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Highly Ordered Metal Nanoribbons

J. M. Duarte[a], J. C. S. Santos[b], D. F. S. Ferreira[c], C. A. B. Silva Jr.[d], J. Del Nero[e]

[a,b] *Programa de Pós-Graduação em Engenharia Elétrica, Universidade Federal do Pará, Belém, 66075-110, Brasil*
[c] *Departamento de Engenharia Elétrica, Universidade Federal de Santa Catarina, 88040-900, Brazil*
[d] *Faculdade de Física, Universidade Federal do Pará, Ananindeua, 67113-901, Brasil*
[e] *Faculdade de Física, Universidade Federal do Pará, Belém, 66075-110, Brasil*

Abstract:

Carbon generates a variety of materials due to its hybridization (sp, sp^2, sp^3) [1]. Since the experimental production of graphene and its applications in nanotechnology, research into carbon allotropes has gained prominence [2]. Among the proposed allotropes, we highlight the planar net-τ network [3], see Figure **1(a)**, a high-order allotrope with 4-5-6-8-10 carbon rings. Figure 1(b) exhibits the unit cell from planar net-τ network with hydrogenated edges, in which we investigated a possible application in nanotechnology. We optimized the geometry of the unit cell with Density Functional Theory (DFT) methodology based on the Generalized Gradient Approximation (GGA) using the Perdew-Burke-Ernzerhof (PBE) and the Single-Zeta Polarized (SZP) basis net in the SIESTA package [4]. We used a convergence criterion of less than 10^{-4} for the self-consistent field (SCF), the lowest energy value for a mesh cut of 400 Ry, 10x1x1 k-points and the interatomic residual force is less than 5.10^{-3} eV/Å. Our results exhibit metallic character as show the band structure (BS) crossing the Fermi Level ($E-E_F = 0$eV) and the Density of States (DOS) presents accessible states at $E-E_F=0$ eV, see Figure **1(c)**. Figure **1(d)** shows the hybrid (zigzag and armchair) net-τ nanoribbon device and its dimensions. The device shows a dual application for the bias window ($0.0\ V \leq V_b \leq 1.0\ V$): (i) $0.0\ V \leq V_b \leq 0.4\ V$ the device behaves like an ohmic resistor and (ii) $V_b > 0.4$ V, the device behaves like a Field Effect Transistor (FET), see Figure **1(e)**. In Figure **1(f)**, the best transmission values are between 0.0*V* and 0.8*V*, from 0.8*V* there is a small drop in transmission values in the region between -0.48*eV* and -0.20*eV* which corresponds to the Highest Occupied Molecular Orbitals (HOMO) region. At 1.0 V is observed a negative differential resistance (NDR) in the differential conductance (-2.97μS).

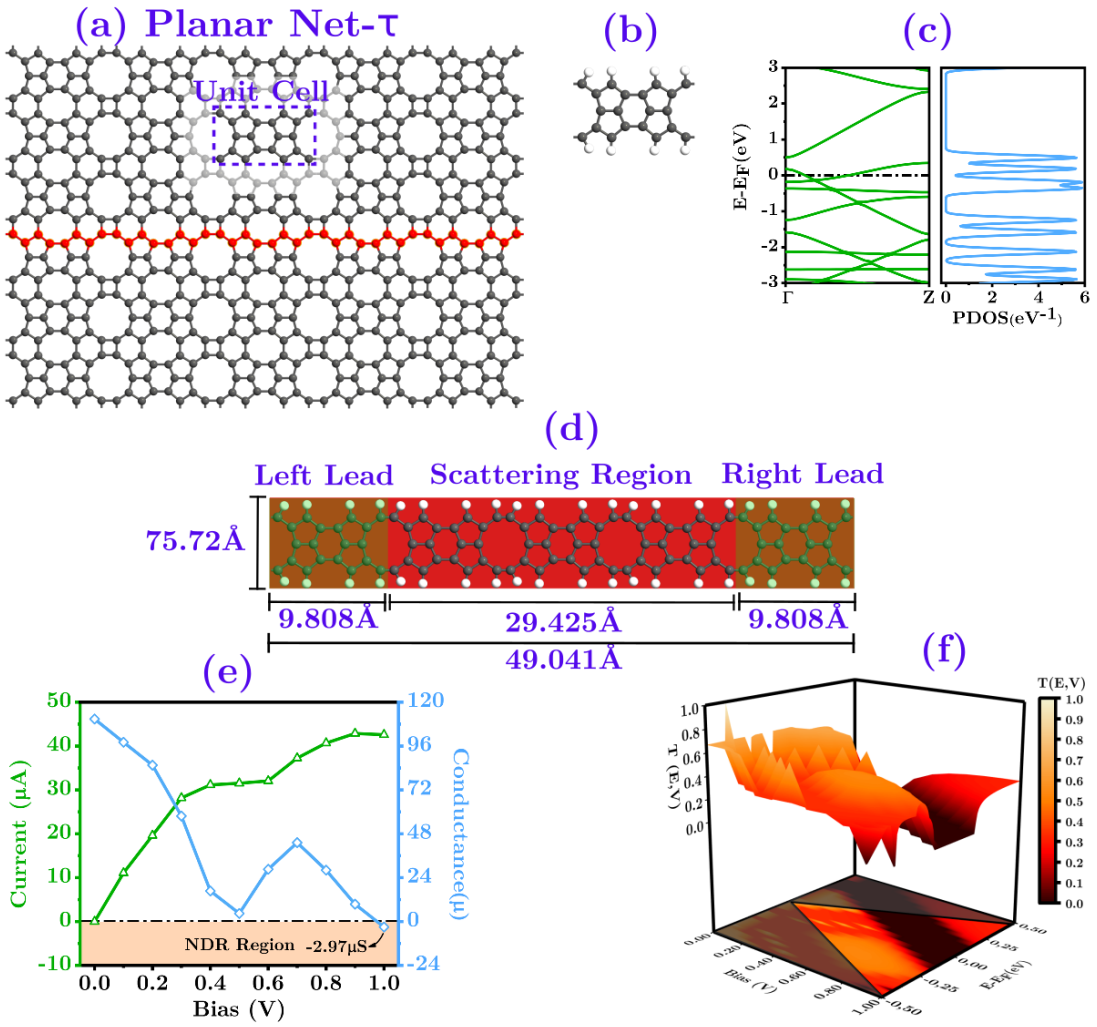

Figure 1: (a) Planar Net-τ (b) unit cell (c) DOS and BS (d) nanoribbon (e) current and differential conductance curves versus V (f) 2D and 3D transmittance versus E,V.

References:

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