ELECTRONIC TRANSPORT IN CARBON NANOWIRES

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The beginning field of nanotechnology, driven by the relentless miniaturization of transistors in the semiconductor industry, has witnessed a surge of interest in recent years. The pioneering work of Aviran and Ratner [1] ushered in a new era of molecular nanoelectronics, expanding the frontiers of this nascent discipline. However, the vast diversity of molecules presents a rich landscape for exploration, encompassing studies on various graphene allotropes for electronic transport [2] and the utilization of diverse molecular structures as electrodes [3]. Given the plethora of potential nanoelectronic devices, further research in this area is imperative. Our study focuses on a simple molecular system comprising an alkyne with a triple carbon bond and 1D carbon wire electrodes (carbynes) see figure **1(a-b)** [4], offering a promising avenue for developing novel transistor alternatives. To delve into the electronic transport properties, band structure (PDOS), density of states (DOS), HOMO, and LUMO of this device and its variants, we employed Density Functional Theory (DFT) and Non-Equilibrium Green's Function (NEGF) methodologies. The Hamiltonian, incorporating donor (D), acceptor (A), and molecular terms, was utilized to model the system. The hybridization of molecular orbitals between the donor and acceptor facilitates the flow of electric current under an applied potential difference. By calculating the current using the Hamiltonian and defining current, charge, and operator for the donor and acceptor electrodes, we confirmed the FET behavior of the molecule. All devices exhibited semiconductor characteristics except for one variant see figure **1(c)**. Additionally, we observed a decrease in current conduction with increasing device size. These findings highlight the potential of this nanoelectronic as a transistor in specific applications where its unique properties offer advantages see figure **1(d-e)**.

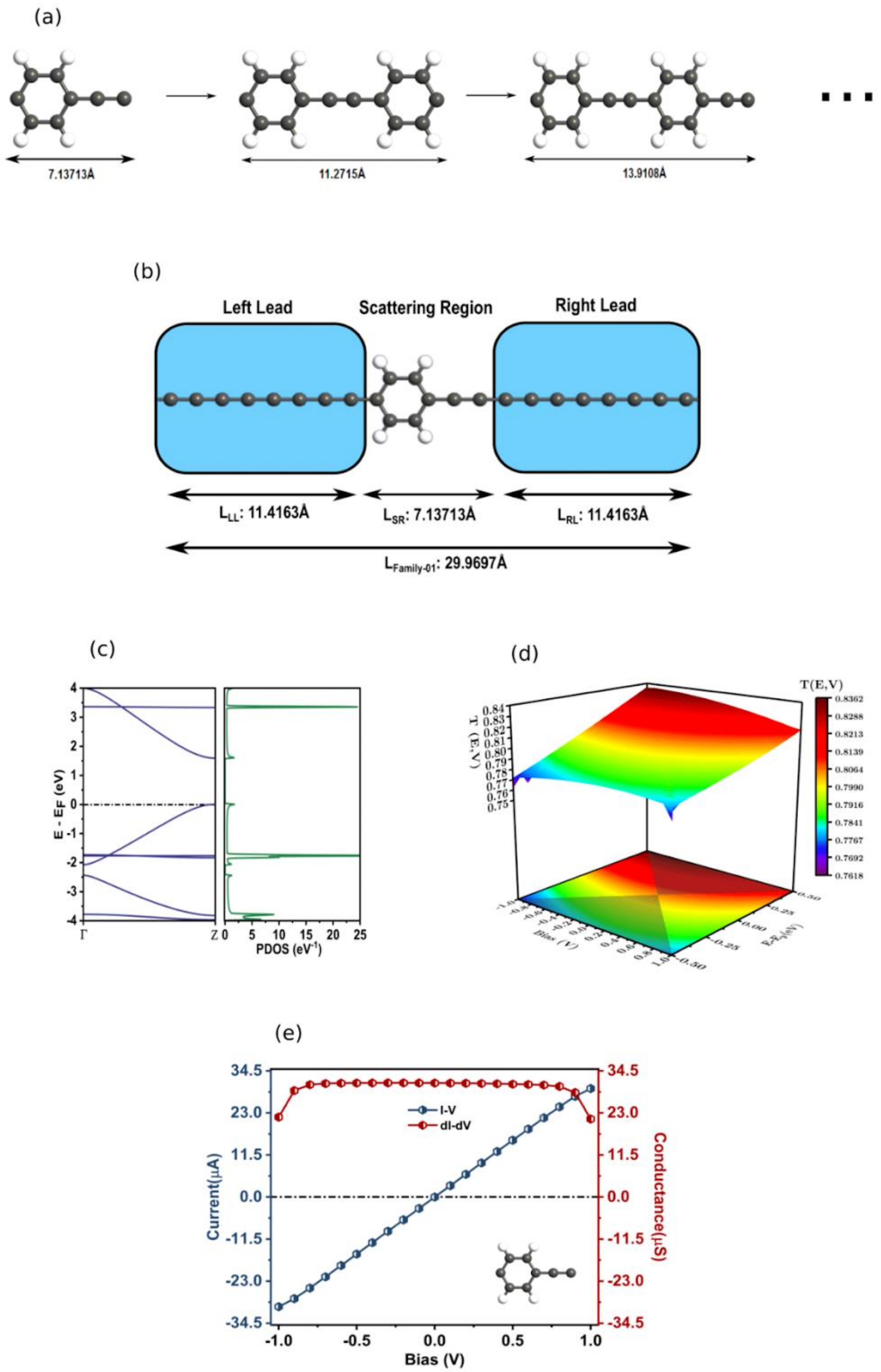

Figure 1: (a) Family variations (b) Family 1 with electrodes (c) BS (violet line) and DOS (green line) (d) Transmittance 2D and 3D (e) *I-V* (blue ball and line) and *G-V* (red ball and line) curves.

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