Quantum-Dot Cellular Automata: An Architecture for Molecular Computing

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***Abstract*—The quantum-dot cellular automata (QCA) paradigm is a revolutionary approach to molecular-scale computing which represents binary information using the charge configuration of nanostructures in lieu of current switching devices. The basic building-block of QCA devices is the QCA cell. Electrostatic interaction between neighboring cells allows the design of QCA wires, logic devices and even simple microprocessors. The geometry of molecular six-dot QCA cells enables the clocking of QCA devices via an electric field generated by a layout of clocking wires. Thus, precise control over the timing and direction of data flow in QCA circuits is possible. The design of QCA circuits now lies not only in the logic structure of the cells, but also in the layout of clocking wires. We discuss the clocking of QCA devices and connect layout to architecture.**

Keywords-architecture; clocking; defect tolerance; molecular QCA

I. INTRODUCTION

Research in the electronics industry has rapidly and consistently reduced semiconductor device sizes and operating currents for several decades. Continued development toward devices on the nanometer scale will be limited not only by process technology, but also by fundamental problems arising from scaling such as quantum-mechanical effects and severe power dissipation. Quantum-dot cellular automata (QCA) [1] is an approach to molecular-scale computing which, rather than using current switching, uses the charge configuration of a set of quantum dots to represent binary information.

Any approach to true single-molecule molecular computing must contend with the difficulties of making contact to individual molecules. On the one hand, if the single-molecule device must be positioned between two or three macroscopic leads, the inherent advantage of single-molecule sizes is lost; the size of the actual device becomes dominated by the size of the leads. On the other hand, if single molecules are to be connected directly to each other, as in the molecular transistor paradigm, then the challenge of "wiring up" vast numbers of molecular interconnects may also prove a defeater. We will see that the molecular QCA approach solves these problems by (1) coupling molecules directly to other molecules to avoid the cost of intervening leads (except of course at the inputs and outputs of the entire array), but (2) uses Coulomb coupling between molecules to provide robust operation without the need for precise control of current flow from molecule to molecule.

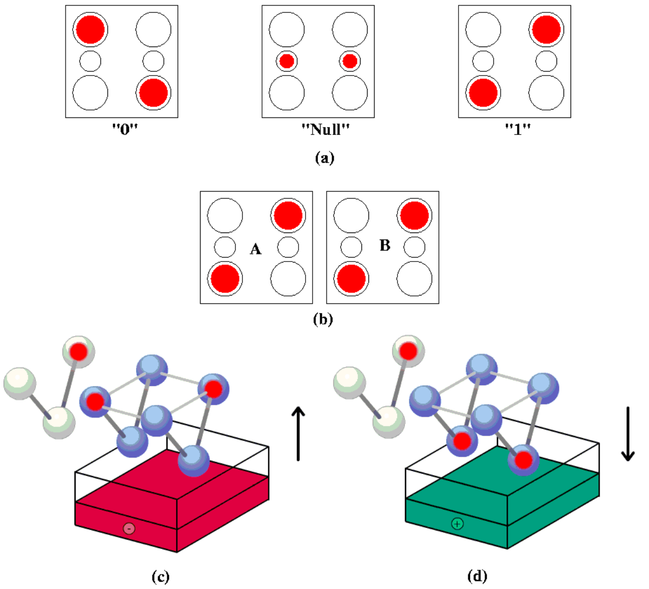

Figure 1. Schematic of six-dot QCA cells. (a) A cell with six quantum dots (black circles) and two electrons (red discs) is shown in three electronic states: "0", "Null", and "1". (b) When cells are juxtaposed, they interact. If cell A is locked in the 1 state and cell B is forced out of the null state, then the ground state for cell B is the 1 state. (c) A cell is placed on a substrate above a negatively charged conductor (red). The perpendicular electric field pushes electrons upward, forcing the cell out of the null state. Electrostatic interaction with the input molecule (white) makes the 1 state the ground state. (d) When the conductor is positively charged, the electric field pulls the electrons down to the null state independent of the input molecule.

