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# Single-Molecule Electronics: From physics to circuits


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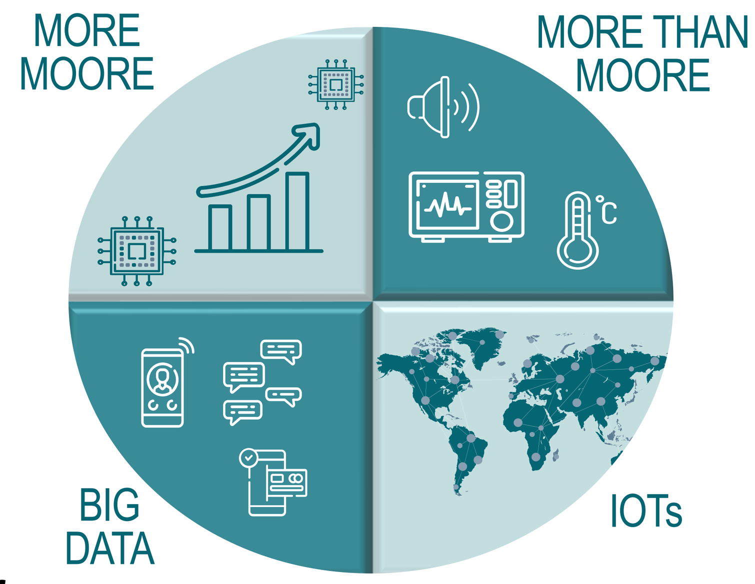
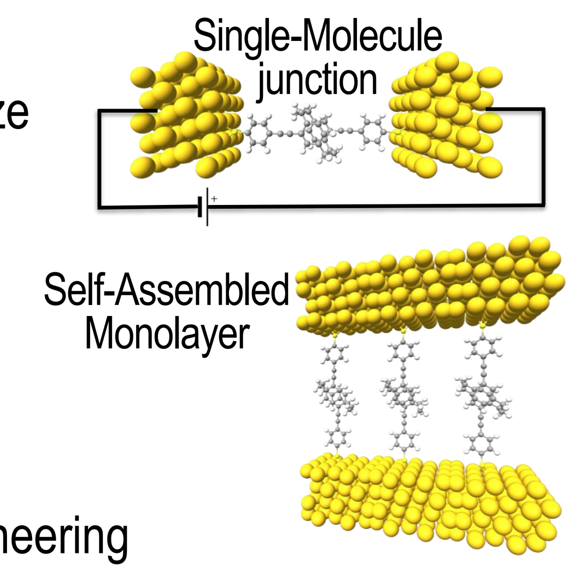
## Research context and motivation

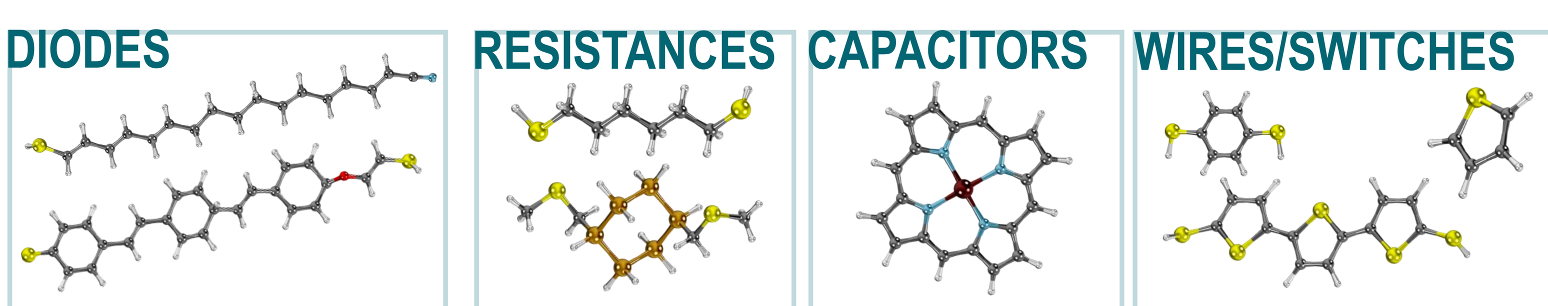
- **Moore's law** is at its ultimate limit, and the ubiquitous paradigm of the **Internet of Things (IOTs),** the pervasive use of **Big Data** and **Artificial Intelligence (AI)** are driving an escalation in demand for heavily scaled, high performing, low-power systems, where **More than Moore (MtM)** paradigm with heterogeneous integration is becoming crucial.




