### **Master theses proposals**

Update: December 2020

NANOLOMPUTING Outer herio (10000001 Protein Giligiane Current Current Protein Believe hericon Gun A duce hime Hour to Umberto Garland





Let's draw a MAP in the NANOCOMPUTING garden



















The NANOCOMPUTING elements





















### Let's explore the garden













# T.MOL.1 Simulation of nano-fabrication processes (1/2)

**Object:** Simulate with Molecular Dynamics technological processes

Molecular devices are so small that the process variations and lattice geometries play a relevant role in the quality of the device.

Simulation of nanofabrication enable linking the technological parameters with the system-level perspective with very high precision, providing feedback to technologists and to designers.





# T.MOL.1 Simulation of nano-fabrication processes (2/2)

**Object:** Simulate with Molecular Dynamics technological processes

- Self-Assembled Monolayers
- Passivation and Nano-Lithography
- Fabrication of patterned devices
- Atomic Layer Deposition

Compare the simulated results with experiments and verify models. Explore the impact at higher level.











### T.MOL.2 Readout systems for MolFCN (1/2) Object: Study new methods to sense the charge of a molecule

 Perform a literature analysis of the molecular charge sensing problem, identifying the techniques already documented in literature

- Study the effects of light on molecules with the aim of finding a way to sense the charge, investigate also alternative ways of doing it.
- Design and simulate a charge sensor exploiting one chosen technique (already present in literature or novel)





DCOMPUTING

photons

### T.MOL.2 Readout systems for MolFCN (2/2) Object: Study new methods to sense the charge of a molecule

Object. Study new methods to sense the charge of a mole

- Extraction of significant figures of merit for the characterization of the readout system performance and robustness
- Study the possible integration of the sensor in electronic circuits to create a CMOS/MolFCN interface
- Study the influence between the measurement system and the molecule under measurement



MolFET-based charge sensor









### T.MOL.3 Study of quantum chemistry calculation for time-dependent molecular properties (1/2)

**Object:** Study of Time-Dependent Ab initio based techniques

In molecular electronics, the dynamic of molecules play a relevant role in the device working principle. Analysis of dynamic molecular properties are as essential as novel in the field of molecular electronics.

- Study of ab initio techniques and tools used to analyse the time-dependent properties of molecules (RT-TDDFT, AIMD, Ehrenfest MD, CPMD)
- Analysis of simple time-dependent properties
- Study of time-dependent electrostatic properties (Electrostatic Potential, dipole moment, molecular charge distribution)



Charge density of a molecule under the effect of electric fields



Time



### T.MOL.3 Study of quantum chemistry calculation for time-dependent molecular properties (2/2)

**Object:** Study of Time-Dependent Ab initio based techniques

A possible application: Molecular FCN

- Study the switching of molecules for MolFCN applications. Study the effect of molecular vibrations.
- Study the propagation of the MolFCN information considering time-dependent parameters. Eventually integrating a dynamic model into the SCERPA algorithm.
- Study the propagation of the information in the presence of an adiabatic clock field and in a clock-wall scenario.





Time-evolution of the 1,4 diallyl-butane Aggregated Charge (Molecular Dynamics)





### T.MOL.4 Design of MOLFCN: Abstraction Level Increase (1/2)

Object: Derive a methodology to create a library of molecular devices

![](_page_20_Figure_2.jpeg)

- Design basic logic devices using the SCERPA algorithm
- Model the device in terms of input/output voltage
- Verify the Safe-Operating area of the model by evaluating possible crosstalk with other devices

![](_page_20_Picture_6.jpeg)

![](_page_20_Picture_7.jpeg)

### T.MOL.4 Design of MOLFCN: Abstraction Level Increase (2/2)

Object: Derive a methodology to create a library of molecular devices

- Connect devices and model possible inter-device interactions
- Design and verify complex circuits
- Insert the model-based device within the SCERPA simulation environment

Future advanced works:

- Exploit FEM (COMSOL/ELMER) Model of robust devices with technological parameters. Process variations and electrical characteristics (power, delay of electrodes).
- Auto-routing

![](_page_21_Picture_8.jpeg)

![](_page_21_Picture_9.jpeg)

![](_page_21_Picture_10.jpeg)

![](_page_21_Picture_11.jpeg)

![](_page_21_Picture_12.jpeg)

![](_page_22_Picture_0.jpeg)

# T.MOL.5 Technological study of MoIFET (1/2)

**Object:** Perform a systematic physical and device level study of the Molecular FET

- Physical characterization of new molecules suitable for conduction (e.g. biodegradable molecules)
- Study of the dependance of channel length on conduction (ohmic, anti-ohmic trends)
- Study of the effects of the anchoring groups

![](_page_23_Picture_5.jpeg)

![](_page_23_Picture_6.jpeg)

![](_page_23_Picture_7.jpeg)

![](_page_23_Picture_8.jpeg)

# T.MOL.5 Technological study of MolFET (2/2)

**Object:** Perform a systematic physical and device level study of the Molecular FET

- Study of the effects of less conventional materials for electrodes (Pt, Graphene, cupped-graphene, ...)
- Study of the dependance of gate/backgate oxide material (HfO2, ZrO2, ...) and geometries on current modulation
- Evaluation of process variations (e.g. torsion, bending, folding of molecule, ...)

![](_page_24_Picture_5.jpeg)

![](_page_24_Picture_6.jpeg)

![](_page_24_Picture_7.jpeg)

![](_page_24_Figure_8.jpeg)

![](_page_24_Figure_9.jpeg)

![](_page_25_Picture_0.jpeg)

## T.MOL.6 Electret: In-Memory Molecular Computing (1/2)

Energy

NANOCOMPUTING

**Object:** Study and characterization of molecular storage devices with computing abilities.

- State-of-art analysis of electret devices
- Study of ab-initio/semiempirical techniques used for static and transient physical analysis of molecules (DFT/EHT + NEG, MD models)
- Physical study with atomistic simulations of trapped atoms within molecular cages, ...)
- Study the influence of different trapped atoms/diatomic molecules (Gd, Ce, ScCl, CaO,...)

![](_page_26_Picture_6.jpeg)

## T.MOL.6 Electret: In-Memory Molecular Computing (2/2)

Object: Study and characterization of molecular storage devices with computing abilities.

- Study of the influence of different molecular cages (C60, C70, C82, ...) and their geometry
- Characterization of the device by figures of merit extraction (write/read times, write/read currents, data retention time, ...)
- Circuital level simulations of the LiM cell and LiM array with EDA tools

![](_page_27_Picture_5.jpeg)

**ATLAB** 

![](_page_27_Picture_6.jpeg)

![](_page_27_Figure_7.jpeg)

![](_page_28_Picture_0.jpeg)

![](_page_28_Picture_2.jpeg)

# T.MOL.7 Molecular Sensor Analysis (1/2)

Object: Investigate the sensing capability of molecular devices

- Literature review on molecular electronic sensors
- Deep study of the physical-chemical model for gas detection and single molecule detection mechanisms
- Device level analyses: detection mechanism, target sensitivity, optimal channel choice, optimal contact material for sensing application, etc...

![](_page_29_Picture_5.jpeg)

$$I = \frac{2q}{h} \int_{-\infty}^{+\infty} T(E) [f_1(E) - f_2(E)] dE$$

Full quantum mechanical treatment (NEGF)

![](_page_29_Figure_8.jpeg)

# T.MOL.7 Molecular Sensor Analysis (2/2)

Object: Investigate the sensing capability of molecular devices

- Extraction of important device-level figures of merit and sensor characterization
- Usage of molecular dynamics analysis techniques to understand the target adsorption mechanism by the device molecular channel
- Study of the effects of the gate on the detection capability
- Equivalent circuit for the developed sensor

![](_page_30_Picture_6.jpeg)