The basic building block of QCA devices is the QCA cell. A QCA cell consists of several quantum dots with two mobile electrons. A quantum dot is a region in the cell structure where charge can localize. Coulombic repulsion between like charges forces electrons in the same cell to occupy dots which maximize their separation. Therefore, when the cell's dots are arranged in a square as in the six-dot cell of Figure 1(a), the electrons will occupy dots at opposite corners of the square. In this square geometry there are two configurations or states in which the electrons can occupy dots at opposite corners. We label these states "0" and "1", and we observe that for an isolated cell these two states are degenerate [2]. For this six-

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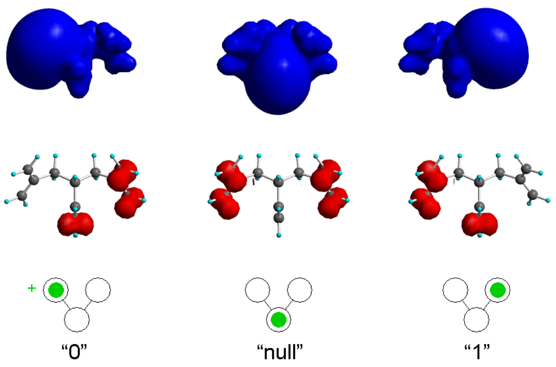

Figure 2. A molecule with three quantum-dot hole sites is shown. Three states of the molecule are depicted schematically (bottom); in a highest-occupied-molecular-orbital diagram (HOMO, middle); and in an isopotential surface diagram (top). Two such molecules form a six-dot QCA cell.

dot cell geometry there is also a "Null" state which stores no information. A cell can be driven to this state by applying the proper electric field.

A cell's charge configuration will be influenced by electrostatic interaction with the charge configuration of any neighboring cells, as represented in Figure 1(b). These electrostatic interactions with neighboring cells can lift the degeneracy of the 0 and 1 states, thereby determining the ground state of the cell [2].

Remarkably, this simple interaction between cells enables general purpose computing using arrays of QCA cells. Wires, logic gates, adders [2], and even simple microprocessors [3] all have been designed within the QCA paradigm. A simple wire consists of QCA cells arranged in rows with intercellular coupling as in Figure 1(b). The majority gate is a three-input logic device which can be implemented using QCA cells. The majority gate is part of a logically complete set [3] and is used in the design of QCA microprocessors.

QCA devices using single-electron switching have been fabricated using small metallic quantum dots at low temperatures [4,5]. Majority gates, wires, and clocked shift registers all have been demonstrated [6-8].

A single molecule can function as a QCA cell. Molecular QCA can be fabricated with a much higher degree of regularity and are on a much smaller size-scale than their metal-dot counterparts. Furthermore, molecular QCA can operate at room temperature [9]. Functioning QCA molecules have yet to be demonstrated, but a molecule first proposed by Aviram [10] and studied by Hush and coworkers [11] has been used as a model system to investigate how a molecular six-dot cell might behave [12]. This molecule, shown in Figure 2, has three quantum dots which serve as localization centers for a mobile hole. It has been shown that a six-dot cell can be formed by juxtaposing two of these molecules [13]. (Note that this molecule has a *hole* as its mobile charge, whereas we assume here mobile *electrons*; appropriate changes in sign can be made.)

