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Investigation of Molecular FCN for Beyond-CMOS

Technology, design, and modeling for nanocomputing

Among the technologies proposed to overextend the CMOS era, the molecular Field-Coupled Nanocomputing (FCN) is one of the most attractive technologies for future digital electronics. It encodes the information in nanometric molecules, following the Quantum-dot Cellular Automata (QCA) paradigm, permitting the realization of tiny and very dense digital devices working at ambient temperature. Furthermore, it propagates and elaborates the information through intermolecular electrostatic interaction at a very high speed. No current flow is involved in the information transport, thus minimizing the power dissipation.

Notwithstanding the increased interest for molecular FCN, fueled by outstanding simulative and theoretical results, a working prototype has not yet been realized, unlike other FCN technologies such as the Nano Magnetic Logic (NML) or the Metallic QCA. Indeed, the difficulties correlated to the need for very high resolution for the nanofabrication of devices and for measuring molecule charges make the realization and the measurement of a working prototype challenging. Besides, the molecular FCN literature investigates the information encoding in molecules from a theoretical perspective and simultaneously employs the two-state approximation typical of the general QCA paradigm to study complex digital architectures. However, few attempts have been made to link the molecular characteristics to the two-state approximation models. Consequently, general QCA simulation tools scarcely consider the effective physics of the molecular interaction, preventing the assessment of molecular FCN technology as a possible candidate for future digital electronics. The literature proposes a vast amount of digital architectures which are supposed to be implemented with molecules, despite a real connection between circuits and molecular nature is still the chain missing link.

This work demonstrates a methodological procedure to fill the gap between the physical molecular perspective and the circuit level. First, it analyses molecules with *ab initio* calculation, considering the effective molecular physics, demonstrating the encoding of the information in the static and dynamic regimes at different temperatures by considering the effect of molecular vibrations. Then, it models the molecule as an electronics device and develops the Self-Consistent Electrostatic Potential Algorithm (SCERPA): an optimized tool that permits the fast simulation of molecular FCN circuits by maintaining a solid link with molecular physics and providing results based on *ab initio* characterization of molecules. The tool is therefore used to analyze molecular FCN circuits and establish the physical-aware design of digital devices by considering the effective physics of the molecules. First, obtained results quantitatively describe the functioning, the stability, the crosstalk, and possible memory effects of molecular FCN devices. Secondly, results give feedback to technologists for the eventual realization of a working prototype, conceiving and demonstrating multi-lines clocked molecular devices, which favors the stability of information encoding and reduces the constraints on the resolution for the nanopatterning.

This work fulfills the aim of filling the gap between the physical molecular perspective and the circuit level. It addresses and motivates the necessity of considering the molecular physics in the design of molecular circuits, intensely motivating the use of a physical-aware design tool and circumscribing the use of the general QCA tools for the design of molecular FCN circuits. Furthermore, this thesis work motivates further research on developing and validating a CAD-integrated physical-aware simulator able to provide reliable analyses of molecular devices and circuits and addresses the essential aspects of molecular FCN technology, making it promising as a candidate for future digital electronics.

The following paragraphs report the organization of the document:

Chapter 1 (Introduction and Background) discusses the state-of-the-art of the molecular Field-Coupled Nanocomputing (FCN): the Quantum-dot Cellular Automata (QCA), the essential devices, and

the clocking mechanism. It describes literature molecules and the realization of write-in, clocking, and readout systems. It also presents experimental techniques promising for fabricating molecular devices. Finally, the chapter introduces the methods and tools used in this thesis to analyze molecular FCN circuits.

Chapter 2 (Theoretical Background) discusses time-dependent/independent computational chemistry theories to analyze molecular problems. Also, it describes the molecular properties fundamental for understanding analyses and models of molecular FCN devices, such as molecular vibrations and polarizability. Finally, it briefly describes the two-state approximation theory to link with the QCA literature.

Chapter 3 (Modelling the molecules and the molecular interaction) models and analyzes molecules proposed for molecular FCN through *ab initio* calculation. It analyses and models monostable and bistable molecules, detailing the effect of electric fields generated by molecules or external electrodes in the static and dynamic regime. This chapter also discusses and validates a model for evaluating molecule ground state energy.

Chapter 4 (Modelling the molecular interaction in FCN circuits: SCERPA) describes the mathematics of the Self-Consistent Electrostatic Potential Algorithm (SCERPA) and discusses the iterative procedure convergence and computational cost. Then, it introduces and assesses approximation techniques for speeding up the calculation, eventually favoring the integration of SCERPA in current CAD tools, and describes the organization and the features of the MATLAB implementation.

Chapter 5 (Molecular FCN circuits) analyses the functioning, the stability, the crosstalk, and possible memory effects of molecular FCN devices. First, the inverters and majority voters are analyzed by addressing the dependencies between molecular nature and circuit-level functioning. Then, this chapter demonstrates a physical-aware design on digital devices by considering the effective physics of the molecules.

Chapter 6 (Conclusion and future perspectives) discusses the thesis outcomes by highlighting the open points which should be investigated to ensure molecular FCN is a possible candidate for future digital electronics, thus providing feedback for the fabrication of a molecular FCN prototype. Also, the future developments of the SCERPA algorithm are discussed, motivating further research on developing a physical-aware simulator able to provide reliable analyses of molecular devices and circuits.