Near zero-energy computing describes the concept of executing logic operations below the \((k_B T \ln 2)\) energy limit. Landauer discussed that it is impossible to break this limit as long as the computations are performed in the conventional, non-reversible way. But even if reversible computations were performed, the basic energy needed for operating circuits realized in conventional technologies is still far above the \((k_B T \ln 2)\) energy limit (i.e., the circuits do not operate in a physically reversible manner). In contrast, novel nanotechnologies like Quantum-dot Cellular Automata (QCA) allow for computations with very low energy dissipation and hence are promising candidates for breaking this limit. Accordingly, the design of reversible QCA circuits is an active field of research. But whether QCA in general and the proposed circuits in particular are indeed able to operate in a logically and physically reversible fashion is unknown thus far, because neither physical realizations nor appropriate simulation approaches are available. In this work, we address this gap by utilizing an established theoretical model that has been implemented in a physics simulator enabling a precise consideration of how energy is dissipated in QCA designs. Our results provide strong evidence that QCA is indeed a suitable technology for near zero-energy computing. Further, the first design of a logically and physically reversible adder circuit is presented, which serves as proof of concept for future circuits with the ability of near zero-energy computing.

CCS Concepts: • Hardware → Reversible logic; Quantum dots and cellular automata; Emerging simulation;

Additional Key Words and Phrases: Emerging technology, field-coupled nanocomputing, reversible computing

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1 INTRODUCTION

In 1961, Rolf Landauer argued that any non-reversible computational process (i.e., each computation in which information is lost) results in a minimum energy dissipation of \((k_B T \ln 2)\) per bit erased (with \(k_B\) being the Boltzmann constant and \(T\) being the temperature of the system’s thermal environment \cite{Landauer1961}). The validity of this thermodynamic limit in computation, also known as Landauer’s principle, has been disputed ever since. Recently, it eventually was experimentally verified in several technologies—confirming that there is a physical limit in non-reversible computation \cite{Berut2012,Hong2016,Orlov2012,Neri2016}.

This significantly affects conventional computation technologies, since they mostly rely on non-reversible operations such as NAND, which non-reversibly transform two input bits into a single output bit and hence lose one bit of information. Although the energy dissipation caused by such information losses (which usually are much larger than Landauer’s lower bound \cite{Gershenfeld1996}) was considered negligible for a long time, the miniaturization of computational devices, as well as improved material and fabrication processes, led to energy dissipations of today’s circuits and systems that come quite close to Landauer’s limit constituted by \((k_B T \ln 2)\) per bit erased. In other words, to continue the ever-increasing reduction of energy consumption as observed in the past decades and thus reach the ability of near-zero-energy computing, complementarily different ways of computation are required, such as computations that can conduct operations without losing information.

Reversible computations are an obvious alternative. Here, all computations are realized through reversible operations, such as bijective functions that map each input pattern to a unique output pattern. Already in 1973, Bennett proved in his seminal work that energy dissipation is reduced or even (theoretically) eliminated if computations are information lossless \cite{Bennett1973}. In fact, he showed that any circuit and system with a (theoretical) energy dissipation of zero must rely on reversible computation. This motivated entire fields of research such as adiabatic computations (e.g., see Zulehner et al. \cite{Zulehner2019}), reversible energy recovery logic (e.g., see Ye and Roy \cite{Ye1996}), or the design and realization of corresponding reversible circuits (e.g., see Zulehner and Wille \cite{Zulehner2018} and Chaves et al. \cite{Chaves2019}). Today, it is seen as a fact that future computation technologies have to be reversible to overcome limitations due to energy dissipation \cite{Frank2017}. Accordingly, technologies are desired that come with low energy dissipation (i.e., with energy dissipation close to the \((k_B T \ln 2)\) energy limit) and, at the same time, can be tweaked to conduct operations in a reversible fashion—eventually allowing for near zero-energy computing \cite{DeBenedictis2016}.

In this regard, Quantum-dot Cellular Automata (QCA) \cite{Lent1997} are a promising candidate. They employ a Field-Coupled Nanotechnology (FCN) in which information is stored in terms of the polarity of small cells and can be propagated to adjacent cells using electrostatic force (Coulomb interaction). This allows for representing and processing information with remarkably low energy dissipation (e.g., see Timler and Lent \cite{Timler2002} and Pitters et al. \cite{Pitters2011}) and makes QCA an interesting candidate for near zero-energy computing.