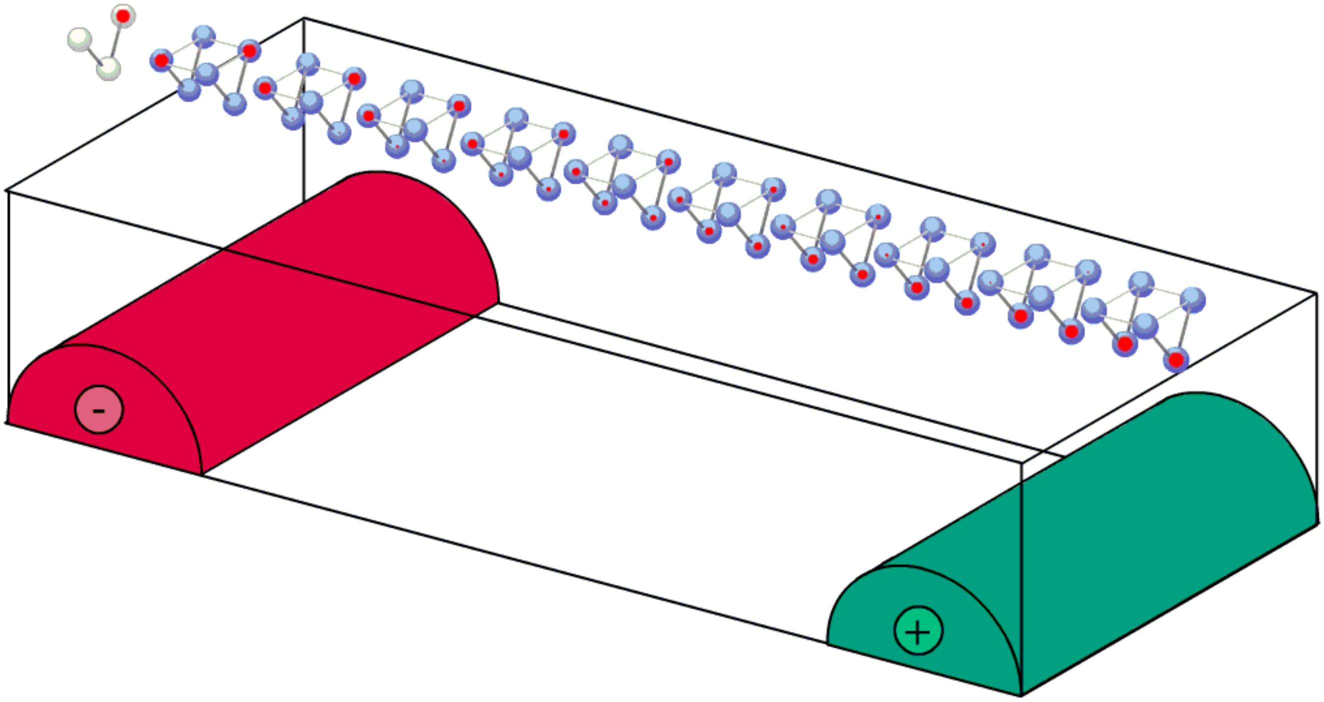

Figure 3. Buried clocking wires create an inhomogeneous perpendicular clocking electric field. Cells with mobile electrons above the negatively charged wire (red) are forced out of the null state and respond to the charge configuration of the white input molecule. Cells above the positively charged wire (green) are forced into the null state and convey no information.

II. CLOCKING A QCA ARRAY

A QCA cell with six dots and two extra electrons can be controlled with a perpendicular electric field [14]. The four dots at the square corners are designated "active dots" and are elevated above the middle dots, which lie on the substrate and are called "null dots". A tunneling path exists between each active dot and a null dot, while direct tunneling between active dots is suppressed. An electric field with a perpendicular component can be used to push the electrons up to the active dots or to pull them down to the null dots. A positive (upward pointing) electric field will pull the electrons down to the null dots, resulting in the "null" configuration as shown in Figure 1(d). On the other hand, a negative (downward pointing) electric field will exert an upward force on the electrons. As we increase the magnitude of the negative electric field from zero, we will reach a point where the cell assumes an active state, either 0 or 1, as in Figure 1(c). Now the field is strong enough that the electrons are locked in their respective active dots. Thus, the cell cannot switch to the other active state (1 or 0, respectively) without first being reset to the null state.

An array of QCA cells can be clocked using clocking wires buried beneath the QCA molecular layer as shown in Figure 3. These wires, when charged according to a multi-phase clocking signal, can create a time-varying, inhomogeneous, smoothly graded electric field across the QCA plane. At any given instant in time, the field will have regions where the perpendicular component is strongly positive or strongly negative. The electrons of any cell in a strongly positive region will be pulled down to the null state. This strongly positive region of the electric field is a null domain. A strongly negative region is an active domain in which the electrons of a cell will be pushed upward and locked into an active state. The null and active domains will be separated by switching regions where the electric field is weak or near zero. Here, cells transition between the null state and active states. The time-variance introduced by the clocking wave will cause the active domains, null domains, and switching regions to move about the QCA plane in a manner dictated by the layout of the clocking wires.