![](_page_30_Picture_7.jpeg)

![](_page_30_Picture_8.jpeg)

![](_page_30_Picture_9.jpeg)

![](_page_30_Picture_10.jpeg)

![](_page_30_Picture_11.jpeg)

![](_page_31_Picture_0.jpeg)

![](_page_31_Picture_1.jpeg)

![](_page_31_Picture_2.jpeg)

# T.MOL.8 Molecular Sensor Systems (1/2)

**Object:** Investigation of CMOS/innovative circuit architectures/topologies for molecular sensor applications

- Study of the basic principle of detection in molecular sensors and device-level meaningful parameters
- Literature review and study of conditioning circuits suitable for molecular sensors signal conditioning and processing

![](_page_32_Figure_4.jpeg)

![](_page_32_Picture_5.jpeg)

![](_page_32_Figure_6.jpeg)

![](_page_32_Figure_7.jpeg)

# T.MOL.8 Molecular Sensor Systems (2/2)

**Object:** Investigation of CMOS/innovative circuit architectures/topologies for molecular sensor applications

- Investigation of architectural and topological solutions for reliable target detection in such kind of sensors
- Design and verification (by means of simulations) of a suitable and reliable conditioning circuit for sensing applications (using Cadence Virtuoso), starting from an equivalent circuit-level model for molecular sensors

MATLAB Custom IC Design Virtuoso cādence

![](_page_33_Figure_5.jpeg)

![](_page_33_Picture_6.jpeg)

![](_page_34_Figure_0.jpeg)

# T.MOL.9 Molecular Neural Systems based on molecular transistors

**Object:** Design of a single-neuron and of a simple neural network with molecular technology

- Literature review of ANNs architectures and molecular devices with particular attention to neural network interesting features
- Development and design of a single neuron and neuron weights by means of a molecular transistor (MOLFET) technology
- Design of a molecular neural network with a hierarchical approach for reliable interfacing of neurons

![](_page_35_Figure_5.jpeg)

![](_page_35_Picture_6.jpeg)
### T.MOL.9 Molecular Neural Systems based on molecular transistors

**Object:** Design of a single-neuron and of a simple neural network with molecular technology

- Integration of the developed structure with conventional and innovative electronic systems and identification of practical application fields
- Investigation of possible solution for molecular FCN-based neurons and investigation of the weightening strategies for molecular FCN technologies



VERY CHALLENGING







### T.MOL.10 Study the effects of magnetic fields on molecules

**Object:** Investigate whether and how magnetic fields (static/dynamic) influence molecule behavior and characteristics

In molecular Field-Coupled Nanocomputing, information encoding and propagation are strictly related to electrostatics. Having the possibility to add other degrees of freedom through magnetic fields may alter molecule characteristics.

- Study of ab initio techniques used to analyse the magnetic properties of molecules and effects of magnetic field on charge distribution (MRCI and CASSCF modules of ORCA)
- Analysis of simple molecules under the effect of static magnetic field
- Analysis of dynamic magnetic fields applied to molecules

ORCA

**Electric field** 









An inner MAP: technologies & applications



### T.MAG.1 Design of an efficient on-chip clocking system

Object: Design and characterization of an efficient on-chip clocking system for the generation of perpendicular fields

- perpendicular Nano Magnetic Logic (pNML) is based on material with strong Perpendicular Magnetic Anisotropy (PMA)
- Usually make in Co/Pt and Co/Ni
- Required a soft PMA spot to control the domain wall nucleation
- Switching is achieve by the superposition of field coupling



### T.MAG.1 Design of an efficient on-chip clocking system

Object: Design and characterization of an efficient on-chip clocking system for the generation of perpendicular fields

- The aim is to design an on-chip coil that requires a simple process and generates an homogenous out of plane field (pNML)
- Simulate the designed clocking system with COMSOL considering power losses with different cladding materials and copper windings
- Evaluate the losses at different operating frequencies. The power losses from the control circuitry when generating positive and negative pulses need to be considered







