An effective algorithm for clocked Field-Coupled Nanocomputing paradigm

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Abstract— Field-coupled nanocomputing (FCN) paradigms offer fundamentally new approaches for digital computing. As one of several FCN paradigms currently under active investigation, Molecular Quantum-dot Cellular Automata (MQCA) is based upon electrostatic interactions among quantum dot cells that does not require charge transport. Hence its energy dissipation is significantly reduced. Moreover, an external clock signal has to be adopted desirably while controlling switch in QCA devices. In this paper, with the aim of analyzing information propagation on clocked molecular QCA device from an electronic point of view, an effective algorithm has been implemented relied on data obtained from ab-initio simulations, electrostatic equations and models of the molecular interaction. The quantitative results generated from the algorithm depict correct behaviors of clocked QCA devices and provide important feedback for future QCA experimental implementation.

I. INTRODUCTION

Molecular Quantum-dot Cellular Automata is the most promising among the emerging technologies for computation, since it is expected to reach very high operating frequencies (THz) associated to reduced power consumption, high device densities and non-cryogenic working temperature [1]. This computation is performed via electrostatic interactions between nearby molecules and does not rely on conduction. As a molecule candidate specifically synthesized for this purpose, the bis-ferrocene is depicted in Fig. 1(A). It contains two ferrocene units (Dot1, Dot2) and a central carbazole group (Dot3). A complete QCA cell can be implemented placing two molecules one near each other. Inside the cell, as depicted in Fig. 1(B), charge can be localized on one of the two dots of a molecule because of external electric field (e.g. input). Then the electrostatic repulsion favors the localization of charge of the nearby molecule in the opposite dot. Positions of charge encode binary information in QCA and such switching in terms of interaction also exists among cells allowing information propagation. An external field called *Clock* is applied for the necessity of controlling the switching phenomena (Fig. 1(C)).

As the fundamental functional block, a molecular QCA wire, is schematically sketched aligning together a group of molecules (Fig. 1(D)). The information propagation has been studied adopting a specific algorithm implemented relying on data obtained using ab-initio simulations and on equations describing the electrostatic interaction between groups of

atoms (Dots). Similarly, for the purpose of realizing adiabatic switching among cells on wire [2], the algorithm also takes into consideration the presence of clock. In addition, the algorithm is then extended for analyzing more complex QCA device, like a 3-input majority voter (Fig 1(F)).

This proposed paper is organized as follows, the clocked molecular QCA behavior will be present in the next section; in the methodology section, the implementation of the algorithm will be described; and finally the results and conclusions are illustrated in Section IV.
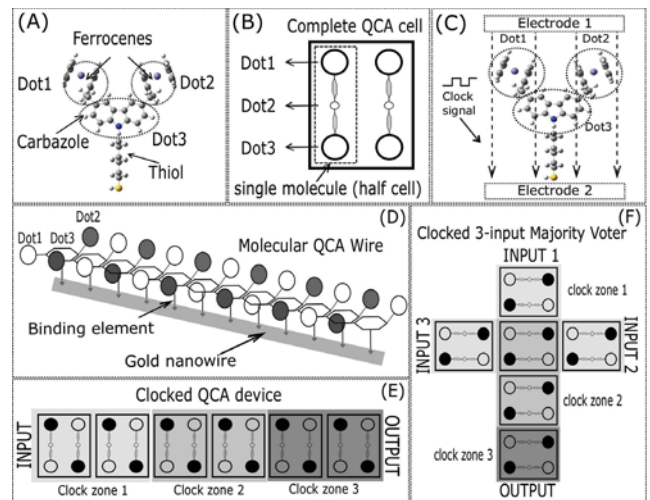

Fig. 1. Molecular Quantum-dot Cellular Automata:(A)Bis-ferrocene molecule structure; (B)Complete mQCA cell; (C)Schematic implementation of clock signal in mQCA structure; (D)Bis-ferrocene mQCA wire; (E)Three different clock zones are applied along wire ensuring information propagation; (F)Structure of clocked 3-input majority voter (top view).

II. CLOCKED MOLECULAR QCA

The clock signal possesses the ability to prohibit or enhance the interaction within or among QCA cells [3]. Depending the direction of applied clock signal, the charge can be focused on the central carbazole group encoding null state of the cell; or released to two ferrocene units making the cell ready to switch its binary information. In the later case, the intensity of clock signal will influence the total amount of charge available on the two ferrocene units, then further affect the quality of electrostatic interaction among molecules inside QCA cell. As for the case of a QCA wire, the clock system could be based on the applied signal to emulate the multi-phase clock system [2]. The multi-phase clock system implies the partition of wire in different clock zones and inside each clock zone several molecules are

found (Fig 1(E)). In particular, each clock zone is assigned for different clock values, thus alternating the clock zones ensures the proper information propagation as well as correct QCA computation for the wire. The clock system for 3-input majority voter is also sketched in principle (Fig. 1(F)).