This motivated the consideration of several reversible QCA designs (e.g., see Chaves et al. \cite{Chaves2015}, Singh et al. \cite{Singh2017}, Mukhopadhyay and Dutta \cite{Mukhopadhyay2015}, Chabi et al. \cite{Chabi2017}, and Goswamia et al. \cite{Goswamia2017}). But all of these previous works considered only the logic level when making the desired function reversible (i.e., the proposed designs indeed realize bijections) but did not address information loss at the gate level (physical level) and either provide no physical realization at all or employ non-reversible gates. This is obviously not enough to enable near zero-energy computing, as it does not address the conceptual problem. Instead, near-zero-energy computing is only feasible if reversibility is kept until the physical level and if energy dissipation remains below \((k_B T \ln 2)\) per
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In this regard, specific clocking strategies as proposed in Lent et al. [2006] and Ottavi et al. [2011] seem much more promising. However, due to the absence of a method for exact estimation of the energy dissipation in QCA designs, the assumptions could not be validated. This restriction holds for all existing proposals, as available simulation approaches do not consider energy dissipation at all (e.g., Walus and Jullien [2006]) or restrict themselves to worst-case scenarios (e.g., Srivastava et al. [2009]) such that they do not allow for a precise estimation of the energy dissipation in QCA designs. As a consequence, it is not known yet whether QCA designs indeed allow for implementing reversibility on the logical and physical level and thus enable operations with near zero-energy dissipation.

In this work, we are going to change this state of the art by delivering strong evidence for this conjecture. To this end, we utilize an established theoretical model that has been implemented in a physics simulator enabling a precise consideration of how energy is dissipated in QCA designs [Timler and Lent 2002; Srivastava et al. 2009; Sill Torres et al. 2018]. For the first time, we are using this approach to explore the capability of QCA designs to operate with near zero-energy consumption.

The results clearly indicate the following:

— Basic QCA building blocks such as wires and primitive logic gates can indeed be operated in a logically and physically reversible way and thus with an energy dissipation below \((k_B T \ln 2)\) per operation.
— The same also holds for more complex QCA designs made up of these reversible building blocks—thereby demonstrating QCA’s general capability to conduct computations with an energy dissipation below the crucial \((k_B T \ln 2)\) energy barrier (and without significant architectural changes as used in Lent et al. [2006] and Ottavi et al. [2011]).
— Design methodologies for QCA as proposed in Huang et al. [2005] or Walter et al. [2019b] can be applied for composing reversible circuits that operate with near zero-energy dissipation.

The remainder of this work is structured as follows. Section 2 reviews the basics on QCA and their energy dissipation. Section 3 analyzes how energy is dissipated by primitive QCA building blocks such as wires or functional gates (like OR) and discusses how these can be operated in a logically and physically reversible way. Based on that, a logically and physically reversible adder circuit is introduced and the results of energy simulations for larger QCA designs are discussed in Section 4—showing that QCA indeed allow for near zero-energy computing. Finally, the article concludes in Section 5.

2 BACKGROUND

In this work, we aim for validating the capability of the QCA technology to operate with near zero-energy dissipation. Since corresponding physical realizations are not available yet, we rely on simulations instead. Therefore, we rest on an established theoretical model that has been integrated in a physics simulator [Timler and Lent 2002; Srivastava et al. 2009; Sill Torres et al. 2018], enabling the precise analysis of energy transfers in QCA. This section reviews the basic concepts of QCA and the physical model for the energy transfer in QCA, and introduces the resulting tool.

2.1 Quantum-Dot Cellular Automata

QCA refers to an emerging FCN that takes an alternative approach to processing information and performing computations that is fundamentally different from today’s established technologies. In fact, information is stored in terms of the polarity of small, square-shaped cells that are arranged
in a grid structure. Within a cyclic process, a cell’s information is regularly erased and a new polarization is determined based on the polarization of the surrounding cells, such as by electrostatic force (Coulomb interaction).

More precisely, a QCA cell is typically composed of (1) four quantum dots situated at the corners of the cell and (2) two free and mobile electrons that are able to tunnel between adjacent dots [Anderson and Bhanja 2014]. The electrons may not tunnel to the outside of the cell due to a potential limit, and also tunneling within the cell can temporarily be prevented—thereby forcing the electrons to remain stationary at one of the quantum dots, thus leading to a stable state. For an illustration of QCA cells with stationary electrons, see Figure 1 where the electrons are represented by black dots.

Electrons experience mutual repulsion due to Coulomb interaction. As a consequence, they tend to locate themselves as far as possible from each other when the intracellular tunneling is prevented and they are being forced to become stationary. Consequently, an isolated cell will assume either of two stable energy states in which the electrostatic forces are minimal. These states are termed cell polarizations and are usually denoted as $P = -1$ and $P = +1$. The described behavior allows for an encoding of binary information by associating each polarization with a binary value. To this end, one usually identifies $P = -1$ with a binary 0 and $P = +1$ with a binary 1 as shown in Figure 1(a).

