Robustness of the In-Plane Data Crossing for Molecular Field-Coupled Nanocomputing

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***Abstract*—Molecular Field-Coupled Nanocomputing (molFCN) offers several advantages compared to other beyond-CMOS technologies, such as the cut of the power dissipation, thanks to the absence of charge transport, and the possibility to work at room temperature. Several circuits have been investigated for molFCN, primarily analyzed from a behavioral standpoint. Also, researchers proposed a few solutions to cross two signals and analyzed them from a logical and ideal perspective. Crossing information is an essential and delicate operation since molFCN is an in-plane technology. Besides, previous works demonstrated the need to consider molecule physics to predict the behavior of a molFCN circuit. This work examines different implementations of the in-plane information crossing interconnection, considering the punctual molecule physics to predict the interconnection functioning. We tune the electrostatic feature of the involved molecules to determine the robustness of the cross-wire against static electrostatic variations, thus providing valuable information for the synthesis of *ad-hoc* molecules for molFCN.**

I. Introduction

In the last decades, researchers investigated new technologies motivated by the impeding physical barrier that modern silicon technologies face, aiming to overcome the scaling limit [1]–[3]. Among the proposed technologies, the molecular Field-Coupled Nanocomputing paradigm (molFCN) exploits the electrostatic interaction between nearby molecules encoding the logic information in the charge distribution [4]. Neighboring molecules interact through electrostatic fields, thus enabling information propagation without charge transport, enormously reducing the power dissipation, which is the challenge that most affects CMOS scaling [5], [6]. Moreover, the electrostatic coupling between molecules is strong enough to work at room temperature [7], [8].

The literature offers several possible designs of the essential devices and interconnections for molFCN [9], [10]. However, the possibility to cross information is the least analyzed in the literature while being a crucial element in designing circuits for in-plane technologies. Furthermore, information crossing has been analyzed mainly from a behavioral standpoint [11]–[13]. Yet, previous works have demonstrated the need to consider the actual molecular implementation since it influences the circuit operation [14].

For these reasons, this work analyzes different implementations of the in-plane information crossing to relate the molecule physics to the expected ideal functioning. Following the same logic of the work in [14], we simulate different designs of the in-plane cross-wire using molecules with different electrostatic footprints. We specifically concentrate on neutral and zwitterionic molecules since it has been demonstrated that purely oxidized molecules are affected by crosstalk [14]. Specifically, we tune the molecule electrostatics and verify how the behavioral functioning of the cross-wire is modified, testing the robustness against static electrostatic variations.

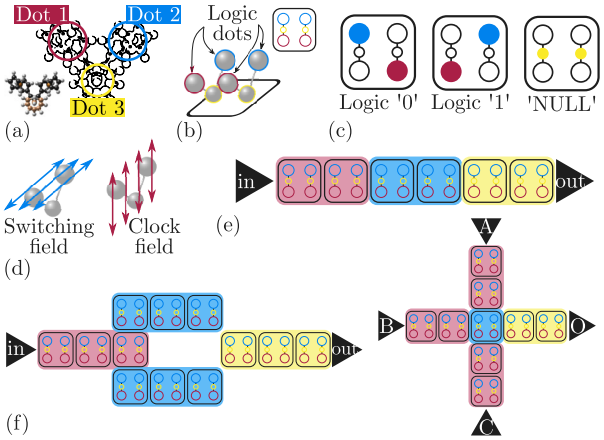

Fig. 1. Basic concepts on molFCN technology: (a) di-ferrocenyl carborane molecule geometry with a schematic view where functional dots are highlighted, (b) schematic unit cell composed of two juxtaposed molecules with the top view of the cell, (c) convention of the logic values, where full dots indicate the presence of a positive charge, (d) the direction of the switching and clock fields referred to the molecule, (e) simple wire, each background color represents a different clock region, (f) double-branch inverter and majority voter layouts for molFCN technology.

