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**ECM\_IM2NP\_GROSSO\_01**

<b>PhD Proposal 2017</b>
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<b>Title: Experimental and theoretical study of 2D semiconductor layers (silicene, germanene) in epitaxy on a graphene template</b>
<b>Scientific field: physics, nanosciences, nanotechnology</b>
<b>Key words: silicene, germanene, graphene, nanotransistor, nanodevice</b>

## **Details for the subject:**

### **Background, Context:**

While conventional silicon-based electronics has experienced rapid and steady growth, thanks to the progressive miniaturization of its basic component, the transistor, this trend cannot continue indefinitely. At the moment, the actual bottleneck for further scaling trends is that, even using bulk materials, the functionality of electronic devices is essentially governed by what occurs at the interface of the semiconductor. In fact, industry has already moved to thin film channel devices with the production of the FinFET, in which a thin film silicon channel is placed vertically. An attractive option for entering the <11 nm nodes is the ultrathin body silicon on insulator (UTB SOI) design that consists of a thin film Si channel placed horizontally. This architecture benefits for low power operation but its scaling down to the <5nm lower nodes will be inherently hindered by both the imperfect interface and non-uniformity of such a very thin film and by quantum confinement effects which increase the effective bandgap.

A radical change of paradigm is therefore required for ultimate thickness scaling beyond the 7-5 nm technology node. This challenging issue could be addressed by using single atomic layers of silicon (or germanium), i.e. new allotropic structures, such as silicene and germanene, with radically different electronic properties compared to Si (Ge) ultrathin films scaled down from the bulk.

The most obvious alternatives for graphene are the group IV elements, i.e. silicon and germanium. Silicene and germanene share several peculiar properties of graphene. They are Dirac materials in which electrons near the K and K' points of the Brillouin zone behave as relativistic massless particles due to the linear dispersion around Fermi level. On the other hand, silicene and germanene show peculiar physical properties which make them better suited than graphene in the race for ultimate thickness scaling of nanoelectronic devices. First of all, they offer perfect compatibility with the current Si-based technology of semiconductor processing. More importantly, the structure of silicene and germanene is more flexible than that of graphene, because of the absence of strong  $\pi$ -bonds enforcing planarity. The larger buckling, as well as the resulting larger spin-orbit coupling, make it easier to create a bandgap in Si and Ge two-dimensional crystals without degrading their electronic properties.

However, there are still several hurdles that have to be overcome for the practical applications of silicene and germanene in microelectronic devices. To date, these materials have been exclusively grown on metallic substrates. On metals, their 2D Dirac character is, in most cases, either altered or completely destroyed due to hybridization of the relevant electronic states near the Fermi level with electronic states of the metallic substrates. Conversely, a wide band gap material would be an ideal template for decoupling silicene and germanene from the underlying substrate. In addition, the fabrication of functional electronic devices necessarily requires non-metallic supports. Thence, a way-around, i.e. transferring silicene on insulating substrates after growth, was needed for the realization of the first silicene field-effect transistor. In order to upscale device production, the challenge is to directly grow silicene and germanene epitaxially on crystalline non-metallic substrates.

### **Research subject, work plan:**

The goal of this PhD thesis is to design epitaxial growth routes which, on the one hand, preserve the honeycomb crystal structure and Dirac cones of free-standing layers and, at the same time, avoid alloy formation typical of metal substrates. As a first milestone, the student will have to demonstrate silicene and germanene epitaxial growth on graphene itself transferred on transparent conductive oxides (TCOs) such as indium tin oxide (ITO) or aluminium zinc oxide, to transport current. These oxides will be fabricated by sol-gel.

Successful growth on graphene will allow subsequent liftoff of silicene/graphene and deposition on SiO<sub>2</sub> for more conventional device fabrication.

In a second step, the student will develop the growth of silicene and germanene on graphene itself on silicon on insulator (SOI). The distribution of epitaxial strain between silicene and graphene will be measured and the conditions of nucleation and growth will be modelled. Results of experiments will be compared to theoretical modelling. These modelling should allow to revisit the mechanism of growth on a self-supported template layer. They should include curvature effects of the deposited ultra-thin layers and the strain sharing in the epitaxial system. Interaction between the template layer, the substrate and the epitaxial silicene and germanene layers will be developed in accordance with the experimental results. In addition, the coupling between strain dynamics and growth will be investigated, in the limit situation of a self-supported graphene/silicene nanomembrane

The student will work partly in the Nanostructures Semiconductor Epitaxy (NSE) team (Aix-Marseille University) which has an impressive range of high technology instruments located in the NanoTecMat clean-room platform and partly in INSP (Université Pierre et Marie Curie, Paris) where he will develop models of the equilibrium structure, nucleation and growth of 2D epitaxial layers.

The collaboration between theory and experiments will bring a unique and specialized training on a very hot topic with outstanding promising applications. With such training the student will acquire skills at the top level, highly sought-after by both industrial companies and academic staff. Commonly, the PhD students of the team find a job before the end their PhD thesis.



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