Sessions: Nanotechnology
Preferred presentation Type: Poster

ELECTRONIC TRANSPORT OF MOLECULAR JUNCTIONS CARBYNE AND TWO-DIMENSIONAL CARBON ALLOTROPES

ROSA DA SILVA[1], A. B.; SAMPAIO-SILVA[1], A.; SILVA JR.[2], C. A. B.; DEL NERO[2], J.

[1]Universidade do Estado do Pará (UEPA), Brazil.
[2]Universidade Federal do Pará (UFPA), Brazil.

Email: alessandre@uepa.br

Abstract

In this work, we present an investigation, via the hybrid DFT-NEGF method [1], on the electronic transport of the molecular junction of carbon wires with a two-dimensional nanoribbon of carbon allotropes [2,3], from various junction configurations. The DFT calculations were performed with the generalized gradient approximation (GGA) and PBE functional, using computational package SIESTA 4.0 [4]. The influence of systematic variation in the bonds between carbyne and the nanoribbon was considered in the calculation. The systems were structurally stable, reaching a lower energy configuration, which was replicated in a device with a scattering region and electrodes. The devices exhibited metallic behavior, with a high probability of transmission. The I-V curve showed a tendency for gap opening with increasing voltage in the various structures, indicating a change in the transport regime. Thus, the systems proved to be very promising for the development of electronic nanodevices.

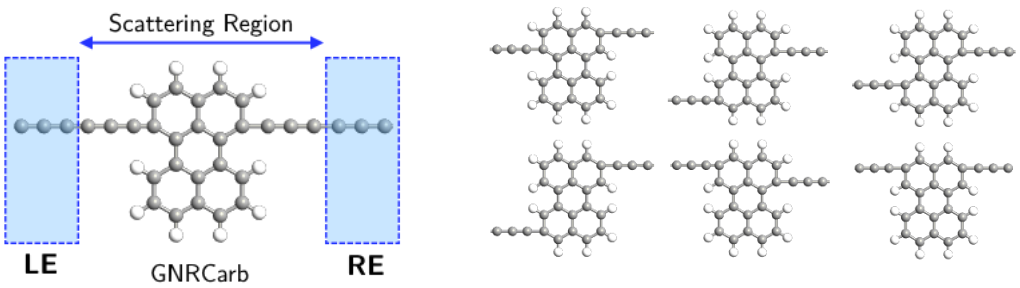

Fig. 1. (a) Molecular configuration of the junction device (GNRCarb). (b) Several configurations of the carbyne-graphene junction studied.

References

[1] A. Sampaio-Silva, D.F. Ferreira, C.A.B. Silva Jr.; J. Del Nero; "Hydrogenation, width and strain effect in Me-graphene devices," *Comput. Materials Sci.*, 210, p. 111456, 2022.
[2] K. S. Novoselov et al.; "Electric Field Effect in Atomically Thin Carbon Films," Science, 306, p. 666, 2004.
[3] R. B. Heimann, S. E. Evsyukov, L. Kavan; "Carbyne and carbynoid structures". *Spr. Sci. & Business Media*, 21, p. 446, 1999.
[4] J. M. Soler, E. Artacho, A. Garcıa, J. Junquera, P. Ordejon, D. S. Portal; "The SIESTA method for ab initio order-N materials simulation," *Jour. Phys. Cond. Matt*. 14, p. 2745, 2002.