

# Ab-initio simulation of quantum transport in nanoscale systems

## Description of the PhD:

The work will be done at C2N within the "Computational Electronics" group composed of 4 researchers and professors. It will be under the supervision of M. Pala and P. Dollfus. A modern computer cluster will be used as main equipment by the PhD student.

## Keywords:

Density functional theory ; Quantum transport ; Non-equilibrium Green's function formalism ; Electron-phonon interaction ; Non-local pseudopotentials ; Plane waves.

## Supervisors:

M. Pala, P. Dollfus

## Profile:

The candidate should have a good knowledge of solid-state physics, electronic transport phenomena, and semiconductor devices, together with a good basis in quantum mechanics. He/she should have a taste for scientific calculation and computing. Knowledge of scientific programming language(s) is also appreciated (Matlab, C, Fortran).

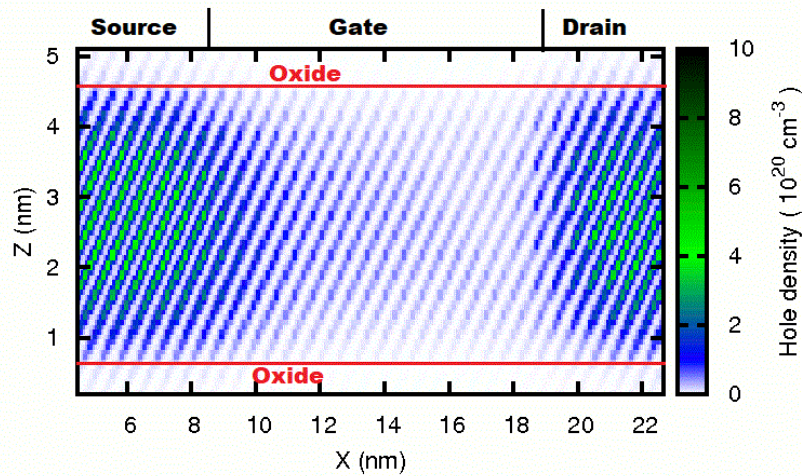
## Detailed presentation in English:

In modern electronic and opto-electronic devices the surface/volume ratio has remarkably increased. Consequently, the transport often occurs along and through interfaces between materials with different physical properties. Examples are the metal/semiconductor junction important to describe the contacts of advanced FETs and the III-V/Si heterostructure used in photonic devices such as lasers and optical modulators. Information on the electronic and transport properties of these devices is often inaccessible from standard characterization techniques and should be achieved by means of predictive simulations based on sophisticated parameter-free models.

In order to accurately model electron transport through such interfaces, it is compulsory to adopt a general approach able to account for quantum tunneling, inter-valley transport, trap-assisted transport (TAT) mediated by phonons or other inelastic mechanisms. Moreover, the accurate description of such systems require the knowledge of the atomic relaxation of different species with significant lattice parameter mismatches as well as the assessment of the impact of non-idealities like interstitial defects, vacancies and roughness at the interfaces.

In this PhD thesis we will develop a full *ab-initio* approach to treat these complex problems. We will exploit density functional theory (DFT) simulations [1] of realistic heterojunctions and interfaces to address a full-band quantum transport analysis within the framework of the non-equilibrium Green's functions (NEGF) method [2]. The DFT calculations will be based on pseudopotential Hamiltonians developed within a plane-waves basis which provide the most rigorous results in terms of atomic position relaxation and convergence of bandstructures. Importantly, we will use these plane-wave Hamiltonians to efficiently compute electronic and transport calculations by using the original approach developed and described in [3]. An example of self-consistently calculated carrier

concentration in a Ge p-MOS is shown in the Figure below, where we observe atomistic scale patterns of the carrier concentration due to the periodic parts of the crystal Bloch functions.



At first, this methodology will be used to study the ballistic regime of transport characterized by elastic tunneling. Further, additional physical complications will be added by considering the inelastic scattering due to electron-phonon interaction as well as the role played by TAT [4]. Eventually, many-body effects will be considered by the addition of nonlocal self-energies based on the GW approximation [5].

A typical system that will be analyzed with this methodology is the heterojunction between materials of groups III-V and IV such as InAs/Si, which is important both in electron devices such as the tunnel-FETs and in optical modulators based on hybrid interfaces [6]. Finally, all the simulations and physical models on this system will be validated by comparison with experimental data which will be supplied by experimental groups working in C2N.

## Objectives:

The final objectives of this theoretical work are: (i) to develop an efficient method to perform ab-initio quantum transport simulations based on pseudopotential Hamiltonians developed in a plane-wave basis, (ii) understand the physics and transport properties of group III-V/IV heterojunctions (iii) possibly propose new efficient electronic and optoelectronic devices for applications in the Internet of Things, autonomous cars and gesture detection.

## Context:

This research will be realized within a scientific collaboration with an experimental group in C2N which will fabricate and characterize III-V/Si heterojunctions.

## Methods:

- DFT methods based on pseudopotentials will be used for bandstructure calculations and the construction of the Hamiltonians used in the transport calculations.
- A full quantum approach will be used to simulate carrier transport within the framework of the non-equilibrium Green's function formalism coupled with Poisson's equation.

- The electron-phonon interaction will be accounted for within the self-consistent Born approximation and the use of DFT self-energies.

### **Valorization:**

The results of this PhD will be published in high profile peer-reviewed journals, belonging to both the microelectronics community (IEEE Electron Device Letters, IEEE Transactions on Electron Devices ...) and the physics/nanosciences community (Nano Letters, Nanoscale, Nanotechnology, Physical Review, Applied Physics Letters ...). They will also be presented at international conferences (e.g., IEDM, IWCN, SISPAD for microelectronics, (E)MRS, APS conferences for physics and nanosciences).

### **References:**

- [1] R. G. Parr and W. Yang, Density Functional Theory of Atoms and Molecules, Oxford University Press, New York, (1989).
- [2] G. Mahan, Many-Particle Physics, Plenum Press, New York, (1990).
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- [4] M. G. Pala and D. Esseni, IEEE Trans. Electron Devices, vol. 60, pp. 2795 - 2801 (2013).
- [5] H. N. Rojas, R. W. Godby, and R. J. Needs, Phys. Rev. Lett. , vol. 74, p. 1827 (1995).
- [6] T. Hiraki et al., Nat. Photonics vol. 11, pp. 482-485 (2017).