Probing graphene-water interactions using hyperfine interactions

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Abstract

The importance of understanding the interaction between graphene and water molecules spans a wide range of applications, not only because it determines the interaction between graphene and a water-based environment but also because adsorbed water molecules directly affect many of graphene's physical and chemical properties (e.g. wetting [1], adhesion [2], electrical doping [3], carrier mobility [4]). Moreover, the structural order of adsorbates on graphene can originate completely new phenomena [5,6].

We present a combination of density functional theory (DFT) calculations and perturbed angular correlations (PAC) experiments dealing with the interaction between graphene, water molecules, and Hg solute atoms/ions. Using PAC, we measure the electric field gradient (EFG) and the magnetic hyperfine field (MHF). By measuring these parameters, and correlating them with DFT calculations, we are able to locally probe the interaction between graphene and the adsorbates, at the atomic scale: structural configuration, stability, and electronic structure. Moreover, by using radioactive probes (^{199m}Hg, in this case) produced at the ISOLDE facility at CERN, we can perform such experiments without the use of external probes (e.g. a tip in scanning probe microscopy) or particle beams (e.g. electron beam in transmission electron microscopy), which can otherwise perturb the probed interactions. As an example of the range of applications of this approach, we discuss the observation of ordered water+Hg structures on the surface of graphene (Fig. 1).

References

[1] Rafiee, J. et al., Nature Mater. 11, 217–222 (2012).
[2] Koenig, et al., Nature Nanotech. 6, 543–546 (2011).
[3] Shim, J. et al., Nano Lett. 12, 648–654 (2012).
[4] Ponomarenko, L. A. et al., Phys. Rev. Lett. 102, 206603 (2009).
[5] Elias, D. et al, Science, 323 (5914), 610−613 (2009).
[6] Nair, R. R. et al, Small, 6 (24), 2877−2884 (2010).

Figures

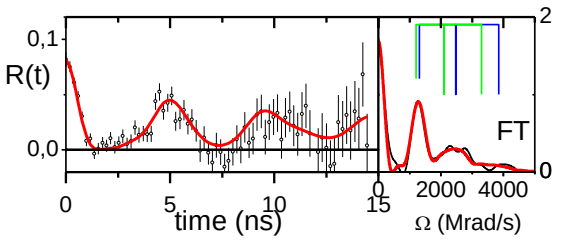

Figure 1: Experimental PAC R(t) function using ^{199m}Hg as a probe for the system Graphene + Water + Hg. The analysis of the Fourier transform (FT) yields two different frequencies (EFGs) associated with two spatial configurations.