Project for long master thesis
Master Nanosciences-nanotechnologies

Modeling the structure and stability of graphene nanoscrolls

Keywords: multilayer graphene, computer modeling, classical molecular dynamics, nanoscrolls

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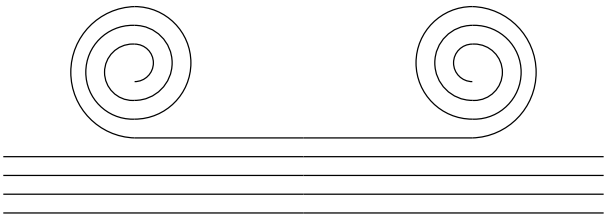
Project description

Experiments have been conducted at Institut Néel (group of J. Coraux) in which graphene multilayers are transferred from the metallic template where they are grown onto a membrane for more convenient spectroscopy and diffraction measurements. Such analyses currently indicate that the edge of the graphite films spontaneously roll to form 'nanoscrolls', but there is no clear evidence about the details of these curved structure would form, or even be stable over longer times.

The goal of the internship is to investigate graphene nanoscrolls by dedicated computer modeling at the atomistic level. In this purpose we will construct realistic candidates for the nanoscrolls involving the upper layer(s) of the graphite sample and leaving them to evolve at various temperatures, with the aim of identifying the possible structural motifs that are most likely to be observed in the experiment, and unravel the structural constraints such nanostructures could exhibit: minimum curvature, number of layers, spatial extent, etc.



Possible nanoscrolls formed by rolling the upper graphene layer of a finite graphite sample

Student profile

Ideally the applicant should be strongly motivated by computational modeling and the use of numerical simulation. Large-scale molecular dynamics code based on the LAMMPS software will be performed on a variety of nanoscroll geometries, for which the initial construction by the candidate will be an initial part of the project.

A taste for programming would also be a welcome addition, in order to analyse the simulation results at later stages of the project.