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XXXIV Cycle

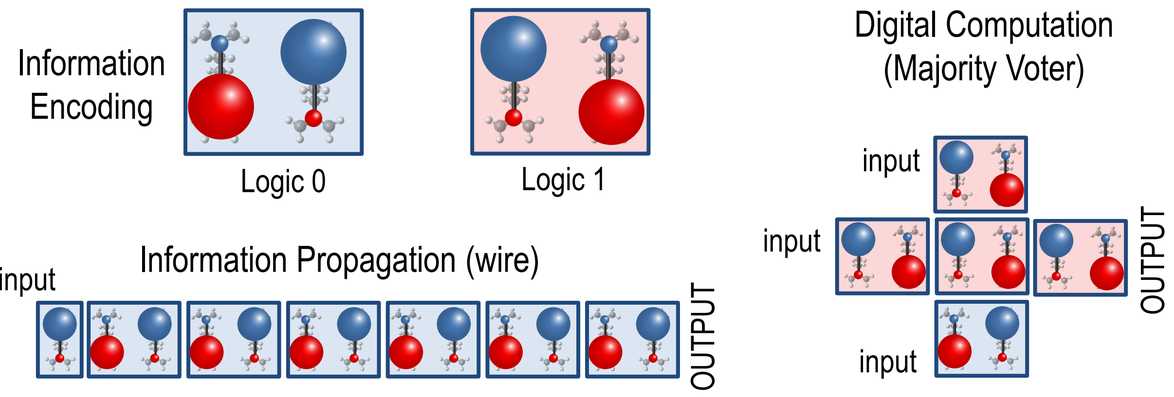
Assessment of molecular technologies for beyond-CMOS

Yuri Ardesi

Supervisor: Prof. Gianluca Piccinini

Research context and motivation

- The size of the state-of-the-art transistor has been reduced so much that its actual behaviour is strongly impinged by the laws of quantum mechanics, arising a list of well-known problems.
- In the last decades, many technologies have been proposed for overcoming the scaling obstacles: the **molecular Field-Coupled Nanocomputing (FCN)** is one-at-a-kind.
- The information is encoded in the charge distribution of molecules and transferred via electrostatic interactions. No charge transport is involved in the information propagation, leading to a drastic reduction of the power dissipation.



Addressed research questions/problems

Low-level perspective:
Physicists and chemists investigated the properties of the single-molecule to understand whether it can encode the information and how it reacts to external electric stimuli.

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High-level perspective:
System-level researchers developed many FCN circuits for digital electronics purpose by considering the molecules as ideal switchable elements.

A significant gap between the two viewpoints exists, making the developing of this new technology difficult. This research aims to shorten the gap between the two perspectives, providing vertical models which facilitate the design of complex digital circuits remaining strongly linked with the physical and technological characters of the molecular device.

- What are the properties molecules must satisfy to ensure the correct encoding and propagation of the information?
- How are molecular and technological parameters connected with system-level features?
- What are the key technological aspects one needs to consider for the realization of a working molecular FCN prototype?

Adopted methodologies

MoSQuiTo (Molecular Simulator Quantum-dot cellular automata Torino): the single-molecule is considered as an electronic device. The molecule interacts with electric fields (input variable) which modify its charge distribution (status variable) and consequently the electric field generated by the molecule (output variable), potentially influencing neighbours.

Ab initio calculations
analyze the electronic structure and the geometry of single molecules

Figures of merit
highlight the key features of the molecule guiding the electrostatic intermolecular interaction