Moreover, when multiple cells are placed close to each other, the polarization of each cell is influenced by the polarization of the others. More precisely, the mutual repulsion causes electrons to avoid a quantum dot if the neighboring quantum dots of adjacent cells are populated by other electrons. This effect can be exploited for the realization of circuit elements, such as the binary OR and AND that can be derived as special cases of the 3-input majority gate shown in Figure 1(b). In the depicted case, a single 0-state from input $a$ competes with two 1-states coming from inputs $b$ and $c$. The output cell $f$ follows the majority of the input states and, thus, is forced to a 1-state in this case. By locking the polarization of one of the three inputs to a constant state, one obtains a binary OR gate (constant 1-state) or an AND gate (constant 0-state), respectively.

To execute these and more complex logic operations, a dedicated clocking is required, which, starting with the initialization of the QCA cells, properly propagates among the cells and avoids metastable states [Liu et al. 2013]. To this end, an external clock is employed that regulates the intercellular tunneling barriers within a QCA cell such that the cell can be polarized (i.e., tunneling is prevented) or not (i.e., electrons may tunnel between adjacent quantum dots within the cell). Typically, the clock consists of four phases. In the so-called relax phase, the cell is depolarized and does not contain any information. During the following switch phase, the interdot barriers are raised, which forces the cell to polarize into one of the two antipodal states (according to the polarization of surrounding cells). In the following hold phase, the cell keeps its polarization and may act as input for adjacent cells. During the final release phase, the interdot barriers are lowered again, thereby removing the previous polarization of the cell.
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To enable the propagation of information among cells, multiple phase-shifted versions of the clock signal are provided [Hennessy and Lent 2001]. Then, the dataflow can be controlled by using appropriately shifted clock signals such that the cells that shall pass their data are in the hold phase at the same time the cells that shall receive the data are in the switch phase. Typically, multiple adjacent cells are grouped to clock zones in which all cells use the same clock signal.

**Example 2.1.** Consider Figure 2 showing a QCA wire consisting of eight cells. The cells are divided into four groups of pairs of adjacent cells that share the same clock signal. Each of these clock zones follows a different clock signal. More precisely, clock zone 2 will be in the switch phase when clock zone 1 is in the hold phase. Thus, in this clock phase, cells in clock zone 2 polarize according to the polarization of the adjacent cells in clock zone 1. During the next clock phase, clock zone 2 changes to hold while clock zone 3 is in the switch phase. Consequently, data are passed from zone 2 to zone 3 (and so on), similar to a pipeline structure.

### 2.2 Modeling the Energy Behavior of QCA Cells

Following the cyclic behavior of the clock signals, the energy behavior of QCA cells can be described in a qualitative way as follows. In the beginning of a clock cycle, the QCA cell is depolarized. Energy is taken from the clock and from neighboring cells to achieve the polarized state induced by the polarization of the neighboring cells. Most of this energy is restored to the clock and also distributed to the neighboring cells until the cell becomes depolarized again at the end of the clock cycle. However, some portion of the energy dissipates to the environment.

To allow for a more precise, quantitative analysis of the energy behavior of QCA cells, one has to make use of the quantum-level modeling of QCA cell behavior discussed in several previous works (e.g., Timler and Lent [2002], Srivastava et al. [2009], Sill Torres et al. [2018], and Rahimi [2016]). In this model, the QCA cell behavior is determined by two three-dimensional energy vectors: \( \vec{\lambda} \) and \( \vec{\Gamma} \). More precisely, the vector \( \vec{\lambda} = (\lambda_x, \lambda_y, \lambda_z) \) denotes the so-called coherence vector and represents the cell’s current state (where \( \lambda_z \) can be identified with its polarization). In a similar fashion, the energy vector \( \vec{\Gamma} = \frac{\hbar}{2} [-2\gamma, 0, \Phi] \), with \( \hbar \) denoting the reduced Planck constant, is related to the cell’s steady-state—that is, a virtual state that characterizes the future behavior of the cell and depends on the current tunneling behavior (\( \gamma \)), as well as the Coulomb force that is induced by neighboring cells (\( \Phi \)).

Using this notation, the instantaneous power \( P \) of a QCA cell is described by

\[
P = \frac{d}{dt} E(t) = \frac{d}{dt} \left( \frac{\hbar}{2} \vec{\Gamma}(t) \cdot \vec{\lambda}(t) \right),
\]

where \( E(t) \) denotes the current energy of the cell at time \( t \) and is essentially given as the scalar product of the two energy vectors at that point in time. Consequently, the total energy dissipation of a QCA cell \( (E_{\text{total}}) \) during a complete clock cycle with period \( T_{\text{clk}} \) is given as