- In this scenario, **MOLECULAR ELECTRONICS** offers:
  - ✓**HIGH INTEGRATION**: intrinsic nanometric molecule size
  - ✓**LOW POWER**: small intrinsic device parasitics
  - ✓**ROOM TEMPERATURE USABILITY**
  - ✓**CHEAP FABRICATION**: self-assembly techniques
  - ✓**UNPARALLEL FLEXIBILITY**: chemical synthesis engineering

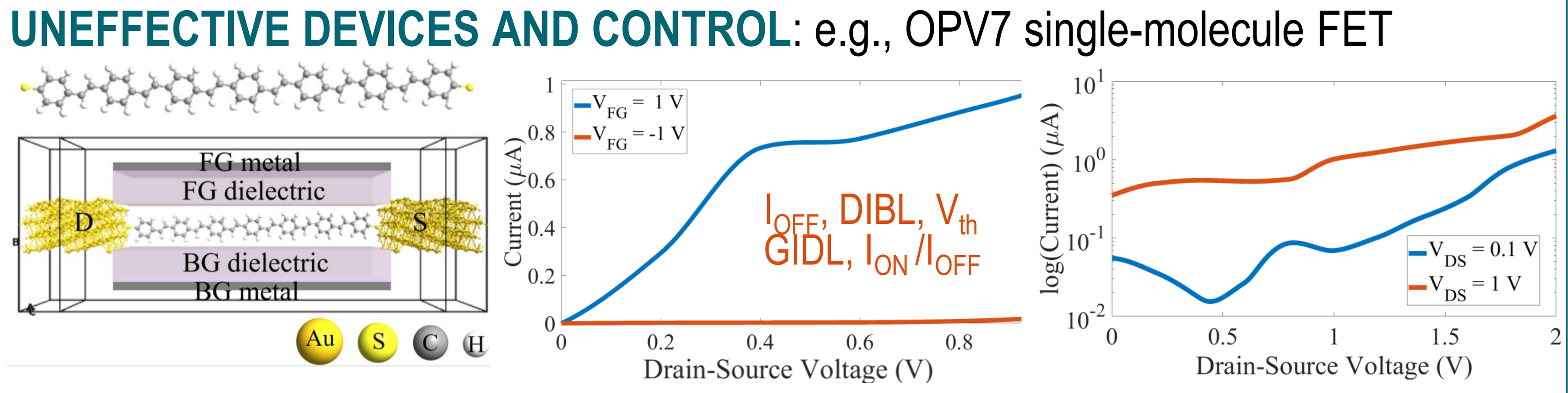



- The electronic properties of molecular devices can be engineered by chemical synthesis with vast degrees of freedom to implement **specific electronic functions**:

