Point defects in graphene systems

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How does the presence of single atomic defects modify the properties of materials? Such a general and fundamental question is addressed by our work for atomic vacancies in graphene systems, where the presence of such defects is expected to have a dramatic impact in its properties due to graphene's pure bidimensionality. Introducing vacancies in graphene-like systems by irradiation has been shown to be an efficient method to vary its mechanical behavior, tune its electronic properties and even to induce magnetism in otherwise non-magnetic samples [1-3]. While the role played by these vacancies as single entities has been extensively addressed by theory [4-7], experimental data available refer to statistical properties of the whole heterogeneous collection of vacancies generated in the irradiation process [1-3]. In this talk I will show how we have overcome this limitation: we first created perfectly characterized single vacancies on graphene layers by Ar+ ion irradiation and then, using low temperature scanning tunneling microscopy (LT-STM), we individually investigated the impact of each of such vacancies in the electronic, structural and magnetic properties of several graphene systems [8-10].

I will first show our results about the role of single isolated vacancies generated in a graphene layer weakly coupled with the substrate as it is the graphite surface [8]. Very recently, it has been predicted that individual carbon vacancies in graphite could even originate room temperature magnetism. Our LT-STM experiments, complemented by tight-binding calculations, reveal the presence of a sharp electronic resonance at the Fermi energy around each single graphite vacancy, which can be associated with the formation of local magnetic moments and implies a dramatic reduction of the charge carriers' mobility. While vacancies in single layer graphene lead to magnetic couplings of arbitrary sign, our results show the possibility of inducing a macroscopic ferrimagnetic state in multilayered graphene just by randomly removing single C atoms.

A fundamental question which naturally follows is: Will properties of this atomically tailored graphene survive in real devices after the unavoidable contact with other materials, in particular with metals? In the second part of the talk, I will show how we combined LT-STM studies with density functional theory calculations to address such a key question, demonstrating that even in weakly coupled graphene/metal systems, the presence of the metal has to be seriously taken into account in order to controllably tune graphene properties by locally modifying its structure [9]. In particular, we have demonstrated that while electronic properties of pristine graphene are basically preserved when adsorbed on Pt(111) surfaces, vacancy sites become reactive leading to an increase of the coupling between the graphene layer and the metal substrate at these points; this gives rise to a rapid decay of the localized state and the quenching of the magnetic moment associated with carbon vacancies in freestanding graphene layers.

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Figures:

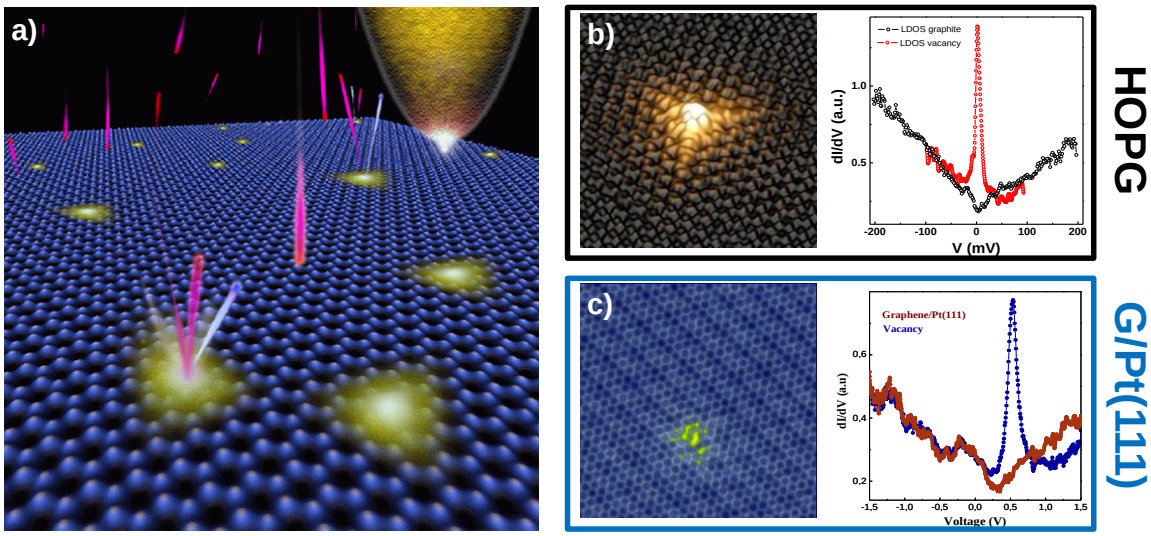

Fig 1: a) Art illustration of a graphene layer atomically tailored by introducing single carbon vacancies. Vacancies are deliberately generated by irradiating the graphene layer with Ar ions (represented by red balls) and its impact in the electronic, structural and magnetic properties of the graphene layer is investigated at the atomic scale by means of a scanning tunneling microscope (represented by the cone-tip at the upper right corner). b) This 3D image (left panel), obtained with a home-made LT-STM, shows a single isolated atomic vacancy artificially created on a graphite surface. A sharp electronic resonance peak has been found on top of each individual vacancy (right panel), which can be associated with the generation of a magnetic moment in this pure carbon system. c) Left panel shows a 3D view of a single isolated vacancy created in the graphene/Pt(111) surface. Right panel corresponds to 6 K STS measurements of the LDOS on a C vacancy (blue circles) and on pristine graphene/Pt(111) showing the existence of a broad electronic resonance above the Fermi energy associated to single C vacancies in this system.