

Double resonant Raman in graphene: all you wanted to know about

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Raman spectroscopy is the most widely used experimental characterization technique to study graphene samples. Raman lines such as the defect-induced D and D', their overtones and the D'+D'', are usually interpreted within the double resonance mechanism. These lines are very well studied since they can be used as an experimental probe of the presence of defects but, also, to determine the presence of a monolayer in few-layers graphene samples.

Several excellent theoretical works already appeared on this topic providing an overall good understanding of the situation. However, the many different approximations used by different authors (e.g. constant electron-phonon matrix elements, resonant phonons are assumed to be on some high symmetry line, in some cases the electronic dispersion is conic, the electronic life-time is a parameter, etc.) and the several debates still going on leave with the unpleasant sensation that something is missing. Besides, some fundamental questions are basically untouched: Which kind of defects are probed by measuring different lines? Does Raman spectroscopy probe the defects which mostly influence electronic transport?

We determined [1] the DR Raman spectra of graphene by using the most precise available electronic bands, phonon dispersions, and electron-phonon coupling matrix elements (obtained by combining ab-initio density functional theory and many-body GW methods). Three different model defects are considered. The method results in a consistent framework to determine the position, the shape, the width and the intensity of the Raman lines as a function of the laser energy and of the defect concentration. Moreover it allows to treat at the same level defect-induced lines and two-phonon lines. The overall agreement with available experimental data is very good.

References

[1] P. Venezuela, M. Lazzeri, and F. Mauri, to be published.