Charge Distribution in a Molecular QCA Wire based on Bisferrocene Molecule

Charge distribution in a molecular QCA wire based on bis-ferrocene molecules

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***Abstract*—Molecular Quantum Dot Cellular Automata (MQCA) are among the most promising emerging technologies for the expected theoretical operating frequencies (THz), the high device densities and the non-cryogenic working temperature. In this work we simulated a molecular QCA wire, based on a molecule synthesized ad-hoc for this technology. The results discussed are obtained by means of iterative steps of ab-initio calculations.**

I. Introduction

Among all the new emergent devices alternative to bulk MOSFET, Quantum-dot Cellular Automata (QCA) is the one that, theoretically, allows to encode binary information without current flow, reaching high operating frequency and lowering the power consumption [1]. As proposed by Lent [2], a QCA cell could be physically implemented by a molecular system with two or more redox centers: the charge configuration within the molecule encodes the logical state and the electrostatic repulsion provides the device-device interaction. The simplest demonstration of logic propagation that could be performed according to this paradigm is a molecular wire (see Fig. 1 (A)). Concerning the physical implementation, all the molecules proposed in literature [3], [4], [6] are ideal systems. Only few experimental attempts have been carried out on a mixed-valence complex [7], [8], even though this molecule is not suitable for real applications. In our previous works [11]–[13], we discussed the functionalities of a bis-ferrocene molecule (Fig. 1 (B)) [9], [10] as an half QCA cell. In this work we emulated a molecular wire, evaluating simultaneously the interaction between two molecules (a complete QCA cell) and the information propagation at different inter-molecule distances.

II. Methodology

A. The single molecule

The bis-ferrocene molecule has been synthesized ad hoc for the QCA technology [9]. The structure is reported in Fig. 1 (B): the two ferrocenes represent the dots, a carbazole bridge provides the isolation between them and the thiol group allows to bind the molecule on a substrate. This molecule is very promising as candidate molecule for QCA computing for many reasons: our early results showed that its bistability properties allow to encode the digital information and that the molecule seems sensitive to a particular electric field, as write-in system [11]–[13]; this molecule is a real system that exists and has already been bonded to a gold substrate [9], [10]. In this work we considered the oxidized molecule: at the equilibrium (no external stimuli) the free positive charge is delocalized between the two main dots (the ferrocenes) and the molecule is in a neutral state.

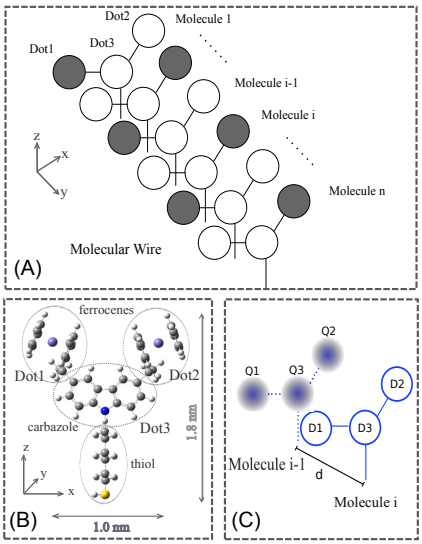

Fig. 1. (A) Schematic view of a MQCA wire of bis-ferrocene molecules. (B) Bis-ferrocene molecule: two ferrocenes linked together by means of a carbazole central group . (C) Section of the wire: the aggregated charges of the *(i-1)th* molecule (Q1, Q2 and Q3) act as a driver for the *Molecule i* varying its dot charges (D1, D2 and D3).

B. The molecular wire

We emulated a molecular QCA wire made of bis-ferrocene molecules by means of iterative simulation steps. In particular, we forced a logic state on the first molecule of the wire (Molecule 1, as shown in Fig. 1 (A)) applying an electric field of 2 V/nm along the ferrocenes axes (as already discussed in [11], [12]). Then we used the charge configuration of this molecule as stimulus for the following cell (Molecule 2). As explained in Fig. 1 (C), at a generic point of the wire we evaluated the response of *Molecule i* to the charge distribution of *Molecule i-1*, assuming that the *Molecule i* is in the neutral state (charge delocalized) and ready to switch [13]. We performed this analysis firstly on a wire in which the distance d between two molecules is 1.0 nm (equal to the width of the molecule, in order to form a square cell) and then setting the distance to 0.8 nm.