II. Background

The molecules used for the molFCN technology have functional groups that can host a charge and are associated with the so-called dots [4]. For example, Fig. 1(a) shows the schematic dot division on the di-ferrocenyl carborane molecule [15]. Following the Quantum-dot Cellular Automata (QCA) paradigm, Fig. 1(b) shows the accepted minimal unit to build devices: a cell composed of two juxtaposed molecules [16]. The unit cell can assume a specific charge configuration associated with a logic state, as Fig. 1(c) shows. Those charge configurations are obtained by applying two independent electric fields, as sketched in Fig. 1(d) [17]. The clock field is applied longitudinally and can cancel binary

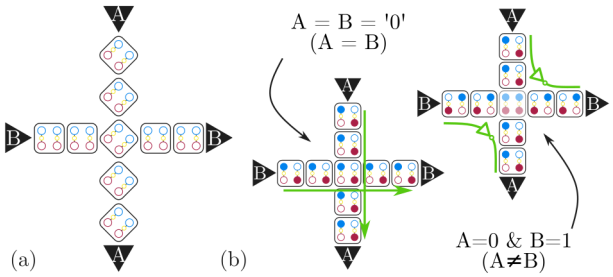

Fig. 2. Layouts of an in-plane cross-wire interconnection: (a) information crossing is obtained by rotating the unit cells on the vertical wire [11], (b) information crossing is obtained without cell rotations. If inputs A and B are equal, all the cells encode the same information: the image at the bottom left shows the example with A = B = '0'. If A and B are different, the central shared cell does not favor any information and the diagonal inverting interactions dominate: the image at the top right shows the example with A = '0' and B = '1'.

logic by confining the charge in the dot 3. In contrast, the switching field drives the charge transversally to obtain a logic '0' or a logic '1'. Since binary logic values are encoded in dot 1 and dot 2, they are usually called "logic dots."

Fig. 1(e) shows a wire that can propagate information divided into virtual regions called clock regions. The subsequent activation of neighboring clock regions guides information packets [18]. Data elaboration is instead derived from specific arrangements of the unit cells. Fig. 1(f) shows two fundamental gates often used in literature, the double-branched inverter and the Majority Voter (MV) [10], [19].

Regarding the cross-wire interconnection treated in this work, two leading solutions exist for in-plane implementations. The hypothesis shown in Fig. 2(a) is technologically arduous to implement since it requires fine control of the unit cell rotation [11]. On the other hand, the solution in Fig. 2(b) exploits the diagonal interaction between input and output wires [9], [13]. Referring to Fig. 2(b), if the information on A and B is the same, all cells will assume the same logic configuration. On the contrary, if A and B encode opposite information, then ideally, the central shared cell does not assume any logic value: charge will be equally distributed in the four logic dots of the cell. In this case, the inverting interaction from the cell on the diagonal dominates, and the outcome is the correct information crossing [9].

The cunning idea reported in Fig. 2(b) does not require structural manipulation. However, it lies on the single-branch inversion that has been demonstrated to be sensitive to molecular physics [14]. Indeed, when input branches encode different logic values, the functioning is strictly dependent on two delicate assumptions: the central shared cell must not assume a logic value, and the single-branch inversion must work properly. This work analyzes the behavior of the implementation of Fig. 2(b), relating it to molecules electrostatics, aiming to define the working limit of that interconnection.

III. Methodology

Generally, molecules are treated through *ab initio* calculations that can precisely predict their electronic behavior

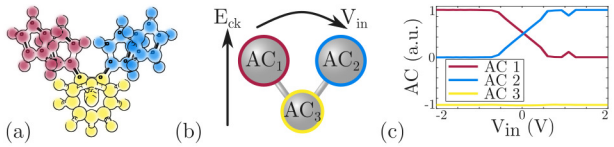

Fig. 3. MoSQuiTo methodology: (a) schematic representation of the atomic charges of a molecule, di-ferrocenyl carborane is used as an example, (b) definition of the principal electrical figures of merit that describe the electrostatic behavior of a molecule, (c) VACT graph for the bis-ferrocene molecule when the clock field equals $2\,\mathrm{V/nm}$.

by solving the Schrödinger equation. However, the required computational effort becomes significant when studying molecular systems with tens or hundreds of molecules, as it could be a molFCN circuit. The MoSQuiTo (Molecular Simulator Quantum-dot cellular automata Torino) methodology has been proposed to solve the trade-off between computation time and precision when dealing with molFCN circuits [17], [20]. In this three-step methodology, the molecule is conceived as an electronic device, where only the physical effects functional to molFCN are considered in the model.

