PhD position 2016-2019

Electron quantum transport simulation of 2D material based devices

KEYWORDS

Two-dimensional materials, numerical simulation, quantum transport, field-effect transistor, tunnel effect

PROJECT DESCRIPTION

Since the discovery of **graphene**, many other layered materials have been synthetized. Among them, we mention the X-enes (silicene…), the X-anes (stanane…) and the **transition metal dichalcogenides** (molybdenum disulfite…). Depending on their composition and layering, these materials have very different properties, such as the presence of a direct or indirect band gap of different width. Together with the excellent electrostatic control due to their atomic thickness, this promotes 2D materials as promising candidates for developing **logic devices for flexible low-power electronics**. The wide variety of 2D materials and of their defects calls for a large exploratory effort, which is still in its early phase. In this context, the **simulation of electron quantum transport** is an essential tool to understand the physics at the origin of the 2D material properties and to design innovative devices based on these original properties.

The goal of the PhD is to **theoretically and numerically investigate these new materials** by exploring their **electron transport properties** and their applicative potential for innovative devices. These systems have an intrinsically quantum behavior, thus requiring the use of a general electron transport approach, such as the **non-equilibrium Green's function** formalism, as well as an atomistic description based on the density functional theory.

The student will be asked to:

- Simulate electron quantum transport in several 2D materials (mainly transition metal dichalcogenides and multilayer structures based on them), in pristine form or with disorder, by using **atomistic Hamiltonians** together with the TB_Sim code developed at CEA.

- Develop a simulation code addressing electron transport in devices exploiting these 2D materials. More precisely, the codes developed at IMEP-LaHC for other devices will be adapted to *k.p* models. These codes make use of the Green's functions formalism, with a self-consistent treatment of the electrostatic potential and of the electron-phonon coupling.

- Simulate electronic devices based on 2D materials, in particular **field-effect and tunnel transistors** (with lateral or vertical junctions), taking into account possible defects (dopants, impurities, structural defects) and their impact on variability.

- Assess the performance of different transistor architectures with respect to their geometry, to the choice of the substrate, and to the electrostatic configuration.

DESIRED SKILLS

- Training in physics and electronics
- Solid knowledge of **condensed matter physics**
- Basic knowledge of **computer programming for numerical simulation**

The candidate must hold a master degree (equivalent to a master M2R in France) or an equivalent university degree eligible for the EEATS Doctoral School of Université Grenoble Alpes.

DETAILS

Thesis supervisors: François TRIOZON (CEA-LETI) and Mireille MOUIS (IMEP-LaHC)

Co-supervisors: Alessandro CRESTI (IMEP-LaHC) and Maud VINET (LETI/CEA)

Funding: PhD grant from "labex MINOS"

Thesis starting date: October/November 2016 Thesis duration: 3 years

ABOUT THE RESEARCH INSTITUTES

IMEP-LAHC (http://www.imep-lahc.grenoble-inp.fr) is a "unité mixte de recherche" involving Grenoble INP, Université Grenoble Alpes, Université Savoie Mont Blanc, and CNRS. It is located within the **Minatec** innovation pole, in Grenoble. The laboratory employs 64 researchers, 18 engineers and technicians, 18 postdoctoral fellows, and 85 PhD students. It has collaborations with several universities and research centers, large industrial groups (ST-Microelectronics, IBM, Motorola, etc.), and preindustrial microelectronics centers (LETI, LITEN, IMEC, Tyndall).

CEA-LETI (http://www-leti.cea.fr) is a research institute for electronics and information technologies employing more than 1000 researchers, engineers, and technicians. It hosts a large technological platform (clean rooms, physico-chemical characterization). It is mainly funded by industrial partnerships (STMicroelectronics, IBM, …). It relies on a strong scientific expertise: partnerships with CEA/DRF (Fundamental Research Division) and academic institutes (CNRS, Universities) via national and European funding.

The PhD student will work within the "groupe Composant MicroNanoElectronique" of IMEP-LaHC and the "groupe Simulation et Modélisation" of LETI.

CONTACT PERSONS AND DEADLINE

Send a CV, a letter of motivation, photocopies of diplomas and academic record with ratings, and two recommendation letters to:

Dr. François TRIOZON, Permanent researcher at CEA-LETI
francois.triozon@cea.fr Tel: +33 4.38.78.21.86

Dr. Alessandro CRESTI, "Chargé de Recherche" at CNRS, IMEP-LaHC
crestial@minatec.inpg.fr tél. +33 4.56.52.95.50

Dr. Mireille MOUIS, "Directeur de Recherche" at CNRS, IMEP-LaHC
mouis@minatec.inpg.fr tél. +33 4.56.52.95.35

The application must be received **before June 27th 2016**. Applications received after this date will be considered only if the funding deadline allows it.