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Molecular QCA: a Write-In System Based on Electric Fields

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Abstract— Molecular Quantum Dot Cellular Automata (MQCA) are an emergent beyond CMOS technology that uses molecular systems as elementary nanoelectronic devices with computational purposes. The binary encoding is provided by the charge localization within the molecule, so that no current flows among the cells. We discuss a method to write a logic state in a molecule synthesized ad hoc for this technology. Our idea is to apply specific electric field to move the electrons inside the molecule, forcing a logic state. A combination of ab-initio calculations and molecular dynamics simulations allowed us to fix the working point of our experimental system and to assess the feasibility of this method, as well as to investigate further experimental solutions for the read-out issue.

Keywords: molecular QCA, molecular computation, nano-gaps.

I. INTRODUCTION

Quantum-dot Cellular Automata (QCA) is a new paradigm for digital computing that, theoretically, is expected to reach very high operating frequencies and significant power consumption reduction [1]. According to the Lent theory [2], a possible implementation of a QCA cell could be physically based on a molecular system with two or more redox-centers, where the charge configuration encodes the binary information (Fig. 1a) and the electrostatic repulsion provides the device-device interaction. As a result, simple logic gates could be implemented, such as a wire or a majority voter (Fig. 1b and 1c). These gates are the building blocks for more complex digital systems [3].

A new molecule has been synthesized by the authors in [8] (in the frame of a collaboration with ST Microelectronics and with the authors of this paper) ad hoc to implement a QCA device with two redox-centers (Fig. 2a): two ferrocenes are separated by a central carbazole bridge, that provides the isolation between the two dots. Though not conductive, this molecule can be influenced by an external electric field in order to change its internal state (HOMO), encoding thus the “0”, “1” and NULL logic values. From an ab-initio analysis, the HOMO of this molecule in its ground state is delocalized along the molecule and mainly on the carbazole (Fig. 2b).

Concerning the physical implementation, in [3 - 5] ideal molecular systems are proposed. In addition, experimental studies have been carried out on a mixed-valence complex [6, 7], even though a molecular QCA prototype is a long way-off.

We present a method to use a bis-ferrocene molecule (Fig. 2) [8] as an half QCA cell and a write-in system (Fig. 3c) based on the application of electrical fields. Results discussed in the following are obtained by means of ab-initio and Molecular Dynamics (MD) simulations.

II. WRITE-IN METHOD SIMULATIONS

A. The Bis-ferrocene Molecule

A new molecule has been synthesized by the authors in [8] (in the frame of a collaboration with ST Microelectronics and with the authors of this paper) ad hoc to implement a QCA device with two redox-centers (Fig. 2a): two ferrocenes are separated by a central carbazole bridge, that provides the isolation between the two dots. Though not conductive, this molecule can be influenced by an external electric field in order to change its internal state (HOMO), encoding thus the “0”, “1” and NULL logic values. From an ab-initio analysis, the HOMO of this molecule in its ground state is de-localized along the molecule and mainly on the carbazole (Fig. 2b).

B. Electric Field Application

Applying an electric field along the x axis, we force a “1” or “0” state (Fig. 3a and 3b, respectively) obtained by the
HOMO localization around one of the two ferrocenes. An electric field applied along the y axis has the effect of localizing the HOMO on the carbazole, forcing the molecule into a NULL state. We found that an electric field in the same direction but with opposite sign localizes the HOMO around the two ferrocenes, enhancing the molecule sensitivity to assume one of the two logical states in presence of a driver (a neighbour identical molecule). These results are important for what concerns clock issues and information delivering [9].

In order to validate the results expressed by the HOMO, we calculated the dipole moment of the molecule with different values of applied electric field along the x axis. We obtained significant variations only on the x component of the dipole moment and this confirmed the electron localization on one of the two dots. Results are shown in Fig. 4a.

The applied electric field used in simulations was on the order of 1 V/nm. As a consequence, it could be easily obtained with a nanogap of about few nanometers. In Fig. 4 the scheme of the planned write-in system is sketched: a bis-ferrocene molecule is bonded between the nanogap electrodes and a voltage drop across them produces an electric field that forces the molecule into a logic state, in this case "1". Varying the applied voltage, and so the electric field, it is possible to change the state of the molecule.

C. Molecular Dynamics Simulations

Since a molecular system is affected by structural changes in time, related both to intrinsic factors (like thermal vibrations) and to external perturbations (like electrical stimuli), we performed several simulations of the bis-ferrocene molecule when different values of electrical field were applied along the x axis. We analyzed the variations of the molecule structure at several time steps and we found that the main differences were in the distance between the two ferrocenes. In particular, when the electrical field is off, the fluctuations are more remarkable, while increased values of electric field seemed to force the molecule into a more stable configuration. In Fig. 4b we reported the trend of the two dots distances varying the applied electric field, in terms of minimum and maximum values obtained during the simulation time for a specific field. The two curves (Dmin and Dmax) seemed to converge towards a similar values and this pinpointed that the range of variation was more and more reduced. The structure is thus expected to "freeze" to a stable configuration with high electric fields.

REFERENCE