# PhD project

## Epitaxy of germanene on silver: theory and simulation

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

Since the discovery in 2004 of graphene, 2D materials have aroused an ever-growing interest. 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. 2D-materials based on group IV elements such as Si (silicene) and Ge (germanene) are promising alternatives. Their production by epitaxy that is both the fundamental paradigmatic growth and a technological lock is thence the focus of different studies [1]. The deposition on metallic substrates revealed possible alloying effects together with self-organization of surface patterns that need to be understood and controlled. The goal of this thesis is to advance in the theoretical modelization of these systems by using kinetic Monte-Carlo (KMC) simulations that is the most suitable tool to describe such systems over the mesoscopic space and time scales, yet including atomistic events and time scales.

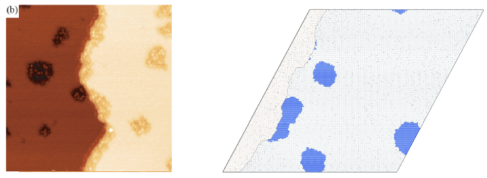

*Figure 1 : Experiments and KMC simulation of Si on Ag(111) reveal inserted islands that coarsen [3]*

We will investigate the growth of germanene on top of a Ag(111) substrate, a system recently investigated in the hosting team [2]. It revealed new growth modes, outside conventional growth patterns, including surface alloying and surface self-organized patterns. To rationalize these growth modes, one needs to describe the out-of-equilibrium behavior that dictates growth morphologies and the dynamics on large scales [3]. We will consider a modelization that incorporates intermixing and surface patterns thanks to fine-discretization of the lattice structure and compositional description. The numerical part will be based on the rejection-free KMC algorithm following Bortz-Kalos-Lebowitz [4]. The algorithm will include different atomic events starting with the fundamental deposition, diffusion and attachment/detachment processes, but will also include intermixing. These processes will be made dependent on different configurations (local height, local neighbourhood …) to account for different effects (ordering, alloying, wetting etc). The energy barriers parameters will be deducted thanks to the comparison between simulation and experimental morphologies and configurations. The possibility of using machine learning methods to systematize the deduction of energy barriers by comparing theory and experience will be investigated. The aim of this coupling between theory and experiment is to gain understanding and control on growth in order to obtain two-dimensional epitaxial deposits of large size and good crystalline quality. The work will be done in close collaboration with the experimental group at INSP.

**Techniques/methods in use**: kinetic Monte-Carlo simulations
**Applicant skills**: solid state physics, analytical and numerical abilities
**PhD supervisor** : Jean-Noël Aqua, aqua.AT.insp.jussieu.fr
**Thesis location**: Jussieu campus

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[3] K. Wang, G. Prévot, J.-N. Aqua, "Anomalous intralayer growth of epitaxial Si on Ag (111)", Sci. Rep. **14** (2024) 2401
[4] Z. Ben Jabra, et al '' Van der Waals heteroepitaxy of air-stable quasi-free-standing silicene layers on CVD epitaxial graphene/6H-SiC'', ACS Nano **16** (2022) 5920