\[
E_{\text{total}} = \int_{t_0}^{t_0 + T_{\text{clk}}} Pdt' = \frac{\hbar}{2} \int_{t_0}^{t_0 + T_{\text{clk}}} \left( \frac{d}{dt} \vec{\Gamma}(t) \cdot \vec{\lambda}(t) + \frac{d}{dt} \vec{\lambda}(t) \cdot \vec{\Gamma}(t) \right) dt'.
\]
The first summand in the integrand of Equation (2) is the scalar product of the derivate of the energy vector of the cell ($\vec{\Gamma}$) and the coherence vector. This term refers to the energy transfer with the clock ($E_{clk}$) and neighboring cells ($E_{IO}$) during a clock cycle [Srivastava et al. 2009; Timler and Lent 2002; Sill Torres et al. 2018]—that is,

$$E_{clk} + E_{IO} = \frac{\hbar}{2} \int_{t_0}^{t_0 + T_{clk}} \left( \frac{d}{dt} \vec{\Gamma} \cdot \vec{\lambda} \right) dt'$$

(3)

with

$$E_{clk} = \frac{1}{2} \int_{t_0}^{t_0 + T_{clk}} \left( \frac{d}{dt} (-2\gamma) \cdot \lambda_x \right) dt'$$

(4)

and

$$E_{IO} = \frac{1}{2} \int_{t_0}^{t_0 + T_{clk}} \left( \frac{d}{dt} \Phi \cdot \lambda_z \right) dt'.$$

(5)

The second summand in the integrand of Equation (2) is the product of the derivate of the coherence vector and the energy vector and captures the energy transfer $E_{env}$ with the environment during a clock cycle. $E_{env}$ is the actually dissipated energy of a QCA cell during a clock cycle and can be determined as

$$E_{env} = -\frac{\hbar}{2\tau} \int_{t_0}^{t_0 + T_{clk}} \left[ (\vec{\Gamma} \cdot \vec{\lambda} + |\vec{\Gamma}| \tan \eta_{th}) \right] dt',$$

(6)

where $\tau$ denotes a technology-dependent relaxation time parameter and $\eta_{th} = \hbar|\vec{\Gamma}| \cdot (2k_BT)^{-1}$ refers to the thermal ratio [Timler and Lent 2002; Srivastava et al. 2009; Sill Torres et al. 2018].

One should note that the proposed model assumes an ideal clock signal that consumes no energy. As discussed in Lent et al. [2006], there indeed occurs some heat dissipation in the clocking circuit due to wire resistances and the clock generation circuitry. However, this is not a fundamental limitation and can be minimized by reducing the residual resistances [Lent et al. 2006; Jeanniot et al. 2016].

### 2.3 Simulating the Energy Dissipation of QCA

Currently, there are two tools available that allow for the simulation of the energy dissipation in QCA circuits—QCADesigner-E [Sill Torres et al. 2018] and QCAPro [Srivastava et al. 2009]. However, the latter is not able to estimate exact values, as it assumes an ideal clock slope and thus only allows for determining an upper limit for the energy dissipation. In contrast, the open source simulation tool QCADesigner-E\(^1\) permits a precise estimation. It is based on the widely applied QCADesigner [Walus and Jullien 2006] and computes the energy terms $E_{clk}$, $E_{IO}$, and $E_{env}$ from Equations (4) through (6) by interpolating the respective integrands. To this end, the required numerical values of the energy vectors $\vec{\lambda}$ and $\vec{\Gamma}$ are obtained by employing the Coherence Vector Simulation Engine (CVSE) that is included in the original QCADesigner tool. This engine implements the state-of-the-art quantum-level modeling of QCA cell behavior discussed in Timler and Lent [2002], Srivastava et al. [2009], and Sill Torres et al. [2018] and determines the evolution of $\vec{\lambda}$ and $\vec{\Gamma}$ by solving the corresponding differential equations using an iterative, fixed timestep approach. The time interval of each iteration step ($T_{step}$) and many other technology and simulation parameters (shown in Table 1) can be adjusted to adapt to a specific physical realization or to increase the precision of the simulation. In fact, as the simulation error that may occur due to inadequate iteration step lengths or rounding is permanently tracked, a simulation run can be repeated with

\(^1\)The tool has been made publicly available as open source at [https://github.com/FSillT/QCADesigner-E](https://github.com/FSillT/QCADesigner-E).
Table 1. Adjustable Technology and Simulation Parameters in the Tool QCADesigner-E

(a) Technology parameters

| Parameter      | Description                                           | Standard Value |
|----------------|-------------------------------------------------------|----------------|
| QD size        | Size of a quantum dot                                 | 5 nm           |
| Cell area      | Dimensions of each cell                               | 18 nm x 18 nm  |
| Cell distance  | Distance between two cells                            | 20 nm          |
| Layer distance | Distance between QCA layers in case of multilayer crossing [Bajec and Pečar 2012] | 11.5 nm        |
| $\tau$         | Relaxation time                                       | 1E-15 s        |
| $\gamma_H$     | Max. saturation energy of clock signal                | 9.8E-22 J      |
| $\gamma_L$     | Min. saturation energy of clock signal                | 3.8E-23 J      |
| $\varepsilon_r$| Relative permittivity of material for QCA system      | 12.9*          |
| Temp           | Operating temperature                                 | 1 K            |
| $r_{\text{effect}}$ | Maximum distance between cells whose interaction is considered | 80 nm†          |

* Relative permittivity of GaAs and AlGaAs.
† Interaction effects between two cells decays inversely with the fifth power of its distance.

