ATOMIC LOCAL STUDIES ON GRAPHENE USING ISOLATED AD-ATOM PROBES

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Abstract

The one-atom-thick crystal - **graphene**, uniquely combines extreme mechanical strength, exceptionally high electronic and thermal conductivities, as well as many other exotic properties, all of which make it highly interesting for fundamental physics and numerous applications. Its properties strongly depend on surface and interface nanoscale interactions, where new physical models should apply aiming their understanding and control.

In the present work we investigate the mechanisms of adhesion of ad-atoms on the surface, alone or when forming clusters, preferably in regions of structural defects (of different kinds), their capture processes, adsorption and migration of atoms. The aim is to investigate electronic, magnetic or catalytic properties. Understanding how the adsorption could be controlled would contribute to the development of innovative devices based on graphene. Experimental works are accompanied by theory and computational models generally based on *density functional theory* and/or molecular dynamics calculations, providing an important support for studying the electronic properties. In this context, our experimental observables are the hyperfine parameters of add-atoms on graphene, measured with the nuclear spectroscopy PAC (*Perturbed Angular Correlations*) technique. PAC allows to probe at the atomic scale the add-atoms interactions without interfering with the graphene electronic structure, thereby providing unique information, which is impossible to obtain by electron spectroscopy and electron microscopy techniques such as, AFM or STM, not exempted from interactions between the tip and the surface test or ad-atoms therein. By PAC measurements it can be determined the electric field gradient (EFG) and magnetic hyperfine field (MHF) at atomic scale, electronic structure and magnetic environment of ad-atoms. The EFG provides structural information, location of the probe, stability, and bond (ionic, covalent bonding, van der Waals). The MHF translates properties correlated with the electronic spin configuration.

In this presentation we will present first results of the PAC hyperfine parameters obtained in graphene grown at different substrates as a function of different temperatures and different probing elements, ^{111m}Cd and ^{199m}Hg. To complement the experimental studies, *ab initio simulations*, using the software *Wien2k* and *VASP*, with the self-consistent LAPW+lo and PAW methods to solve the Kohn-Sham

equations and GGA/LDA approximations, have been implemented to simulate the charge density distribution of ad-atoms on graphene for different probe isotopes. This is the first step to attain the next objective that is to understand the Cd, and Hg (our PAC probes) interactions at the graphene layer. Minima of energy for the ideal bond-length, the hyperfine parameters and the charge distributions in the unit cells will be presented.

These are preliminary experimental and simulation results of a large portfolio of experiments and ideas, which are envisaged to come.

References

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Figures

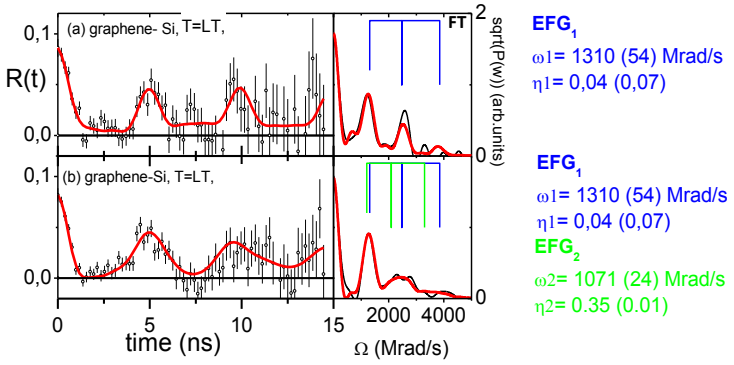

Fig.1 – First *PAC* results, on graphene/Si with ^{199m}Hg probe. We can observe 2 different local environments, characterized by EFG_1 and EFG_2.

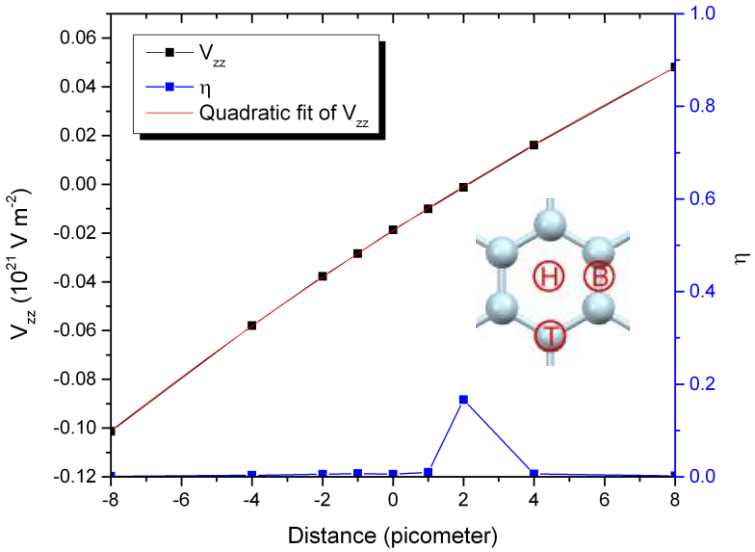

Fig.2 – *Ab initio simulation* with VASP. Variation of principal component of electric field gradient, V_{zz}, and asymmetry parameter, $\eta = (v_{yy}-v_{xx})/v_{zz}$, of Cd (at the H site) as a function of displacement relative to the equilibrium position, along the c axis. It is possible to assign a linear behavior for V_{zz}, which is sensitive to variations of the order of picometer.