

Fullerene and Nanotube-like electronic states experimentally observed in [5,5]-C₉₀ fullertube molecules.

Ó. Jover,^{*1,2} A. Martín-Jiménez,² H. M. Franklin,³ R. M. Koenig,³ J. I. Martínez,⁴ N. Martín,^{2,5} K. Lauwaet,² R. Miranda,^{1,2,6} J. M. Gallego,⁴ S. Stevenson³ and R. Otero.^{1,2,6}

¹ Dep. De Física de la Materia Condensada, Universidad Autónoma de Madrid, 28049 Madrid, Spain

² IMDEA Nanoscience, 28049 Madrid, Spain

³ Purdue University Fort Wayne, Dep. Of Chemistry and Biochemistry, Fort Wayne, Indiana 46805, United States

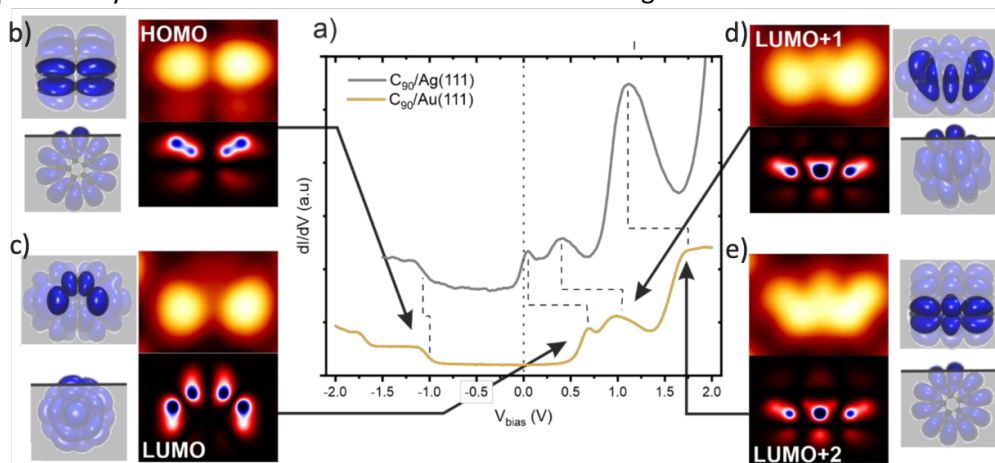
⁴ Instituto de Ciencia de Materiales (ICMM), CSIC, 28049 Madrid, Spain

⁵ Dep. De Química Orgánica, Facultad de Ciencias Químicas, Universidad Complutense de Madrid, 28040 Madrid, Spain

⁶ IFIMAC, Universidad Autónoma de Madrid, 28049 Madrid, Spain.

* oscar.jover@imdea.org

Fullertubes, defined as a carbon nanotube moiety capped by hemifullerene ends, have emerged as new and promising carbon structure whose properties are expected to show both fullerene and carbon nanotube traits. Although there might be expected electronic states with resemblance to those of the extended CNT, such correlation has not yet been described. Here we show an STM and STS characterization of the adsorption, self-assembly and electronic structure of two-dimensional arrays of [5,5]-C₉₀ fullertubes on Ag(111) and Au(111). Our results demonstrate that the shape of the MO's of the adsorbed molecules corresponds closely to those expected for isolated species on the grounds of DFT calculations. Moreover, comparison between the electronic density profiles in the bands of the extended [5,5]-CNT and C₉₀ reveals that some of the frontier orbitals of the [5,5]-C₉₀ can be described as the result of the quantum confinement imposed by the hemifullerene caps to the delocalized valence and conduction band states in the extended CNT. Our work thus provides a conceptual framework for the rational design of custom fullertubes with new and interesting electronic behavior and can potentially become a cornerstone in our understanding of these new carbon nanoforms.



a) Mean dI/dV curves recorded on C₉₀ fullertubes area adsorbed on Ag(111) and Au(111). Both curves show similar spectral distribution with peaks positions shifted with respect to each other. STM images for each peak's energy observed in (a) (red-orange scale images) correspond well with the areas in which the calculated wave functions of HOMO, LUMO, LUMO+1 and LUMO+2 of isolated molecules shows the topmost lobes (grey-blue scale images). As an addition calculated 2D maps of the wave-function modulus at a given height over the molecular axis (red-blue scale images).