

## Highly Ordered Metal Nanoribbons

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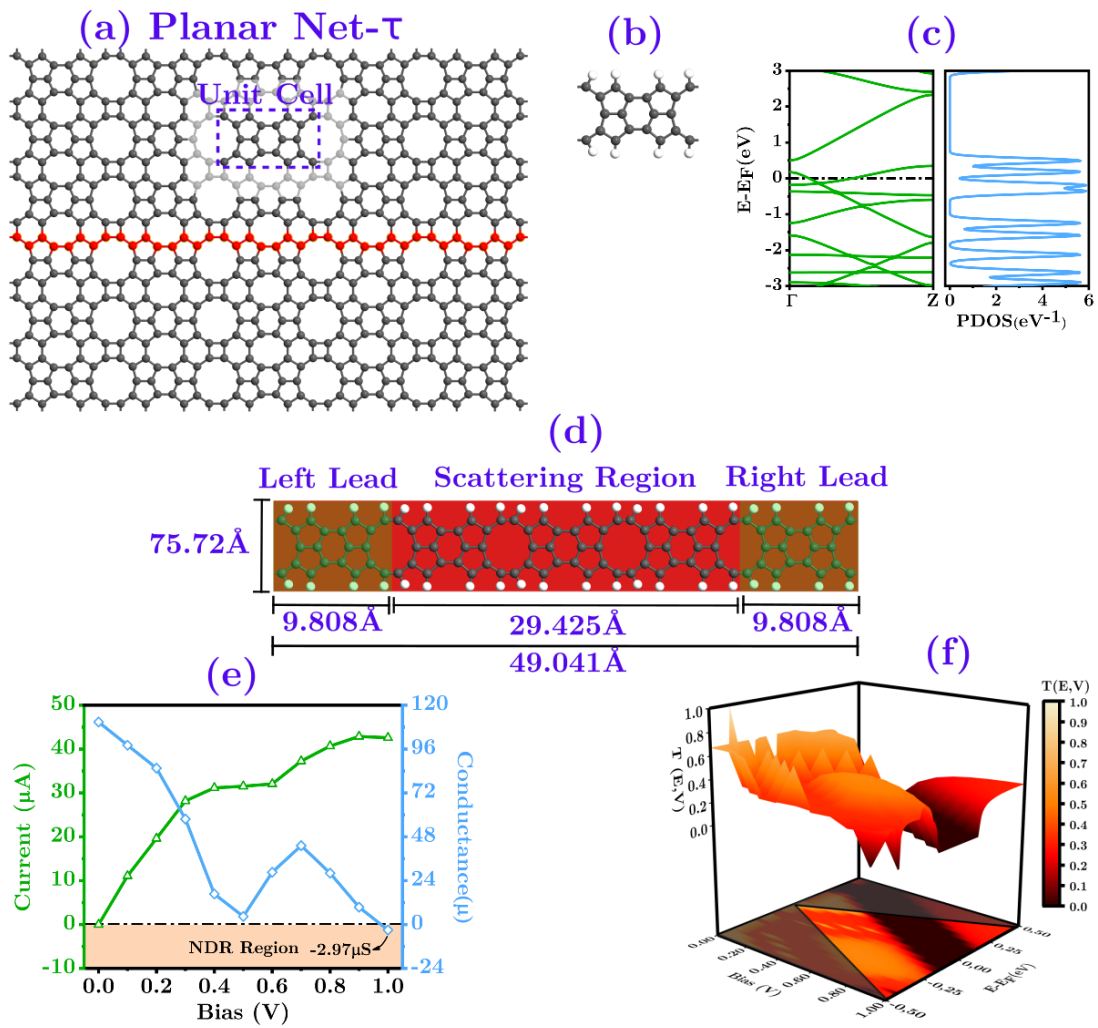
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### Abstract:

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- $\tau$  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- $\tau$  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 set 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,  $10 \times 10 \times 1$  k-points and the interatomic residual force is less than  $5 \cdot 10^{-3}$  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- $\tau$  nanoribbon device and its dimensions. The device shows a dual application for the bias window ( $0.0 \text{ V} \leq V_b \leq 1.0 \text{ V}$ ): (i)  $0.0 \text{ V} \leq V_b \leq 0.4 \text{ V}$  the device behaves like an ohmic resistor and (ii)  $V_b > 0.4 \text{ V}$ , the device behaves like a Field Effect Transistor (FET), see Figure 1(e). In Figure 1(f), the best transmission values are between  $0.0 \text{ V}$  and  $0.8 \text{ V}$ , from  $0.8 \text{ V}$  there is a small drop in transmission values in the region between  $-0.48 \text{ eV}$  and  $-0.20 \text{ eV}$  which corresponds to the Highest Occupied Molecular Orbitals (HOMO) region. At  $1.0 \text{ V}$  is observed a negative differential resistance (NDR) in the differential conductance ( $-2.97 \mu\text{S}$ ).



**Figure 1:** (a) Planar Net- $\tau$  (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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