First, the isolated molecule of interest is analyzed through *ab initio* calculation. At this stage, the description of the molecule is strictly related to the atomic configuration, as schematically represented in Fig. 3(a). The successive methodology step is in charge of extracting new figures of merit that adequately describe the electronic state of the molecule. In this context, the dot aggregated charge (AC) is defined as the sum of the atomic charge of each atom belonging to the same dot. Also, we define the input voltage (V_{in}) as the integral along the shortest path between dot 1 and dot 2 of the electric field resulting from the combination of the switching fields of nearby molecules. Fig. 3(b) shows a schematic view of the defined figures of merit and the positive clock field direction (E_{ck}). The above mentioned figures of merit are often related in graphs named V_{in}–AC Transcharacteristic (VACT) [20]. As an example, Fig. 3(c) shows the VACT of another established molecule, i.e., the bis-ferrocene [21]. As a final step, we use the figures of merit just calculated in SCERPA (Self-Consistent ElectRostatic Potential Algorithm) to perform circuit-level simulations by evaluating the electrostatic interaction between the several molecules making up circuits [9], [19], [22].

The figures of merit defined by the MoSQuiTo methodology are sufficient to describe the electrostatic behavior of a molecule for the molFCN scope. Since this work studies the behavior of the cross-wire when the electrostatics of the involved molecules vary, we shape different VACTs, and we use them to simulate the cross-wire interconnection from a behavioral standpoint using SCERPA. Using synthetic VACT grants the efficacy of eventual comparisons since variations are restricted to electrostatics only.

IV. Results and Discussion

This work considers different implementations of the cross-wire interconnection to verify in which conditions it works. First, we examine different layout patterns, starting

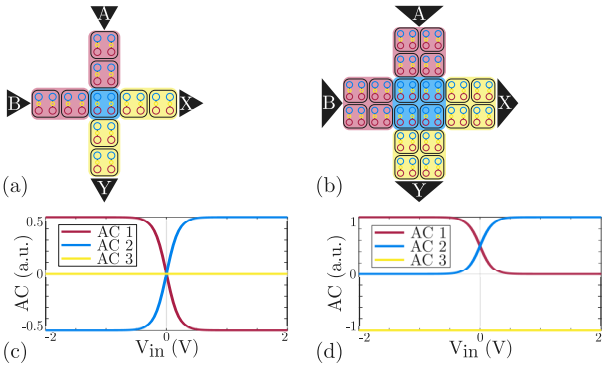

Fig. 4. Features of the simulated structures: (a) layout of a single-line cross-wire interconnection highlighting the signals name and clock regions through background colors, (b) layout of a 2-line bus cross-wire interconnection highlighting the signals name and clock regions through background colors, (c) VACT graph for a neutral molecule that follows equation (1) with $w = 10\,\mathrm{V}^{-1}$, and when the clock field is favoring the logic information, (d) VACT graph for a zwitterionic molecule that follows equation (2) with $w = 10\,\mathrm{V}^{-1}$, and when the clock field favors the logic information.

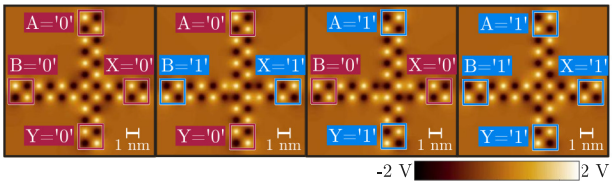

Fig. 5. SCERPA simulation of a single-line cross-wire interconnection implemented with neutral molecules: the four images represent the electrostatic potential of the last propagating step, evaluated 2 Å above the logic dot plane.

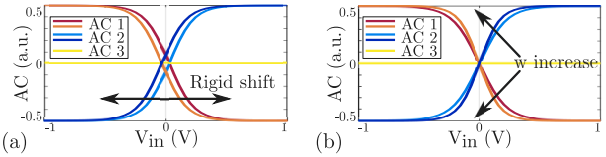

Fig. 6. VACT variation ranges for the cross-wire interconnection to continue working: (a) application of rigid shifts to the VACT, the maximum allowed shifts equal $\pm 30\,\mathrm{mV}$, (b) change of the slope of the VACT, w in equation (1) can vary in the interval $[9; 12]\,\mathrm{V}^{-1}$.

from the single-line interconnection of Fig. 4(a), then moving to the 2-line bus circuits shown in Fig. 4(b). Increasing the number of lines that compose each wire strengthens the information stability during the propagation [9]. Also, it simplifies the fabrication process by reducing the need for nano-patterned structures [9]. Secondly, we simulate the mentioned systems using neutral and zwitterionic molecules, considering the same equations of the work in [14]. Equation (1) and equation (2) individually describe the AC behavior for dot 1 in neutral and zwitterionic molecules, where the parameter w is an indication of the curve steepness. Fig. 4(c) and Fig. 4(d) show the VACT of neutral and zwitterionic molecules when $w = 10\,\mathrm{V}^{-1}$.

$$\text{neutral} \rightarrow AC_1 = \frac{1}{1 + e^{w \cdot V_{in}}} - 0.5 \tag{1}$$

$$\text{zwitterionic} \rightarrow AC_1 = \frac{1}{1 + e^{w \cdot V_{in}}} \tag{2}$$

The first case we consider is the single-line cross-wire of Fig. 4(a) implemented with the neutral molecules whose VACT is shown in Fig. 4(c). By simulating the circuit in SCERPA, we verify how information propagates, and we find that the circuit only works if the output wires are in the same clock region as the central cell. Specifically, Fig. 5 shows the electrostatic potential of the last propagating steps of the four possible input combinations. White spots represent positive charge localization, whereas black dots indicate localization of negative charge. Looking at the simulations, we notice that the two logic data are correctly crossed and propagated in all four cases. From the simulation for case $A \neq B$, we can observe that the central shared cell encodes a specific logic value even if the final configurations are correct. This last aspect is still coherent with the expected functioning. Indeed, when the clock field starts switching on output cells, the central cell does not encode any information. So the output branches follow the inverting interaction coming from the diagonals. Though at the end of the propagation, the input voltages on the central molecules are no more null, so even the central cell assumes a logic value.

We then simulate the same circuit of Fig. 4(a) changing the molecule VACT, to test the robustness of the propagation. We try rigid horizontal shift of the neutral VACT and variations of the steepness w. Fig. 6(a) illustrates the shift range on the VACT acceptable to continue having a working interconnection. If the rigid shift is bigger than $\pm 30\,\mathrm{mV}$, then at least one configuration propagates the wrong data. That means that the charge difference at equilibrium ($V_{in} = 0\,\mathrm{V}$) between dot 1 and dot 2 must be smaller than $\Delta AC_{MAX} = 0.15\,\mathrm{a.u.}$ when $w = 10\,\mathrm{V}^{-1}$. On the other hand, Fig. 6(b) shows the range of slopes leading to a correctly behaving cross-wire, i.e., for $w \in [9; 12]\,\mathrm{V}^{-1}$.

The case just analyzed is optimal since the circuit comprises only one type of molecule and can also retain some variations of the electrostatic behavior. However, single-line devices are challenging to fabricate since they require nanometric patterning of the hosting substrate. Consequently, we also simulate the system of Fig. 4(b). It comes out that the crossing mechanism no longer works with any clock distribution. Indeed, when $A \neq B$, since the central region is made up of several molecules, those molecules influence each other enough to encode a clear logic value, thus impeding the functioning of the interconnection.

Besides, suppose we implement the single-line cross-wire interconnections using the zwitterionic molecules with the VACT of Fig. 4(d). In that case, Fig. 7 shows that the system does not work. Indeed, even if the single-diagonal interaction can invert the logic signal in some circumstances, the adjacent interaction is more energetically favorable [14]. This time, varying the slope of the VACT or introducing a shift does not help the propagation. Moreover, more than changing the geometrical position of dot 3 to reinforce the diagonal interaction is required for this implementation, contrary to the example of the single-branch inverter shown in [14].

