

## Theoretical studies of novel graphene based nanostructures

A PhD position is open in the “Groupe de Modélisation et Théorie” at SPEC (UMR 3680 CNRS – CEA Saclay).

This theoretical work is dedicated to the study of new carbon materials like graphene nano-meshes (perfectly periodical network of sized holes within the lattice) shape/size controlled graphene flakes and graphene nanoribbons. All these structures are of crucial interest in several modern issues like optics, nanoelectronics and spintronics.

It consists in the study of both atomistic and electronic structures of these new materials, aiming to determinate electronic transport and optical properties.

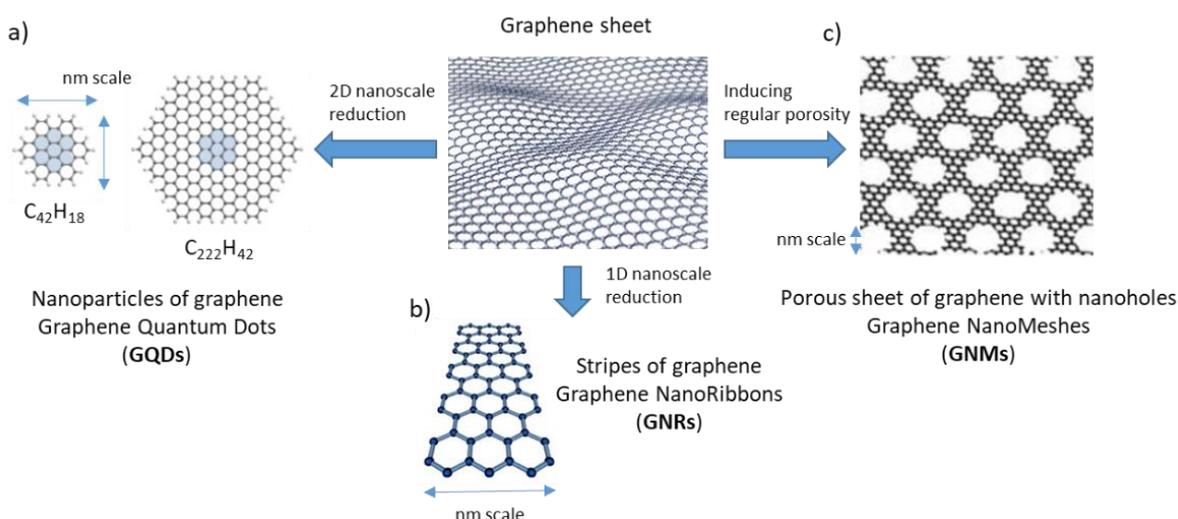
Investigations will be performed with Density Functional Theory (DFT) and tight-binding models. The goal is to determine electronic structure at different levels of accuracy, enabling robustness of predictions for a large range of systems sizes. From this well established electronic structure, the transport properties will firstly be determined within a Green functions formalism. Scanning tunneling microscopy (STM) images as well as tunnel current spectroscopies will also be simulated, in order to compare and analyze experimental data.

Optical response of these materials will be studied from previous DFT results. Absorption or luminescence properties will be calculated help to a combined DFT/tight-binding formalism. A large part of the work here will consist in the development of the tight binding model needed to study the largest structures.

The research performed during this project will be performed within a long-time collaboration network involving experimental teams located in the Saclay area: chemistry groups at CEA-Nimbe and ICMMO, STM/STS at ISMO and optics measurements at LAC.

The PhD student theoretical work will then be performed within this collaboration, ensuring excellent experiment/theory feedbacks and comparisons.

The candidate must have followed condensed matter studies, with a numerical and theoretical background. He/she also should show interest in experimental techniques involved in this project.



### Contacts:

Yannick Dappe  
Sylvain Latil

[yannick.dappe@cea.fr](mailto:yannick.dappe@cea.fr)  
[sylvain.latil@cea.fr](mailto:sylvain.latil@cea.fr)