[O7B.2]

New high-pressure fullerene structures

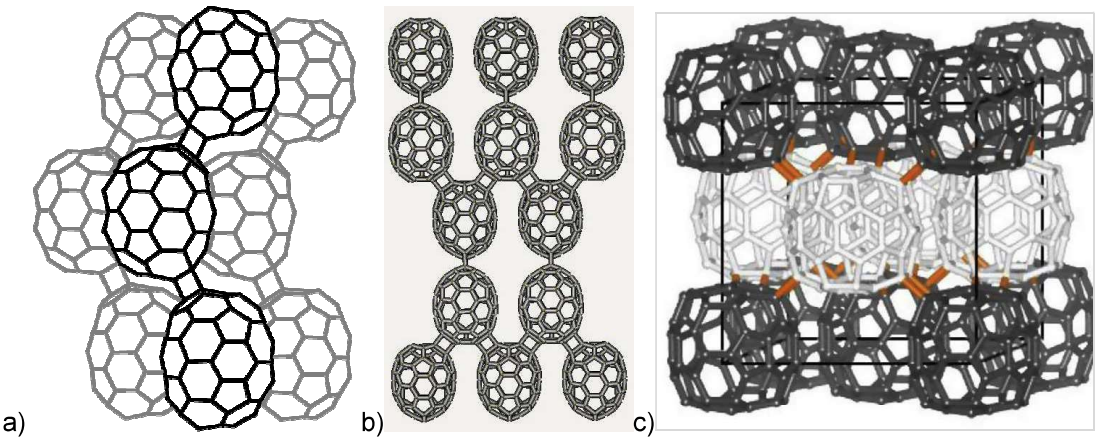
J. Laranjeira, L. Marques*

Departamento de Física and Ciceco, Universidade de Aveiro, Portugal

New polymerized phases of fullerenes were prepared under high pressure and high temperature. Their crystal structures were determined through a combined experimental-theoretical effort; x-ray diffraction methods, laboratory and synchrotron, complemented by density functional theory (DFT) modeling, were employed.

Two novel C_{70} phases were prepared at 10GPa-270ºC and 7GPa-600ºC [1-3]. The first of these structures consists of one-dimensional (1D) zig-zag polymer, while the second structure consists of buckled-hexagon two-dimensional (2D) polymerized planes (see fig.1).

A new C_{60} face centered cubic (fcc) phase, with a short lattice constant, was prepared at 9.5GPa and 550ºC [4]. DFT calculations showed that the short interfullerene distances corresponds to polymeric 56/56 2+2 cycloaddition bonds. This bonding type forms between molecules having different standard orientations, although no covalent bond forms between similarly oriented molecules. Several ordered 3D polymerized C_{60} structures, based on the well-known ordered binary-alloy structures, were constructed. They display lower symmetry than the experimentally observed fcc structure suggesting that this should be a disordered/frustrated structure.



a) b) c)

Figure 1. New crystal structures of C_{70}, a) and b), and of C_{60} , c).

The electronic properties of these novel fullerene structures were investigated by DFT. While the 1D and 2D C_{70} structures are semiconductors the 3D C_{60} polymers show metallic behaviour [4].

[1] L. Marques et al. Carbon 82, (2015) 599-603.

[2] L. Marques et al. Phys. Stat. Sol. RRL 9, (2015) 535.

[3] L. Marques et al. Materials Today: proceedings 4 (2017) 11564-11569.

[4] J. Laranjeira et al. Carbon 137, (2018) 511-518.

[5] J. Laranjeira et al. Phys. Stat. Sol. RRL 11 (2017) 1700343.

Ackowledgment: This work was supported by projects POCI-01-0145-FEDER-031326 financed by FCT and co-financed by FEDER and CICECO-Aveiro Institute of Materials, FCT

Ref. UID/CTM/50011/2019, financed by national funds through the FCT/MCTES. J. Laranjeira acknowledges a PhD grant from FCT (SFRH/BD/139327/2018).

Keywords: fullerenes, high-pressure, x-ray diffraction, modeling