In order to do this, we defined a new figure of merit for our

analysis, the *aggregated charge* of the dots, simply summing up the charge of the atoms that constitute the dot [12]. In addition, for each step of our simulation we emulated the driver molecule (Molecule i-1) with a system of point charges built placing the aggregated charge Q1, Q2 and Q3 in the same position of the dots, as shown in Fig. 1 (C). In this way, we computed the aggregated charges (D1, D2 and D3) of the nearby molecule (Molecule i), that became the driver system in the following step *Molecule i+1*). Iterating this method for all the molecules of the wire, we simulated the information propagation through the wire. All the results reported here were obtained by means of ab-initio simulations.

III. Results

In Fig. 2 the charges of the two main dots (dot1 and dot2) are reported: for sake of brevity, we focused on the first part of the wire, considering only five molecules. As depicted in Fig. 2, in the ideal case (distance equals to 1.0 nm) the charge displacement between the two dots (empty points) decreases with increasing number of molecules. We could consider the logic signal valid only for the first three molecules, while from the fourth molecule on the state is not defined. On the other hand, when the molecules are placed 0.8 nm far from each other, the difference of charge between the two dots is still huge enough to consider the molecule in a defined logic state (see Fig. 2, filled points). In both the cases, the switching of the molecule along the wire is preserved, since the polarity of the dots is inverted at each stage.

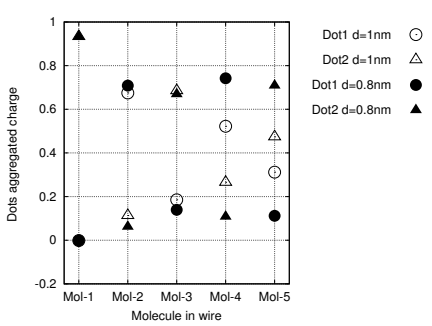

Fig. 2. Dot charges along the wire, as function of the distance *d*.

As additional figure of merit for our analysis, we computed the *electric field* generated by a charge system by means of mathematical calculations. In particular, each molecule along the wire, depending on its logic state, generates an electric field whose absolute value is maximum near the occupied dot. Fig. 3 show a top view of the electric field (computed basing on the aggregated charges of Fig. 2) generated by the first five molecules of the wire for two different inter-molecule distances (*d=0.8 nm* top and *d=1.0 nm* bottom). Both the pictures show how the peak of the electric field moves following the position of the free charge in the molecule. However, in the bigger distance case the peak become smoother along the wire.

These results are notable because they reveal the strength of the logic signal in two MQCA wires. In particular, the one with the ideal distance for the bis-ferrocene molecule (*d=1.0 nm*) shows a degradation already at the fourth molecule, while in case of *d=0.8 nm* the molecules interacts properly and the signal is preserved. This represents an important feedback to the technological process for the fabbrication of a bisferrocene wire.

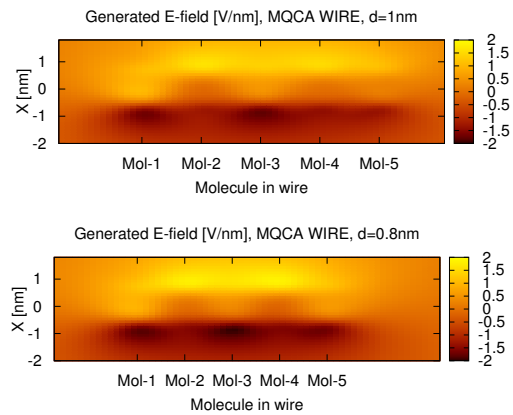

Fig. 3. Electric field generated by the charge distribution along the wire, when molecules are placed at *d=0.8 nm* (top) and *d=1.0 nm* (bottom)

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