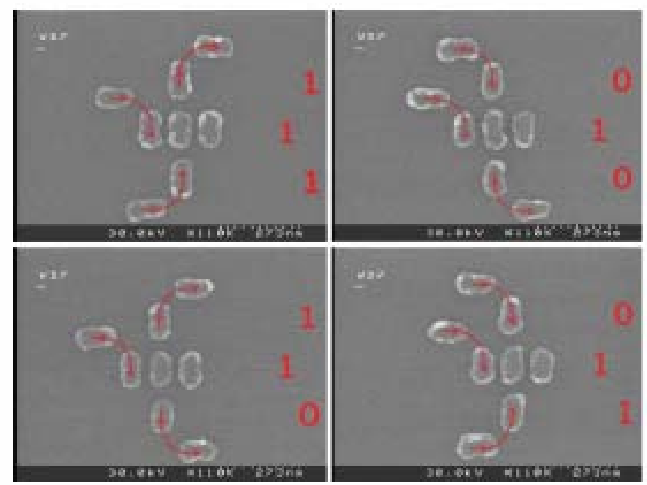
Majority Logic Gate for Magnetic Quantum-Dot Cellular Automata

A. Imre,[1*] G. Csaba,[2] L. Ji,[1] A. Orlov,[1] G. H. Bernstein,[1] W. Porod[1]

We describe the operation of, and demonstrate logic functionality in, networks of physically coupled, nanometer-scale magnets designed for digital computation in magnetic quantum-do cellular automata (MQCA) systems. MQCA offer low power dissipation and high integration density of functional elements and operate at room temperature. The basic MQCA logic gate, that is, the three-input majority logic gate, is demonstrated.

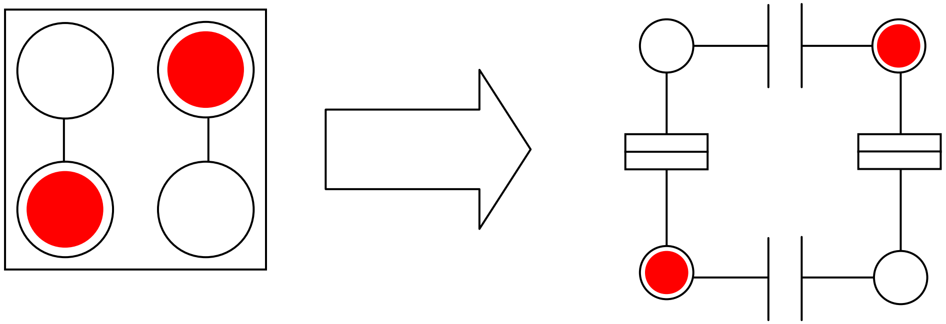


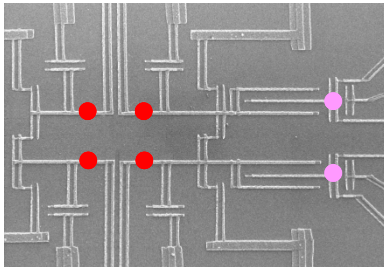
- Dots defined by magnetic domains
- Room temperature operation



Molecular QCA

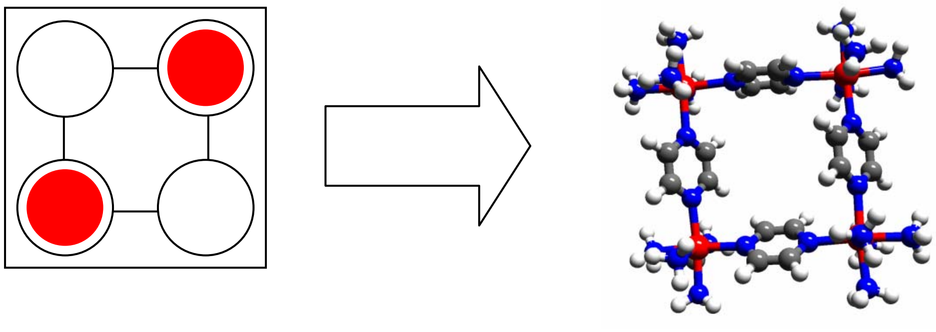
Metal tunnel junctions





“dot” = metal island

70 mK



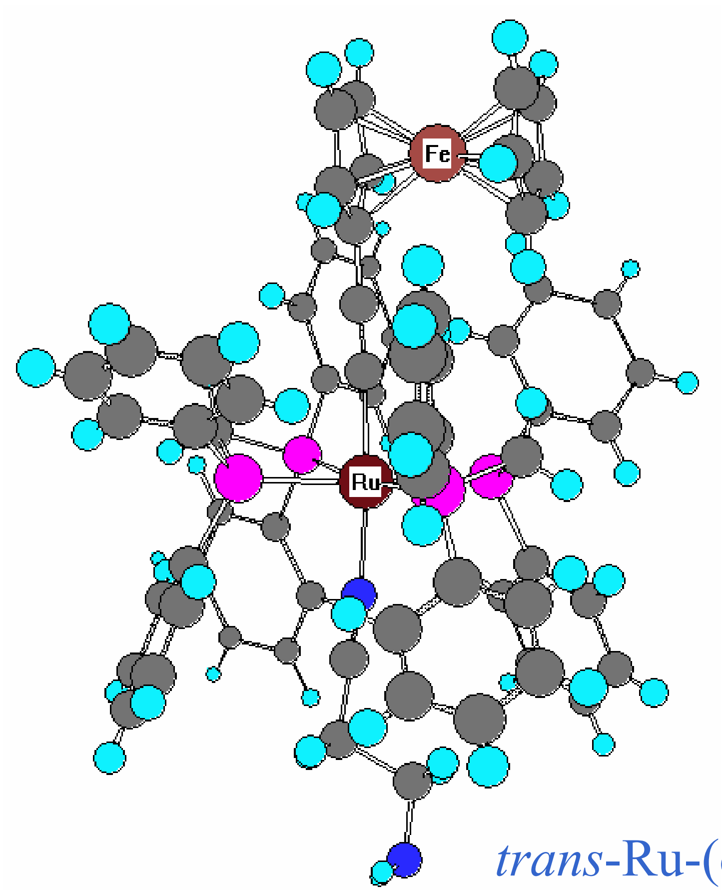
“dot” = redox center

Mixed valence compounds

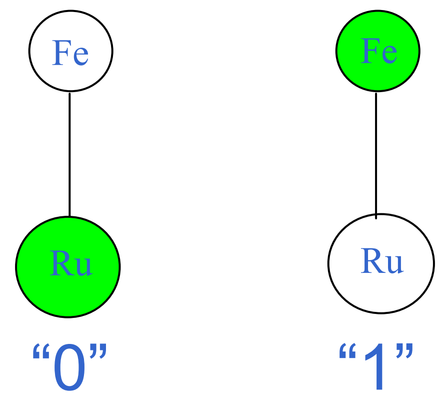
room temperature+

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

Experiments on molecular double-dot



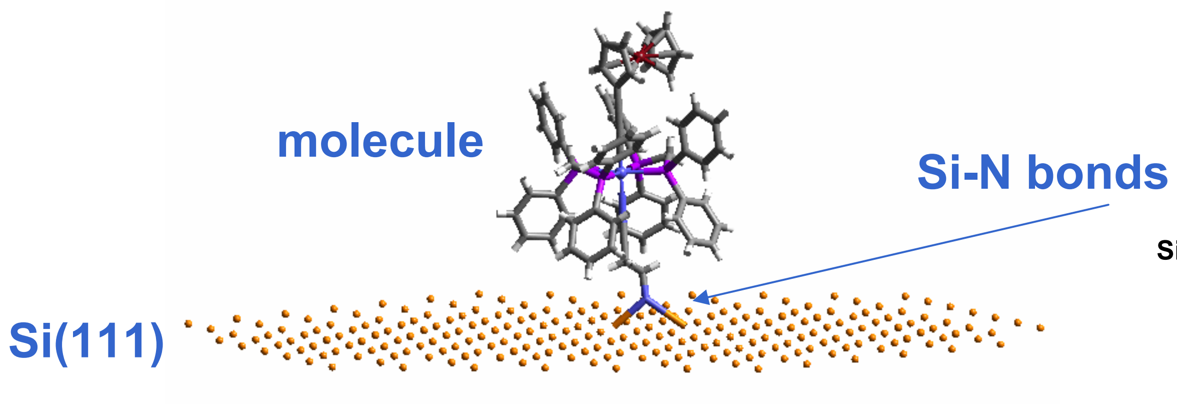
Thomas Fehlner *et al.*
(Notre Dame chemistry group)
Journal of American Chemical Society, 125:15250, 2003

