Isomerization Effects on the Electronic Transport Properties of Carotenoid Derivatives

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Abstract

In the last decades, single atoms and molecules have been widely studied and suggested as electronic devices in nanoscale [1-4]. In 1974, Aviran and Ratner purposed the first single-molecule device, a molecular diode [1]. Since then, theoretical and experimental advances have arisen to analyze these nanodevices with details. One notable advance in nanoscale devices is the low cost to synthesis, once some of these molecules there exist in the nature. There is little need for synthesis, for molecular devices based on natural single-molecules. In the present work we have studied retinol (A vitamin) derivatives as molecular devices. Using the ballistic approximation, we studied the 11-*cis*-retinol and *all-trans*-retinol. To study theoretically these molecules as single-molecular devices we used the DFT-NEGF methodology [5,6]. These molecules were attached between Au(111) electrodes and their current-voltage curves were obtained. In low applied bias (from -0.4V to 0.4V) 11-*cis*-retinol has symmetric current-voltage curve, while *all-trans*-retinol has a diode behavior. The results suggest that a simple isomeric effect modulates the transport properties. These changes can be induced by an external applied field and the system changes from ohmic behavior to diode with potential application as Molecular Field Effect Transistor (MFET), due the positioning of energy levels relative to the bias window.

Key-words: Retinol, Molecular Electronics, DFT-NEGF, Molecular diode.

References:

[1] A. Aviram and M. A. Ratner. Chemical Physics Letters 29, 277 (1974).
[2] C. Guo, *et al.* The Journal of Physical Chemistry C 116, 12900 (2012).
[3] M. Siqueira, *et al.* Journal of Molecular Modeling 21, 317 (2015).
[4] A. Batra, *et al.* Nano letters 13, 6233 (2013).
[5] J. Taylor, H. Guo, and J. Wang. Physical Review B 63, 245407 (2001).
[6] B. K. Nikolić, *et al.* Journal of Computational Electronics 11, 78 (2012).