NEW ROUTES FOR RATIONAL SYNTHESIS OF NANOSTRUCTURES: ON-SURFACE SYNTHESIS AT WORK

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Abstract

Creating or connecting together organic molecules, as polycyclic aromatic hydrocarbons (PAH), by chemical reactions readily on surfaces is the first step to a true advance in the field of molecular electronics. On-surface chemistry has become one of the most important strategies for bottom-up assembly of new nanostructures from their constituent molecular building blocks. Although diverse compounds have been formed in recent years using this methodology, a limited knowledge on the molecular machinery operating at the nanoscale has so far disallowed to control the reaction outcome.

We combined advanced in-situ surface techniques as STM, high-resolution XPS and NEXAFS with theoretical ab-initio (DFT) calculations to achieve a complete understanding of the self-assembling of organic molecules on metallic surfaces and to follow different coupling reactions between them. Thus, nanostructures of different dimensionality can be assembled “a la carte” just by choosing the adequate molecular precursor, temperature and the suitable surface termination.

Thus, in this talk, by merging information from these techniques and different single-crystal metal substrates, we report on the thermal controlled competitive intramolecular and intermolecular dehydrogenative processes respectively called cyclodehydrogenation and dehydrogenative polymerisation, which operate in the on-surface synthesis of N-doped fullerene, nanographene, polyaromatic network, single molecule polymers, membranes or graphene.

Keywords: STM, DFT, on-surface chemistry, dehydrogination

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