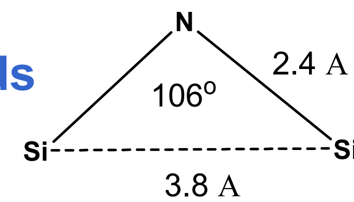


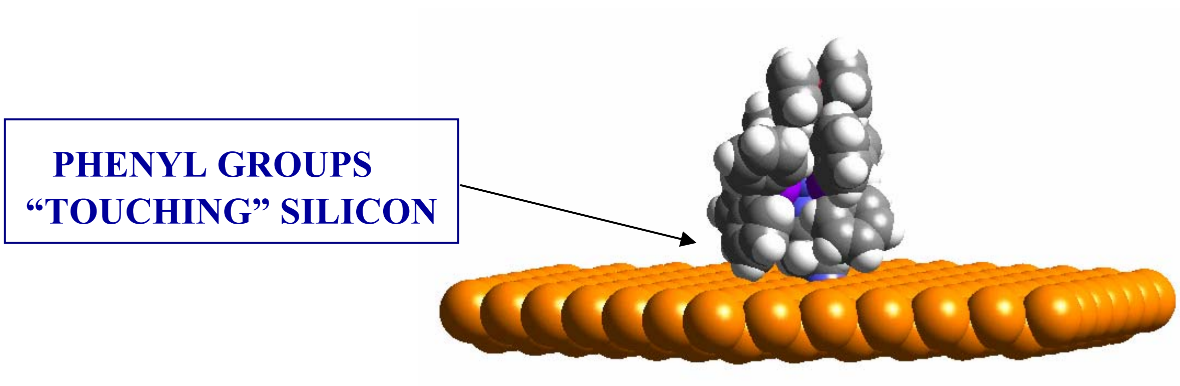
trans-Ru-(dppm)$_2$(C≡CFc)(NCCH$_2$CH$_2$NH$_2$) dication

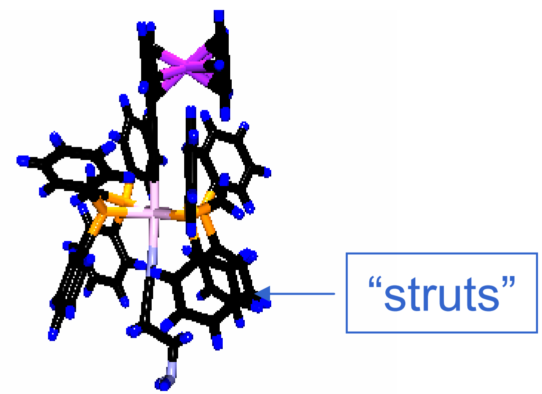
Fe group and Ru group act as two *unequal* quantum dots.

Surface attachment and orientation







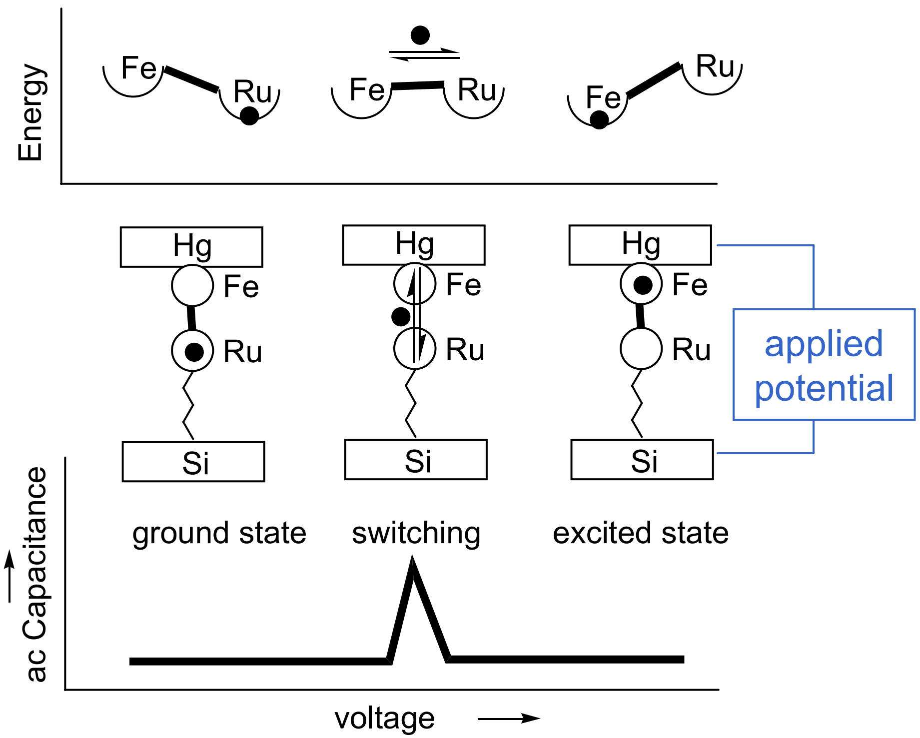


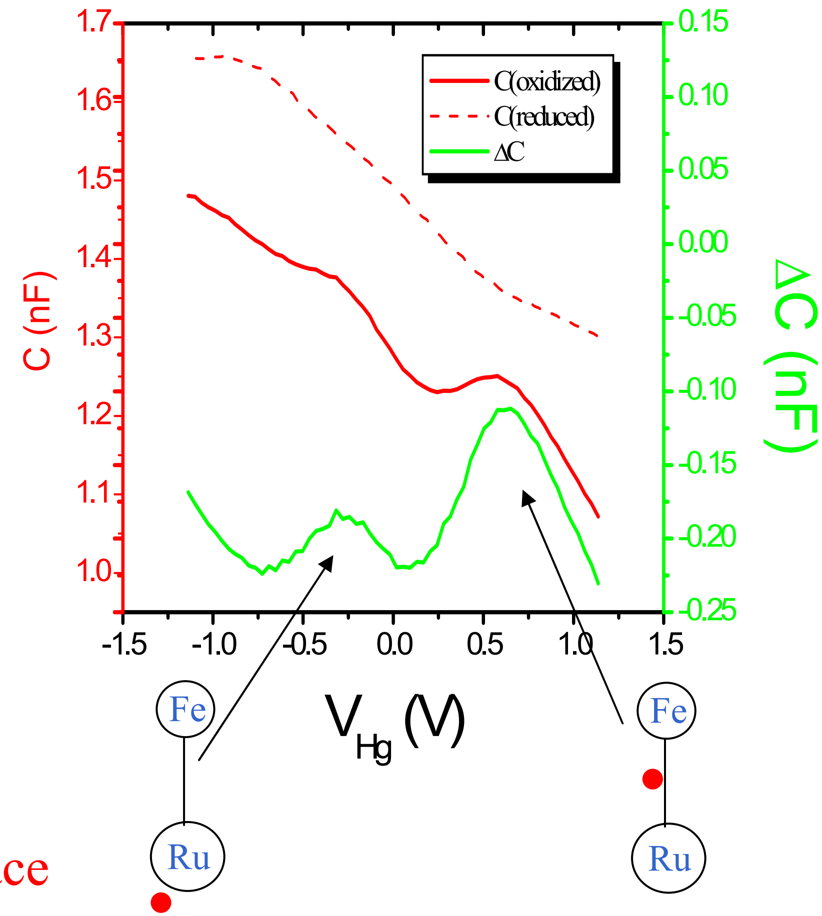
Molecule is covalent bonded to Si and oriented vertically by "struts."

Measurement of molecular bistability

layer of molecules

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

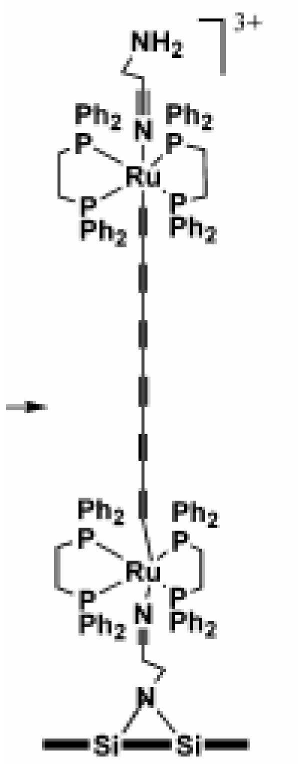




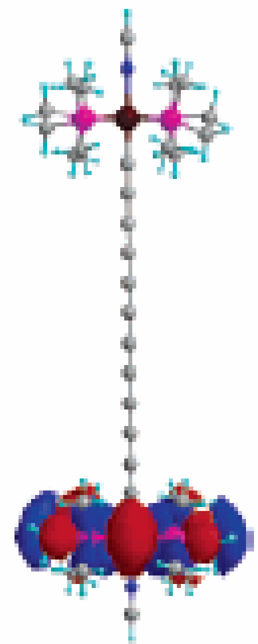
When equalized, capacitance peaks.

