Doctoral positions
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Thesis supervisor

Name: AQUA Jean-Noël

Location: INSP - 4 place Jussieu, 75005 Paris – Tour 22 étage 4 ; 22-12-415

Group: Physico-chimie et dynamique des surfaces

E-mail: aqua@insp.jussieu.fr

Phone : +33 (0)1 44 27

Group website: http://www.insp.jussieu.fr/-Aqua-Jean-Noel-

Thesis topic Silicene and germanene growth on non-metallic substrates

The recent discovery of the stability of 2D materials, has revolutionized the physics and potential technology of semiconductors thanks to their ability to confine carriers. Graphene, a single free-standing layer of sp^2 hybridized carbon atoms was found to be stable because of the anharmonic coupling between stretching and bending modes resulting in intrinsic corrugations of the layer [Novoselov2004]. Graphene has outstanding properties, such as the Dirac-cone-shaped energy band and high carrier mobility. However, despite the huge efforts devoted to open its bandgap, graphene remains gapless, which makes it useless for field-effect applications.

The most obvious alternatives based on the group IV elements, are silicene and germanene that share several peculiar properties with graphene. Free-standing silicene and germanene do not exist in nature but their synthesis has been reported on metallic substrates. However, their properties were found to be strongly affected by the coupling with their substrates. An alternative is to directly use a non-metallic substrate, that was done using synthetic graphite [Persichetti2016, DeCrescenzi2016].

The PhD work will concern the experimental and theoretical study of the formation mechanisms of silicene and germanene on HOPG and graphene substrates. The experimental study will consist in the molecular beam epitaxy of layers in a ultra-high-vacuum environment. Diverse approaches will be followed to optimize the growth process and obtain wafer scale silicene and germanene layers. In order to achieve this goal, the major parameters determining the growth behavior, namely the temperature, flux and strain will be investigated. The experimental work will be done in the NanoTecMat platform at IM2NP in Marseille in the group of Isabelle Berbezier.

The theoretical understanding of the growth of silicene and germanene will be done in INSP in Paris under the supervision of Jean-Noël Aqua. It will be based on appropriate kinetic frameworks that will encompass the specific film/substrate interactions. They will be based on kinetic Monte-Carlo simulations and the classical nucleation theory, where strain will be described in an efficient Green's function formalism [Liu2017]. These frameworks will describe the important atomistic features revealed both by experiments and by *ab-initio* molecular dynamics (AIMD) studies done with a collaborating group.

The PhD work is embedded in a project to ultimately fabricate a prototype transistor device based on such 2D materials.

References:

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Unité mixte de recherche 7588 – CNRS / Université Pierre et Marie Curie
Campus Jussieu – Tours 22 et 23 – Case courrier 840
4 place Jussieu – 75252 Paris Cedex 5 – France
Tél. : +33 (0)1 44 27 63 72 – Fax : +33 (0)1 44 27 46 09 – www.insp.upmc.fr