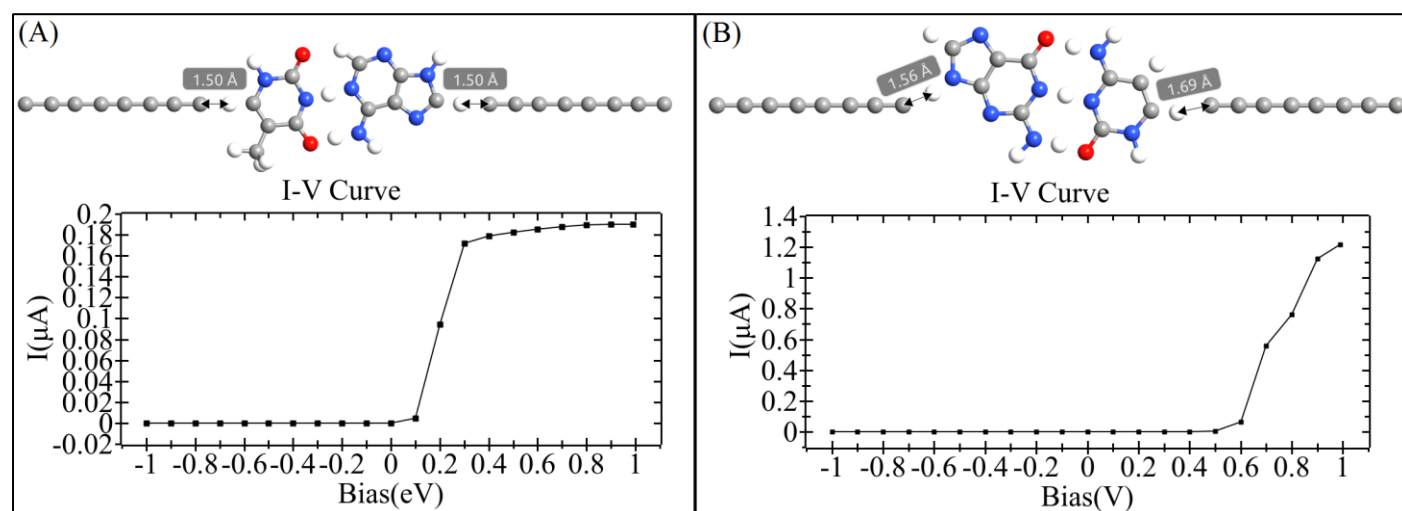


## The Characterization of DNA Fragments by means Electronic Transport

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## ABSTRACT

The electronic transport of the nitrogen-based pairs Adenine-Thymine (A-T) and Guanine-Cytosine (G-C) were studied in order to propose a new sensor for the identification of genetic sequencing of DNA strands. The Carbyne electrodes were placed at a distance of approximately 1.5 Å from the central region composed by the base pairs, without effective binding, so that the electronic transport occurred by tunneling and, thus, the I-V curve of the nanodevice can be generated. Initially, the central region was optimized with DFT/B3LYP/6-311G(d) calculations implemented in the Gaussian 09W package. The nanodevice (central region and electrodes) was optimized again with DFT/LDA/SZP calculations implemented in the SIESTA package, where the minimum power configuration for the device was obtained. The electronic transport was obtained with EHT/NEGF calculations implemented in Virtual Nanolab package, where the T-V, I-V and G-V curves were obtained. The results show that there is no reverse polarization transport for both nitrogen-based pairs. In direct polarization, the A-T base exhibits a slight increase in the current from 0 to 0.1 V, then increasing linearly and intensively, in the range of 0.1 V to 0.3 V, slowly stabilizing to values greater than 0.3 V, thus, the characteristic of the I-V curve is a Field Effect Transistor (FET). For the G-C base, transport occurs only for values of bias greater than 0.5V, increasing abruptly up to 1.0V, with small variations in the growth rate, thus, the characteristic of curve I-V is of a Light Emitting Diode (LED). The results show that Carbyne electrodes can be used, via electronic tunneling, as a sensor to identify the base pairs A-T and G-C, since the resulting devices have distinct and well-defined characteristic curves of FET and LED, respectively.



**Figure 1:** Nanostructure and I-V curve: (A) Adenine-Thymine. (B) Guanine-Cytosine.

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