# T.MAG.2 Development of the racetrack logic technology

Object: Design of threshold logic gates by controlling dynamically the magnetic anisotropy

- Study CoFeB/MgO stacks
- Study the behavior of Artificial Nucleation Centers on magnetic island
- Design and characterization of the developed logic gates
- Investigate potential applications that can benefit from this highly structure performing bit-wise operations







R. Bläsing *et al.*, "Magnetic Racetrack Memory: FromPhysics to the Cusp of Applications Within a Decade," Aug.2020









### T.MAG.3 Development of a Compact Model for Spinwaves Simulatons

Object: Development of a compact model in Verilog-A for the simulations of circuits based on Spinwaves

Inputs

B

0

A

Outputs

C

0

S

1

 Study the spinwave technology for its applicability for logic computation

a Ground state

b Excited state

High energy

Excited state

- Develop a compact model in Verilog-A (Cadence Virtuoso) of every building blocks
- Model validation and performance evaluation of complex systems with respect to state of the art CMOS

B = 0



Wang, Q. et al. A magnonic directional coupler for integrated magnonic half-adders. *Nat Electron* (2020)

Output S

Output C



Custom IC Design

Virtuoso







# T.MAG.4 Characterization and modeling of standard blocks for skyrmion logic

Object: Definition and study of standard basic blocks for skyrmion computing systems

- Study of state of the art devices based on skyrmion for logic purposes
- Definition of a complete set of operations for logic based on skyrmion
- Simlation and characterization of the basic blocks of the defined set

#### Advanced work:

 Analytical modeling of the defined basic blocks









NANOCOMPUTING

OR



### T.MAG.5 Hybrid PNML-Skyrmion systems

Object: Design and evaluation of complex logic in memory skyrmion magnetic systems for in-memory computing

- Exploration of ferromagnetic materials hosting skyrmion and compatible with PNML technology
- Simulation and modelling of interface device in the chosen material
- Algorithm exploration suitable for hybrid spintronic systems
- Evaluation of performance of one or few case study







Logic













#### **Quantum Information**

- Quantum Information is a discipline of Information Theory related to the analysis and the design of computational and communication protocols based on a unit of information, named qubit, encoded onto a quantum physical quantity.
- Quantum physical properties as superposition and entanglement permit to define faster computation and safer communication protocols.



#### **Quantum Computational Advantage**

- Superposition permits to simultaneously evaluate multiple data
- Entanglement can assist in fast converging to the problem's solution.

They **both** permit to define, for some hard problems, algorithms with computational costs **lower** than the best corresponding classical ones.



#### Hardware for Quantum Computing

- Quantum Computing technologies can significantly differ in terms of:
  - temperature;
  - magnetostatic fields;
  - bandwidth of EM signals employed for the implementation of quantum gates;
  - non-ideality (e.g. decoherence and relaxation) timescales;
  - native gates;
  - fabrication and maintenance costs.
- A system capable of evaluating the quality of a quantum circuit/algorithm on different quantum computers, taking always into account their pros and cons, is required. (a)  $i \phi$  (c)  $\phi$



#### Methodology for analyzing a QC technology

- Perspective: development of a software tool for designing and comparing the execution of quantum circuits with different technologies.
- Description for each technology of a compact model involving its main physical properties.
- An optimized simulator for non-ideal quantum circuits is required.
- Current infrastructure is based on MATLAB.





### T.QC.1: QC with Silicon Quantum-Dots

- Solid-state technology encoding quantum information on electron spins.
- Higher operating temperature than superconducting qubits (IBM).
- Potential easier interface with a classical computer and to photonic links.
- A two-qubit architecture of TU Delft is already programmable via-cloud.







