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Edge geometry and bias control of resonant transport in M-graphene nanoribbons

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Abstract:

M-graphene, an allotrope composed of alternating pentagon and heptagon rings, is metallic and mechanically stable in its two-dimensional form, but how zigzag and chiral nanoribbon cuts differ in their bias-dependent conduction had not been mapped in a single, internally consistent study. We report a comparative first-principles study of electronic transport in M-graphene nanoribbons with zigzag and chiral edge terminations for widths W = 1-4, using density functional theory combined with non-equilibrium Green's-function (DFT+NEGF) calculations of relaxed geometries, band structures, bias-dependent transmission spectra, and two-terminal current-voltage characteristics, supported by a diagnostic suite comprising Fowler-Nordheim and Millikan-Lauritsen transforms, WKB estimates, power-law fitting, transmission eigenchannel decomposition, and first-principles inelastic electron tunneling spectroscopy (IETS).

Narrow nanoribbons display sharp, bias-tunable transmission resonances that localize on specific ring motifs and produce abrupt increases in differential conductance, while wider nanoribbons exhibit a smoother bias dependence consistent with field-assisted tunneling and progressive barrier thinning. For the zigzag family, the leading transmission eigenvalue $\tau 1$ shows sharp, width-dependent peaks at intermediate bias for the narrower widths, reaching above 0.998 at zero bias before collapsing to about 1.2×10^{-3} once the dominant channel is driven off resonance, with sudden drops at higher bias that match the negative-differential-resistance and switching trends already reported for M-graphene; the chiral family instead shows a generally smoother eigenvalue evolution, though its narrowest member still displays a discrete jump, from $\tau 1 = 0.50$ at zero bias to 0.98 at 0.5 V. IETS signatures correlate closely with these eigenchannel reorganizations, providing independent vibrational corroboration of resonance-assisted conduction at the same bias values where the Fowler-Nordheim and Millikan-Lauritsen transforms change slope.

Extracted device metrics, including the threshold bias for resonance, the peak differential conductance, and the bias evolution of the leading transmission eigenvalue, map directly onto measurable two-terminal observables and indicate that M-graphene nanoribbons are promising candidates for nanoscale switching and resonant-tunneling elements. The convergence of independent diagnostics, spectral, eigenchannel, and vibrational, onto the same set of bias values across both edge families demonstrates that ring topology, rather

than extrinsic disorder, is the primary variable controlling device-relevant transport in this allotrope, and it establishes edge orientation as a practical selector between smooth, field-assisted conduction and sharp, resonance-dominated switching.

References:

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