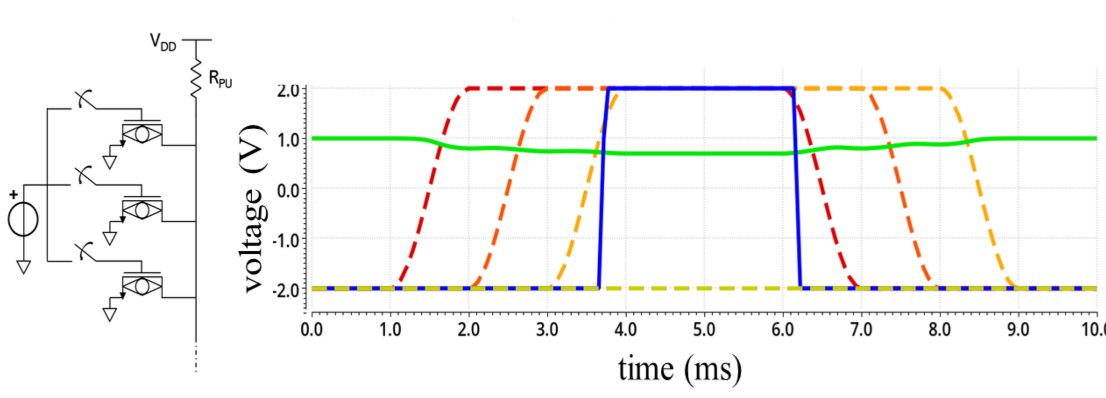



## Addressed research questions/problems

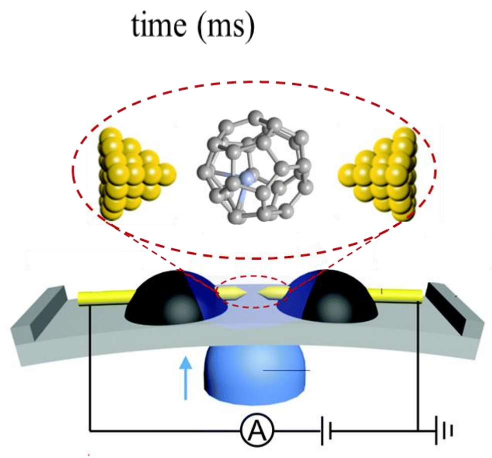
- In the last two decades, a substantial effort has been spent to experimentally demonstrate and theoretically model single-molecule electronic devices. Nevertheless, molecular electronics is still in its **infancy stage** because of the following **open issues** addressed in this research:
  - **UNEFFECTIVE DEVICES AND CONTROL**: e.g., OPV7 single-molecule FET




  - **LACK OF CIRCUITAL AND SYSTEM -LEVEL STUDIES**
    - Functionality
    - Power
    - Delay
    - Area

