Metrology for precise detection of functional groups in graphene by in-situ Raman spectroscopy

Julio C. Chacón-Torres
Philipp Vecera, Thomas Pichler, Stephanie Reich, Himadri R. Soni, Andreas Görling, Konstantin Edelthalhammer, Herwig Peterlik, Frank Hauke, Andreas Hirsch

Yachay Tech University, School of Physical Sciences and Nanotechnology, Urcuquí, Ecuador

jchacon@yachaytech.edu.ec

The mechanism and metrology for an unequivocal assignment as well as the detection of covalent and ionic sites in the lattice of functionalized graphene was elusive, and remained a major challenge for years in the fields of chemistry and materials science. Answering this challenge requires the know-how on performing simultaneously time-dependent in-situ synthesis and characterization of molecular reactions. In this work, we have developed this unique knowledge by conducting an in-situ Raman spectroscopy study of chemically functionalized graphene surfaces.[1] We found several new bands appearing in the D-region of the spectrum, which can be directly assigned to particular structural changes in the graphene lattice and the presence of sp3 site formations. By complementary DFT calculations, we were able to identify the vibrational changes in the close proximity of the addend bearing lattice carbon atoms and assign them to interatomic bonding environments as observed in the Raman spectrum. This work represents an important step in understanding the chemistry of graphene as well as a remarkable metrology system towards the standardization of graphene surface quality measurements via combined in-situ spectroscopy plus computational simulations.

References

[1] Vecera, Philipp; Chacon-Torres, Julio C.; Pichler, Thomas; et al., Nature Comm., 8 (2017) 15192

Figures

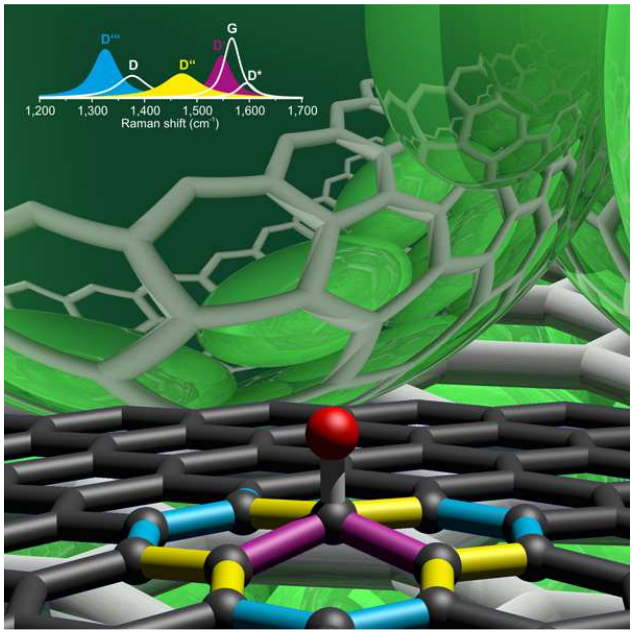

Figure 1: Section of a graphene network with chemically bound hydrogen atom: the spectral vibrational signature of the single carbon-carbon bonds adjacent to the bound hydrogen atom is highlighted in different colors. © Frank Hauke 2017.