Contribution ID: **35** Type: **Poster**

HYPERFINE TECHNIQUES STUDIES OF GRAPHENE USING ISOLATED AD-ATOM PROBES

Wednesday 2 December 2015 18:20 (2 hours)

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 aim investigating the mechanisms of adhesion of ad-atoms on the surface, their capture processes, adsorption and migration of atoms, alone or intermediated by water and defects. The later aim is to investigate electronic, magnetic and catalytic properties resulting from such "dopant"like interactions. 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, 111mCd and 199mHg. To complement the experimental studies, ab initio simulations, using the software Wien2k, with the self-consistent LAPW+lo method 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.

Author: DA SILVA FENTA, Abel Eduardo (University of Aveiro (PT))

Co-authors: GOTTBERG, Alexander (CERN / CENBG / CSIC); MARTINS CORREIA, Joao (Instituto Superior Tecnico (PT)); SANTOS GONCALVES, Joao Nuno (University of Aveiro (PT)); JOHNSTON, Karl (CERN); DA COSTA PEREIRA, Lino Miguel (KU Leuven (BE)); AMARAL, Vitor (Universidade de Aveiro); KADI, Yacine (CERN)

Presenter: DA SILVA FENTA, Abel Eduardo (University of Aveiro (PT))

Session Classification: Poster Session