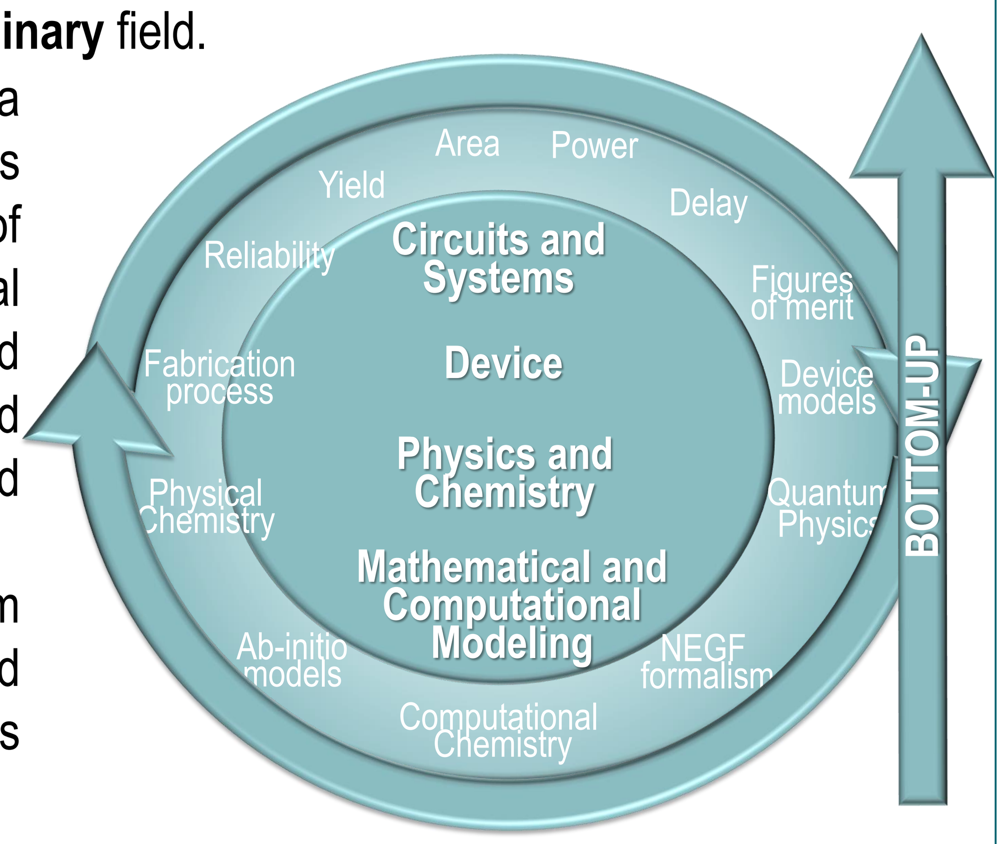



  - **DIFFICULTIES IN ON-CHIP INTEGRATION**
    - Massively parallel nanogap formation
    - Molecules anchoring
    - Different molecules for each device



