In-situ Raman spectroscopy as a tool for precise detection of doping and functional groups in carbon allotropes

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The precise detection of ionic, and covalent functional groups attached to the graphitic lattice in diverse carbon allotropes can easily be carried out by Raman spectroscopy. Nevertheless, the unequivocal assignment and resolution of individual vibrational modes associated with the covalent binding of addends was puzzling up to now. Here I will present an in-situ Raman study of a controlled doping, plus functionalization of potassium intercalated graphite, graphene, and carbon nanotubes revealing several new bands appearing in the D-region of the spectrum and a general benchmark for doping. [1,2,3] The development of these defect-related bands as a function of functionalization, from low to restrained levels, provides the basis to deconvolute different components that help in the quantization of sp3 functional groups attached to the graphene surface. By complementary DFT calculations, we were able to identify the vibrational changes in the close proximity of the addend bearing lattice carbon atoms and to assign them to specific Raman modes. This work represents an important step towards an improved understanding of the chemistry of graphene, and intercalation compounds and a remarkable metrology for the accurate assignment of the Raman modes in functionalized graphene and further carbon allotropes.

[1] P. Vecera, et al., Nature Communications, DOI: 10.1038/ncomms15192

[2] J.C. Chacón-Torres, et al., Phys. Status Solidi B, DOI: 10.1002/pssb.201451477

[3] J.C. Chacón-Torres, et al., Carbon, DOI: 10.1016/j.carbon.2016.04.016