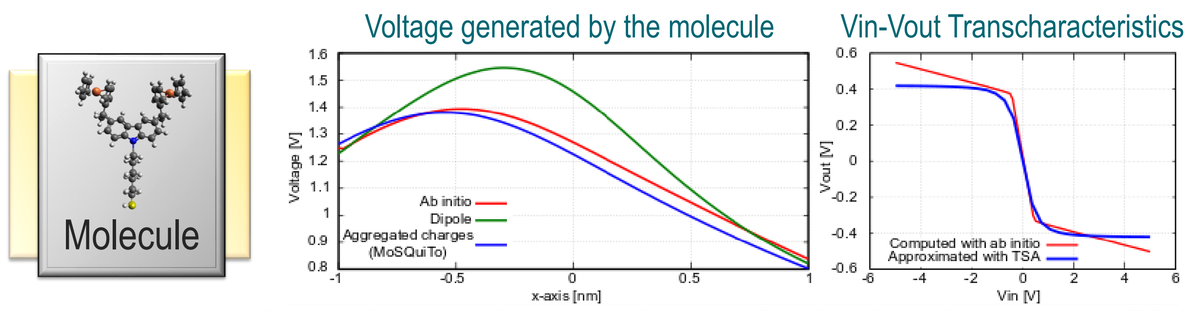
SCERPA
a Self Consistent Electrostatic Potential Algorithm evaluates the charge distribution in molecules of FCN circuits.

Submitted and published works

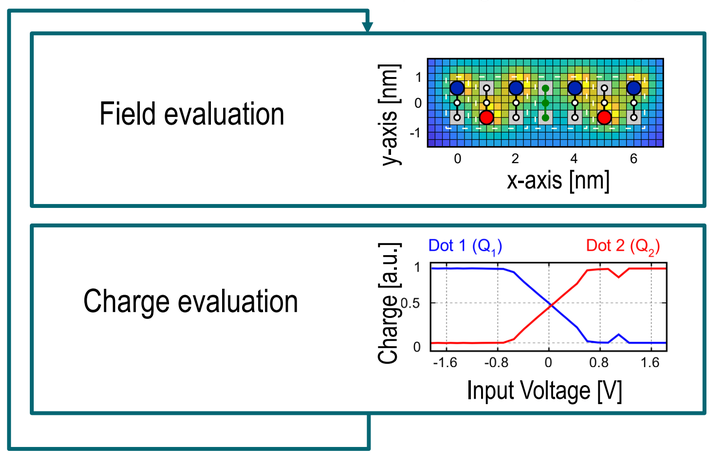
- Ardesi, Y., Wang, R., Turvani, G., Piccinini, G., *"SCERPA: a Self-Consistent Algorithm for the Information Propagation Evaluation in Molecular Field-Coupled Nanocomputing"*, IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems, (Submitted 2019).
- Ardesi, Y., Gnoli, L., Graziano, M. Piccinini, G., "*Bistable Propagation of Monostable Molecules in Molecular Field-Coupled Nanocomputing*", 15th Conference on PhD Research in Microelectronics and Electronics (PRIME), Lausanne (SWITZERLAND), 2019, pp. 225-228.
- Liang, X., Lopez, M., Aiello, J., Langone, N., Vottari, S., Ardesi Y., "*Public engagement in urban innovation: towards the concept of inclusive mobility*", CERN IdeaSquare Journal of Experimental Innovation, vol. 3, no. 1, 2019, pp. 16-21.
- Graziano, M., Wang, R., Roch, M.R., Ardesi, Y., Riente, F., Piccinini, G., "*Characterisation of a bis-ferrocene molecular QCA wire on a non-ideal gold surface*", Micro & Nano Letters, vol. 14, no. 1, 2019, pp. 22-27.
- Ardesi, Y., Graziano, M., Piccinini, G., "*System-level bistability of molecular Field-Coupled Nanocomputing*", Poster at 9th International Conference on Molecular Electronics (ELECMOL), Paris (FRANCE), 2018.
- Ardesi, Y., Pulimeno, A., Graziano, M., Riente, F., Piccinini, G., "*Effectiveness of Molecules for Quantum Cellular Automata as Computing Devices*", Journal of Low Power Electronics and Applications, vol. 8, no. 3, 2018, pp. 24.

Novel contributions

- Improvement and evaluation of the Methodology: how does MoSQuiTo compare with other available methodologies?