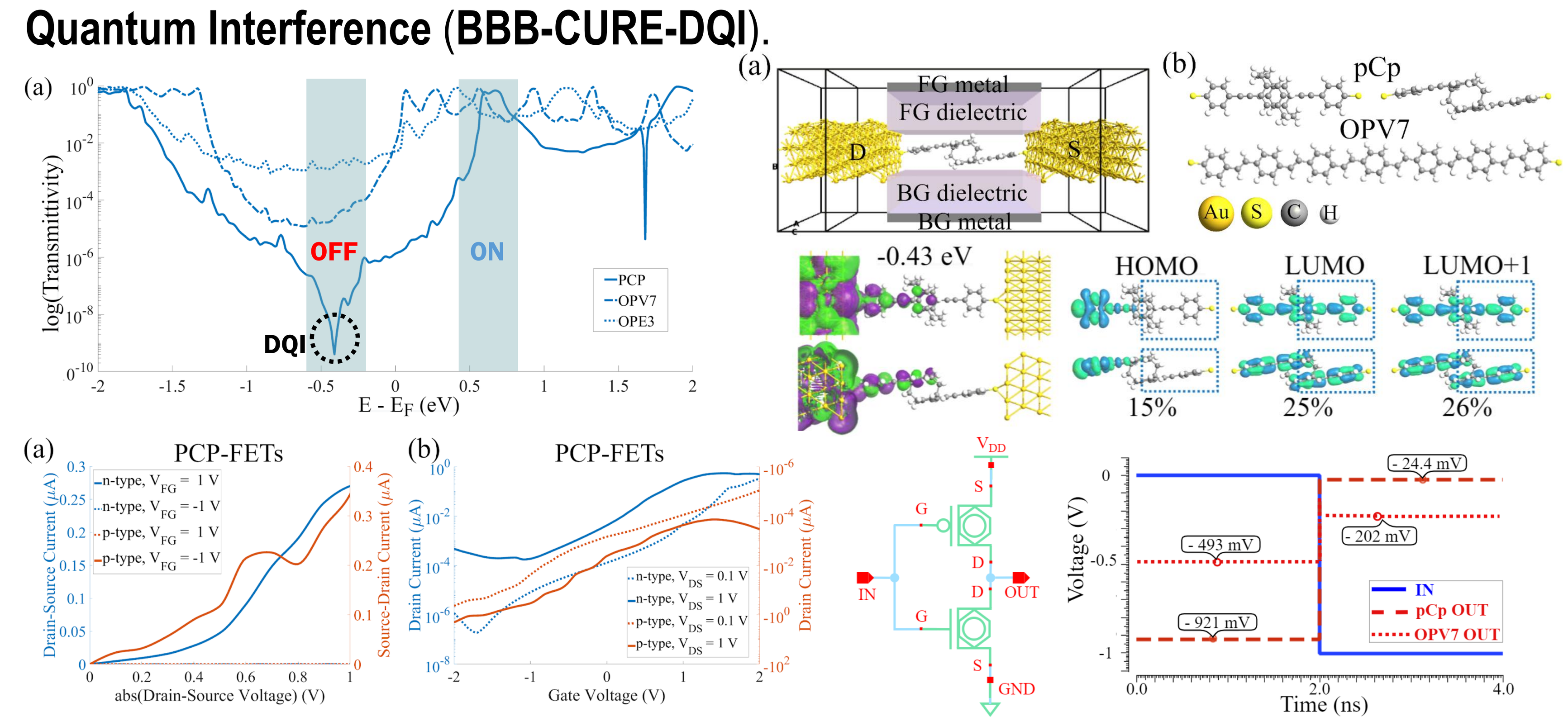
## Adopted methodologies

- Molecular electronics is a **multidisciplinary** field.
- In this research, we adopt a **delocalized perspective** that joins together the localized perspectives of mathematical and computational modeling, quantum and applied physics, physical chemistry, and electronics at the device, circuital and system levels.
- A **bottom-up approach** starting from the chemical and physical levels and going up to the system level is employed in a **feedback** way.

