

FULLERENES FORMATION FROM AROMATIC PRECURSORS BY A SURFACE CATALYSED CYCLODEHYDROGENATION PROCESS.

J.A. Martín-Gago, G. Otero¹, G. Biddau², C. Sánchez-Sánchez¹, R. Caillard¹, M. F. López¹, C. Rogero³, F. J. Palomares¹, N. Cabello⁴, M. A. Basanta², J. Ortega², A. M. Echavarren⁴, J. Méndez¹, R. Pérez², B. Gómez-Lor¹

1.-Instituto de Ciencia de Materiales de Madrid (CSIC). Cantoblanco, 28049-Madrid, Spain 2.- Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, 28049-Madrid, Spain 3.-Centro de Astrobiología – CSIC-INTA. Ctra. de Ajalvir Km.4, 28850 -Torrejón de Ardoz, Madrid, Spain 4.-Institute of Chemical Research of Catalonia (ICIQ), Av. Països Catalans 16, 43007-Tarragona, Spain

gago@icmm.csic.es

Controlled synthesis of fullerenes and heterofullerenes on surfaces is a preceding step towards the development of a true fullerene-based molecular electronics. New methods are required for the rational, size-controlled synthesis of fullerenes, heterofullerenes, and endohedral fullerenes that cannot be accessed by the current method of graphite vaporization. Recently, pioneering experiments have shown that C₆₀ fullerene can be formed by flash vacuum pyrolysis of a trichlorinated precursor C₆₀H₅₇Cl₃. However, this precursor was prepared in 11 steps from commercially available materials and the final dehydrogenation/dehydrochlorination proceeds in the gas phase in ca. 0.1-1.0% yield¹. Here we report a highly efficient (<100%) dehydrogenation mechanism leading to the formation of fullerene C₆₀ and the first triazaful fullerene C₅₇N₃ in a one-step from the corresponding planar polycyclic aromatic precursors by a surface catalysed process². We have visualized the whole process by in-situ Scanning Tunneling Microscopy (STM) and X-Ray Photoemission spectroscopy (XPS). The cyclodehydrogenation has been confirmed by the thermal desorption of HD and D₂ from hexadeuterated 1-d₆ precursors, by the mass-spectrometric detection of C₆₀ in the platinum-catalysed dehydrogenation, and the whole process followed by first principles DFT calculations.

The process is catalysed by reactive substrates, as Pt, which favour strong surface-molecule interactions. The mechanism we describe opens the door to size-controlled production of fullerenes and heterofullerenes, it could allow the encapsulation of different atomic and molecular species to form endohedral fullerenes and to the formation of different carbon-based nanostructures, such as doped graphene, which nowadays are not readily available on surfaces by other methods.

References:

[1] Scott, L.T. *Science* **295**, (2002)1500.

[2] G. Otero, G. Biddau, C. Sánchez-Sánchez, et al. *Nature*, in press

Figures:

