PACKING C60 IN CARBON NANOTUBES: AN ATOMISTIC MOLECULAR DYNAMICS STUDY

Karla S. Troche[1], David D. Chinellato[1], Vitor R. Coluci[1,2], Scheila F. Braga[1], Fernando Sato[1], Sergio B. Legoas[2], and Douglas S. Galvão[1]
[1]Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas
CP 6165, 13083-970 Campinas, SP, Brazil
[2]Departamento de Física, Universidade Federal do Amazonas
69077-000, Manaus, AM, Brazil
E-mail: galvao@ifi.unicamp.br

The encapsulation of C60 molecules in carbon nanotubes (CNTs), sometimes generically named nanopeapods, has received great theoretical and experimental attention in the last years [1-3]. More recently [4], packing of C60 in boron nitride nanotubes has also been obtained. Very unusual diameter dependent configurations have been observed including linear, helical, and hollow core.

Several theoretical studies have been carried out for these systems, including Monte Carlo [3] and simulated annealing [2], sometimes with conflicting results. In this work we report a fully atomistic molecular dynamics study for different nanotubes (zig-zag, chiral, and arm-chair) of different diameters and at different temperatures. We have used classical molecular dynamics methodologies with standard molecular force fields [5,6].

Our results show the existence of chiral and achiral phases, depending on the tube type, diameter and temperatures. We have obtained diameter dependent configurations (Fig. 1) such as linear, helical (Fig. 2), etc.. The obtained patterns are very similar to the ones observed in boron nitride nanotubes [4]. Spontaneous chiral symmetry breaking were observed, but not following exactly the model of cylindrically confined hard spheres [7]. These results are discussed in terms of previous works addressing the origin of discrepancies among different methodologies.

References:

[1] B. W. Smith, M. Monthioux, and D. E. Luzzi, Nature (London) **396** (1998) 323.
[2] M. Hodak and L. A. Girifalco, Phys. Rev. B **67** (2003) 075419.
[3] M. Hodak and L. A. Girifalco, Phys. Rev. B **68** (2003) 085405.
[4] W. Mickelson, S. Aloni, W.-Q. Han, J. Cumings, and A. Zettl, Science **300** (2003) 467.
[5] R. H. Baughman and D. S. Galvão, Nature (London) **365** (1993) 735.
[6] Universal 1.02 Molecular Force Field, available from Accelrys, Inc. as part of the Cerius suite programs. http://www.accelrys.com.
[7] G. T. Pickett, M. Gross, and H. Okuyama, Phys. Rev. Lett. **85** (2000) 3652.

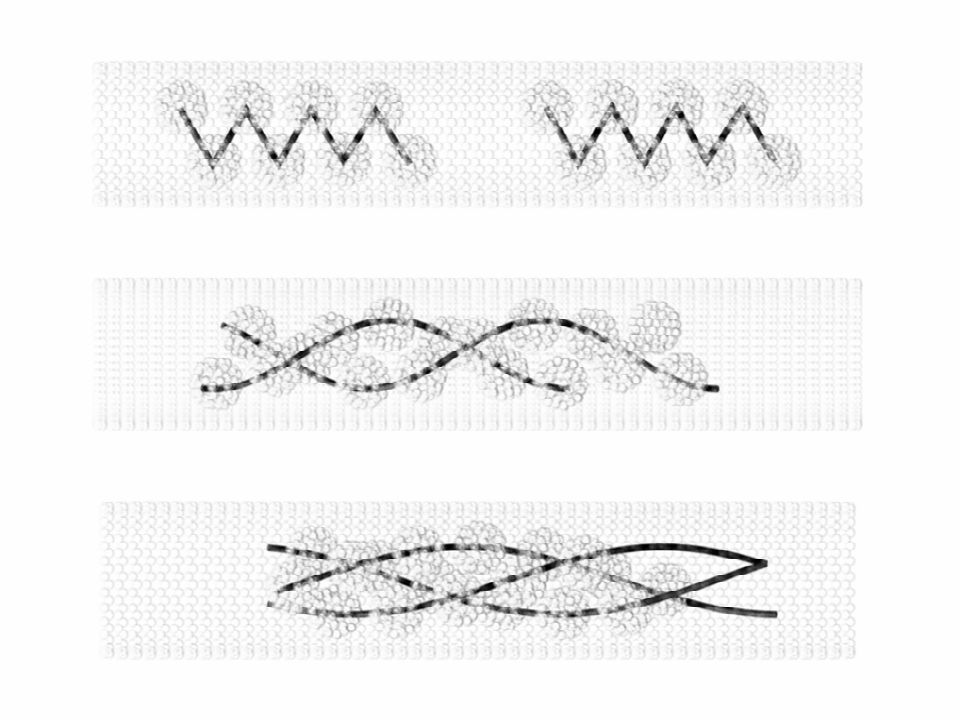

Figure 1. Structural arrangements of C60 inside carbon nanotubes: zig-zag, double and triple helices conformations were observed.

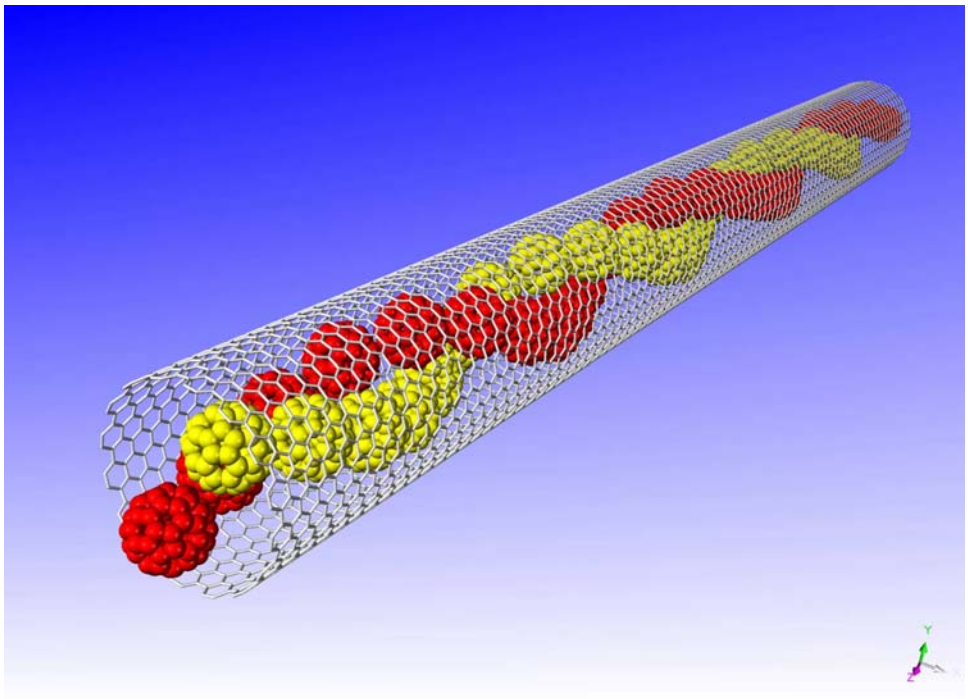

Figure 2. Illustrative example of double helix formation. The C60 were colored with different colors in order to help the visualization of the helical pattern.

Work supported in part by the Brazilian Agencies FAPESP, CNPq, IMMP/MCT, and CAPES.