2 counterion charge configurations on surface

Longer molecular double-dot

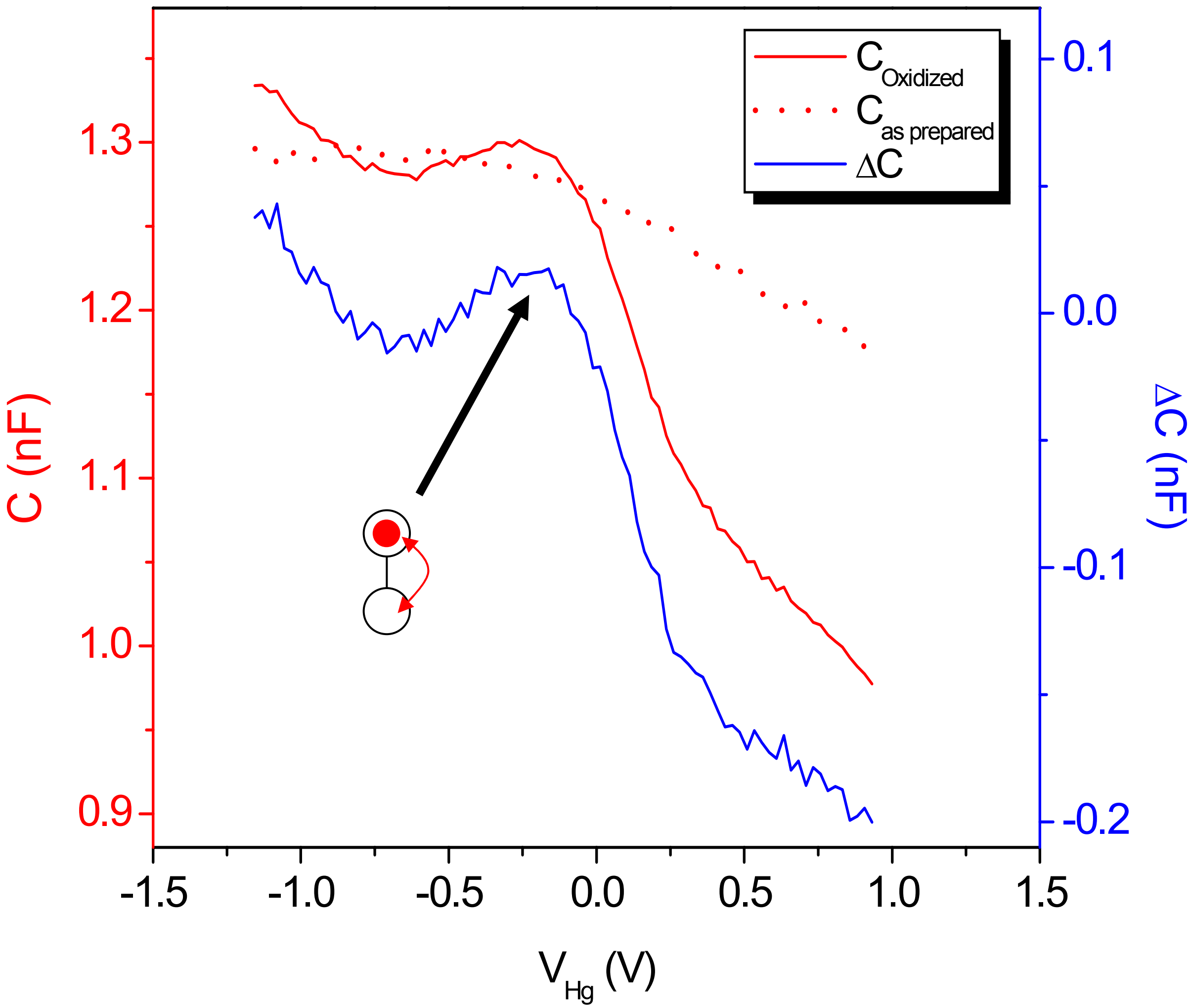


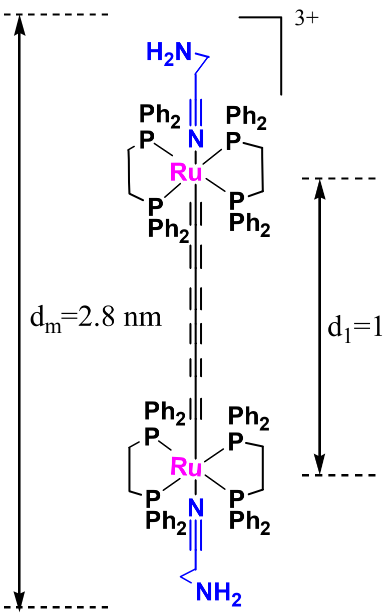
Isopotential surface



HOMO orbital

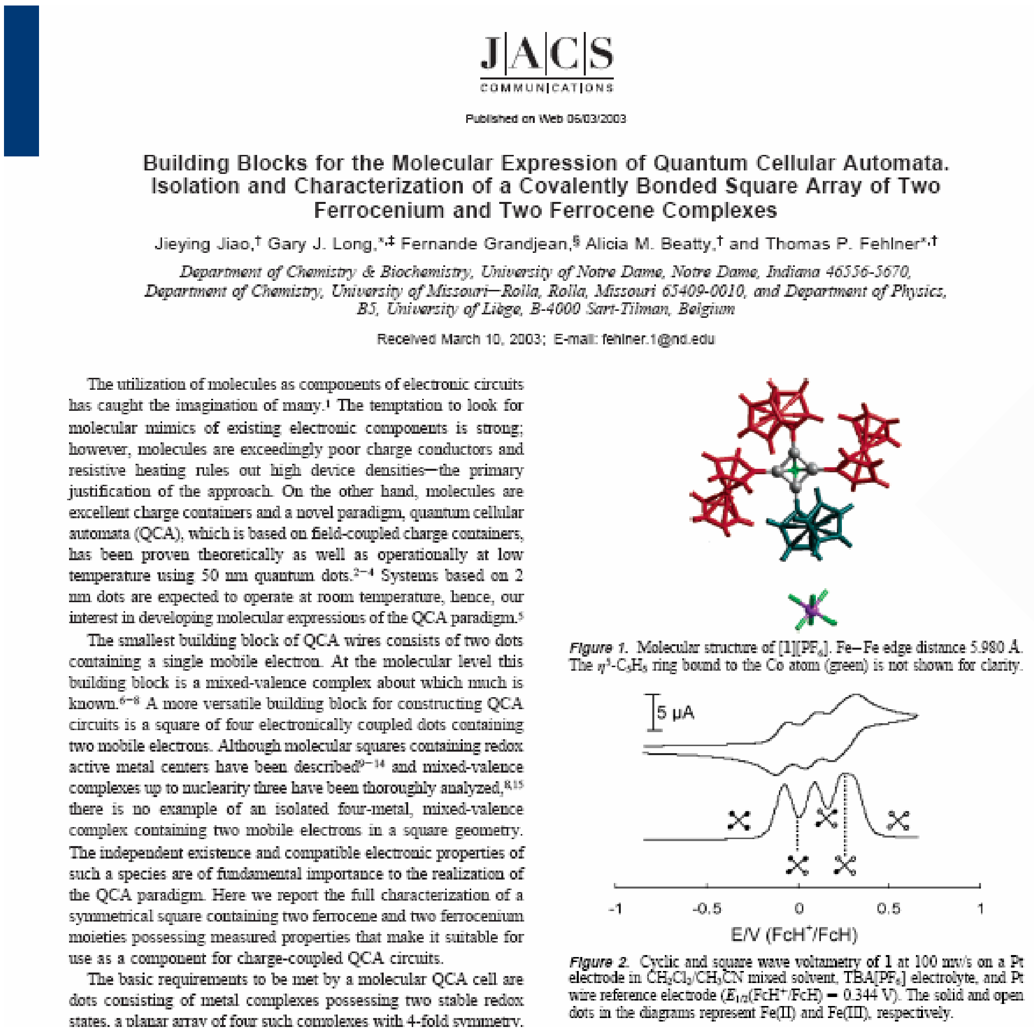
Double-dot click-clack





Hua & Fehlner

Square 4-dot QCA molecules


J|A|C|S COMMUNICATIONS

Published on Web 06/03/2003

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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Received March 10, 2003; E-mail: fehlner.1@nd.edu

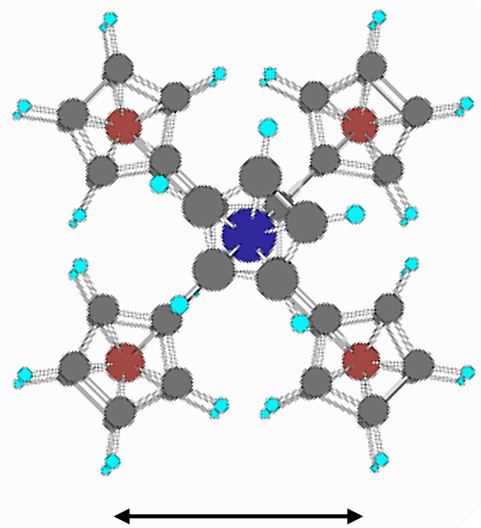
The utilization of molecules as components of electronic circuits has caught the imagination of many.[1] The temptation to look for molecular mimics of existing electronic components is strong; however, molecules are exceedingly poor charge conductors and resistive heating rules out high device densities—the 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.

