ECHAHID HAMMA LAKHDAR UNIVERSITY - EL-OUED
Under the Supervision of the DGRSDT and in collaboration with the CRTI
International Pluridisciplinary PhD Meeting (IPPM'20)
1st Edition, February23-26, 2020
Theme: Synthesis, characterization, applications, and challenges of new materials

Theoretical Study of the Effect of Pentagon/Heptagon Defects on the Electronic Behaviour of Coiled Carbon Nanotubes: A Review

Lina Linda Bechohra*, Safia Kellou-Tairi*, Hamza Azzaz **

*Laboratoire de Physico-Chimie Théorique et Chimie Informatique,USTHB, BP 32 Bab Ezzouar, Algerie.
**Laboratoire des Sciences et de Génie des Matériaux, USTHB, BP 32 Bab Ezzouar, Algerie.
Email: lynabechohra@gmail.com

Abstract

Coiled carbon nanotube (CCNT) structure is the result of the periodic insertion of the pentagon and heptagon pairs (defect) into the carbon hexagonal network of the nanotube causing positively and negatively curved surface. Based on theoretical studies, regular coiled nanotubes exhibit exceptional electronic, mechanical, electrical, optic and magnetic properties due to the combination of their peculiar helical morphology and the fascinating properties of nanotubes.
Although coiled carbon nanotubes provide attractive features, there is little both theoretical and experimental research. In the present work, we attempted to clarify essential aspect of the electronic behaviour of CCNTs and summarize results obtained until now.

***Keywords*:** coiled carbon nanotube, pentagon/heptagon pairs (defect), carbon hexagonal network, structure, electronic properties.

1. Introduction

The existence of coiled carbon nanotubes (CCNTs) was first predicted by Ihara et *al*. and Dunlap in the early nineties [1, 2] and a few years later a Belgian research group reported their experimental observation [3]. Carbon nanotube with regular coiled structure can be generated through a periodic incorporation of pentagon and heptagon pairs into a hexagonal carbon framework. CCNTs are predicted to have excellent electro-magnetic properties, although their structure, formation mechanism and theoretical aspects are still subjects of scientific discussions. So far, only few studies have discussed the electronic structure of CCNTs. Different structural models of helically coiled carbon nanotubes (HCCNT) has been considered where the tight-binding method was used to calculate the band structure.

In this work we attempted to review the results obtained so far about the electronic properties of CCNTs and see the influence of the proposed structural models on the electronic behavior, also the impact of changing the positions of pentagon/heptagon defects on the band structure.

2. Structural and electronic properties

A systematic method to form helically coiled cages and tube helices as shown in Figs. 1(a), 1(b), and 1(c) proposed by Ihara et *al* [1] is to draw a map of the development on the perfect graphite layer. The electronic structure of the proposed models is calculated using a simple tight-binding method.

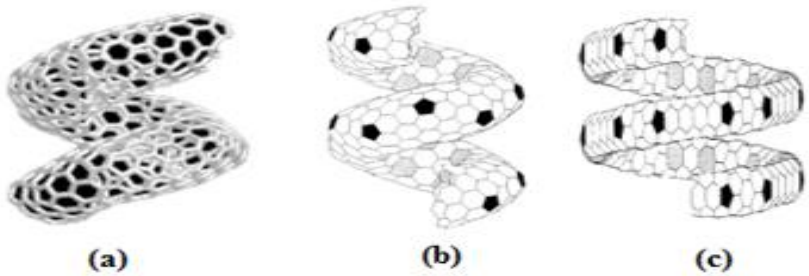


Fig.1. (a) the structure of a helically coiled cage of graphite layer determined by molecular dynamics simulation [4], **(b)** model of uniform tube helix C_{360} and **(c)** model of nonuniform tube helix C_{540} [5] based on development maps method.