(b) Simulation parameters

| Parameter | Description                                           | Standard Value |
|-----------|-------------------------------------------------------|----------------|
| $T_\gamma$| Period of the clock signal                           | 10E-12 s       |
| $\gamma_{\text{rise}}$ | Rise and fall time of the clock signal slopes       | 1E-10 s        |
| $\gamma_{\text{shape}}$ | Shape of clock signal slopes [RAMP/GAUSSIAN]       | GAUSSIAN       |
| $T_{\text{in}}$ | Period of the input signals                         | 10E-12 s       |
| $T_{\text{sim}}$ | Total simulation time                                | 80E-12 s       |
| $T_{\text{step}}$ | Time interval of each iteration step                | 1E-17 s        |

Higher resolution if the error grows too large. However, as demonstrated and validated in Sill Torres et al. [2018], using the standard simulation parameters of the tool (listed in Table 1) one can in general expect high quality results with simulation errors below 5%.

3 ENERGY DISSIPATION IN QCA BUILDING BLOCKS

Using the simulator reviewed earlier as a basis, this section describes the obtained energy dissipation for common QCA building blocks. The main subject of our study is to validate whether QCA designs that are expected to be reversible indeed allow for operating below the $(k_B T \ln 2)$ energy limit or not. To this end, we investigate a single QCA wire and an elementary logic operation (namely, an OR) as proper representatives. Although the wire inherently is reversible at the logic level, the OR operation obviously is not. However, findings summarized in Lent et al. [2006] suggested a corresponding QCA design that is expected to achieve reversibility, both logical and physical. This design is, of course, also considered within this study. Please note that the issue of cooling will be ignored in the following, keeping in mind that this work is a theoretical analysis exploring whether the actual concept of QCA enables near zero-energy dissipation computing. Extrapolating any costs for cooling costs could easily yield to misleading conclusions.
3.1 Energy Dissipation in QCA Wires

As discussed in Section 2.2, there is an energy transfer among QCA cells (denoted by $E_{IO}$), from the clock to the QCA cells (denoted by $E_{clk}$) and from the QCA cells to the environment (denoted by $E_{env}$). Timler and Lent [2002, 2003] discussed that energy coming from the clock is used to restore the signal strength of internal signals and compensate energy dissipated to the environment. This shall be detailed in the following example.

**Example 3.1.** The top of Figure 3 shows a QCA wire composed of cells in three clock zones. The corresponding energy transfer between cells, clock, and environment is summarized in the bottom of Figure 3. To obtain these numbers, the wire has been simulated with the QCADesigner-E tool using its standard parameters (listed in Table 1).

The symbols $E_{in}$ and $E_{out}$ represent the energy entering ($E_{in}$) and leaving ($E_{out}$) the QCA cell. In case of the depicted wire, the value for $E_{IO}$ follows from the difference between $E_{out}$ and $E_{in}$. Further, positive values mean that energy has been transferred to the environment ($E_{env}$), to the clock ($E_{clk}$), and to the cell ($E_{IO}$), whereas negative values mean the opposite. To neglect any effect due to the ideal signal source (marked as IN) whose behavior is to some extent artificial, the energy of QCA cells in zone 1 (highlighted in green) shall be ignored. Nevertheless, the behavior of all cells has been fully simulated.

As can be seen, energy is transferred from the clock to the QCA cells to compensate energy transferred to the next cell. This can been seen, for example, at cell $c_{10}$, which receives 0.19 meV from its left neighbors and passes 0.64 meV to its right neighbors located in the next clock zone. The resulting difference of $-0.45$ meV is then compensated by the clock signal. Similarly, all energy not transferred to neighboring cells is sent back to the clock. For example, cell $c_{11}$ receives 0.64 meV from its left neighbors but passes only 0.18 meV to its right neighbors. The difference of 0.46 meV is returned to the clock. As expected, the amount of energy $E_{env}$ that is transferred to the environment is negligible and clearly stays below the $\left(k_B T \ln 2\right)$ energy limit of 0.06 meV, a mandatory requirement for designing circuits that are able to operate with near zero-energy dissipation.

