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Fully *ab initio* calculation of the resonant one-phonon Raman intensity of graphene[1] SVEN REICHARDT, Physics and Materials Science Research Unit, University of Luxembourg; JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, LUDGER WIRTZ, Physics and Materials Science Research Unit, University of Luxembourg — We developed a fully *ab initio*, many-body perturbation theory approach for the calculation of resonant, one-phonon Raman spectra. Our general approach is applicable to any material and here we present its application to the case of graphene. Our diagrammatic, first-principles approach allows us to go beyond and improve on an earlier theoretical study by Basko [1], which relied on an analytical calculation in certain limits. We investigate the dependence of the G peak intensity on both the excitation energy and Fermi level. Furthermore, our method allows us to identify the relevant electronic quantum pathways and to demonstrate the importance of the contributions from non-resonant electronic transitions. We also applied our approach to the calculation of the resonant one-phonon Raman spectrum of MoS_2, with our results being in good agreement with experimental data. Ref.: [1] Basko, D. M. *New. J. Phys.* **11,** 095011 (2009)

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