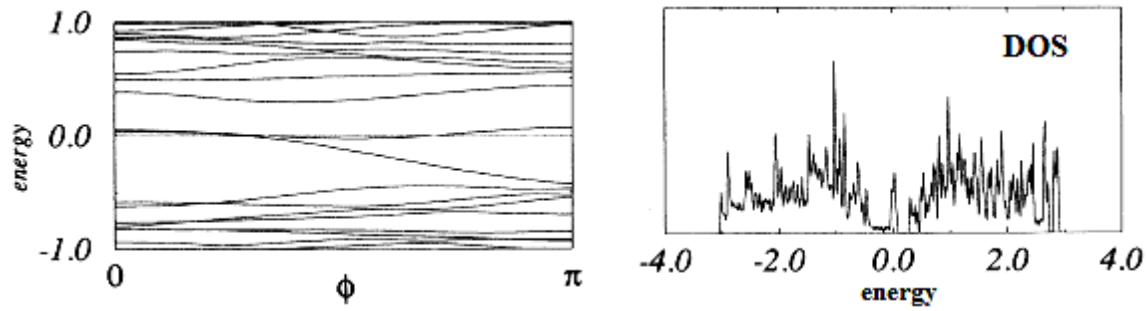


Fig.2. The energy bands and the densities of states (DOS) for helically coiled cages [5].

Depending on the placement of the 5- and 7-membered rings on the structure of development map, the coiled cage can behave as metallic, semiconducting (with direct or indirect band gap) and unlike the straight carbon nanotubes, the CCNT can even show a semi-metallic character due to the high density of states at the Fermi level [4, 5]. Such a sharp peak at the Fermi level may result in interesting properties such as the superconducting ones [4].

Few years later Milosevic and coworkers have studied the electronic band structure of HCCNT where different structural models have been considered. The electronic properties were calculated by fully symmetry based density functional tight binding method (DFTB) implemented in POLSym code. Simpler models of structures are proposed with different chiral angles and diameters Fig.3(d) and where atoms are forming only hexagons, being slightly deformed in a way to produce helical coil without introducing pentagon/heptagon defects [6, 7, 8].

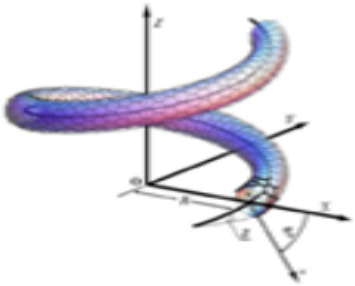
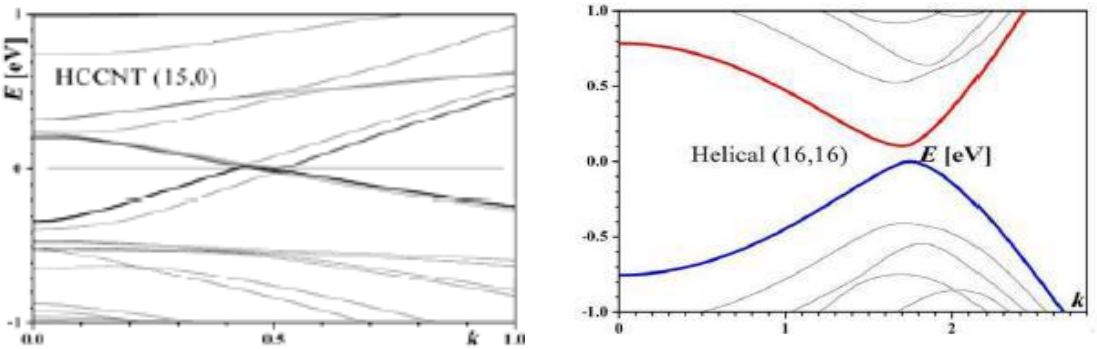


Fig.3. (d) simple model of CCNT without introducing pentagon/heptagon defects [6,7,8].



