New high-pressure fullerene structures

J. Laranjeira*, L. Marques*
Departamento de Física and CICECO, Universidade de Aveiro, 3810 Aveiro, Portugal

New polymerized phases of fullerences 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\textsubscript{70} phases were prepared at 10GPa-270°C and 7GPa-600°C [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\textsubscript{60} face centered cubic (fcc) phase, with a short lattice constant, was prepared at 9.5GPa and 550°C [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\textsubscript{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.

![Figure 1](image1.png)  
**Figure 1. New crystal structures of C\textsubscript{70}, a) and b), and of C\textsubscript{60}, c).**

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

Acknowledgment: 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).