WREN 2017
The Workshop on Renewable Energy and Nanotechnology

ELECTRONIC TRANSPORT IN MOLECULAR TUNNELING JUNCTION COMPOSED BY CENTRAL ATOM AND CARBYNE ELECTRODES.

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ABSTRACT

Nanoscale science and technology have attracted considerable attention in recent years. Research and development, in nanotechnology, aim to manipulate nanoscale structures and integrate them to form larger components and systems [1]. Organic nanomaterials are widely used for the development of nanoscale research. The potential of carbon-related materials has long been attracting much attention, because of their flexibility to make both the sp^2 and sp^3 bond networks [2]. Carbon allotropes discovered more recently, such as fullerenes, nanotubes and graphene (all composed of sp^2 -hybridized carbon) each also show unique properties, often different from those of either diamond or graphite [3] . Next in the series of carbon-atom hybridization from sp^3 - to sp^2 -is *sp*-hybridization and the least well-known of the carbon allotropes, carbyne [4], it’s considered as a linear carbon allotrope of *sp*-hybridized carbon atoms [4-6]. Interest in carbyne and its potential properties remains intense because of, at least in part, technological breakthroughs offered by other carbon allotropes, such as fullerenes, carbon nanotubes and graphene [4]. This work presents a theoretical study of the properties of electronic transport at a molecular tunneling junction for a device formed by a Central Sodium atom located between Carbyne electrodes and without effective binding between the central atom and the electrodes (Figure 1), aiming to investigate the characteristics in the electrode-atom interaction via molecular tunneling. The electron transport calculations were performed using the SIESTA/TRANSIESTA package [7-8] that uses the Density Functional Theory Methodology combined with the Non-Equilibrium Green's Function and the Landauer-Büttiker formalism [9]. The results shows the behavior of the system when a bias voltage is applied using the current curve and conductance differential and also the effect of quantum tunneling through the Eigenchannels.

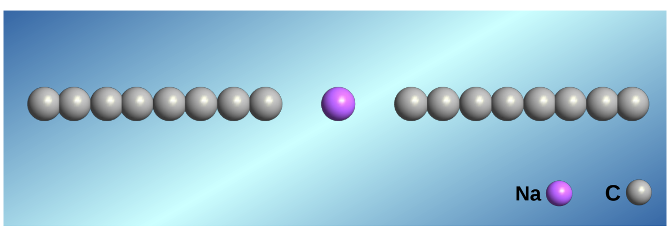

Figure 1- Schematic representation of the studied system composed by a central atom (Na) and Carbyne electrodes without effective bonding.

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