Structure, electronic configuration and molecular interactions of organic layers on surfaces

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The fundamental of molecular electronics lies in the use of the strongly non-linear transport characteristics through single molecules or molecular layers in order to induce effects like rectification of an electric current or negative-differential resistance, crucial for the operation of logic devices. On the first grounds such non-linear effects are a consequence of the orbital structure of the molecules. When adsorbed on a metal surface, molecular states become localised resonances so far the molecules are weakly interacting with the electrodes contacting the molecule. Scanning tunnelling microscope is an ideal tool to investigate the structure and the transport characteristics of "molecular devices". On the one hand it provides a detailed characterization of the molecular orientation, conformation and contact with the substrate electrode, which allows us to resolve the role of molecular interactions within the layer. On the other hand, the spectroscopic mode of STM can provide information about transport mechanisms, including resonant tunnelling, and tunnelling mediated by molecular vibrations.

In this presentation I will resume the basic principles of molecular self organization, in which the structure of molecular layers and nanostructures formed at the surface of a "weakly interacting" metal (gold) can be rationalised as a balance between intermolecular interactions and molecular-surface interaction. In the second part of this presentation I will illustrate the concept of scanning tunnelling spectroscopy (STS) applied to the resolution of molecular states (molecular orbitals) and how are they interacting with the metal surface. In addition to this STS is also sensitive to tunnelling processes involving the excitation of molecular vibrations by tunnelling electrons. As molecular vibrational modes are a fingerprint of the chemical nature of a molecule, this resolution allows us not only to see and measure molecules, but to say what are the atoms forming the molecule.