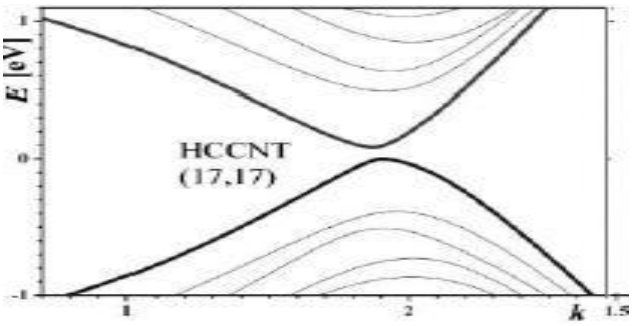


Fig. 4. Electron bands of zig-zag and armchair HCCNTs [6,8]

It has been shown Fig.4. that vast of majority of the relaxed CCNTs are found to be conductive with finite density of states at Fermi level while the armchair ones are quasi-metallic (narrow gap semiconducting).

Dmitrovic et *al* studied the effect of how by stretching a coil CCNTs its electro-optical properties can be changed [9].

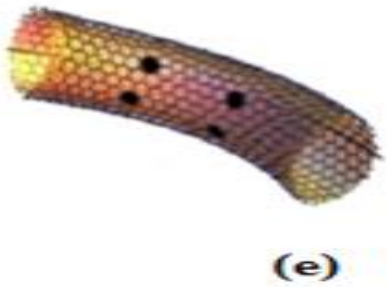


Fig.5. (e) structure of monomer of HCCNT constructed by the triple connected graph of pentagons, hexagons and heptagons [10].

The same team investigated the influence of the local structure Fig. 5(e) on the electronic properties of HCCNT Fig.6.and found that changing positions of pentagons and heptagons within a monomer, transitions between metallic, semi-metallic, quasi-metallic, and semi-conducting structures can be made [10].

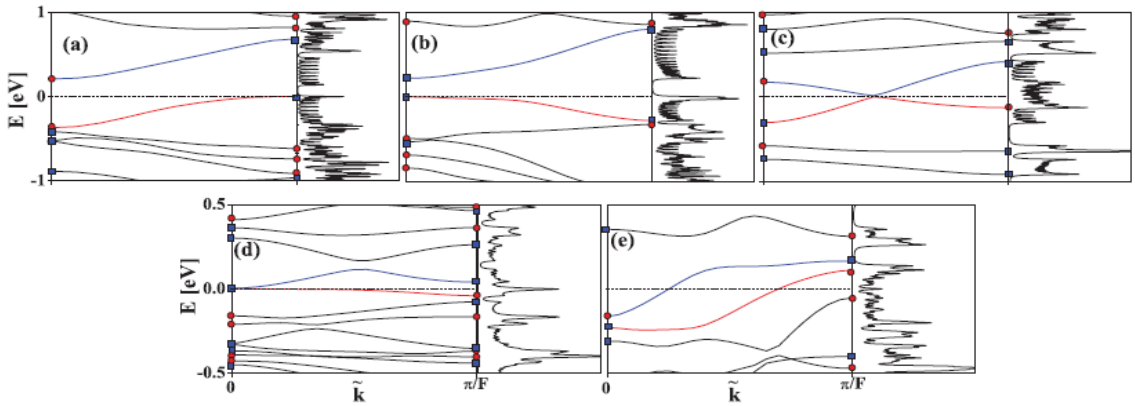


Fig.6. Five types of electronic band structure and corresponding density of states of HCCNTs [10].

3.Conclusion

According to these theoretical studies, coiled CNTs can be classified as metals, quasi-metals, semiconductors with direct or indirect band gap and also semi-metals character which is impossible for the case of straight nanotubes. Moreover, it is predicted that the topological structure of CCNTs governs the electronic behavior around the Fermi level.

However, these previous studies need further theoretical exploration using different atomic scale computer programs to study the influence of all the geometric parameters of CCNTs in their properties calculation.

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