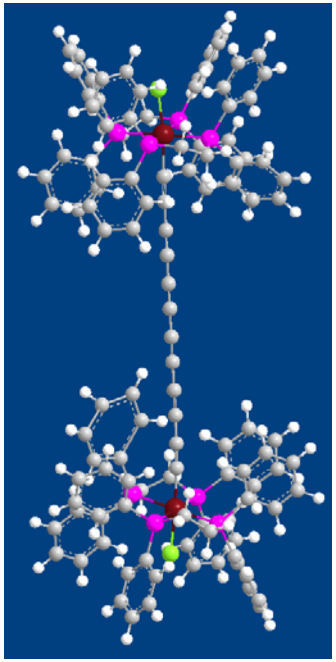
Figure 2. Cyclic and square wave voltametry of **1** at 100 mv/s on a Pt electrode in CH_2Cl_2/CH_3CN mixed solvent, TBA[PF_6] electrolyte, and Pt wire reference electrode ($E_{1/2}$(FcH^+/FcH) = 0.344 V). The solid and open dots in the diagrams represent Fe(II) and Fe(III), respectively.



0.6 nm

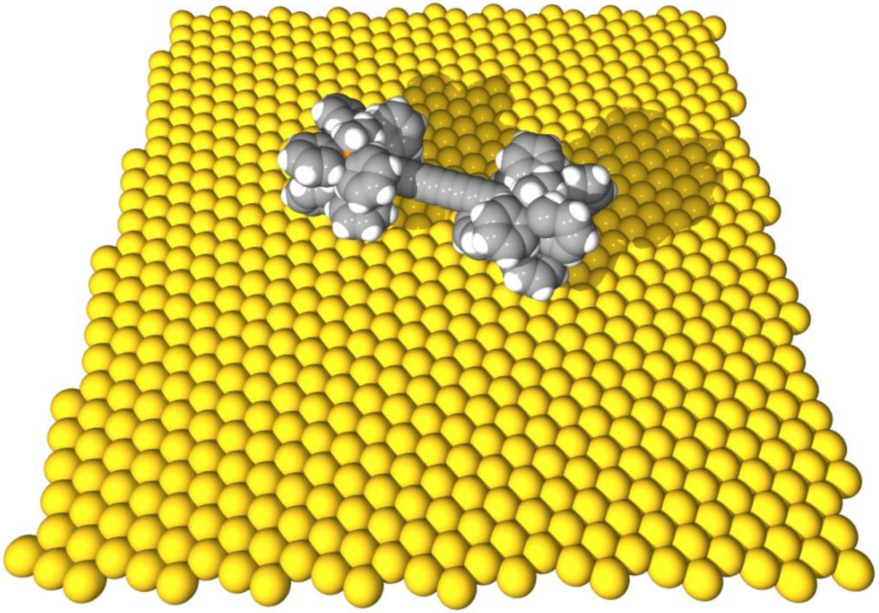
Imaging molecular double-dot

Kandel group



structure

toluene solution



Goal: single-molecule imaging on surfaces

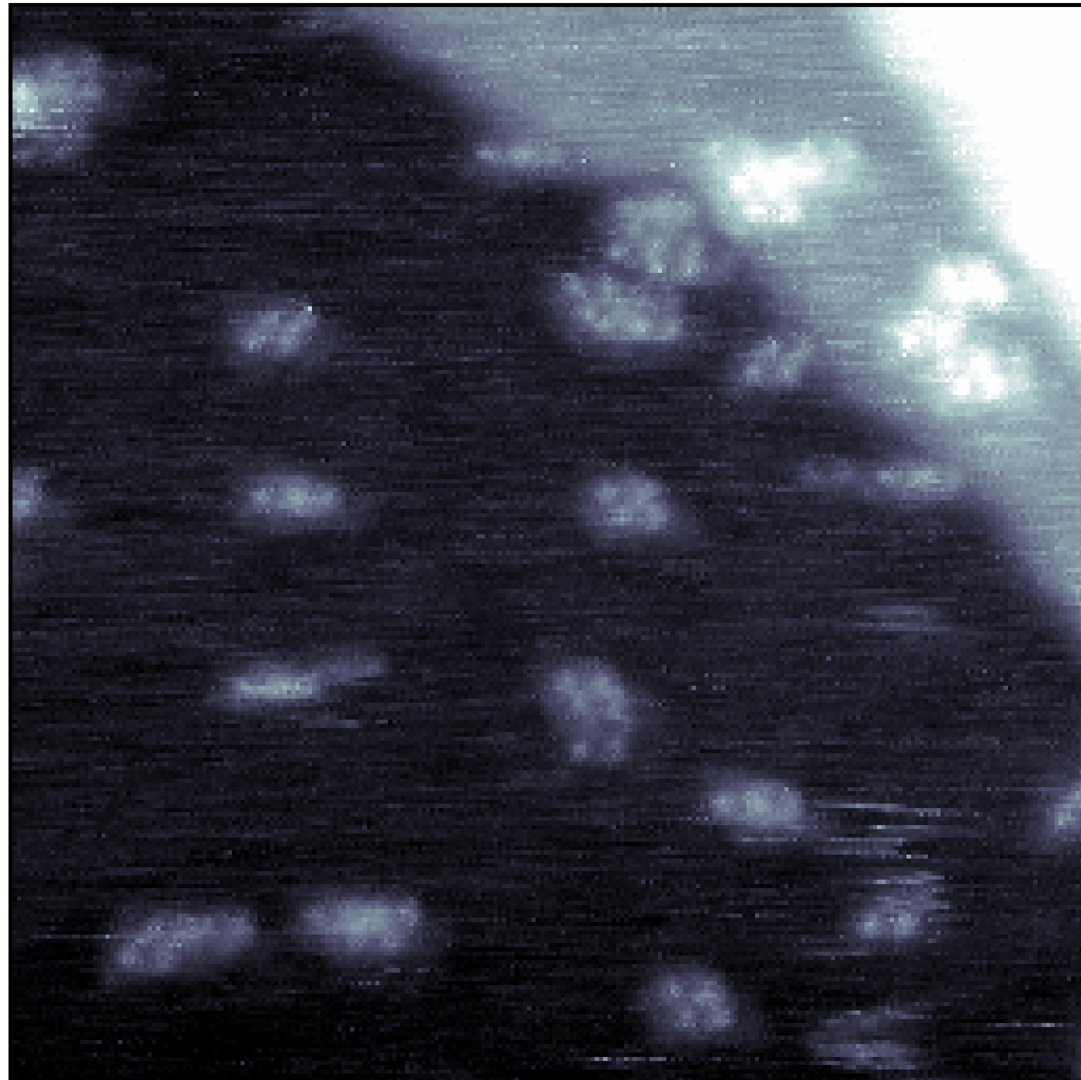
Molecules are pulse-injected from solution into vacuum onto a clean, crystalline gold [Au(111)] surface.

Ru-Ru molecule with no surface binding. Not mixed-valence species.

Ru_2 clustering

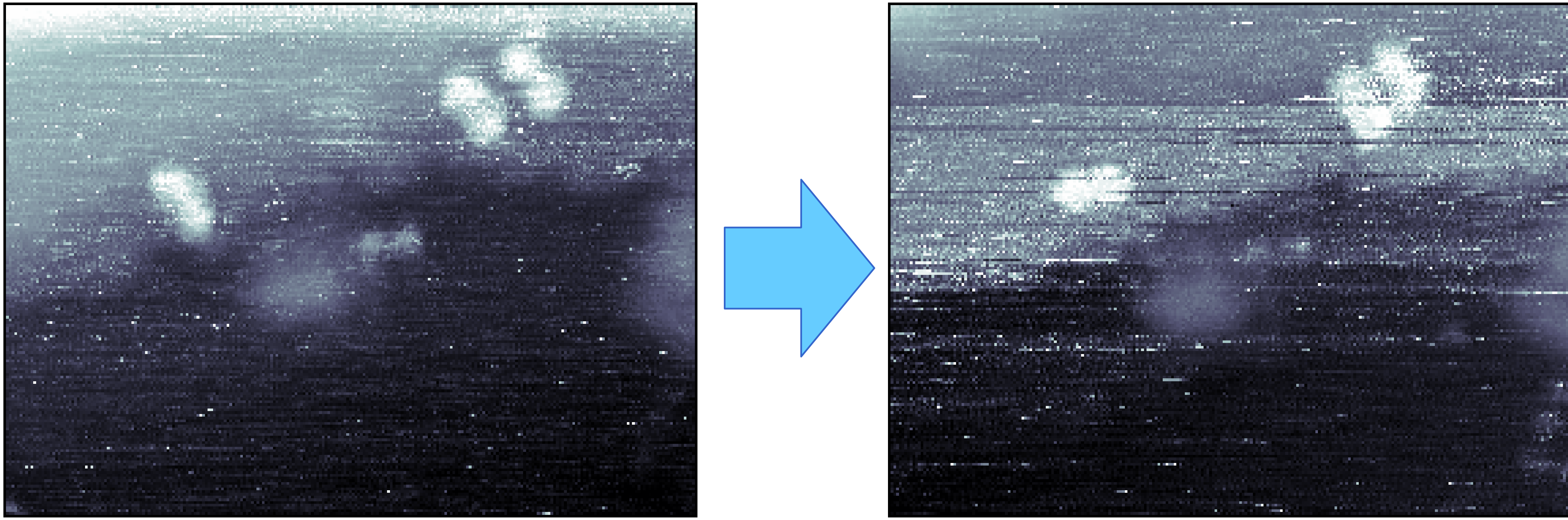
Some clustering and alignment of molecules occurs automatically during deposition. (50 nm image shown.)

