How Atomic Edges Turn Carbon into Nanoscale Electronics

Jordan Del Nero
Faculdade de Física, UFPA, Belém, PA, 66075-110, Brazil

Abstract

The recent body of our work systematically demonstrates how atomic-scale geometry and edge configuration in newly proposed two-dimensional carbon allotropes and their derived nanoribbons control electronic structure and transport, enabling tunable resonant tunneling, negative differential resistance (NDR), and transitions between resonant and quasi-ohmic behaviour. Using first-principles electronic structure calculations combined with quantum transport (density functional theory + non-equilibrium Green's functions or equivalent methodologies), these studies uncover robust, reproducible mechanisms by which geometry and topology produce device-relevant signatures suitable for nanoelectronic applications.

A recurring motif across the papers is the central role of edges and boundaries. In the 2D net-τ allotrope examined by Duarte et al., chiral edge states emerge as active channels that drive a pronounced NDR in appropriately terminated ribbons. The work shows that by tuning boundary termination (the atomic arrangement at the ribbon edge), one can selectively enable or suppress chiral edge modes that align energetically with transmitting resonances. When bias moves these chiral channels through energy windows that favor transmission, a sharp increase in current is followed, at larger bias, by a suppression of available resonant channels, producing a negative differential resistance region in the I–V trace. This chiral edge-driven mechanism is presented as an architecture-level knob for producing NDR without relying on heterojunctions or doping gradients.

Complementary studies on net-t nanoribbons (Duarte et al., Surfaces and Interfaces) emphasize the power of width modulation as a practical design parameter. Systematic variation of ribbon width reveals distinct transport regimes: narrow ribbons show discrete, sharp resonances associated with quasi-one-dimensional subbands and localized states, which produce strong resonant tunneling and well-defined NDR features; wider ribbons evolve towards broadened conduction features and quasi-ohmic behaviour as subband spacing shrinks and coupling between localized states and leads increases. The net-t results therefore supply a straightforward engineering rule: width tuning can switch a device between NDR-dominated and near-linear conduction responses, opening the door to multi-functional nanoelectronic elements derived from a single material family.

Investigations of zigzag M-graphene nanoribbons integrate band topology into the design picture. Their work demonstrates geometry-controlled switching: topological characteristics of the bandstructure (for instance, whether specific edge bands are topologically protected or accidental) directly influence the formation and energy alignment of resonant states that mediate tunneling. This link between topology and resonant transport implies that one can engineer switching devices, resonant tunneling diodes and transistors, by choosing edge orientation and unit-cell geometry to produce desired band inversions or protected edge channels. The implication is a route to robust device operation that leverages topology rather than fine chemical doping.

A broader methodological and conceptual thread appears in the comparative study of edge configuration effects (Reis, Mota, Fileti, Del Nero): different edge terminations (zigzag, armchair, mixed/chiral) produce predictable shifts in bandgaps, emergence or suppression of localized edge states, and changes in coupling to metallic leads. Through

a combination of band structure analysis, density of states mapping, and conductance spectra, that work presents a practical toolkit for predicting how a proposed ribbon will behave under bias, enabling device designers to anticipate resonant energies and optimize contacts, gating, or geometric constraints.

The PHOTH-G nanoribbon study (Baia Reis & Del Nero) examines the continuum from sharp resonant peaks to broad conductance bands. Their calculations show how small structural modifications, edge roughness, unit-cell reconstruction, or inter-site coupling changes, can broaden formerly sharp resonances into overlapping bands. This transition is critical: while sharp resonances enable high ON/OFF contrast and pronounced NDR, broader bands favor stable, low-resistance conduction desirable for interconnects or channel materials. Understanding the parameters that control this evolution (coupling strength, symmetry breaking, and dimensional crossover) is thus essential for matching material design to specific circuit needs.

Collectively, these studies outline a set of design principles for carbon-based nanoelectronics: (1) edge engineering is a primary control handle, atomic termination type governs the presence and energy of localized and chiral states; (2) geometric parameters such as ribbon width and unit-cell pattern determine whether transport is dominated by discrete resonances or extended bands; (3) band topology provides an additional, robust lever to create protected channels or topologically mediated switching; and (4) resonant tunneling and NDR can be achieved intrinsically by single-material architectures through careful boundary and width control, avoiding the need for heterostructures.

From an applications perspective, the demonstrated phenomena map naturally to resonant tunneling diodes, high-contrast switches, memory elements (leveraging NDR hysteresis under circuit load), and compact oscillators. The authors emphasize the potential for multifunctional device platforms where different operational modes (resonant/NDR vs. quasi-ohmic) are selected by geometric tuning rather than different materials, simplifying fabrication and integration. Important next steps highlighted implicitly across the papers include experimental realization (synthesis and atomic control of edges), interface engineering with metallic contacts and gates, and assessment of disorder, temperature, and many-body effects on the sharpness of resonances.

In sum, these five papers constitute a coherent research program that elevates edge and geometry as foundational design variables for emergent carbon nanoarchitectures. By connecting atomic-scale structure to band topology and non-equilibrium transport signatures, they provide both predictive understanding and practical design rules for future carbon-based resonant electronic devices.

[1] Duarte JM, Ferreira DFS, da Silva CAB, Del Nero J. Chiral edge-driven negative differential resistance in net-τ: 2D carbon allotrope with tunable boundaries. *Physica B: Condensed Matter*. **2026**;721:418037.

[2] Reis FB, Del Nero J. Geometry-controlled switching: Band topology and resonant tunneling devices in zigzag M-graphene nanoribbons. *Physica B: Condensed Matter*. **2026**;723:418120.

[3] Duarte JM, dos Santos JCS, Ferreira DFS, da Silva CAB, Del Nero J. Metallic Net-t nanoribbons for nanoelectronics: Width modulation of NDR, quasi-ohmic behavior, and resonant tunneling. *Surfaces and Interfaces*. **2026**;80:108242.

[4] Reis FB, Mota EAV, Fileti EE, Del Nero J. Adjusting electronic properties and device behavior of new carbon nanoribbons using edges configuration effect: A first-principles study. *Computational Materials Science*. **2026**;264:114479.

[5] Reis FB, Del Nero J. Resonant tunnelling and conductance evolution in PHOTH-G nanoribbons: From sharp resonances to broad bands. *Computational Condensed Matter*. **2026**;46:e01223.