P01 - 3D C60 POLYMERS WITH ORDERED BINARY-ALLOY TYPE STRUCTURES INVESTIGATED VIA DFT

J. Laranjeira[a*], L. Marques[a], N. M. Fortunato[a], M. Melle-Franco[b], K. Strutyński[b] and M. Barroso[c]

[a] Departamento de Física and CICECO, Universidade de Aveiro, 3810 Aveiro, Portugal.
[b] Departamento de Química and CICECO, Universidade de Aveiro, 3810 Aveiro, Portugal.
[c] Departamento de Física and I3N, Universidade de Aveiro, 3810 Aveiro, Portugal.
[*]Corresponding Author: jorgelaranjeira@ua.pt

Three-dimensional (3D) C60 polymerized structures with each molecule adopting one of the two standard orientations, have been studied via density functional theory methods (DFT). Well-known ordered binary-alloy (AB) structures - AuCuI, Au_3Cu, CuPt, "A_2B_2" - , have been used as prototypes, in which one standard orientation corresponds to atom A and the other orientation corresponds to atom B. In all the studied structures there is no bond between molecules with the same orientation but between molecules with different orientation there is the formation of a 56/56 2+2 cycloaddition polymeric bond. It, thus, corresponds to an orientational antiferromagnetic interaction and the system can be mapped onto Ising fcc antiferromagnet. The bonding type, 56/56 2+2 cycloaddition, is different from the 66/66 2+2 cycloaddition characteristic of the low-dimensional, 1D and 2D, C60 polymers, as it is formed between intramolecular single bonds of neighboring molecules and not between intramolecular double bonds.

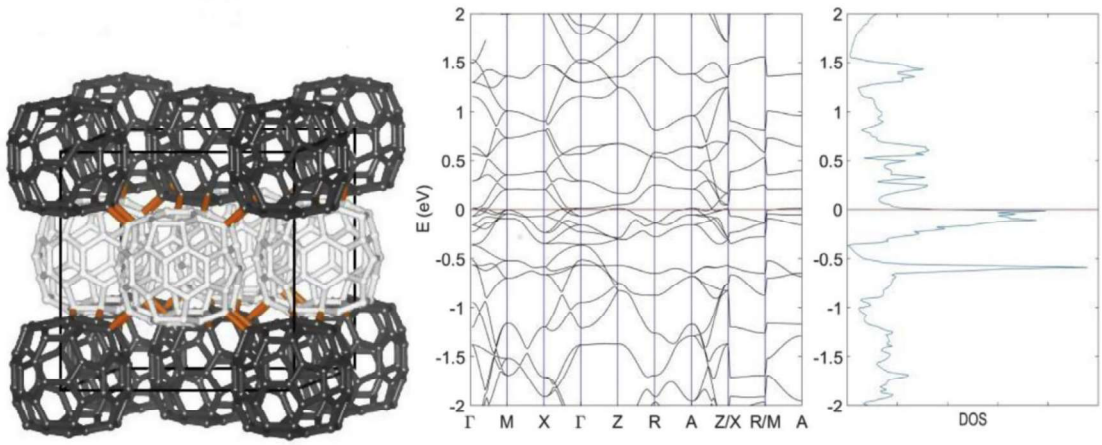

Figure 2 crystal structure, electronic band structure and density of states of the AuCuI-type C60 polymer structure.

These 3D polymer structures are candidates to be obtained experimentally at high pressure once the observed frustration could be relieved [1]. Their structural, elastic and electronic properties were calculated at room pressure and at 9.5 GPa and all of them show a metallic behavior [2].

References

[1] J. Laranjeira, L. Marques, M. Mezouar, M. Melle-Franco, K. Strutyński, Phys. Stat. Sol. RRL, 11, 1700343 (2017).
[2] J. Laranjeira, L. Marques, N. Fortunato, M. Melle-Franco, K. Strutyński, M. Barroso, Carbon, 137, 511-518 (2018).