We should be able to *compare* isolated molecules with those in larger clusters.



Experimental conditions: 0.5 V, 20 pA, 298 K

Molecular motion



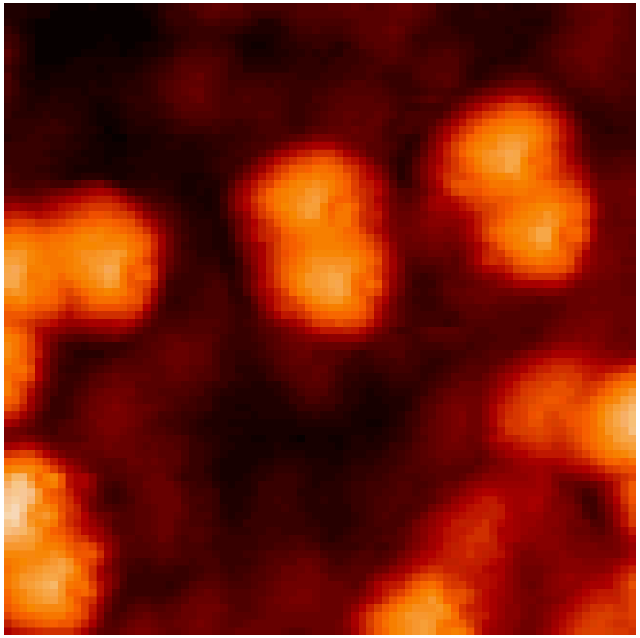
Changing tunneling conditions (from 1.0 V, 20 pA to 1.0 V, 100 pA) increases tip/molecule interaction.

We observe a change in orientation for one Ru_2 molecule.

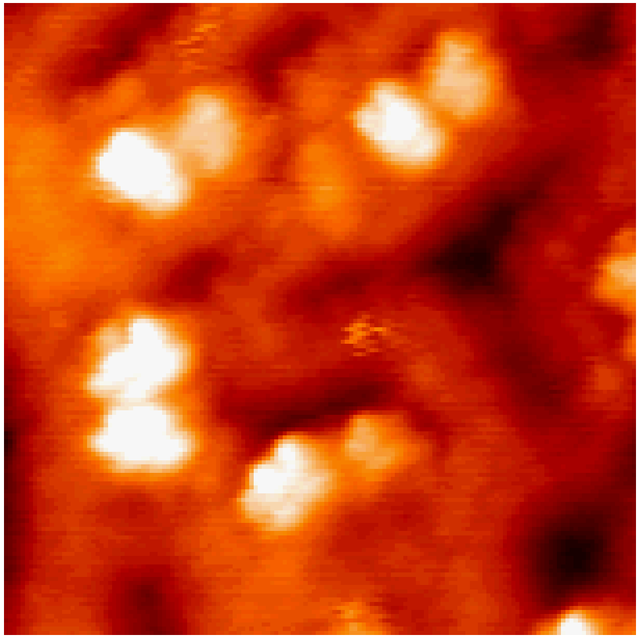
This suggests the possibility of using the STM tip for *controlled manipulation* of these molecules on the surface.

Experimental conditions: 250 × 180 Å, 1.0 V, 20 (100) pA, 298 K

Imaging charge localization



Neutral molecules



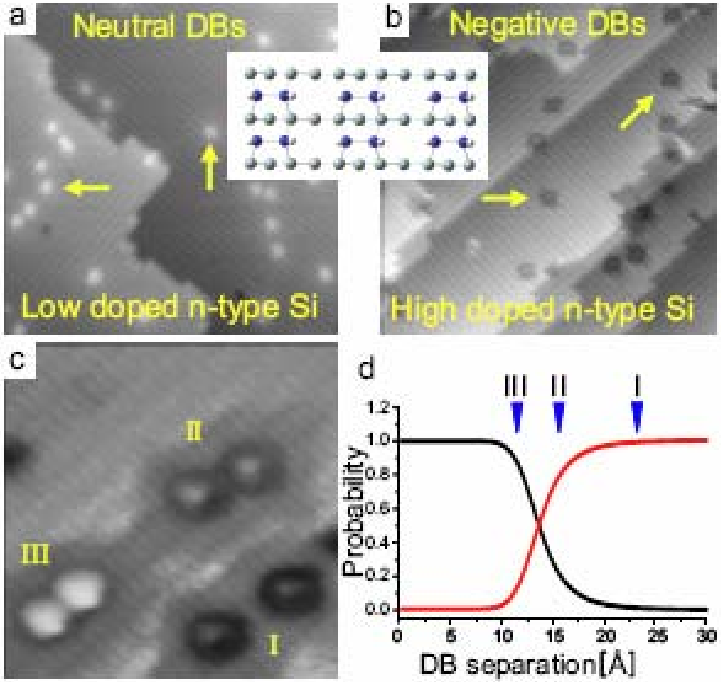
Mixed-valence molecules

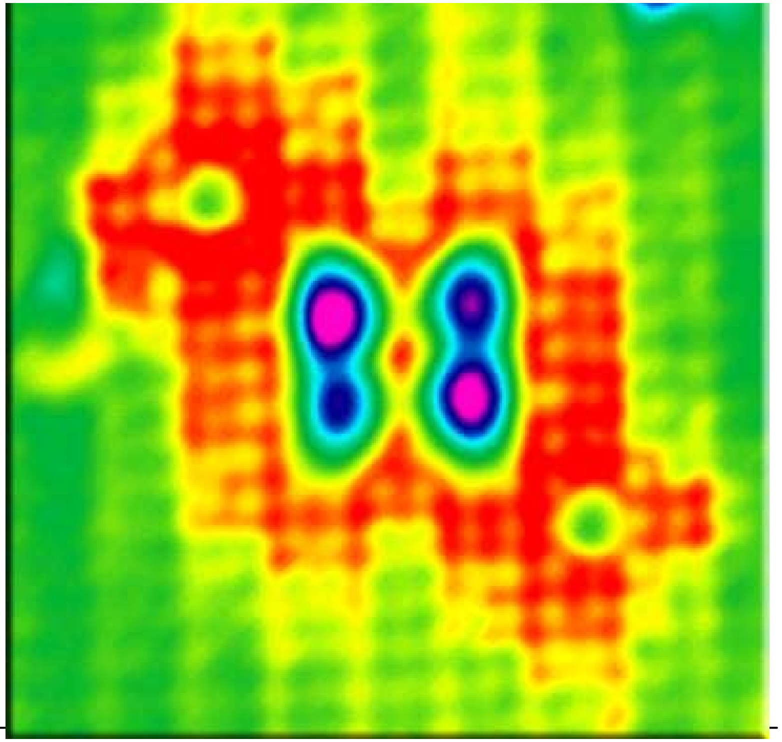
Preliminary results for Fe-Fe fabricated by Claude Lapinte (Rennes)

Single-atom quantum dots

Controlled Coupling and Occupation of Silicon Atomic Quantum Dots at Room Temperature

M. Baseer Haider†,* Jason L Pitters,† Gino A. DiLabio, Lucian Livadaru,* Josh Y Mutus,* and Robert A. Wolkow*
National Institute for Nanotechnology, National Research Council of Canada
11421 Saskatchewan Drive, Edmonton, Alberta T6G 2M9, Canada‡
(Dated: October 11, 2008)





