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Ab initio calculation of double-resonant Raman spectra for bilayer graphene PAOLA GAVA, LSI - Ecole Polytechnique, MATTEO CALANDRA, MICHELE LAZZERI, FRANCESCO MAURI, IMPMC - Universite Paris 6 — The discovery that the application of an external electric field induces a band gap opening in bilayer graphene attracted a lot of interest on this system, due to important applications in nanoelectronics [1]. Raman spectroscopy is one of the most important experimental techniques for the characterisation of carbon based materials, providing informations on carriers concentration [2], disorder [3], number of layers on multi-layers graphene systems [4], and phonon properties. Most of the theoretical studies on multi-layers graphene are performed using a Tight Binding (TB) model, and full calculation of Raman matrix elements to obtain frequencies, intensities and linewidths of Raman bands has not been performed up to now. The developpement of a fully ab initio theoretical tool to compute Raman spectra is therefore higly desirable and particularly relevant for systems where a simple TB parametrization of the electronic structure and of the electron-phonon interaction is not available. In this talk I will discuss a recently developped methodology to compute fully ab initio double-resonant Raman spectra and I will present results for bilayer graphene.

[1] Ohta et al, Science **313**, 951 (2006), [2] Malard et al, PRL **101**, 257410 (2008), [3] Lucchese et al, Carbon **48**, 1592 (2010), [4] Ferrari et al, PRL **97**, 187401 (2006)

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