As can be seen from Equation (6) and as already discussed before in Srivastava et al. [2009] and Timler and Lent [2002], the energy dissipation of a QCA cell mainly results from the difference between its current state (represented by the coherence vector $\vec{\lambda}$) and its steady state (represented by the energy vector $\vec{\Gamma}$). As outlined in Section 2.2, this difference results from changing polarizations of neighboring cells, leading to changing Coulomb forces, as well as from the varying tunneling barrier, both directly related to the clock signal. As a consequence, the inclination of the slope of the external clock signal has a considerable impact on the energy transfer to the environment (i.e., the total energy dissipation of the QCA cell). In other words, the slower the clock signal
changes, the easier it is for the cell to follow the (accordingly changed) steady state and the less energy is dissipated. This behavior has already been discussed by Bhanja et al. in Srivastava et al. [2009] and is illustrated by the following example.

Example 3.2. Figure 4 depicts the relation between the slope of the external clock signal $\gamma_{\text{slope}}$ and the energy transfer to the environment $E_{\text{env}}$ of the wire shown in Figure 3. The numbers were generated using the QCADesigner-E tool and the standard parameters (listed in Table 1(a)). The results indicate an exponential relation between the clock slope $\gamma_{\text{slope}}$ and $E_{\text{env}}$. It follows further that clock slopes longer than 10 ps lead to operations with energy dissipation below the $(k_B T \ln 2)$ limit.

Overall, the conducted case studies confirm that the QCA wire indeed can be operated below the $(k_B T \ln 2)$ limit, a fundamental requirement for building circuits that are logically and physically reversible.

3.2 Energy Dissipation in QCA Gates

Next, we consider the realization of QCA gates—with an OR operation as representative. The OR is a non-reversible logic operation that may cause information loss and hence yields an energy dissipation above Landauer’s limit. Lent discussed that this process can be turned reversible for a specific cell, if first a copy of the information (bit) is made [Lent et al. 2006]. When the cell is then actually losing its information, that copy would act as a Demon—a hypothetical model introduced by Maxwell in 1875 [Lent et al. 2006]—and thus would allow to return the cell to a null state without thermodynamical energy loss.

Timler and Lent [2003] discussed that in case of QCA, the information erasure happens during the release phase—that is, when the interdot barriers are lowered and the polarization of the QCA cell is removed (see Section 2.1). Further, they observed that a neighboring QCA cell can act as the Demon (i.e., as a holder of the copy of the bit that is stored as polarization).

The results presented in Timler and Lent [2003] and in Example 3.1 confirm this observation. One can observe that during the release phase, all cells within the same clock zone lose their polarization (i.e., the stored information). However, for the QCA wire, there is no energy transfer to the environment (i.e., this erasure process happens in a reversible fashion).

In case of a standard QCA OR gate, it is not possible to ensure for all possible input patterns that such a copy always exists—that is, that neighboring cells possess the same information. The following example shall detail the consequences.
Example 3.3. Consider the standard QCA OR gate depicted in Figure 5(a), which has been simulated with the QCADesigner-E tool using the standard parameters listed in Table 1(a) for the case \( a = 0 \) and \( b = 1 \). Figure 5(c) shows the integrand \( P_{en} \) of the energy dissipated to the environment (see also Equation (6)), the polarization, and the related clock signal for the cell \( c_1 \). These results indicate that during the release phase, the polarization of cell \( c_1 \) changes abruptly—leading to a high energy transfer to the environment and consequently to an energy dissipation that is above the \( (k_B T \ln 2) \) limit.

However, following the concept of demon cells discussed earlier, the high energy dissipation can be prevented by using a modified OR that echoes both inputs to the output of the cell. This approach originally was proposed in Lent et al. [2006] and is expected to result in a reversible...
erasure with an energy dissipation below the \((k_B T \ln 2)\) limit. However, the actual energy behavior of the proposed design has not been evaluated with precise simulations yet.

**Example 3.4.** Figure 5(b) shows the modified OR gate as proposed in Lent et al. [2006]. Simulating this gate with the QCADesigner-E tool using the same settings as reported in Example 3.3 leads to results as summarized in Figure 5(c). Here, it can be seen that during the *release* phase, no abrupt change of the polarization of cell \(c_2\) occurs. Consequently, the energy transfer to the environment is considerably lower. In fact, an energy dissipation can be observed that is always below the \((k_B T \ln 2)\) energy limit—that is, the computation of the reversible QCA OR gate is indeed logically and physically reversible.

For the first time, these results confirm the hypotheses of Lent et al. [2006] and Huang et al. [2006] with precise simulation results and, by this, validate the general capability of QCA to implement logic operations reversibly at both the logic and physical levels—that is, a logically reversible operation can be conducted with an energy dissipation below the \((k_B T \ln 2)\) limit. Next, we evaluate whether physical reversibility can also be achieved for larger QCA designs.

