A Roadmap for Molecular Field-Coupled Nanocomputing Actualization

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Federico Ravera[1,*], Giuliana Beretta[1], Yuri Ardesi[1], Maciej Krzywiecki[2], Mariagrazia Graziano[3], and Gianluca Piccinini[1]

***Abstract*—In molecular field-coupled nanocomputing, electrostatically-coupled molecules encode the logic information in their charge distribution, promising extremely low power consumption, room temperature operation, and THz frequency operations. Besides the impressive theoretical predictions and simulation confirmations, a working prototype must still be fabricated. This work discusses the most crucial aspects that hinder the fabrication of a working prototype and defines a roadmap to address and guide the procedure to fabricate a working proof of concept. Accurate physical simulations support each point of the roadmap.**

I. Introduction and Background

Molecular Field-Coupled Nanocomputing (molFCN) is one of the most appealing technologies proposed for future digital electronics. Fig. 1(a) shows the unit cell made with the bis-ferrocene molecules, which have been proposed for implementing molFCN [1] and the two minimum-energy configurations associated with logic states encoded in the molecule charge distributions [2]. Information propagation is obtained thanks to intermolecular electrostatic interactions of nearby molecular cells following the quantum-dot cellular automata paradigm [2], as shown in Fig. 1(b). In the same way, positioning molecules precisely according to specific layouts permits the implementation of logic gates and circuits, such as the NOT gate in Fig. 1(c) or the majority voter in Fig. 1(d). The current-less working principle of the molFCN paradigm guarantees minimal power dissipation [3]. In addition, molFCN ensures room temperature operations and THz operating frequencies [4].

Given the impressive advantages, researchers propose interesting molecular architecture analyzed with functional simulations that consider molecular cells as ideal QCA elements. The results fuel the interest in molFCN research, however, to address the crucial aspects hindering the working prototype realization it is necessary to consider molecular physics in the simulation engine. For this reason, we proposed a comprehensive methodology named MoSQuiTo (Molecular Simulator Quantum-dot cellular automata Torino) [5]. It analyzes candidate molecules using *ab initio* calculation and models their behavior as electronic devices, permitting circuit design and simulation

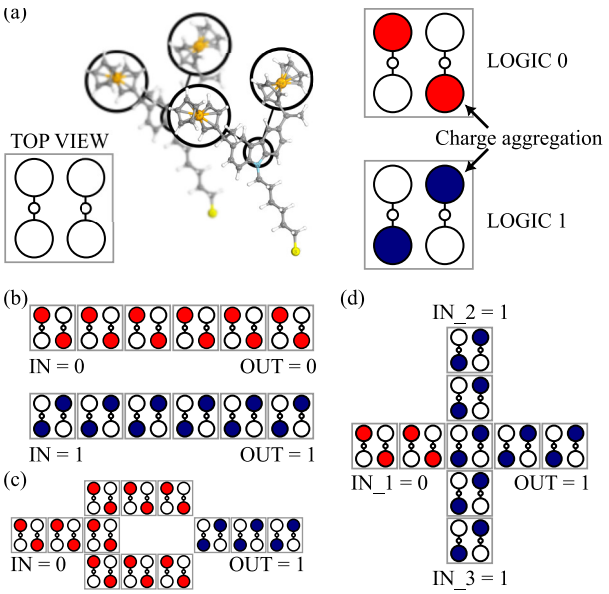

Fig. 1. Molecular field-coupled nanocomputing paradigm: (a) molFCN cell composed by two juxtaposed bis-ferrocenes and its schematic representation of the logic states '0' and '1', (b) wires propagating logic '0' and logic '1', (c) NOT gate layout, (d) majority voter gate layout.

with the SCERPA (Self-Consistent ElectRostatic Potential Algorithm) tool [6], [7]. MoSQuiTo links molecule physics to circuit characteristics, thus favoring the study of cross-implication between molecular physics and logic functionalities [8]. It also permits assessing the impressive advantages of molFCN devices, which, supported by the recent improvement of nanofabrication methods, renew and fuel the interest in prototyping a molFCN device.