Outline of presentation

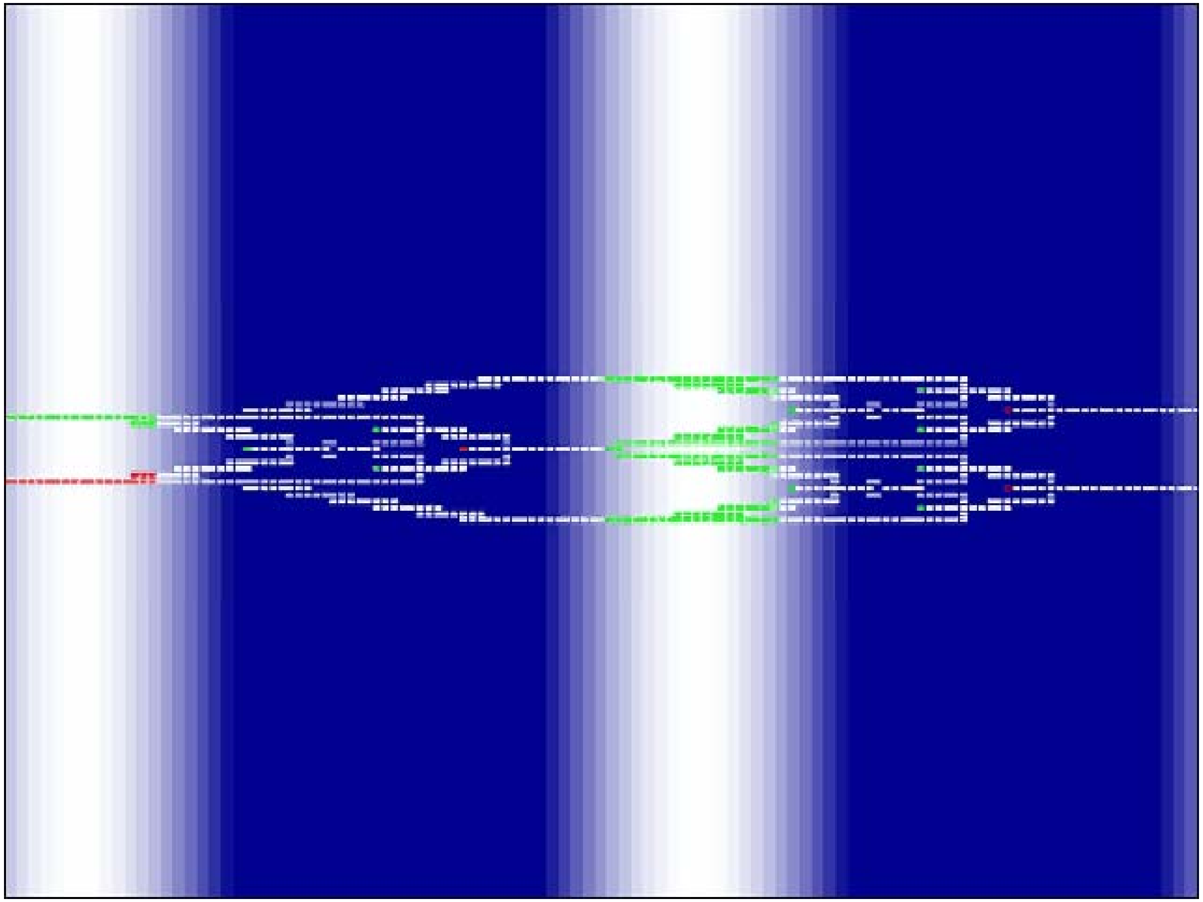
- Introduction and motivation
- QCA paradigm
- QCA implementations
  - Metal-dot
  - Semiconductor-dot
  - Magnetic
  - Molecular
- Circuit and system architecture
- Summary

