ScuDo
Scuola di Dottorato ~ Doctoral School
WHAT YOU ARE, TAKES YOU FAR

XXXVI Cycle

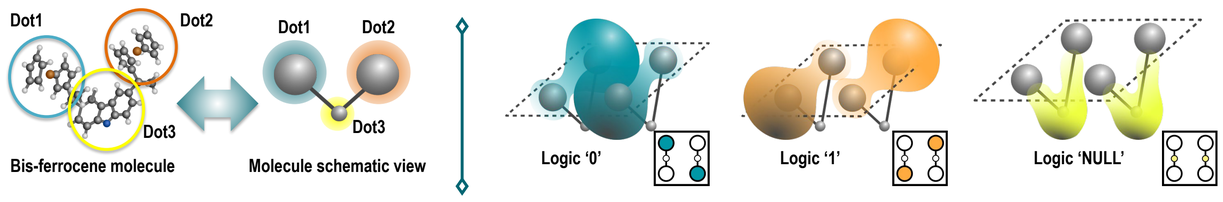
Modeling and analysis of molecular nanotechnologies for digital applications

Giuliana Beretta

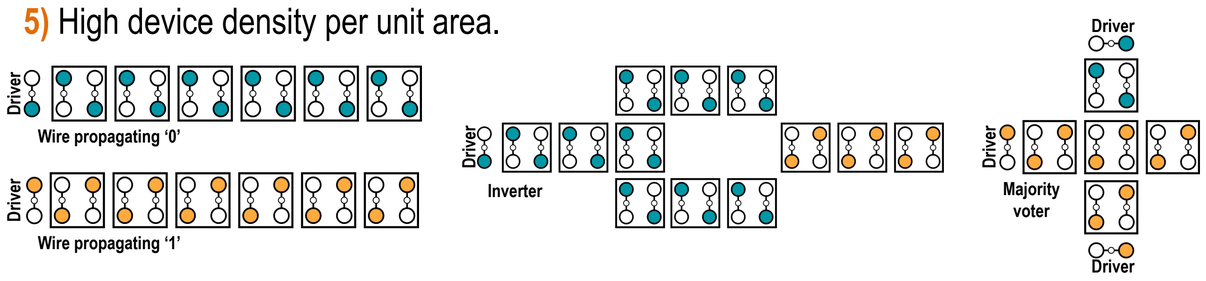
Supervisor: Prof. Gianluca Piccinini, Prof. Guido Masera

Research context and motivation

- In the wide scenario of the proposed Beyond-CMOS technologies, the **molecular** implementation of the **Field-Coupled Nanocomputing (molFCN)** paradigm is promising.
- In molFCN paradigm, the logic information is encoded in the charge distribution of ad-hoc molecules and propagation is enabled by the interaction of the electric fields generated by that charge.

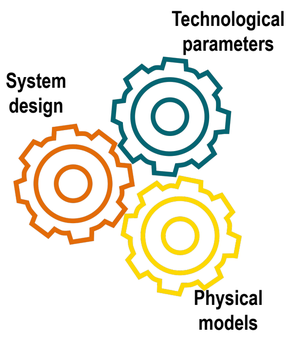


- Logic functions are obtained through specific layout placement of the involved molecules.
- The **advantages** offered by molFCN technology are: **1)** Low power dissipation, **2)** Operating frequency up to THz, **3)** Room temperature operation, **4)** Bottom-up fabrication, **5)** High device density per unit area.



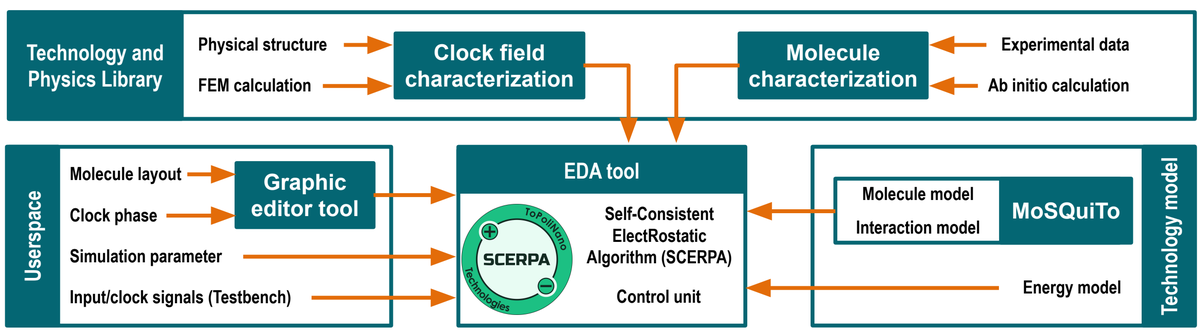
Addressed research questions/problems

- The current literature barely considers the effective molecule behavior. Generally, researchers use quantum approximations of the QCA theory and approximate molecules as ideal two-state quantum-mechanical systems.
- The **physical models**, the **technological parameters**, and **system design** are still far apart, arising difficulties in the design, validation, and realization of molFCN arithmetic circuits.