#### T.QC.1: QC with Silicon Quantum-Dots

#### Article

#### Universal quantum logic in hot silicon qubits

https://doi.org/10.1038/s41586-020-2170-7 Received: 22 October 2019 Accepted: 22 January 2020

Published online: 15 April 2020

Check for updates

L. Petit<sup>1</sup>, H. G. J. Eenink<sup>1</sup>, M. Russ<sup>1</sup>, W. I. L. Lawrie<sup>1</sup>, N. W. Hendrickx<sup>1</sup>, S. G. J. Philips<sup>1</sup>, J. S. Clarke<sup>2</sup>, L. M. K. Vandersypen<sup>1</sup> & M. Veldhorst<sup>1</sup><sup>23</sup>

Quantum computation requires many qubits that can be coherently controlled and coupled to each other<sup>1</sup>. Qubits that are defined using lithographic techniques have been suggested to enable the development of scalable quantum systems because they













T = 1.1K

### T.QC.1: QC with Silicon Quantum-Dots

Object: development of compact models for QC with silicon quantum-dots.

- Analysis of physical principles ruling the quantum device and the quantum system.
- Definition of an initial MATLAB compact model.
- Model validation based on the comparison with reference models and experimental data.
- Potential improvements of the compact model.
- Integration in the simulation infrastructure under development at VLSI Lab.





NANOCOMPUTING



Analysis of physical principles Development of a compact model

Model validation and integration



### T.NDA.1 A new tool for fast process simulation of nanosystems

Object: Design a new tool for the simulation of technological processes

Current tools to perform process simulation are computationally expensive.

- Use a graphical library (TBD: blender, python, matlab) to develop a tool to draw 3D processes (etching, deposition, oxidation, ...).
- Create functional simulation of technological processes (without any physical model) for nanosystems. E.g. Atomic Layer Deposition (ALD).
- Study physical models for processes, eventually validating them with literature or simulative results.
- Integrate physical models into the framework.
- Simulate the design-flow of some devices (e.g. FinFET).









# T.NDA.2 Device-level modeling of advanced transistors (1/2)

Object: Development of device-level suitable models for innovative technologies

 Choice of an innovative technology among: Semiconductor-based novel devices (FD-SOI, FinFET, GAA-FET, Si-NW-FET, ...), T-FET, Graphene-FET, GNR-FET, CNT-FET, Molecular-FET, ...

(ONLY 1 TECH TO BE INVESTIGATED!)

and study of suitable device-level modeling techniques for such a technology

Device-level modeling with MATLAB





**MATLAB** 





# T.NDA.2 Device-level modeling of advanced transistors (2/2)

Object: Development of device-level suitable models for innovative technologies

- Validation of obtained results by means of physical simulators (Sentaurus-TCAD & QuantumATK)
- TAMTAMS framework for extraction, evaluation, conception of device figures of merit for performance evaluation











# T.NDA.3 Technology impact on system performance (1/2)

Object: Development of suitable models for evaluation of system-level performance

 Several (or even all) innovative technologies should be considered and then compared, they include: Semiconductor-based novel devices (FD-SOI, FinFET, GAA-FET, Si-NW-FET, ...), T-FET, Graphene-FET, GNR-FET, CNT-FET, Molecular-FET, ...













# T.NDA.3 Technology impact on system performance (2/2)

Object: Development of suitable models for evaluation of system-level performance

- Development of system-level models for evaluation of performance
- Validation of developed models with circuit implementations (Synopsys & Virtuoso)
- Complex systems performance evaluation and comparison among different technological choices with the help of TAMTAMS framework







📣 MATLAB









### T.NDA.4 Hybrid CMOS/Emerging Devices Design Flow

- Study and exploration of existing hybrid design flow (identify advantages and limitations)
- Develop a methodology for hybrid simulations of CMOS and emerging devices (e.g. magnetic circuits) taking into account the physics of the technology
- Apply the hybrid methodology to some case study technologies (e.g. MTJ/Skyrmions/pNML CMOS)








## **Questions?**

## www.vlsilab.polito.it

The theses presented here are ready now and available in the next few months. However other related or prosecutions will be available later.