Field-clocking of QCA wire: shift-register

Computational wave: majority gate

Computational wave: adder back-end

Permuter

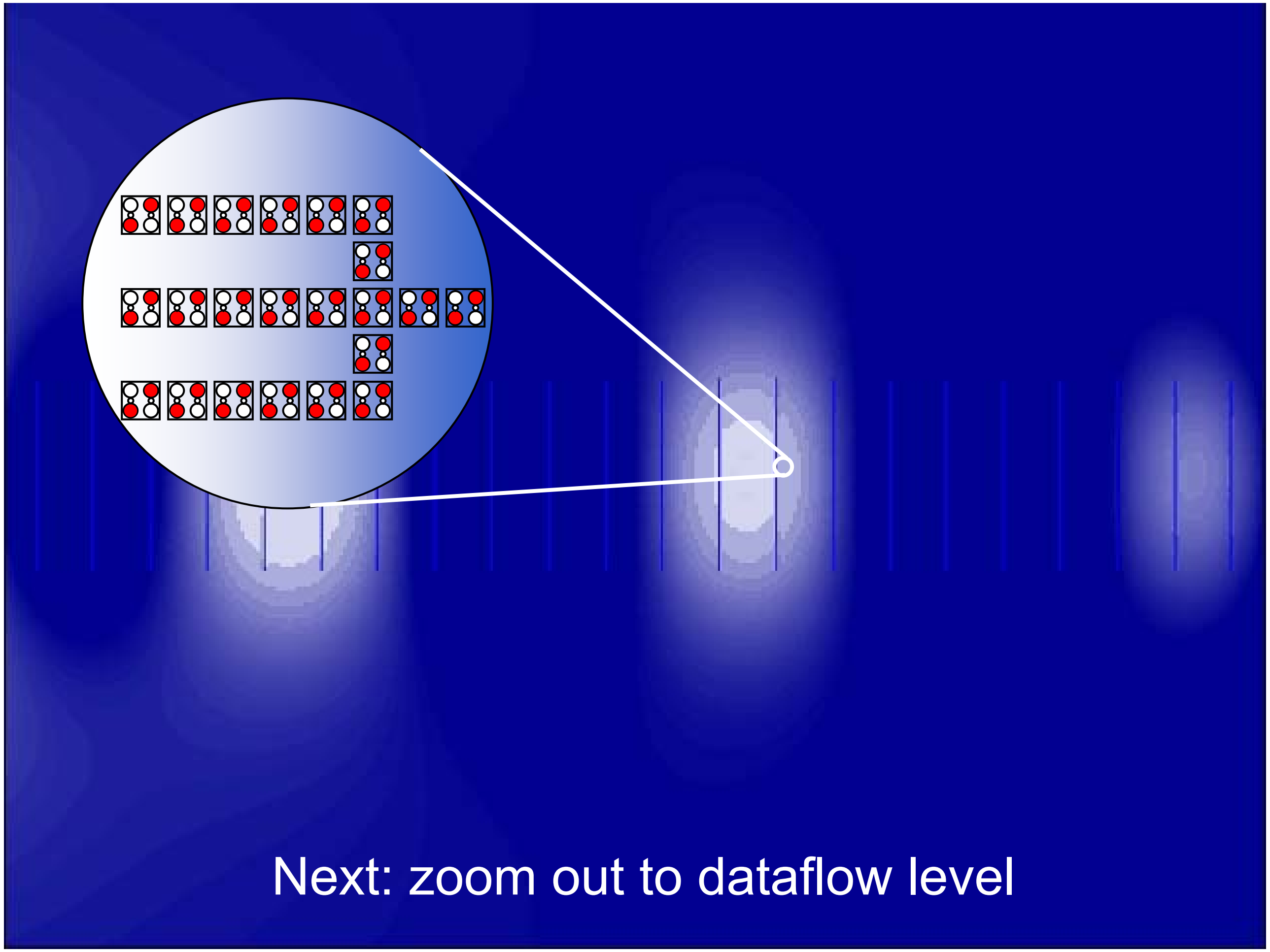


Deep pipe-lining at very small scale

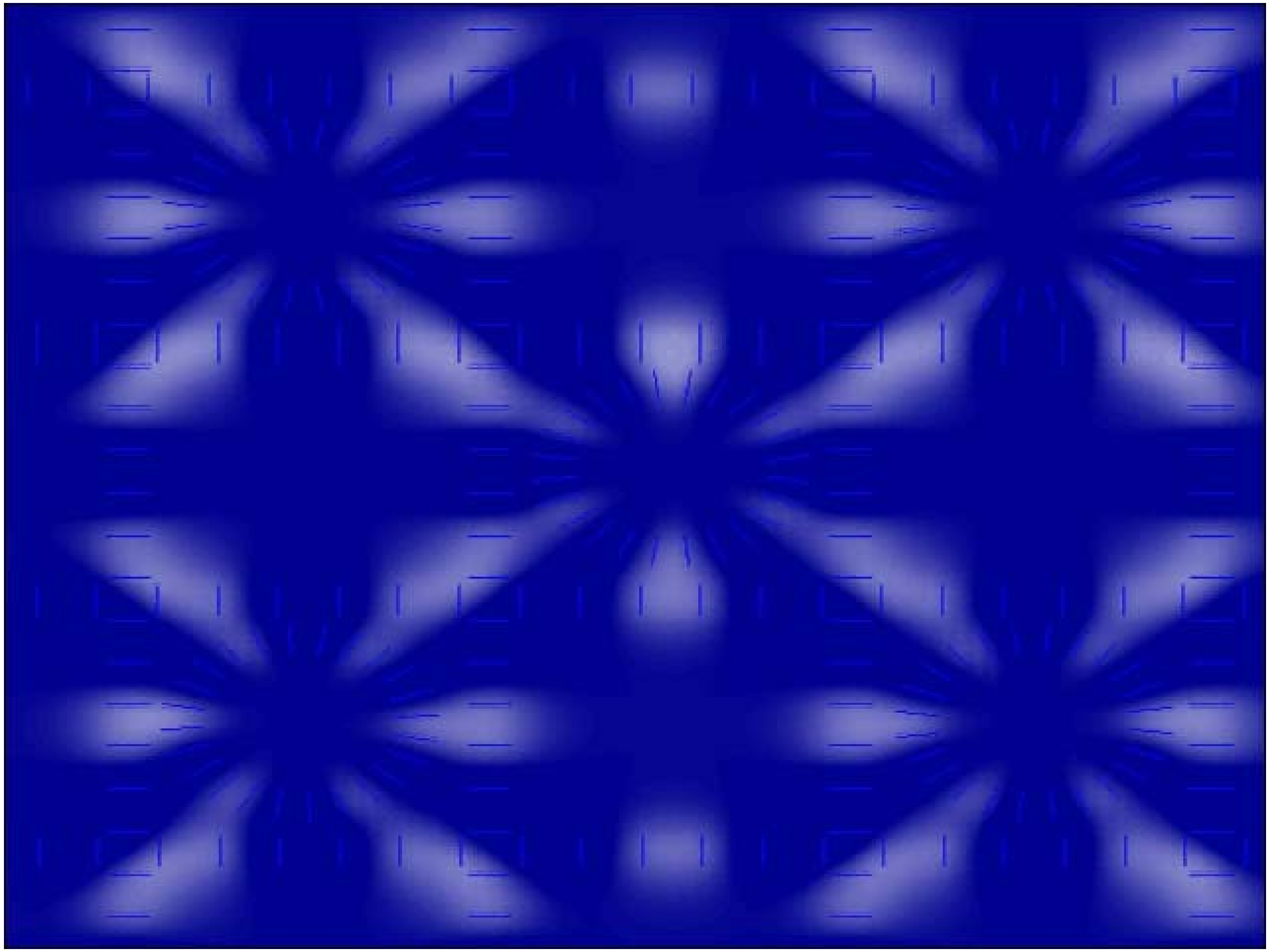
Wider QCA wires

Redundancy results in defect tolerance.

Molecular circuits and clocking wires

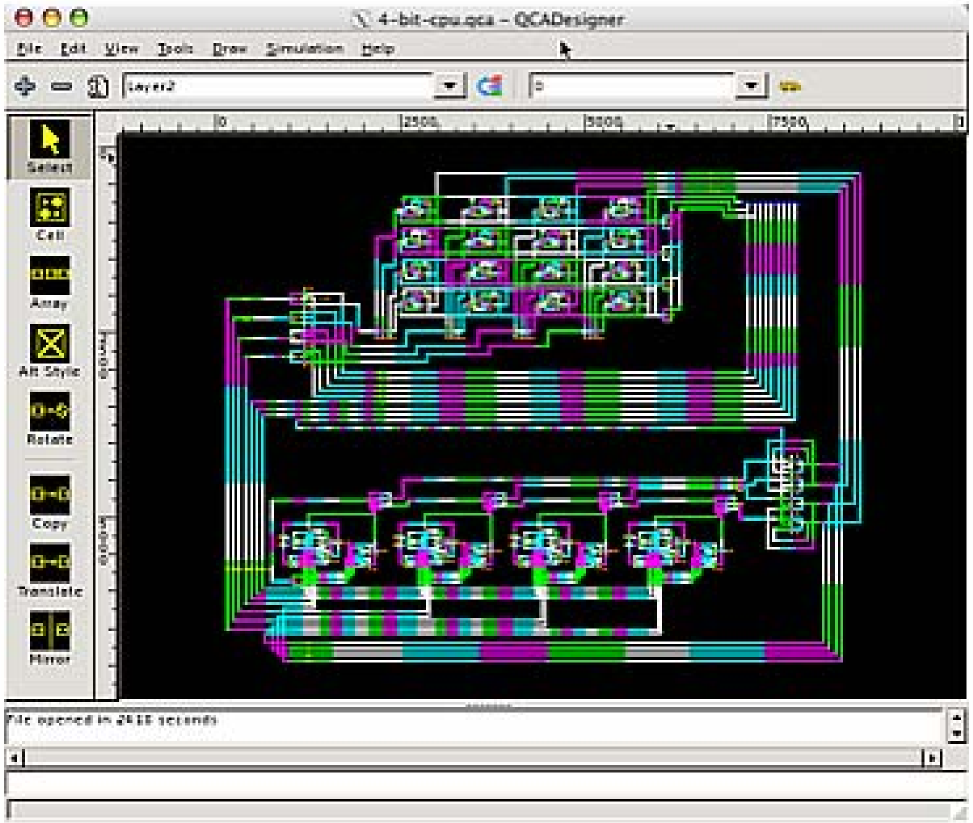


Universal floorplan



Peter Kogge

QCA design tools



QCADesigner

Konrad Walus
U. British Columbia

QCA*Designer* screenshot showing a simple 4-bit processor layout.

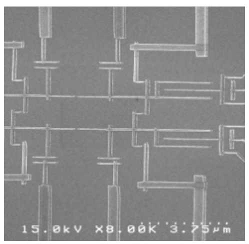
Design tools are starting to enable new systems ideas.