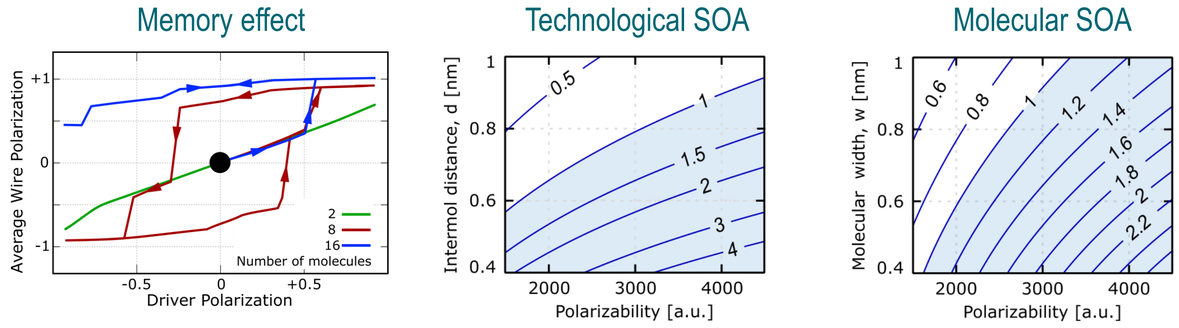
- A computationally efficient algorithm for the evaluation of molecule polarizations in FCN circuits. How can we evaluate the propagation in large molecular circuits?



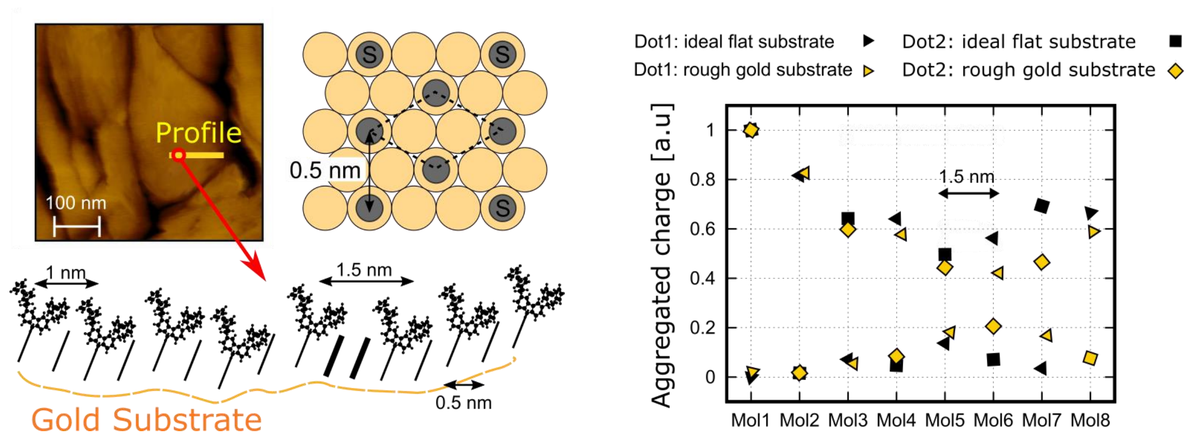
Computational cost reduction of the single evaluation from $O(n^2)$ to $\sim O(1)$

MATLAB

- Characterization of the propagation in monostable molecules and definition of a first safe-operating area (SOA): can we obtain bistable propagation from monostable elements?



- Analysis of robustness with respect to substrate roughness: how does the information propagate when the molecules are anchored on a real substrate?



Future work

- Study of the fabrication and characterization of molecular FCN devices, initially with a simulative and analytical approach and eventually from a practical perspective.
- Exploration of computation paradigms alternative to standard digital logic for novel applications of molecular technologies in electronics.
- Study of new molecules for the eventual prototyping of the technology and the assessment of the MoSQuiTo methodology.

List of attended classes

- 02LWHRV – Communication (21/08/2019, 5 hours)
- 03SGVRV – Entrepreneurship and start-up creation from University Research (4/07/2019, 40 hours)
- 01SFURV – Programmazione scientifica avanzata in matlab (27/03/2019, 28 hours)
- 01QSXRU – The measurement of electrical impedance (5/03/2019, 5 hours)
- (UniTO: CHI0056) – Chimica Computazionale (14/02/2019, 30 hours)

POLITECNICO DI TORINO

PhD program in
Electrical, Electronics and Communications Engineering