Session: Nanotechnology
Preferred presentation type: Poster

Edge termination as a switch between near-ballistic conduction and negative differential resistance in ZP-graphene nanoribbons

J. M. Duarte[a], M. Moura-Moreira[b], J. Del Nero[c]

[a] *Faculdade de Engenharia de Minas, UFOPA, Juruti, 68170-000, Brazil*

[b] *Departamento de Física, UEPA, Cametá, 68400-000, Brazil*

[c] *Faculdade de Física, UFPA, Belém, 66075-110, Brazil*

Abstract:

ZP-graphene, a two-ring carbon allotrope, combines square and pentagonal motifs into a parent lattice whose nanoribbons have not previously been mapped across edge terminations. We present a first-principles investigation of ZP-graphene nanoribbons using the DFT+NEGF methodology, with SIESTA for electronic structure and TranSIESTA for quantum transport, computing band structures, density of states, and bias-dependent transmission spectra and current-voltage characteristics for five distinct hydrogen-passivated ZPGNR terminations. Each device was modeled as a two-probe system, with left electrode, central scattering region, and right electrode all constructed from the same fully relaxed ribbon segment, so that the transport response reflects the intrinsic properties of each termination rather than contact mismatch, and the results are placed in the context of the broader carbon-nanoribbon literature by comparison with representative hydrogen-passivated systems from related allotrope families.

Across the five terminations studied, transport behavior spans a remarkably broad and termination-sensitive landscape. Some edge cuts sustain near-ballistic conduction over an extended bias window, with transmission close to the maximum allowed per channel and current-voltage curves that stay close to linear, while others develop pronounced negative differential resistance, with current peaks followed by sharp drops in conductance as specific transmission resonances are driven out of alignment with the electrochemical window of the two electrodes. This range of behavior, from near-ballistic to strongly non-linear, is obtained from a single parent lattice simply by changing which atoms terminate the ribbon edge, without any change in ribbon width, doping, or applied gate field. Comparison across terminations shows that the NDR-active cuts are precisely those whose edge geometry localizes a transmission resonance close to the Fermi level at zero bias, so that a modest applied voltage is sufficient to sweep it out of the transport window, while the near-ballistic terminations instead keep their dominant channel far from any band edge across the whole bias range studied.

These results place edge termination on equal footing with width and strain as an independent, purely geometric design parameter for two-ring carbon nanoribbons, and they show that a single ZP-graphene parent sheet can be cut, without any chemical doping, into either a near-ballistic interconnect or a room-temperature-relevant negative-differential-resistance switching element. This termination-selectable duality is a practical route toward

carbon-based resonant-tunneling and logic devices built from a single, synthetically accessible two-dimensional allotrope, and it narrows the geometric search space that future bottom-up synthesis of ZP-graphene ribbons would need to target.

References:

1. Duarte, J. M.; Moura-Moreira, M. M.; Del Nero, J. Topology-Driven Transport Diversity in ZP-Graphene Nanoribbons: From Near-Ballistic Conduction to Negative Differential Resistance via Edge Termination Engineering. FlatChem 2026, 58, 101068.

2. Son, Y.-W.; Cohen, M. L.; Louie, S. G. Energy Gaps in Graphene Nanoribbons. Phys. Rev. Lett. 2006, 97, 216803.

3. Soler, J. M.; Artacho, E.; Gale, J. D.; García, A.; Junquera, J.; Ordejón, P.; Sánchez-Portal, D. The SIESTA Method for ab Initio Order-N Materials Simulation. J. Phys.: Condens. Matter 2002, 14, 2745–2779.

4. Zhang, J.; Ghawri, B.; Dutta, D.; Fasel, R.; Calame, M.; Borin Barin, G.; Perrin, M. L. Bottom-up-Synthesized Graphene Nanoribbons for Nanoelectronics. Nat. Rev. Mater. 2026, 11, 194–212.