Adopted methodologies

- Definition of **five abstraction layers** to guarantee vertical handling of the design: Characterisation Layer, Fabrication Layer, Molecule Modelling Layer, Interaction Modelling Layer, Design Layer.
- Definition of a **framework** that facilitates the design and analysis of molecular circuits. The framework is subdivided into four main sections: **Technology and physics library**, **Technology model**, **Userspace**, and **EDA**.



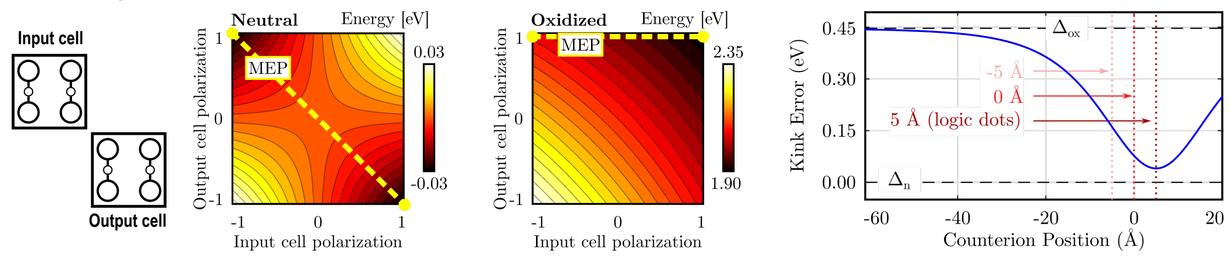
- Combination of Density Functional Theory (DFT) calculation to characterize the molecule, Finite Element Modelling (FEM) to analyze the technological aspects, and theoretical validation of simulations through energy maps.
- The Self-Consistent Electrostatic Potential Algorithm (SCERPA) is linked to the ToPoliNano EDA software to provide **computation capabilities**.

List of attended classes

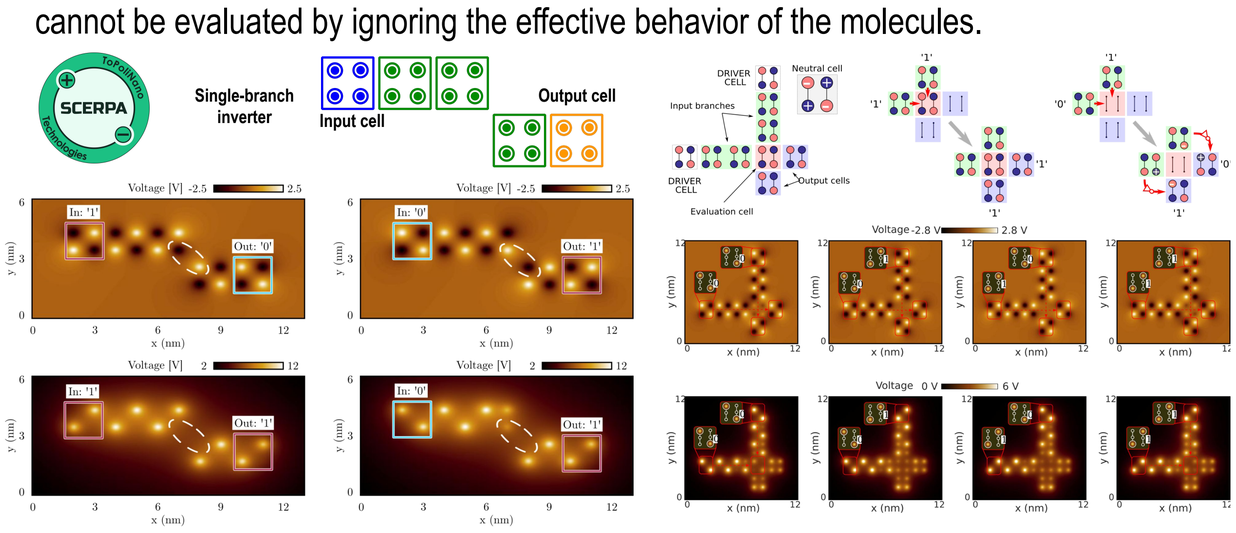
- 02LWHRV – Communication (10/4/2021, 1)
- 05APMNX – Dispositivi elettronici (26/2/2021, 6)
- 01SHMRV – Entrepreneurial Finance (21/6/2021, 1)
- 01SHORV – Nano & Quantum Computing (16/12/2021, 8)
- 01TCPRV – Nano and molecular electronics (15/9/2021, 8)
- 01UNVRV – Navigating the hiring process: CV, tests, interview (4/3/2021, 1)
- 02SFURV – Programmazione scientifica avanzata in matlab (27/4/2021, 6)
- 08IXTRV – Project management (12/4/2021, 1)
- 01RISRV – Public speaking (19/1/2021, 1)
- 01SYBRV – Research integrity (1/5/2021, 1)
- 01SWQRV – Responsible research and innovation, the impact on social challenges (5/5/2021, 1)
- 02RHORV – The new Internet Society: entering the black-box of digital innovations (14/6/2021, 1)
- 01UNXRV – Thinking out of the box (22/11/2020, 1)
- 01SWPRV – Time management (12/1/2021, 1)

