Sessions: Nanotechnology.
Preferred presentation Type: Poster.

Title. A New DNA Sensor Based on Electronic Transport Using Carbyne Electrodes

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Abstract: The electron transport by tunneling was carried out in nanodevices made of carbyne electrodes and a nucleotide monomer A-T or G-C, in order to propose new nanodevices to be applied in the field of molecular electronics, and establishing a sensor that provides the genetic sequencing of a DNA chain based on the similarities of the electrical properties analyzed. For the carbyne optimization, the DFT/B3LYP/6-31++G(d) methodology was implemented, and for the DNA monomers the DFT/M062X/6-311G(d,p) ones, both applied in Gaussian 09W. For the nanodevices optimization, the DFT/LDA/SZ methodology was implemented in SIESTA package [1]. In order to obtain the electronic transport, the NEGF methodology was implemented in the TranSIESTA package [2]. The results show that both nanodevices can be applied in the field of molecular electronics, since they present the behavior of a FET or LED in one of the voltage ranges analyzed, which have in good agreement with experimental results for direct bias voltage [3]. Furthermore, they present different I-V curves, allowing us to establish a new DNA sensor based on electronic transport using carbyne electrodes.

Keywords: DNA Nanodevice, DNA Sensor, Carbyne, DFT, NEGF.

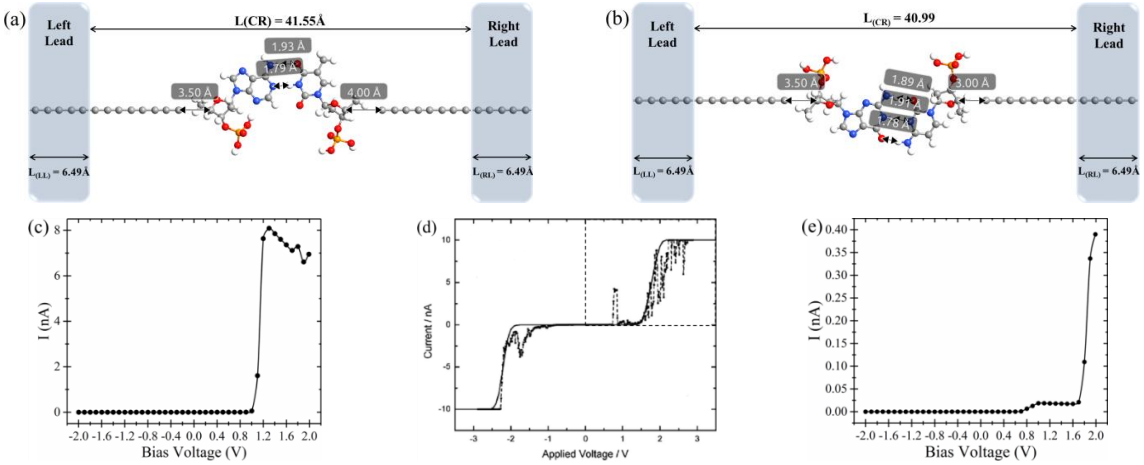

Figure 1: DNA nanodevices and current-voltage results: a) A-T nanodevice. b) G-C nanodevice. c) A-T I-V curve. d) Experimental I-V results. e) G-C I-V curve.

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