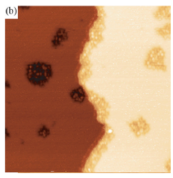
# Master thesis proposal

INSP / 4 place Jussieu, Paris 5e
Director: Massimiliano Marangolo

**Title**: Epitaxy of germanene on silver: a kinetic Monte-Carlo study

**Keywords**: 2D materials, kinetic Monte-Carlo, out-of-equilibrium

**Scientific description**:
Since the discovery in 2004 of graphene, 2D materials have aroused an ever-growing interest since different atoms form 2D layers: carbon, silicon, transition metal dichalcogenides... Graphene has shown remarkable properties, such as the Dirac-cone-shaped energy band and high carrier mobility. However, despite significant efforts, there has been no reproducible method to open up its bandgap while preserving high carrier mobility. 2D-materials based on group IV elements such as Si (silicene) and Ge (germanene) are promising alternatives. Manufacturing good quality, quality-controlled such 2D crystals is thence of major importance from both fundamental and applied perspectives. Their growth by epitaxy that is both the fundamental cleanest way and a technological lock is thence the focus of different experimental studies. The growth on some metallic substrates revealed possible alloying effects that need to be understood and controlled. The goal of this internship is to advance in the theoretical understanding of these systems by using kinetic Monte-Carlo (KMC) simulations that is the most suitable tool to describe these systems over the relevant space and time scales, yet including atomistic time scales.



We will investigate the growth of germanene on top of Ag(111) substrates. A significant experimental work was performed in the hosting team on this system. It revealed new growth modes, outside conventional growth patterns. To rationalize these growth modes, one needs to describe the out-of-equilibrium behavior that dictates growth morphologies and regimes, and thence the dynamics and self-organization on large scales. We will consider a modelization that will incorporate alloying effects and the possibility of intermixing so as to describe surface alloys revealed by experiments. We will also include surface effects in the dynamics that were shown at INSP to be at work during the growth of silicene on Ag(111). The numerical part will include the derivation of rejection-free KMC simulations following the Bortz-Kalos-Lebowitz algorithm. The algorithm will include different atomic events starting with the fundamental deposition, diffusion and attachment/detachment processes. These processes will be made dependent on different configurations (local height, local configuration …) to account for different effects (segregation, alloying, wetting etc). Energy barriers will be derived both thanks to experimental and ab-initio results, but also thanks to the analysis of the simulation and experimental morphologies. The aim of this coupling between theory and experiment is to gain control on the growth procedure in order to obtain two-dimensional epitaxial deposits of large size and good crystalline quality. The internship will be done in close collaboration with the experimental group at INSP.

**Techniques/methods in use**: kinetic Monte-Carlo simulations
**Applicant skills**: numerical abilities, solid state physics
**Industrial partnership**: No
**Internship supervisor** : Jean-Noël Aqua, aqua@insp.jussieu.fr, 01 44 47 57 97
**Internship location**: 22-32 4th floor, Jussieu campus
**Possibility for a Doctoral thesis**: Yes