If we recall the ideal working principle explained in

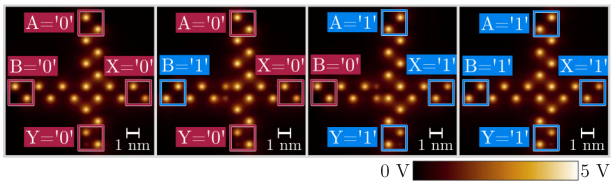

Fig. 7. SCERPA simulation of a single-line cross-wire interconnection implemented with zwitterionic molecules with $w = 10\,\mathrm{V}^{-1}$: the four images represent the electrostatic potential of the last propagating step, evaluated 2 Å above the logic dot plane.

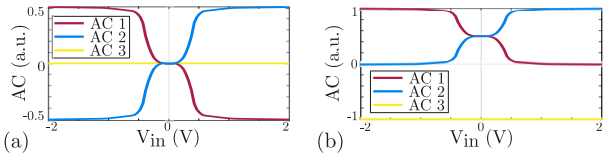

Fig. 8. VACT of the molecules used to favor the crossing mechanism, synthesized getting inspired by the 1,5,9-decatriene cation behavior: (a) neutral version, (b) zwitterionic version.

section II, we observe that we need a central cell that does not polarize when the inputs are different and assumes a logic value for equal inputs. When inputs are different, the charge is ideally equally distributed on the logic dots, meaning that the expected input voltage on the involved molecule would be nearly zero. On the contrary, if both inputs are equal, the charge distribution would be well-defined on one of the two diagonals, meaning that the expected input voltage on the involved molecule would be higher than zero (considering absolute values). With this mechanism in mind, we realize that one way to facilitate the crossing mechanism is to have a molecule with a constant charge distribution on logic dots for a small V_{in}, similar to the behavior of the 1,5,9-decatriene cation [20], [23]. To remain coherent with the work presented here, instead of directly using the VACT of the 1,5,9-decatriene cation, we again synthesize the VACT and create a neutral and zwitterionic version of this molecule, shown in Fig. 8(a) and Fig. 8(b), respectively. We use these molecules in the central shared region of the cross-wire interconnections, i.e., in the cells with a blue background in Fig. 4(a)-(b), giving us circuits implemented with more than one type of molecule [24].

For the multi-molecule cross-wire interconnection, we first consider the single-line implementation. Fig. 9(a) demonstrates that if the system is implemented with neutral molecules, it works even with the clock phase distribution of Fig. 4(a). Moreover, the interconnection propagates the data precisely, even with zwitterionic molecules, given that the single-branch inversion works correctly [14]. Indeed, Fig. 9(b) shows the correct behavior for zwitterionic molecules whose dot 3 is at 5 Å from the logic dot plane. In addition, this implementation is now very stable against electrostatic variations as demonstrated by the wide working range, i.e., $w \in [6; 13]\,\mathrm{V}^{-1}$. On the other hand, Fig. 9(c) shows a non-working interconnection implemented with zwitterionic molecules whose dot 3 is at 10 Å from the logic dot plane, demonstrating that a correct single-branch

