

Hydrogen interaction and dynamics in defective graphene

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Abstract

In this work [1,2], we performed a detailed study of the hydrogen interaction with defective graphene obtained via thermal expansion of graphite oxide (TEGO), part of which was enriched with about 0.7 wt % hydrogen by a further thermal annealing at 1273 K under H₂ flux at ambient pressure (H-TEGO). The macroscopic availability (grams) of such graphene made possible the investigation with techniques requiring bulk amount of samples, such as Solid State Nuclear Magnetic Resonance (SSNMR), Inelastic Neutron Spectroscopy (INS) and Muon Spectroscopy (μ SR). While the first two are extremely sensitive to hydrogen dynamics, the third can probe the interaction of muonium (an isotope of hydrogen) with graphene[3]. A thermally activated H dynamics is shown by NMR while hydrogen diffusion on the graphene plane is suggested by μ SR. The neutron spectra, on the other hand, reveal the characteristic lines of C-H vibrational modes. Using ab-initio simulations, these signatures allow characterising qualitatively and quantitatively the local environment of the C-H bonds, e.g. at the external edges of the

carbon planes, or located inside in-plane voids. The temperature dependence of the C-H bending modes region of the neutron spectra suggests that the hydrogen atoms environment changes with increasing temperature. We attribute this observation to the onset of atomic H diffusion at surface defects promoted by tunnelling effects.

References

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Figures

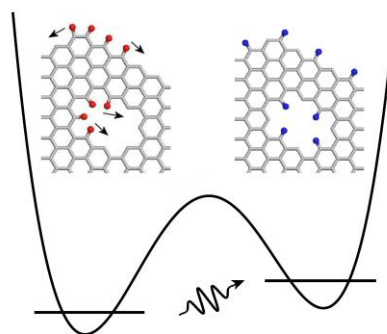


Figure 1: Local reorganization of H atoms in an Asymmetric Double Well Potential: C-H arrangements including dangling bonds are proposed as local stable minima.