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HYPERFINE STUDIES ON GRAPHENE USING ISOLATED AD-ATOM PROBES

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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.
The aim of this work is to use radioactive ad-atoms attaching to graphene to investigate several aspects:
The first motivation concerns the investigation of adhesion mechanisms of atoms alone or when forming clusters, their adsorption, migration and interaction with surface defects. Understanding how and if adsorption could be controlled could contribute to the development of innovative devices based on graphene, such as quantum detectors of single molecules with applications in catalysis and nucleation of clusters in nanostructures, ballistic transistors and spintronic devices.
The second motivation of our experimental, concerning the probing of fundamental electronic properties, relies on the type of experimental observables, which are the hyperfine fields measured by ad-atoms on graphene. The experimental method is the nuclear spectroscopy Perturbed Angular Correlations (PAC) technique that allows probing at the atomic scale the ad-atom/graphene interactions without further interference with the graphene electronic structure, other than its atomic bonding. We believe that any electronic perturbation at the level of the graphene intrinsic properties, either electric or magnetic will reveal at the highly sensitive hyperfine parameters, thereby providing unique local, single atom, information, which is impossible to obtain by other techniques like 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.
In this brief communication 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, 111mCd and 199mHg. To complement the experimental studies, ab initio simulations, using the software Wien2k and VASP, with the self-consistent LAPW+lo method to solve the Kohn-Sham equations and GGA approximation, 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 hiperfiines 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.

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