II. The Roadmap

This work establishes a roadmap addressing the most crucial challenges to be faced to realize a working prototype. Considering the schematic representation of Fig. 2(a), we identify three main targets for the roadmap. First, the roadmap guides the design of molecules by determining the requirements they ought to satisfy to provide correct functioning. Secondly, the roadmap explores physical and structural requirements that must be followed to fabricate sub-nanometric molecular patterns. Finally, the roadmap addresses the hybrid integration between molFCN and CMOS.

A. Molecule specifications

Molecules are the building blocks of the molFCN technology, and previous works already demonstrate the strict

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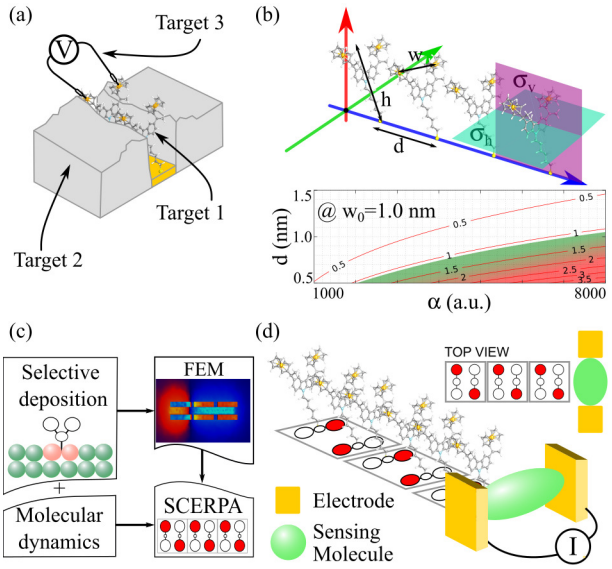

Fig. 2. Roadmap targets: (a) schematic representation of a hypothetical system structure highlighting the three main elements addressed by the roadmap, (b) representation of some requirements the molecules ought to satisfy, (c) proposed framework for the fabrication analysis, (d) possible interface between molecules and a charge transducer for the integration in conductive circuits.

link between molecular physical characteristics and their effects on the behavioral functioning of the circuits [8], [9]. We start by examining the molecules already proposed in the literature, and by exploiting theoretical analyses, we identify and define the quantities involved in the circuit functioning. By performing parametric simulations of various circuits using SCERPA, we find the boundaries of the working region for several parameters, such as the molecule electrostatic nature, the size, and the polarizability. Fig. 2(b) shows as an example the dimensions and symmetry planes on the bis-ferrocene and the molecular safe operating area obtained by evaluating the so-called bistable factor, defined in [9], as a function of molecule polarizability (α) and intermolecular distance (d). Once known the constraints, chemists can address the synthesis of molecules that satisfy all the requirements.

B. Layout and substrate

Properly designing sub-nanometric molecular patterns enables the correct functioning of molFCN circuits. Therefore, achieving a working mFCN prototype requires atomic precision control of the deposition process. The roadmap investigates recent nanofabrication techniques, such as area-selective atomic layer deposition, that may permit the deposition of molecules on precise patterns [10]. Supported by the framework schematized in Fig. 2(c), we analyze the deposition features with molecular dynamics simulations and possible device nanostructures for the realization of electrodes with FEM calculation [6]. The results are used in SCERPA to evaluate propagation characteristics and to identify possible fabrication pathways, thus paving the way for the fabrication of a molFCN prototype.

C. Integration with other technologies

The peculiarity of the molFCN technology comes from the absence of current during information propagation and processing. On one side, this aspect provides minimum power consumption, yet it complicates the interface with established technologies based on conduction. The transduction of the information encoded in the charge distribution becomes crucial for validating a prototype and enabling hybrid integration with CMOS. Recently, literature proposed using asymmetric molecules that vary their vibrational behavior as a function of the molecule charge distribution [11]. We also investigate the interaction between molFCN and single-molecule junctions to demonstrate the transduction of charge-encoded logic information into an electrical quantity. Fig. 2(d) shows a schematic representation of charge transduction based on single-molecule junction sensors [12].

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