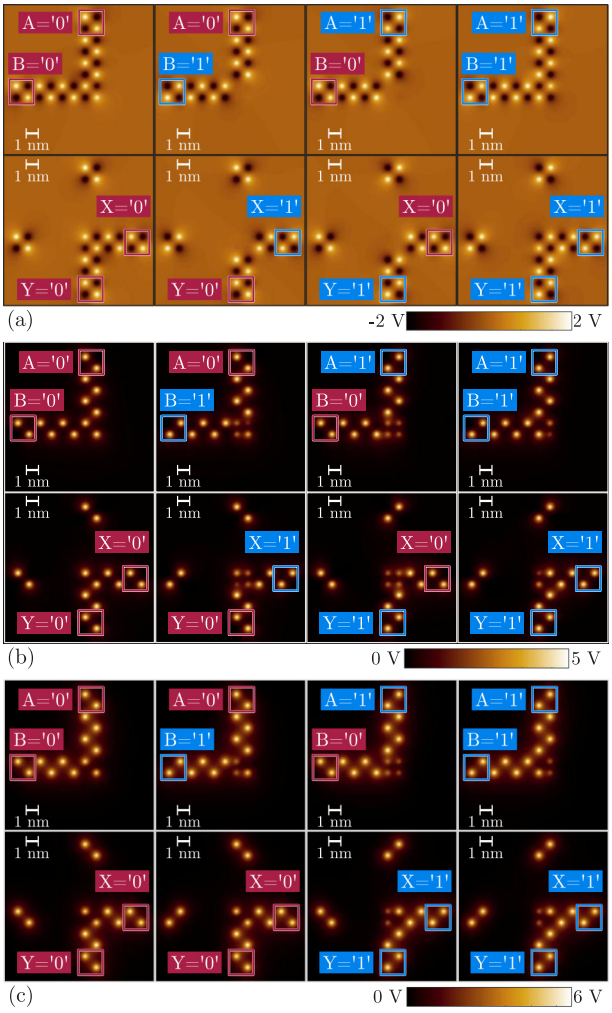

Fig. 9. Electrostatic potential evaluated 2 Å above the logic dot plane and obtained by SCERPA simulations of a single-line cross-wire interconnection. The top and bottom images of every sub-figure show two subsequent propagation steps. The circuit is implemented with molecules with $w = 10\,\mathrm{V}^{-1}$ and the following features: (a) neutral molecules, (b) zwitterionic molecules with dot 3 5 Å far from the logic dots plane, (c) zwitterionic molecules with dot 3 10 Å far from the logic dots plane.

inversion is the essence of the functioning.

Even in the case of multi-molecule systems, we simulate bus interconnections. Since we have seen that implementations with neutral molecules are straightforward, we now concentrate on the realization with zwitterionic molecules, which is more peculiar. For the bus cross-wire, we find that the interconnection behaves correctly only when $w = 6\,\mathrm{V}^{-1}$ or $w = 7\,\mathrm{V}^{-1}$, and Fig. 10 shows the SCERPA simulation for this last case. For higher values of w, the electrostatics is sufficiently strong to polarize the central cells when $A \neq B$. On the contrary, for smaller values of w, the electrostatics is not strong enough to induce the inversion when $A \neq B$.

V. Conclusion

Molecular Field-Coupled Nanocomputing is a promising solution among emerging technologies, offering low-power consumption and room-temperature operation. Though, one feature coming with this technology is the structural difficulty

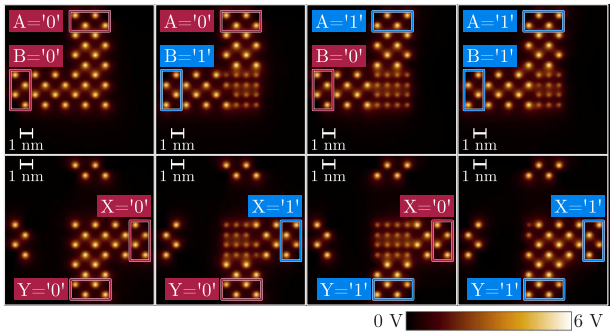

Fig. 10. Electrostatic potential evaluated 2 Å above the logic dot plane obtained by SCERPA simulations of a 2-line bus cross-wire interconnection. The top and bottom images of every sub-figure show two subsequent propagation steps. The circuit is implemented with zwitterionic molecules with $w = 7\,\mathrm{V}^{-1}$.

of using the third dimension for interconnections, leading to an in-plane technology. Hence, information crossing is a crucial aspect to investigate.

This work concentrates on a cross-wire solution that exploits single-branch inversion between input and output to cross-propagate different information. To validate the operating range of this implementation, we simulate the cross-wire with the SCERPA tool focusing on the effects of electrostatic variations. We study single-line and 2-line cross-wires implemented with neutral and zwitterionic molecules. However, we obtain the correct behavior only with single-line cross-wire implemented with neutral molecules. Thus, we further propose an all-electrostatic solution to toughen up the propagation in various cases by combining different molecule species in a circuit. In this way, we enhance the functioning and favor information crossing: using different molecule types enables the correct operation of both the considered layouts.

This work once again demonstrates that molecule physics is a two-edged sword. Indeed physics must be considered during the design process to predict the electrostatic footprint on devices precisely, but it can be tuned to offer singular features and be a beacon in reverse engineering processes.

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