This results in "computational waves" – data in active domains flowing throughout the circuitry, moving and interacting with other data. Bits of data will exist only within active domains. The movement of a given active domain about the QCA plane will cause the bits of data contained therein to move as well. Data can be carried along wires and processed through logic devices designed to process the data. Clocked, controlled computation occurs when switching regions pass through logic devices and interact. The active ground state of the switching cells is determined by the logical structure of the device and by the bits contained in the adjacent active domains.

III. CLOCKED QCA DEVICES

Several clocked QCA devices have been designed and simulated in time using this logic-clocking architecture. Simulations involve a device, which is nothing more than an array of QCA cells, and a layout of clocking wires to clock the device. To simulate a cell array in time, we assume that cell behavior is adiabatic and that the state of the QCA array at time *t* is very close to the instantaneous ground state of the array under the influence of the clocking field at time *t*. At each time *t* of interest, we iteratively solve the time-independent Schrödinger equation (TISE) for the ground state of each cell in the array until a self-consistent solution is found for the entire array at time *t*. Each solution of the TISE takes into account the electrostatic potential due to both the clocking electric field and interactions with neighboring cells. Therefore, this process requires: using Gauss' Law to calculate the electric field at time *t* across the QCA plane due to the layout of clocking wires; calculating the electrostatic potential at each quantum dot from this clocking electric field; and calculating the electrostatic potential at each quantum dot of each cell due to the charge configurations of neighboring cells.

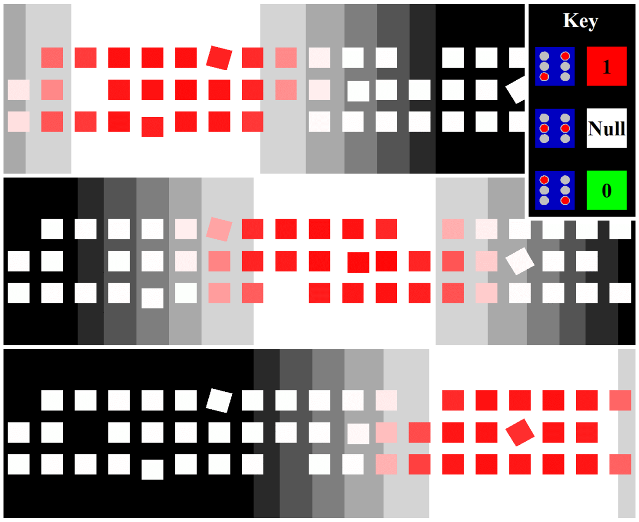

Figure 4. A three-cell-wide shift register exhibits defect tolerance. Defects in this shift register include missing cells, rotated cells, and translated cells. Nonetheless, a 1 bit successfully shifts rightward with the active domain on the register, as shown in the three simulation snapshots.

Here we describe the clocked shift register and the clocked majority gate. We also include a description of the back end of a single-bit adder, which is an example of a device implemented by several majority gates.

A. The Shift Register

A shift register is implemented by first burying a set of parallel clocking wires in a layout like the ties of a railroad track. Next, we lay QCA cells out in a row forming a QCA wire above and parallel to the path created by the clocking wires. The clocking wires can be used to shift data in active domains along the wire in a controlled manner. This is a shift register, the means by which we move data from one point to another. It is an important part of any clocked QCA circuit.

B. The Majority Gate

The majority gate is a three-input, single-output device which can be used in the design of more complex logic devices. Three input bits are shifted in active domains along three separate shift registers toward a cell or set of cells which acts as a majority gate. The three inputs each have equal influence over the output of the device. When all the inputs are