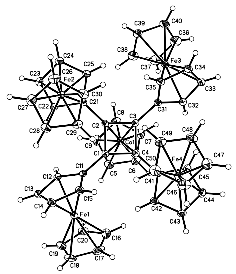
System + Application Architectures

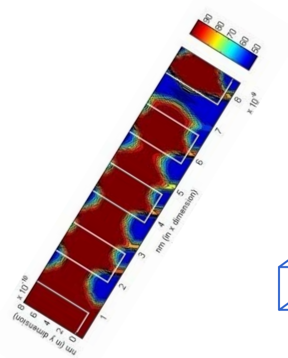
Mike Niemier

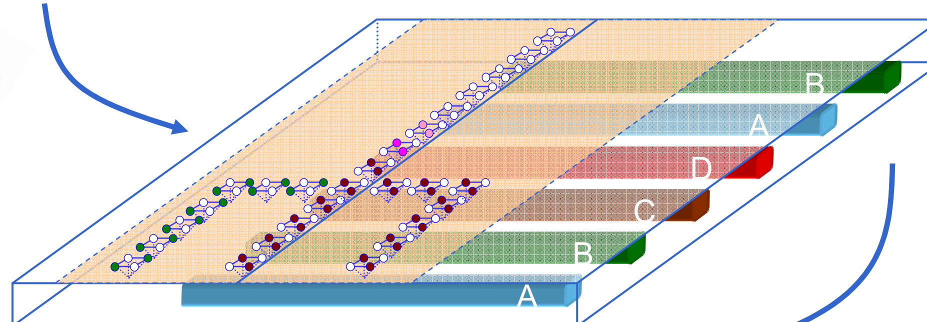
Grounded in device physics & simulation

Incorporate clock driven dataflow



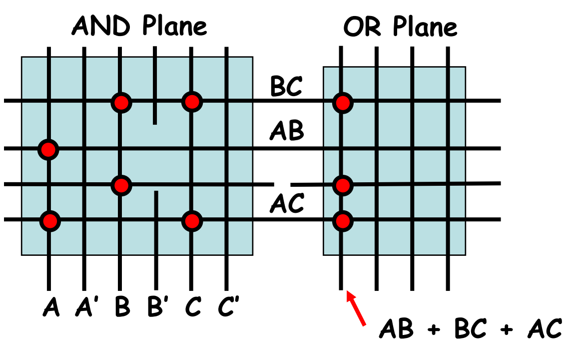




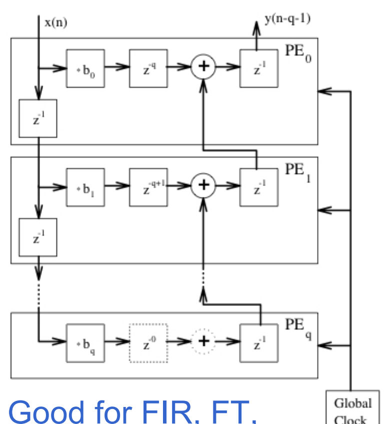


Device architecture maps well to many system architectures…

Reconfigurable

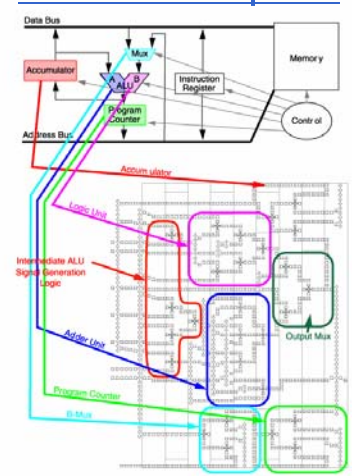


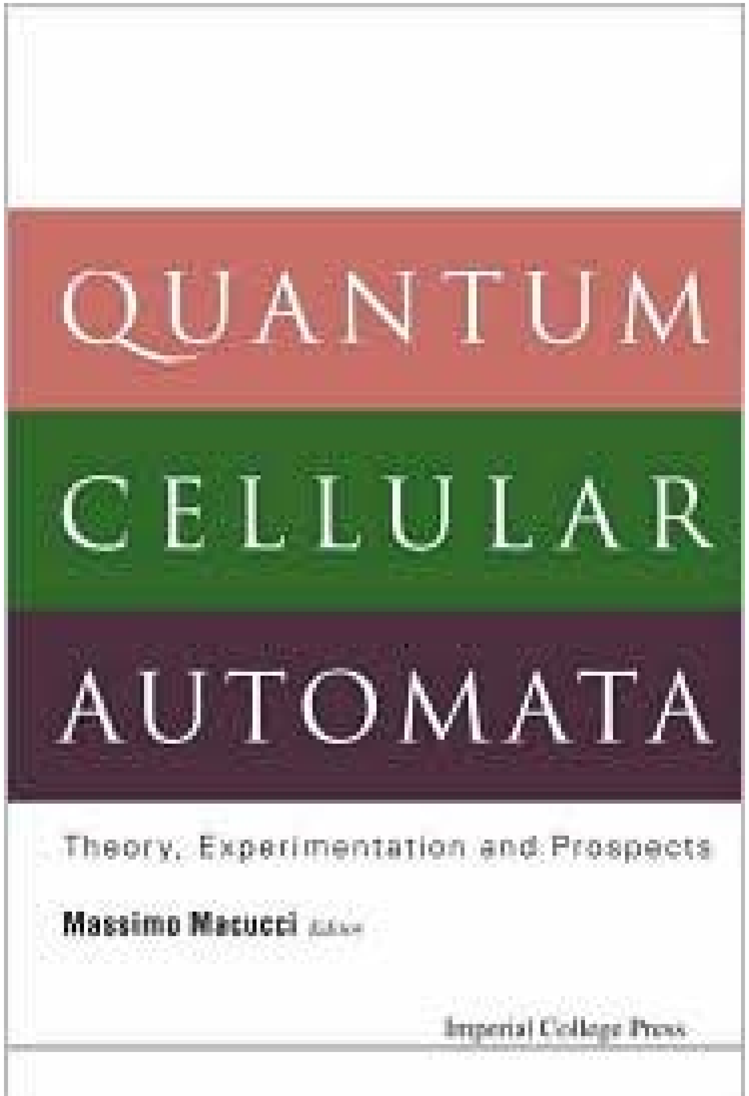
Systolic

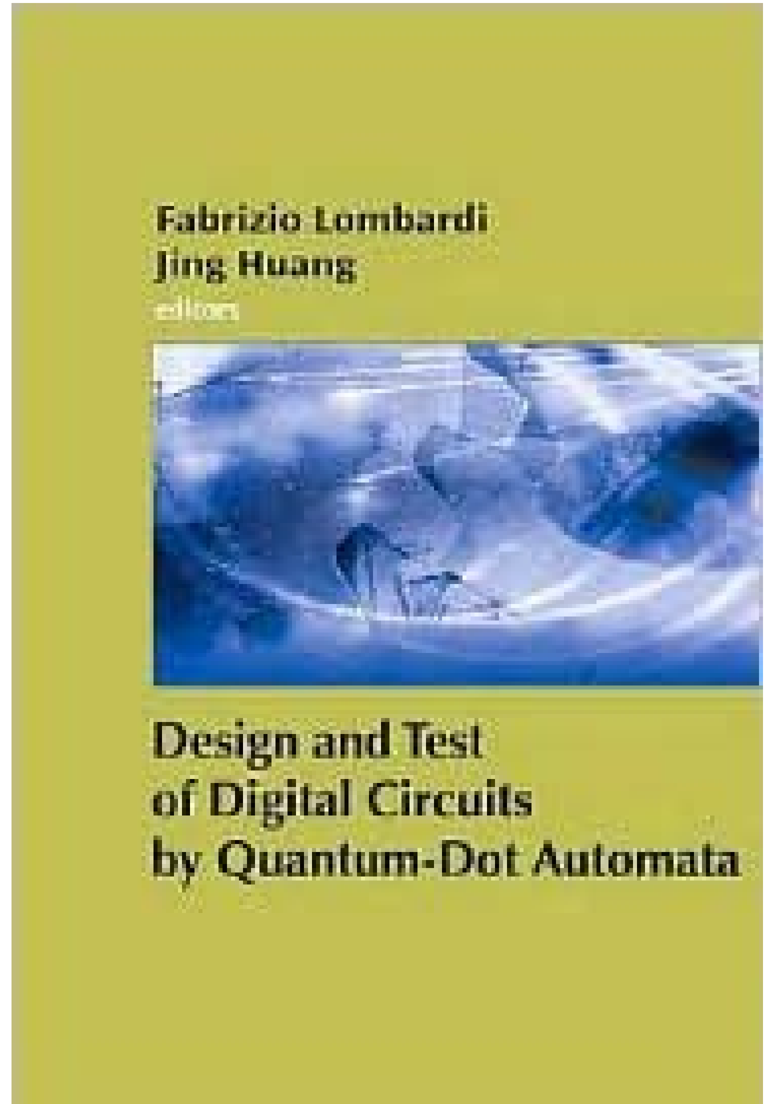


Good for FIR, FT, Matrix multiply, graph algorithms, etc.

General Purpose




QUANTUM
CELLULAR
AUTOMATA
Theory, Experimentation and Prospects
Massimo Macucci
Imperial College Press


Fabrizio Lombardi
Jing Huang
editors
Design and Test
of Digital Circuits
by Quantum-Dot Automata

J Electron Test (2008) 24:313–320
DOI 10.1007/s10836-007-5052-0

Scalability of Globally Asynchronous QCA (Quantum-Dot Cellular Automata) Adder Design

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The Robust QCA Adder Designs using Composable QCA Building Blocks

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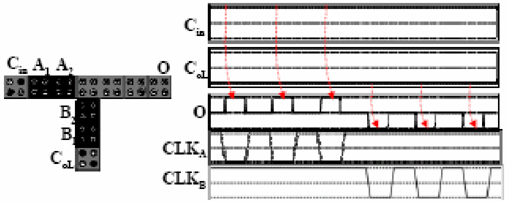

Figure 14: The schematic of a multiplex using clock gating

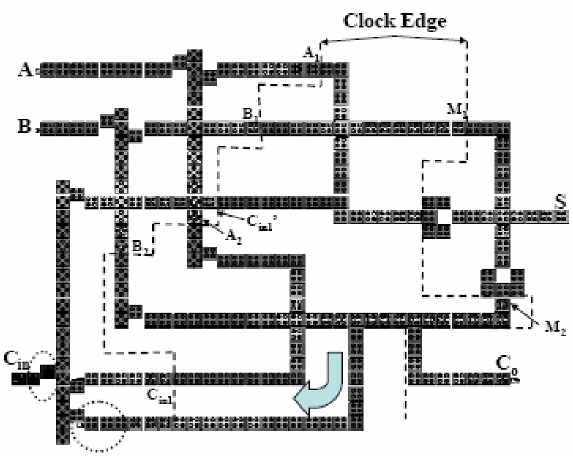

Figure 15: The schematic of a serial adder

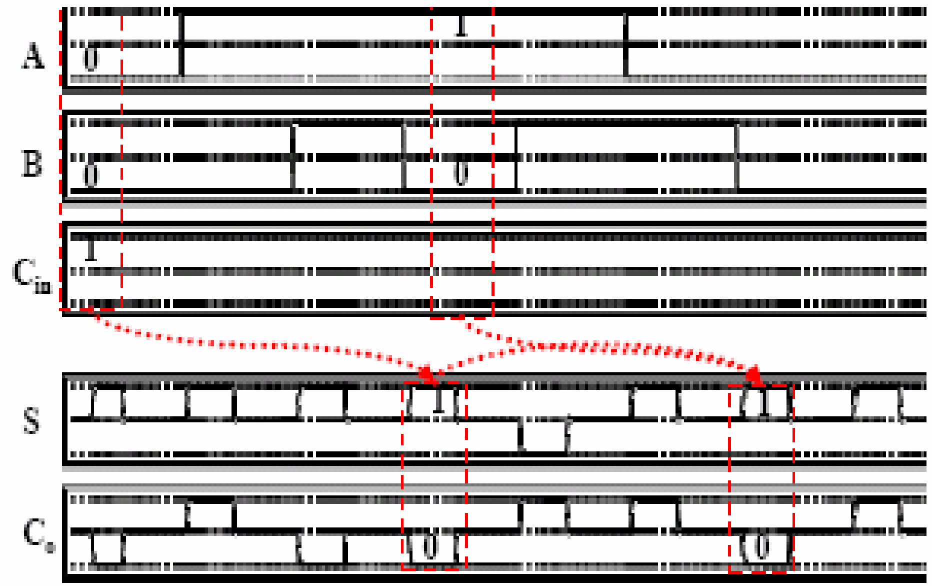

Figure 16: The simulation of the serial adder

Quantum-dot Cellular Automata Design Guideline

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The Fastest Single-Layer Robust QCA Adder

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Designing layout–timing independent quantum-dot cellular automata (QCA) circuits by global asynchrony

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Available online 14 January 2007

Summary

- QCA offers possible path to limits of downscaling – molecular computing.
  - General-purpose computing
  - New architecture
  - Low power dissipation which is essential
- Single-electron metal-dot QCA devices exist.
- First steps in molecular-scale QCA
- Clear path but much research remains to be done.
  - Rethinking architecture to match problem
  - Chemistry, physics, electrical engineering, computer science

Thanks for your attention.