

Electron Transport in Graphene-Phagraphene Mixed Structures

J.C.S. SANTOS¹; D.F.S. FERREIRA¹; S.M. CORRÊA²; M.R.S. SIQUEIRA³; KAZUKO, R. NISIOKA³; JÚNIOR, C.A.B.S²; DEL NERO, J^{1,2,5}.

¹ Graduate Program in Electrical Engineering, Federal University of Pará, Belém-PA, Brasil.

² Faculty of Materials Engineering, Federal Universidade of Pará, Ananindeua, PA, Brazil

³ Faculty of Physics, Federal University of Amapá, Macapá-AP, Brasil.

⁴ Faculty of Physics, Federal Universidade of Pará, Ananindeua, PA, Brazil

⁵Department of Physics and Quantum Theory Project, University of Florida (UF), Gainesville, FL, USA

contacts: ¹julio.santos@icen.ufpa.br; ²smcufpa@gmail.com, jordan@ufpa.br ;
marcelo.siqueira@unifap.br; cabsjr@ufpa.br.

Abstract

The nanoelectronics is today a strong new front of development, providing findings about new properties in a large range of materials. Among different ways to approach nanodevices based technologies there is the molecular electronics [1]. The first design for molecular electronic device was attributed to Aviram and Ratner [2]. New nano materials that have similar properties as conventional electronic devices are the most interesting [3]. Among these materials, graphene based devices have called attention of researchers around the world, due electrical, mechanical and thermal properties and high Fermi velocity in low temperatures [4]. Recently, Z. Wang *et al.* have suggested a new allotropic form of carbon, the phagraphene, a bi-dimensional material composed by carbon rings with 5-6-7 atoms, with sp^2 hybridization and comparable in energy with graphene, but most favorable in energy than other allotropic forms [5]. In this work, we have proposed a phagraphene based nanoelectronic device with metallic graphene leads. To perform electron transport calculations we have used the DFT-NEGF methodology in the Landauer-Büttiker formalism as implemented in the TRANSIESTA [6] code. Properties as current-voltage, transmission through the system compared with molecular orbitals shows interesting results and suggests phagraphene as promising material in nanoelectronics.

Key-words: Electron Transport; Graphene; New allotropic forms; Phagraphene;

References

- [1] CUEVAS, Juan Carlos; SCHEER, Elke. **Molecular electronics: an introduction to theory and experiment**. World Scientific, 2017.
- [2] AVIRAM, A. ; RATNER, M. A. Molecular rectifiers. **Chemical Physics Letters**, v. 29, p. 277, 1974.
- [3] FERREIRA, Marystela et al. **Grandes áreas da nanociência e suas aplicações**. Elsevier Brasil, 2016.
- [4] SAFARI, Ali et al. Graphene based electronic device. **World Acad. Sci. Eng. Technol. Int. J. Electr. Comput. Energ. Electron. Commun. Eng**, v. 8, p. 1232, 2014.
- [5] WANG, Zhenhai et al. Phagraphene: a low-energy graphene allotrope composed of 5–6–7 carbon rings with distorted dirac cones. **Nano letters**, v. 15, p. 6182, 2015.
- [6] SOLER, José M. et al. The SIESTA method for ab initio order-N materials simulation. **Journal of Physics: Condensed Matter**, v. 14, p. 2745, 2002.