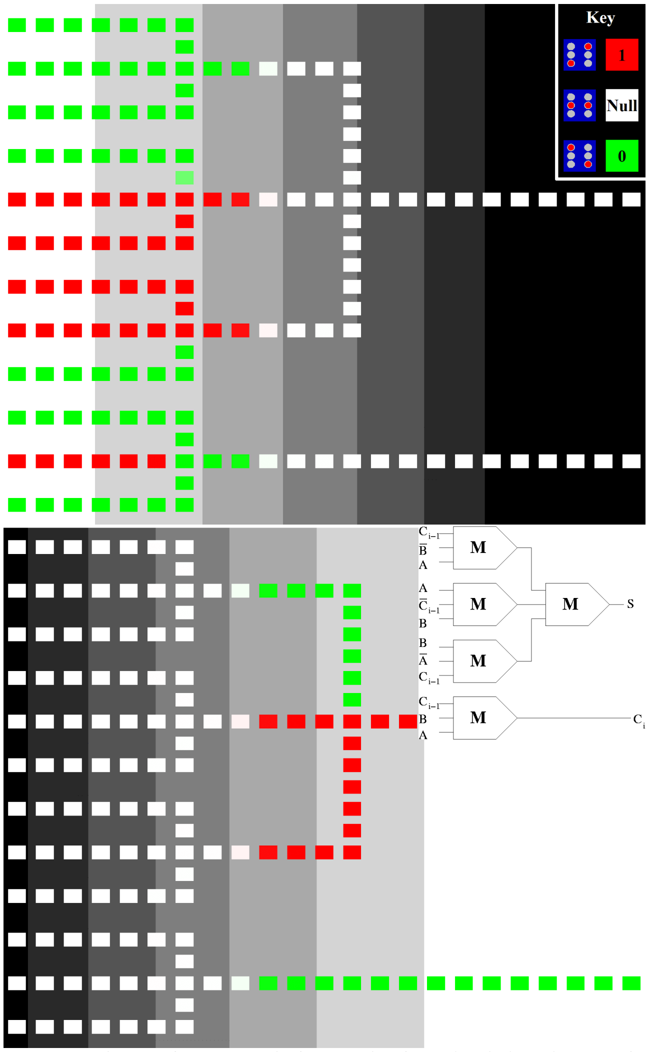

Figure 5. The two frames are "before" and "after" simulation pictures of a clocking wave carrying data through a single-bit adder where it is processed. Cells are represented by white or colored squares with the clocking field in the background. The light region in the background represents an active domain. The dark region represents a null domain. As the active domain sweeps by the adder, it carries data with it. The data reaches the device, and computation occurs. Here, the inputs $A = 0$, $B = 1$, and $C_{i-1} = 0$ are passed through the adder by the rightward propagation of the active domain and switching region. The resulting output is a sum $S = 1$ with carry $C = 0$.

the same, there is no conflict, and the output of the majority gate is dictated in unison by the three inputs. A set of conflicting inputs will include two like bits, which comprise a majority, and one incongruous bit in the minority. The influence of the majority dominates over that of the minority, and the output will be dictated by the majority. As the bits reach the majority gate, the gate assumes the state dictated by the majority. This bit is the device output and can then be shifted away from the gate for further computation.

C. The Single-Bit Adder

The single-bit adder is a three-input, two-output device based on the majority gate. Three single-bit inputs, A, B, and C_{i-1} (the carry from the previous addition operation), are shifted to the front end of the adder, which distributes the inputs and their complements to the back end for computation. The back end of the adder is implemented using five majority gates. The adder outputs the sum S and carry C_i of A, B, and C_{i-1}. A simulation of the back end of the adder is shown in Figure 4.

IV. DEFECT TOLERANCE

Defects are unavoidable in molecular electronics. Incorporating redundancy into the design of QCA devices to make them more defect tolerant [15-17]. The simple improvement of making a shift-register three cells wide provides intrinsic triple-modular redundancy at each stage. A simulation of such a defect-tolerant shift register is shown in Figure 5.

V. POWER GAIN

Power gain is an essential component of any successful digital electronics technology. Unavoidable dissipative processes cause energy in the signal path to leak out to the environment. If there is no way to restore this energy the signal will degrade from stage to stage until it is lost in the thermal background. In conventional electronics, the power supply provides the energy necessary to restore the signal integrity. In clocked QCA, the energy from the clocking field provides this energy. If the signal in a cell is reduced, the clocking field must do extra work to copy the bit to the nearby cells. The cells automatically absorb sufficient energy from the clock to restore the signal. Power gain in clocked QCA has been analyzed theoretically for molecular QCA [18] and measured experimentally for metal-dot QCA devices [19].

VI. CONCLUSION

The QCA paradigm is a revolutionary alternative to current-switching devices that holds promise for molecular electronics. QCA is a paradigm in which general-purpose computing is possible. The ability to clock QCA yields precise control over the timing of computation in QCA circuits. Clocking by means of buried clocking wires defines the data flow in QCA circuits.

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