## 4 ENERGY DISSIPATION IN LARGER QCA DESIGNS

The investigations summarized earlier showed that QCA building blocks indeed allow for (1) the realization of established functional building blocks in a reversible fashion (including maintaining reversibility at the physical level) and hence (2) an energy dissipation that is below the \((k_B T \ln 2)\) energy limit. Now, these findings are employed to investigate whether similar results can also be observed for larger QCA designs as well. In this section, we first summarize the case studies that have been conducted to evaluate this. Afterward, the obtained results are presented and discussed.

### 4.1 Conducted Case Studies

As larger QCA designs, we considered the realization of QCA implementations from the following three categories:

- **Standard QCA Designs**, which are QCA implementations that have been commonly used for QCA designs. More precisely, the standard OR gate, the standard AND gate, and the standard majority gate are considered as representatives for this category.

- **Logically (but not physically) Reversible QCA Designs**, which are implementations as proposed in related works that implement reversible logic functions but, as discussed in Section 1, have either no or only a "conventional" (i.e., non-reversible) physical implementation. More precisely, an implementation of the Feynman gate [Chaves et al. 2015; Singh et al. 2017], a logically reversible T-FlipFlop (T-FF) [Mukhopadhyay and Dutta 2015], a testable adder implemented in reversible logic (T-adder) [Goswamia et al. 2017], and a circuit based on multiplexers and XOR gates implementing a random reversible function (Rev-Func) [Chabi et al. 2017] are considered as representatives for this category.

- **Logically and Physically Reversible QCA Designs**, which are implementations based on the schemes discussed in Lent et al. [2006] and reviewed in the previous section that are reversible and, at least from a theoretical point of view, can be operated below the \((k_B T \ln 2)\) energy limit.

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2 Note that to achieve reversibility at the logic level, the primary inputs are echoed to the primary outputs of the design. This increases the number of primary outputs to three. But still, the gate does not seem to be reversible at the logic level (there are now more outputs than inputs), and thus Landauer’s principle seems to contradict the physical reversibility determined by our simulations. However, this contradiction is resolved if the locked cell is interpreted as a third—but constant—primary input [Zulehner and Wille 2017].
Fig. 6. Considered logically and physically reversible QCA designs.

Further, we propose an implementation of a logically and physically reversible half adder (see Figure 6(b)) that, for the first time, utilizes exclusively logically and physically reversible circuit elements, such as as introduced by Lent et al. [2006] and in this work. The wire crossings (indicated by QCA cells containing crosses in Figure 6(b)) are realized via the multilayer approach discussed

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3 The reversible AND gate is nearly identical to the reversible OR gate depicted in Figure 5(b), except for the constant input that is instead locked to the 0-state.

4 The difference in the number of inputs (3) and outputs (4) does not change the fact that this gate can be understood as reversible circuits. This follows from Landauer’s observation that the fundamental energy dissipation is defined by the change of entropy—that is, the difference between initial entropy $S_i$ (before operation) and final entropy $S_f$ (after operation) [DeBenedictis et al. 2016]. In case of the proposed gate, both entropies $S_i$ and $S_f$ are identically, as each possible output state is related to one and only one input state, whereas all remaining output states have a probability of zero.
Table 2. Energy Dissipation in Larger QCA Designs

| Circuits | Energy Dissipation [meV] for an Input Signal Combination |
|----------|--------------------------------------------------------|
|          | 000 | 001 | 010 | 011 | 100 | 101 | 110 | 111 |
| **Standard QCA Designs** |      |      |      |      |      |      |      |      |
| Inverter | 0.001 | 0.001 |      |      |      |      |      |      |
| OR (standard) | 0.082 | 0.709 | 0.712 | **0.001** |      |      |      |      |
| AND (standard) | **0.001** | 0.711 | 0.709 | 0.081 |      |      |      |      |
| Majority (standard) | **0.001** | 0.709 | 0.714 | 0.711 | 0.709 | 0.714 | 0.711 | **0.001** |
| **Logically (but not physically) Reversible QCA Designs** |      |      |      |      |      |      |      |      |
| Feynman [Chaves et al. 2015] | 0.817 | 1.645 | 1.645 | 0.867 |      |      |      |      |
| Feynman [Singh et al. 2017] | 0.393 | 0.064 | 0.839 | 1.376 |      |      |      |      |
| T-FF [Mukhopadhyay and Dutta 2015] | 1.053 | 0.397 | 2.072 | 2.200 | 2.993 | 1.424 | 1.050 | 1.138 |
| RevFunc [Chabi et al. 2017] | 1.190 | 0.742 | 0.753 | 0.353 | 1.537 | 0.130 | 0.684 | 0.074 |
| T-adder [Goswamia et al. 2017] | 1.565 | 1.565 | 2.458 | 2.493 | 1.315 | 1.315 | 2.493 | 2.458 |
| **Physically Reversible QCA Designs** |      |      |      |      |      |      |      |      |
| OR (reversible, Figure 5(b)) | **0.002** | **0.003** | **0.002** | **0.002** |      |      |      |      |
| AND (reversible) | **0.002** | **0.002** | **0.003** | **0.002** |      |      |      |      |
| Majority (reversible, Figure 6(a)) | **0.003** | **0.003** | **0.003** | **0.003** | **0.003** | **0.003** | **0.003** | **0.003** |
| Half adder (Figure 6(b)) | **0.022** | **0.025** | **0.029** | **0.022** |      |      |      |      |