III. METHODOLOGY

The implementation of the algorithm for case of a mQCA wire is introduced here. The trans-characteristic (charge vs. applied E-field) of a bis-ferrocene molecule obtained from ab-initio simulations is adopted in the algorithm for modeling interactions between nearby molecules [2]. Starting from the first molecule, every molecule (Mol i) along the wire will, following its trans-characteristic, arrange its charge distribution according to the superposed effects E_{ji} (*Cause*) generated by all its neighbors Mol j (j≠i). Such re-arranged charge affects again in its turn its neighboring molecules Mol j (j≠i) generating new E_{ij} (*Effect*) thus propagating the information. Then iterating the *cause and effect* procedure of interaction in a sequence of molecule, e.g. their positions located along the wire, until the newly generated effects E_{ij} reach convergence making successive molecular interactions negligible. The flow chart of the algorithm is shown in Fig. 2(D). Eventually the *aggregated charge distribution* of molecules along the wire is obtained as output considering all calculated interactions [4]. Different clock values have different trans-characteristics of the molecule. Thus when multi-phase clock zones are applied on QCA wire, the algorithm chooses relevant trans-characteristic for computing interactions among molecules inside the same clock zone. Concerning more complicated structure, e.g. a 3-input majority voter, once the sequence of molecule is defined throughout the whole structure, the algorithm can be used by the same logic rendering aggregated charge distribution.

IV. RESULTS AND CONCLUSION

Results correspond to the clocked bis-ferrocene molecule performance and the algorithm are reported as follows.

Clocked bis-ferrocene molecule: Fig. 2(A) shows the molecular behaviors in presence of an enhancing or an inhibiting clock signal. The curves represent the energy of the ground states (bottom) and the first-excited states (top) of bis-ferrocene molecule as a function of the polarization of driver. The associated molecular orbitals are also plotted for same conditions, as *HOMO/LUMO* indicated in Fig. 2(A).

MQCA wire: Fig. 2(B) depicts the results of a clocked QCA wire. As shown in Fig. 1(E), along the wire there distribute 3 different clock zones, and alternating them guarantees the correct wire performance. From Fig 2(B), it can been seen that the logic information is propagated following the setup of the clock zones.

3-input majority voter: The aggregated charge distribution of 3-input majority voter is sketched in Fig. 2(C). Giving the three inputs defined logic states "010", the output (dashed box) takes their majority which is, as expected, logic "0". Meanwhile the multi-phase clock zones are also adopted by the same logic as wire condition.
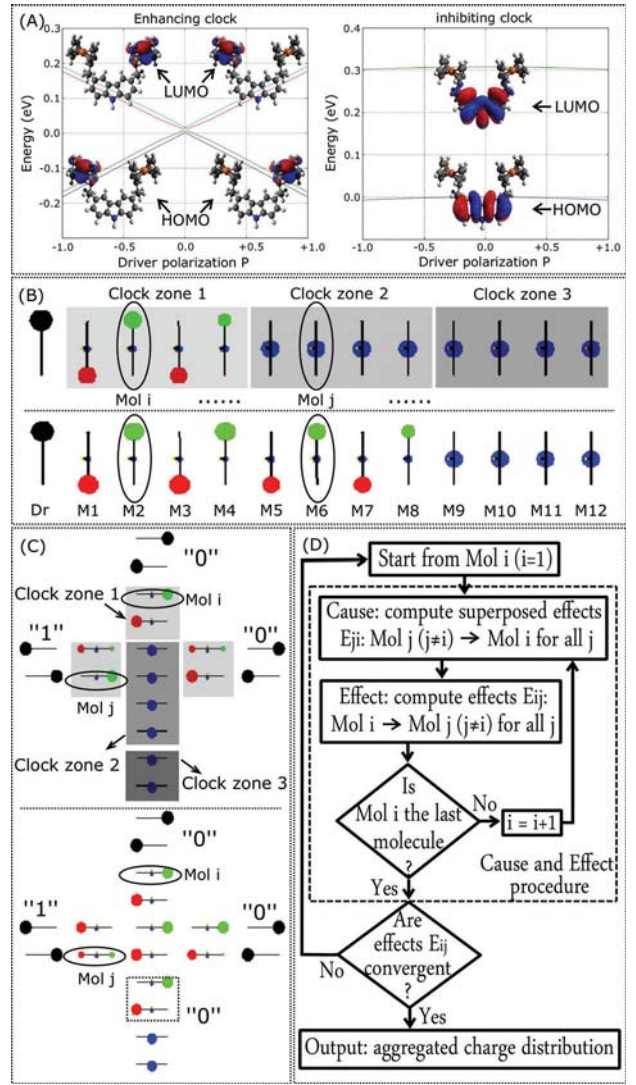

Fig. 2. (A)Energy levels of the bis-ferrocene molecule as a function of the polarization of the driver, both enhancing (left) and inhibiting (right) clock signal are considered; Aggregated charge distribution of: (B)Clocked QCA wire; (C)Clocked 3-input majority voter; with $0.8nm$ as inter-molecule distance and $2V/nm$ as clock; (D)Flow chart of the designed algorithm.

In conclusion, an efficient algorithm has been implemented superposing all possibly existed electrostatic interactions among molecules in QCA devices. The generated results show the charge distributions and the ability of clock to control switching of logic information in mQCA devices. These results are convincing and could provide important feedback for eventual fabrication of mQCA technology.

REFERENCES

[1] Y.Liu, Molecular quantum-dot cellular automata: From molecular structure to circuit dynamics, App. Physics, v. 102, 2007.
[2] R. Wang, et al, Effect of a Clock System on Bis-ferrocene Molecular QCA, DOI: 10.1109/TNANO.2016.2555931, 2015.
[3] V. Vankamamidi, M. Ottavi, F. Lombardi, Clocking and Cell Placement for QCA, IEEE-NANO, vol. 1, pp. 343- 346, 2006.
[4] A. Pulimeno, et al. Bis-ferrocene molecular QCA wire: ab-initio simulations of fabrication driven fault tolerance, IEEE Transactions on Nanotechnology, vol. 12, 2014.