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DFT study of novel 3D C_{60} polymers

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Abstract

New three-dimensional (3D) C60 polymerized structures, in which each molecule adopts either one of the two standard orientations, have been investigated using the density functional theory (DFT) method. Ordered binary-alloy type structures (AuCuI, Au_3Cu, CuPt, "A_2B_2") were used as prototypes in constructing 3D C60 polymerized structures, one standard orientation corresponding to the A atom and the other orientation to the B atom. DFT structural optimizations show that intermolecular bonds, 56/56 2+2 cycloaddition, form between molecules with different orientations but no intermolecular covalent bond is formed between similarly oriented molecules, and, thus, the intermolecular covalent bonding can be mapped on to the antiferromagnetic interaction. This intermolecular bonding type forms between two intramolecular single bonds of neighbouring molecules and differs from the more common 66/66 2+2 cycloaddition that forms between intramolecular double bonds.

The electronic and elastic properties of these polymerized structures were also calculated, within the general gradient approximation framework, at room pressure and at 9.5 GPa. All these structures show metallic behaviour [1] and their bulk moduli range from 88 to 132 GPa [2]. These 3D polymerized structures are likely to be prepared at 9.5 GPa and 550ºC, although the observed fcc structure points to a disordered/frustrated structure, which is characteristic of the Ising antiferromagnetic interactions in the fcc lattice [3].

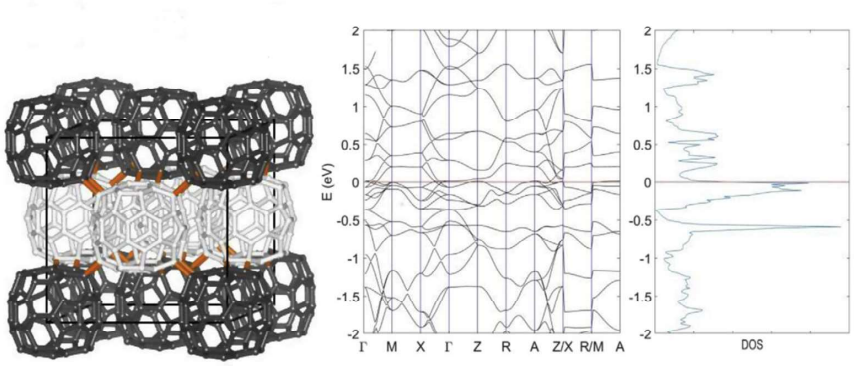

Figure 1 crystal structure, electronic band structure and density of states of the AuCuI-type C60 polymer structure

References

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

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