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ATOMIC LOCAL STUDIES ON GRAPHENE USING ISOLATED AD-ATOM PROBES

The one-atom-thick crystal - graphene, uniquely combines many exotic properties such as huge mechanical strength with high electronic and thermal conductivities, among others, which make it interesting for fundamental physics and applications. Its properties strongly depend on surface and interface nanoscale interactions, where the 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 based on density functional theory, quite adequate for simulating the electronic properties and the hyperfine parameters which consist of our experimental observables, as measured with the nuclear spectroscopy Perturbed Angular Correlations (PAC) technique. PAC allows probing at the atomic scale the add-atoms interactions without interfering with the graphene electronic structure, thereby providing unique information. PAC measures the electric field gradient (EFG) that provides structural information, location of the probe, stability, and bond (ionic, covalent bonding, van der Waals), and the magnetic hyperfine field (MHF) that translates properties correlated with the electronic spin configuration.
We will present some results of the PAC hyperfine parameters obtained in graphene grown at different substrates using199mHg as a probe. 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. This is the first step to attain the next objective that is to look for the bonding of isolated ad-atoms at the graphene surface there brought by soft landing (evaporation) of the radioactive probe under UHV ambient.

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