Application 2021

Spectroscopic study of C-H vibrational modes in hydrogenated graphene

Chiara Cavallari

Institut Laue Langevin and University of Parma, Grenoble

The recent development of chemical methods to produce graphene by thermal exfoliation of graphite oxide [Chemical methods for the production of graphenes S. Park and R. S. Ruoff, Nat. Nano 4, 217 - 224 (2009)] has allowed the

production of gram-scale quantities of samples. This new discovery has paved the way to investigations using bulk techniques, which are not applicable to single atom layers and, at the same time, has encouraged the experimental research towards more concrete and scalable

applications, as in the field of hydrogen storage. Graphene produced by thermally exfoliated graphite oxide (TEGO) is far from the ideal

honeycomb graphene lattice: it is highly defective because of the synthesis process and shows different in-plane defects and corrugations, which make the surface very reactive. We have already performed an extended characterization of TEGO, synthesized in different conditions and treatedin hydrogen atmosphere using Muon Spin spectroscopy (uSR) [Muons Probe Strong Hydrogen Interactions with Defective Graphene M. Riccò et al. Nano Lett., 2011, 11 (11), pp 49194922 (2011)], Neutron Spectroscopy (INS) [C. Cavallari et al. in preparation], Nuclear Magnetic Resonance (NMR) [Evidences of hydrogen diffusion in chemically produced graphene D. Pontiroli et al. (2013), submitted]and Density Functional Theory (DFT) calculations [C. Cavallari et al. in preparation].

Our studies have witnessed the effectiveness of defects in dissociating the molecule of hydrogen and trapping atomic hydrogen, which is chemisorbed at the graphene surface.

We propose to carry out a IR microspectroscopy study to further back up our understanding of the dynamical properties of hydrogen on graphene with improved energy resolution. FTIR spectroscopy, thanks to its sensitivity to C-H modes, will help us to better understand the configuration of H at the graphene plane and will integrate neutron data-set. The modes in different region of the spectrum will be attributed to

specific H-Csp2/H-Csp3 configurations, as supported by DFT ab-initio calculations, already done to reproduce neutron spectra.

Moreover, while neutron measurements give averaged information over a cm-sized area of the sample, FTIR spectroscopy can allow to isolate the spectral responses coming from different graphene flakes et to locally characterize the samples.

As it is important to handle the TEGO samples in the as grown condition preventing any

exposure to air, we will perform all the measurements in controlled atmosphere , as already discussed with the local contacts.