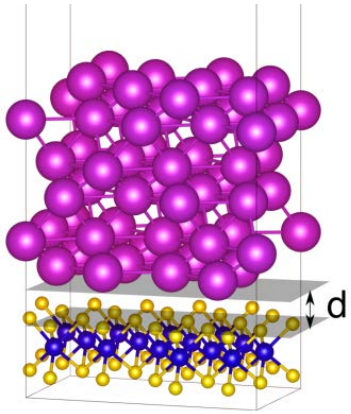
Co-tutored PhD Position at Università degli Studi di Udine (IT) and Université Paris-Saclay (FR): "First principle quantum transport for an atomistic engineering of nanoscale devices and interfaces".
Funded by the Università Italo-Francese (UIF)/Université Franco-Italienne (UFI).



Background: This PhD position is funded by the UIF/UFI (https://www.universite-franco-italienne.org) and the PhD fellow will be co-tutored by Prof. **David Esseni** at the University of Udine (Udine, Italia) and by Dr. **Marco Pala** at the Centre de Nanosciences et de Nanotechnologies (C2N), Université Paris-Saclay (Palaiseau, France).

The PhD project will cover *ab-initio* simulations investigating the electrical and transport properties of nanoelectronic devices. The work will encompass theoretical developments and numerical implementations of methods for quantum transport based on first principles, which will then be used for the design of nanoscale devices based on novel materials such as two-dimensional (2D) semiconductors. The primary working premises for the PhD fellow will be the University of Udine, where the nanoelectronics group offers an international working environment and the involvement in stimulating research projects in the field of nanoscale devices and new computational paradigms, such as the European Union funded H2020 project BeFerroSynaptic, "BEOL technology platform based on ferroelectric synaptic devices for advanced neuromorphic processors" (http://www.beferrosynaptic.eu/home/), and the PRIN project funded by the Italian MIUR Five2D "Five challenges towards electronics based on 2D materials". During the 3-year PhD program the PhD fellow will spend 12 months in the Paris region, at the Centre de Nanosciences et de Nanotechnologies, Université Paris-Saclay. The PhD activities will be part of the framework of a well-established and scientific collaboration between the nanoelectronics group at the University of Udine (https://nanoelectronics.uniud.it/) and the computational electronics group at C2N (https://comics.c2n.universite-paris-saclay.fr/). The PhD student will benefit from top scientific research guidance in the field of first-principle calculations, quantum transport techniques and nanoelectronic device design, and will be involved in joint activities, technical meetings, dissemination of results and technical reports for international projects.

PhD Project Description: The specific objectives of this PhD project include theoretical aspects and an effective numerical implementation related to the development of a first-principle, quantum transport simulation environment with far-reaching applications going from material science to nanoelectronic devices. The project will also encompass the analysis and design of nanoelectronic devices and physical systems based on the above-mentioned simulator, including leakage currents flowing through 2D insulators, the contact resistance between 2D semiconductors and bulk metals, as well as the transport in horizontal and vertical Van-der-Waals heterostructure of 2D materials. The device design activities will be developed in collaboration with international partners having fabrication and characterization facilities.

The skills and competences developed by the PhD student during the PhD program will be highly multi-disciplinary and expendable in several fields including nanoelectronic devices, synaptic devices for neuromorphic computing, and nanostructured material science. The program may also

include material level experimental activities at the synchrotron in Trieste, that will be arranged by submitting to the synchrotron an appropriate project proposal.
The PhD fellow will find an ideal and complementary tutoring from the different research groups involved in the project, covering first-principle material property calculations, cutting-edge electron transport methods based on the Non-Equilibrium Green's Functions approach, and a sound background in electron devices engineering. It is a goal of the PhD project to make the first-principle simulation environment available in the Quantum ESPRESSO platform, which will result in a high visibility of the project. This activity will be carried out under the guidance of Prof. **Paolo Giannozzi**, who is one of the main developers of Quantum ESPRESSO.

Candidate Profile: The candidate should hold a M.Sc. (Laurea Magistrale) in electronical engineering, solid-state physics or material science. Specific experience with Matlab, Fortran, C++ and Python programming is an advantage. The candidate is expected to have the proper qualifications to perform this work as part of a PhD program, including presentations of the work at conferences and publications in scientific journals.

Doctoral position: The research activities will be carried out at the Dipartimento Politecnico di Ingegneria e Architettura dell'Università degli Studi di Udine, Udine, Italy, and 12 months will be spent in Paris at the C2N, Université Paris-Saclay. The fellow will be co-supervised by **Prof. David Esseni** (see Nanoelectronics at University of Udine: https://nanoelectronics.uniud.it/) and by **Dr. Marco Pala**.
The doctoral fellow will be hired on a 36 months fellowship and enrolled in the PhD Programme of Industrial and Information Engineering: https://phd.diegm.uniud.it/iie-phd/ .

For more information about the PhD project and about the call for applications, please contact:

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