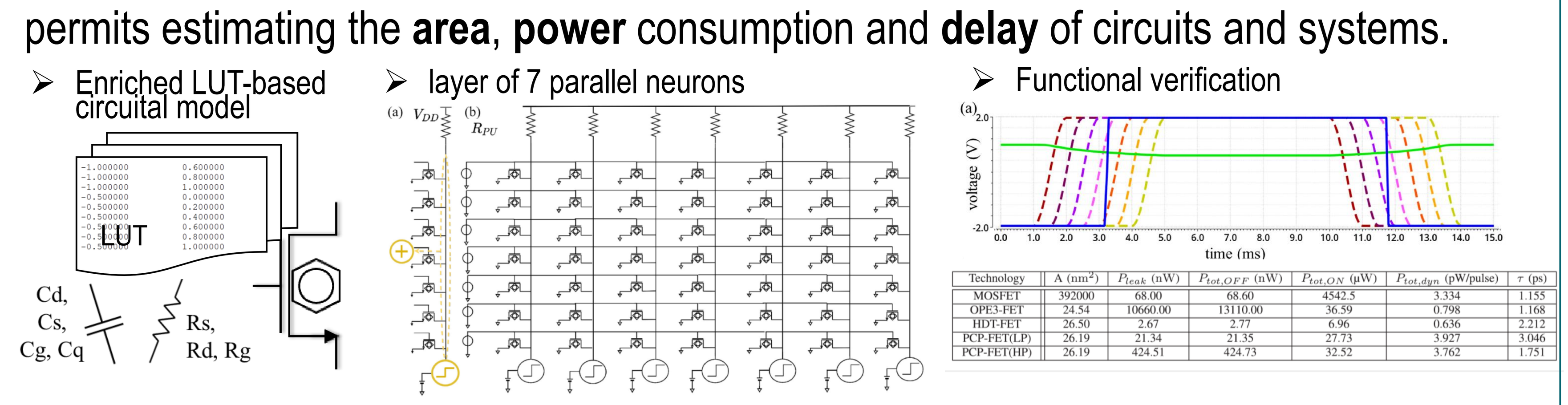



## Novel contributions and results

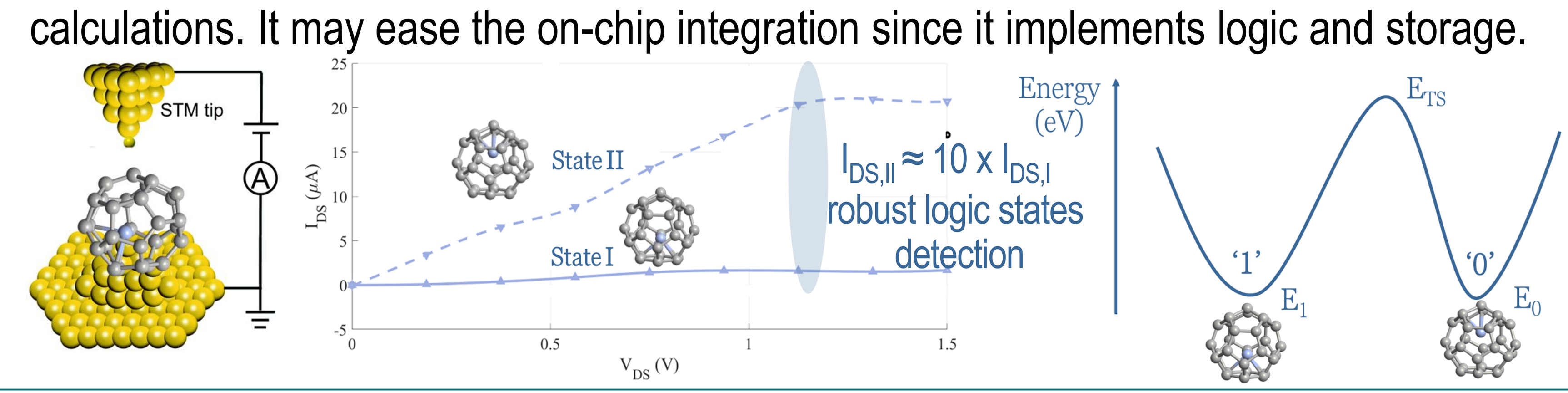
- In [3], we conceive an effective Back gate Biasing-based **method for the ON/OFF CUrrent Ratio Enhancement** of the **single-molecule FET** via the control **of Destructive Quantum Interference** (**BBB-CURE-DQI**).




- In [1], we develop a simple and effective **circuital model for single-molecule FETs** that permits estimating the **area**, **power** consumption and **delay** of circuits and systems.




- In [4], we investigate a **single-molecule amperometric AFB1 sensor** through DFT calculations to enable the **More Moore** paradigm in molecular-based chips.
- In [2], we investigate a **single-molecule device** for **Logic-in-Memory** (LiM) through DFT calculations. It may ease the on-chip integration since it implements logic and storage.




## Future work

- Amelioration of the circuital model for single-molecule devices
- Design of a programmable multipurpouse single-molecule device
- STM-BJ or MBJ experiments

## Submitted and published works


- [1] Mo, F., Spano, C., Ardesi, Y., Piccinini, G., Graziano, M. "*Beyond-CMOS Artificial Neuron: A simulation-based exploration of the molecular-FET*". IEEE TRANSACTIONS ON NANOTECHNOLOGY, vol. 20, pp. 903-911, December 2021
- [2] Spano, C., Mo, F., Ardesi, Y., Ruo Roch, M., Piccinini, G., Graziano, M. "*Electronic Transport Study of Bistable Cr@C28 Single-Molecule Device for High-Density Data Storage Applications*". 13th International Conference on Nanotechnology: Fundamentals and Applications (ICNFA'22), Praga (CZ), August 2022. ISBN: 978-1-990800-11-5.
- [3] Spano, C., Ardesi, Y., M., Piccinini, G., Graziano, M. "*Enhancing the On/Off Current Ratio in Single-Molecule FET via Destructive Quantum Interference*". IEEE TRANSACTIONS ON ELECTRON DEVICES, vol. 69, pp.1-7, September 2022.
- [4] Mo, F., Spano, C., Ardesi, Y., Ruo Roch, M., Piccinini, G., Graziano, M. "*Single-molecule Aflatoxin B1 Sensing via Pyrrole-based Molecular Quantum Dot*". 22nd IEEE International Conference on Nanotechnology (IEEE-NANO 2022), Palma de Mallorca (ES), July 2022.


## List of attended classes

- 01UDAPE – Technology for Nanoelectronic Systems (26/01/21, 6 CFU)
- 01TZFOQ – Engineering Empathy (06/07/21, 6 CFU)
- 01TCPRV – Nano and Molecular Electronics (15/09/21, 8 CFU)
- 01MLHKG – Microscopia a scansione di sonda per la fisica e l'ingegneria (03/22, 6 CFU)
- 01SZPKG – Introduzione alla microscopia elettronica (07/22, 4 CFU)
- 01SHORV – Nano and Quantum Computing (09/22, 8 CFU)
- 10 Soft-skills classes (01/21, 10 CFU)

POLITECNICO DI TORINO

PhD program in
**Electrical, Electronics and Communications Engineering**