Probing nanostructures with forces and currents: From atomic-scale contrast on graphene and carbon nanotubes to heterofullerene synthesis with planar aromatic precursors

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In this talk, we focus on the application of Scanning Tunneling (STM) and Frequency-Modulation Atomic Force (AFM) microscopy [1] to carbon nanostructures (graphene, carbon nanotubes and fullerenes). The simple honeycomb structure shared by these materials represents both a perfect testing ground and a fundamental challenge for scanning microscopy imaging. STM can achieve atomic resolution in graphite even in ambient conditions but, after 25 years of research, still there is no consensus whether the maxima in the atomic scale images correspond to atoms or to the hollow sites. To tackle this long-standing problem, we have performed complex first-principles calculations of forces and currents between a tip and carbon nanostructures. Our results explain the rich variety of image patterns observed in both AFM and STM experiments in terms of two factors: (i) the tip-sample distance and (ii) the chemical reactivity of the tip [2]. Based on this work, we have explored the electronic properties of epitaxial graphene on metals, both in the case of the pristine layer and in the presence of carbon vacancies, where the calculations help to correlate the structure of the defect with the experimental STM images [3]. These calculations also shed light on the possible magnetic state associated with these defects, predicted but not experimentally confirmed, in graphite [4].

Finally, we'll discuss the microscopic mechanisms behind the different steps involved in our recent proposal for a controlled synthesis of heterofullerenes based on a surface-catalysed cyclo-dehydrogenation process [5, 6]. With this approach it is possible to transform with an almost 100% efficiency polycyclic aromatic hydrocarbons like C60H30 and C57N3H33, deposited on Pt(111) surfaces, into C60 fullerenes and triazafullerenes C57N3.

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