# Study of the geometric and energetic properties of carbon nano-onions with vacancy defects produced by ionizing radiation

*Ronaldo Méndez Hernández* [1], *Daniel Codorniu Pujals* [1], *Maykel Márquez Mijares* [1]

[1] Instituto Superior de Tecnologías y Ciencias Aplicadas (InSTEC), Universidad de La Habana, Ave. Salvador Allende No. 1110, Plaza de la Revolución, Cuba

mmarquez@instec.cu

Carbon Nano-Onions (CNOs) has allowed the development of multiple applications due to their remarkable physicochemical properties [1-3]. Since the discovery of these nanostructures, one of the main phenomena that has startled the scientific community has been the obtaining of practically spherical nano-onions from polyhedral particles using intense electron beams [4-6]. Today the rigorous explanation of this phenomenon continues to be a pending issue, among other things, because it has not been possible to achieve a model capable of explaining it.

Using the computational method based on the Density Functional Theory with Thight-Binding Approximation (DFTB+), the geometries of fullerenes of order $n \leq 6$ (2160 atoms) were optimized and the different energetic and geometric parameters of fullerenes and polyhedral CNOs were calculated. From the induction of mono and divacance defects in these nanostructures, the possible structural deformations caused in these arrangements were analyzed, as well as the formation energies.

[1] Castagnino, J. M. *"Técnicas, materiales y aplicaciones en nanotecnología"*. Acta bioquímica clínica latinoamericana, 41 (2007) 189-191.

[2] Delgado, J. L., Herranz M. A., and León, N. M. *"Nanoestructuras de carbono: un nuevo desafío científico"*. Anales de Química de la RSEQ, 103 (2007) 5-5.

[3] Palkar, A., et al. *"Reactivity differences between carbon nano onions (CNOs) prepared by different methods"*. Chemistry–An Asian Journal, 2 (2007) 625-633.

[4] Ugarte, D. *"Curling and closure of graphitic networks under electron-beam irradiation"*. Nature, 359 (1992) 707-709

[5] Ugarte, D. *"Formation mechanism of quasi-spherical carbon particles induced by electron bombardment"*. Chemical physics letters, 207 (1993) 473-479.

[6] Ugarte, D. *"Onion-like graphitic particles"*. Carbon nanotubes, (1996) 163-167.

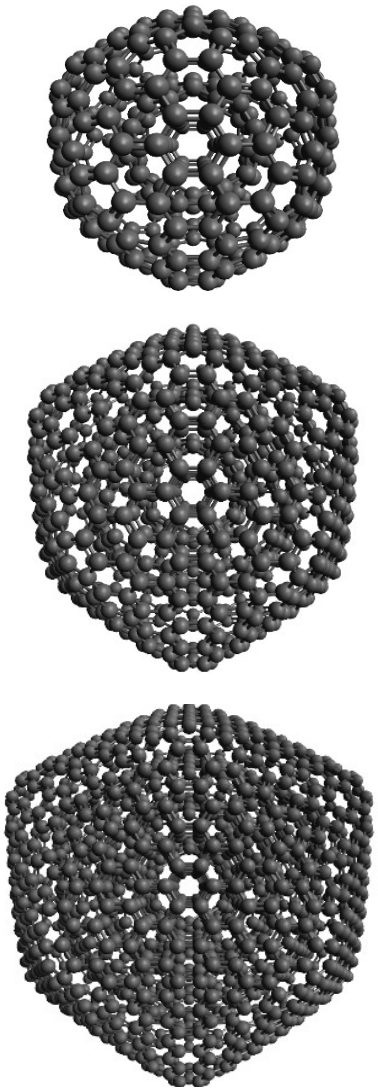

Figure 1: *The structures of some CNOs obtained after being optimized with DFTB+ at 300K are shown. From up to down (C60@C240, C60@C240@C540, C60@C240@C540@C960).*