(k_B T ln 2) energy limit is at 0.06 meV (values marked in bold are below this limit). Simulations executed with Gaussian-shaped clock slope of \( \gamma_{\text{slope}} = 100 \) ps and Temp = 1 K.

in Bajec and Pečar [2012].\(^5\) The design of this circuit is based on a tile-based design approach as proposed in Huang et al. [2005], which facilitates an automatic implementation as, for example, shown by Walter et al. [2018], Wille et al. [2019], and Walter et al. [2019a].

All evaluations have been executed with the same method and settings as done before for the case studies in Section 3—that is, with the tool QCADesigner-E [Sill Torres et al. 2018] reviewed in Section 2.2 using its standard parameters listed in Table 1(a). The clock slope was set to \( \gamma_{\text{slope}} = 100 \) ps, following from the observations in Section 3.1 and Figure 3. The time interval \( T_{\text{step}} \) of each iteration step was set to 0.01 fs—leading to simulation errors of \( \epsilon_{\text{env}} \leq 1\% \). As proposed in Sill Torres et al. [2018], we cascaded the artificial input signals by placing a few buffer cells between the stimulated inputs and the actual inputs of the considered design (to allow for a realistic energy analysis). The same is done for the outputs, which are as well connected to a few buffer cells.

### 4.2 Results and Discussions

Table 2 lists the obtained energy dissipation for each input signal combination (in million electron volts). Values marked in bold indicate an energy dissipation below the \( (k_B T \ln 2) \) energy limit (which is at 0.06 meV). These results allow for the following conclusions:

— Already the standard and the logically reversible QCA designs allow, in very few cases, for an energy dissipation below the \( (k_B T \ln 2) \) barrier. This, however, is only the case when input assignments are employed that do not yield to an information loss. This, for example, is the case for the OR implementation with the input assignment ‘11’ (e.g., see Figure 5(a)).
— In all other cases, we could confirm that logical reversibility is not sufficient to operate below the \( (k_B T \ln 2) \) energy barrier. As discussed earlier, this is because these realizations

\(^5\)Despite the fact that multilayer design is not trivial, the concept has been explored in several previous works with a very favorable conclusion regarding its feasibility [Bajec and Pečar 2012; Gin et al. 1999]

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are based on non-reversible structures (e.g., standard AND, OR, majority gates) and hence employ a “conventional” (i.e., non-reversible) physical realization. As a consequence, only for few selected input assignments that, similar to ‘11’ for the OR gate, do not cause any information loss, an energy dissipation below the \((k_B T \ln 2)\) limit is possible. For all other cases, the limit can never be broken, which is also confirmed by the reported results.

— In contrast, we are able to confirm that logically and physically reversible implementations indeed allow for an energy dissipation below \((k_B T \ln 2)\) per operation and thus near zero-energy computing. In fact, for all corresponding implementations, energy dissipations that are clearly below the \((k_B T \ln 2)\) barrier are reported. This is also the case for the proposed reversible majority gate and the half adder circuit. By this, for the first time, we could show with precise simulations that it is indeed possible to implement QCA designs that satisfy the requirements for physically reversible circuits and hence allow for near zero-energy computing.

— Furthermore, as we could show that it is possible to implement all fundamental Boolean operations (i.e., AND, OR, and inversion) in a logically and physically reversible manner, one can conclude that all Boolean logic functions can be designed as logically and physically reversible QCA designs.

5 CONCLUSION

In this work, we validated that it is possible to design QCA circuits that are logically and physically reversible and thus allow for near zero-energy computing. To this end, we conducted dedicated case studies on corresponding QCA designs for primitive building blocks such as wires or functional gates (like OR), as well as larger QCA designs. Furthermore, we applied reversible building blocks and a common design methodology for QCA to develop the first logically and physically reversible QCA adder circuit. The obtained results confirm the general capability of QCA designs to compute with near zero-energy dissipation. This constitutes an essential result that further motivates the consideration of QCA as an alternative to overcome physical limitations of conventional computation technologies. Future work is defined by confirming these findings on physically built QCA designs—the results obtained in this work deliver a strong motivation toward this path.

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