

Nanopit formation induced on surfaces by molecular deposition

M. Pedio

*TASC national Laboratory INFN-CNR
Basovizza, 34012 Trieste, Italy*

The mechanism of large C-molecule anchoring on surfaces is due to a balance of intermolecular binding forces and of molecule-substrate interaction involving a large number of sites. This can result in either displacive substrate reconstructions, involving extensive mass transport, and/or in complex structural deformation of the adsorbed molecules. The molecule-substrate system must be taken into account as a whole and it is not possible to simply transfer molecular functionalities, deduced in their isolated state, to the adsorbed case. Adsorption of complex carbon based molecules on metal and semiconductor interfaces may lead to the formation of highly ordered nano-structuration through molecule-substrate bonding. Novel artificial structured materials with tailored properties are under study and these molecules can then be exploited, in principle, for the fabrication of surface supported nanostructures, as molecular building blocks confined to two-dimensional systems.

In this context C_{60} is considered a prototype nanomolecule [1] with its spherical shape and its interaction with surfaces is a model system: the presence of strong directional π molecular states, together with the capability of being an acceptor or donor of electrons, allows fullerene to establish different kinds of interaction, ranging from van der Waals to ionic and to covalent bonding, through the C atoms that are in direct contact with the substrate.

This contribution aims to give an overview on the fullerene/surface systems. The mechanism of molecular and local substrate deformation induced by chemisorption substrates has been studied by Surface X-ray diffraction, compared with C K-edge absorption spectroscopy and Inverse Photoemission spectroscopy results. All our studies [2,3,4] have shown that the adsorption of C_{60} molecules induces large an unpredicted reconstruction deeply modifying the substrate original structure [5]. The energy, necessary to displace a large number of surface atoms from their original “bulk like” position, is due to the strong interaction between the π molecules orbitals and the substrate electrons. Density Functional Theory simulations indicate that the strong directional interaction between fullerenes and topmost surface atoms induces the formation of nanoscopic pits hosting the molecules. This phenomenon can have general implications on the adsorption of complex carbon based molecules on metal surfaces and could lead to the revision of some interaction mechanisms determined by STM analysis.

/1/ P. Rudolf, G. Gensterblum and R. Caudano, *Journal de Physique IV (Colloque)* **7**, 137 (1997)

/2/ M. Pedio, R. Felici, X. Torrelles, et al., *Phys. Rev. Lett.* **85**, 1040 (2000)

/3/ M. Hinterstein, X. Torrelles, R. Felici et al., submitted to *Phys. Rev. Lett.*

/4/ R. Felici, M. Pedio, F. Borgatti, et al., *Nature Materials* **4**, 688 (2005)

/5/ See also X. Torrelles, J. Rius, O. Bikondoa, et al., *ESRF Newsletter* **39**, 17 (2004)