


**Internship proposal 2011-2012**

<p><b>Laboratory : IMPMC</b></p> <p><b>Address : 4 Place Jussieu, 75005 Paris</b></p> <p><b>Laboratory director : Bernard Capelle</b></p>	
<p><b>Internship supervisor : Francesco Mauri</b></p> <p><b>Phone : 01 44 27 27 64</b></p> <p><b>e-mail: francesco.mauri@impmc.jussieu.fr</b></p>	

**Ultimate mobility of graphene**

The outstanding structural and electronic properties of graphene promote graphene as a promising material for a wide range of nanoscience and nanotechnology applications. In particular, free standing (isolated) graphene exhibits 2D mobilities up to 200000 cm<sup>2</sup>/Vs. The corresponding conductivity, for carrier density larger than 10<sup>12</sup> cm<sup>-2</sup> surpasses that of silver, making graphene the best known conductor at room temperature.

For technological applications, graphene should be supported by a substrate. Supported graphene flakes still exhibit very large 2D mobility but with a reduced value compared to the free standing case. The measured mobility depends on the specific substrate: up to 60000 cm<sup>2</sup>/Vs for graphene on hexagonal BN, and typically 20000 cm<sup>2</sup>/Vs on silica.

The optimization of the conducting properties of unsupported and supported graphene requires knowing and controlling the mechanisms that limit its mobility. However such mechanisms are still much debated. For unsupported graphene, a precise estimation of intrinsic acoustic phonon scattering is still missing. For supported graphene, remote phonon scattering (the scattering of graphene electrons by the polar phonons of the substrate) has been invoked to explain the substrate dependence of the mobility, but, also in this case, a direct experimental or theoretical evaluation of the importance of such mechanism is missing.

In this stage, and in the following thesis, we propose to use first-principles density functional theory calculations to obtain a precise estimation of the mobility-reduction due to acoustic graphene phonons and to remote phonon scattering on different substrates. This will establish the value of the ultimate mobility of supported graphene in undefected samples (in absence of defect scattering).

A fellowship is already available to support a thesis on this subject.

Selected publications of the group on graphene:

*Breakdown of the adiabatic Born-Oppenheimer approximation in graphene*  
S Pisana, M Lazzeri, C Casiraghi, KS Novoselov, AK Geim, AC Ferrari, F Mauri  
Nature Materials 6, 198 (2007)

*Doped Graphene as Tunable Electron-Phonon Coupling Material*  
C Attacalite, L Wirtz, M Lazzeri, F Mauri, A Rubio  
Nano Letters 10, 1172 (2010)

*Transport properties of graphene in the high-current limit*

A Barreiro, M Lazzeri, J Moser, F Mauri, and A Bachtold  
Physical Review Letters 103, 076601 (2009)

**Techniques in use :**

First-principles calculations based on Density Functional Theory of phonons, electrons and of electron-phonon interaction.

**Applicant skills :**

Condensed matter theory, quantum mechanics

**Granted internship :** yes ( about 400 €/month)

**C'nano IdF laboratory (France only) :** yes

**Possibility for a thesis :** a IDS-FunMat fellowship is already available to start a thesis in 2012