Abstract Submitted
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Theory of double-resonant Raman spectra in graphene: intensity and line shape of defect-induced and two-phonon bands PEDRO VENEZUELA, Universidade Federal Fluminense - Brazil, MICHELE LAZZERI, FRANCESCO MAURI, Université Pierre et Marie Curie - France — We calculate the double resonant Raman spectrum of graphene associated to both phonon-defect processes (such as the D and D' lines), and two-phonons ones (such as the $2D$, $2D'$ and $D + D''$ lines). For an excitation energy of 2.4 eV, the agreement with measurements is very good and calculations reproduce the relative intensities among phonon-defect or among two-phonon lines and the measured small widths of the D, D', $2D$ and $2D'$ lines. We determine how the spectra depend on the excitation energy, on the light polarization, on the electronic linewidth, on the kind of defects and on their concentration. The intensity ratio between the D and D' lines depends on the kind of model defect, suggesting that this ratio could be used to identify actual defects. The present analysis reveals that, for both D and $2D$ lines, the dominant DR processes are those in which electrons and holes are both involved in the scattering. The most important phonons belong to the $\mathbf{K}\rightarrow\ \mathbf{\Gamma}$ direction (*inner* phonons) and not to the $\mathbf{K}\rightarrow\mathbf{M}$ one (*outer* phonons), as usually assumed. The small $2D$ line width at $\epsilon_L = 2.4$ eV is a consequence of the interplay between the opposite trigonal warpings of the electron and phonon dispersions.

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