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CAROTENOIDS AS NEW MATERIALS IN MOLECULAR ENGINEERING

A. GUEDES *1*, M.R.S. SIQUEIRA *1*, S.M. CORRÊA *1*, R.M. GESTER *2*, A.M. Chaves Neto *1* and J.DEL NERO *1*

1 Programa de Pós-Graduação em Física, Universidade Federal do Pará, Belém-PA, Brasil.
2 Faculdade de Física, Universidade Federal do Pará, Marabá, Brasil.
amguedes@ufpa.br

Abstract

Advances in electronics have been performed in the sense of the miniaturization in circuits elements. These new electronic devices are made ever smaller and they are going to molecular and atomic scale [1]. Several works have studied organic compounds as molecular devices. Between these compounds are aromatic structures as graphene, opioids and oxides[1,2]. The characteristics of some group of molecules are interesting in the molecular engineering. The aim is innovation and low energy cost. Carotenoids are very interesting to study because this is a new front in the development of molecular electronics, once these molecules are not studied as electronic device. In this work, single-molecule devices based in carotenes were studied and the behavior of the electronic current, transmission and energy levels were obtained. To perform these calculations, we have used the NEGF-DFT methodology and the Landauer-Büttiker [3] formalism as implemented in the SIESTA/TRANSIESTA package [4]. The results shows diode and Field Effect Transistor behavior when the transmission and energy levels are analyzed in low bias voltage.

References

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