Novel contributions

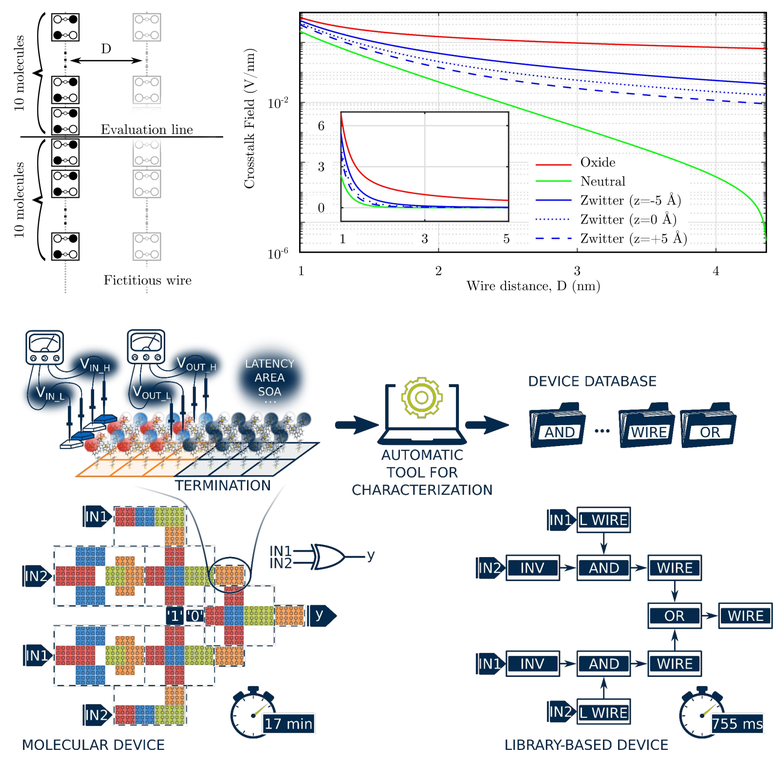
- **Molecule electrostatics** depends on the molecular species (neutral, oxidized, zwitterionic) and impacts the cell-to-cell interaction.



- **Logic gate behavior** is affected by the molecule type used to implement the device, often leading to contradictory gate implementations. The final behavior of molFCN circuits cannot be evaluated by ignoring the effective behavior of the molecules.



- Logic devices interact and the design must take into account for unwanted **crosstalk** polarization.
- The simulation tool used for the design must take into account the effective molecular characteristics, as the proposed framework does. We are thus able to **simulate** and build **circuits considering** the effective **physical behavior**. Then we can store simulations in a library and use those results for future simulations.



Future work

- Derivation of **time-variant molecule models** at the physical level (RT-TDDFT and Ehrenfest molecular dynamics) and **integration in the framework** of those models to simulate circuits in the time domain.
- Populate the **library** of gate-level models, aiming to **automate the design** of complex circuits implemented in molFCN.

External activities

- 15th European School on Molecular Nanoscience (ESMolNa2022), Tordesillas, Valladolid, Spain
- 59th Design Automation Conference (DAC) - Young Fellows Program, San Francisco, CA, USA
- Internship at the Nanoscience Research Center - CIC nanoGUNE, San Sebastian, Spain (**from October 2022**)

Submitted and published works

- Ardesi, Y., Garlando, U., Riente, F., Beretta, G., Piccinini, G., and Graziano, M., "*Taming Molecular Field-Coupling for Nanocomputing Design*", ACM Journal on Emerging Technologies in Computing Systems (JETC), **JUST ACCEPTED**
- Beretta, G., Ardesi, Y., Graziano, M. and Piccinini, G., "*Multi-Molecule Field-Coupled Nanocomputing for the Implementation of a Neuron*", IEEE Transactions on Nanotechnology, vol. 21, 2022, pp. 52-59
- Ardesi, Y. , Beretta, G., Vacca, M., Piccinini, G. and Graziano, M., "*Impact of Molecular Electrostatics on Field-Coupled Nanocomputing and Quantum-Dot Cellular Automata Circuits*", MDPI Electronics, vol. 11, no. 2, 2022, pp. 276
- Ardesi, Y. , Beretta, G., Fabiano, C., Graziano, M. and Piccinini, G., "*A Reconfigurable Field-Coupled Nanocomputing Paradigm on Uniform Molecular Monolayers*", IEEE International Conference on Rebooting Computing (ICRC 2021), Los Alamitos, CA, USA, 2021, pp. 124-128
- Ardesi, Y. , Gaeta, A., Beretta, G., Piccinini, G. and Graziano, M., "*Ab initio Molecular Dynamics Simulations of Field-Coupled Nanocomputing Molecules*", Journal of Integrated Circuits and Systems (JICS), vol. 16, no. 1, 2021, pp. 1-8

Politecnico di Torino

PhD program in
Electrical, Electronics and Communications Engineering