Abstract Submitted
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Calculation of the Raman intensity in graphene and carbon nanotubes[1] MARCUS MOUTINHO, PEDRO VENEZUELA, Universidade Federal Fluminense — Raman spectroscopy is one of the most important experimental techniques for characterization of carbon materials because it can give a lot of information about electronic and phonon structure in a non destructive way. We use a third-order quantum field model to obtain the theoretical Raman intensity for graphene and carbon nanotubes (CNT). The most important Raman peaks in graphitic materials comes from to the iLo and iTo phonon branches near to Γ and **K** points and, in this work, we focus our attention on some of these peaks, like the G, D and 2D bands, as a function of laser energy. The electronic and phonon dispersion used in our calculations reproduces the graphene *ab initio* results with GW corrections and the zone folding method is used to obtain the CNT ones. Our results show that the experimental G band Raman excitation profile for CNT can be reproduced if we use the proper electronic and phonon dispersions. We also show that the phonon dispersion may influence the shape of the graphene D band and the dispersive behavior of the 2D band for graphene and CNT.

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