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Edge-ring selection as a design parameter for quantum transport in X-graphene nanoribbons

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Abstract:

X-graphene, a two-dimensional carbon allotrope whose unit cell combines pentagonal, hexagonal, and heptagonal rings, offers a non-hexagonal alternative to graphene in which boundary chemistry, rather than lateral confinement alone, can be engineered to control charge transport. We present a first-principles study, combining density functional theory with the non-equilibrium Green's function formalism (DFT+NEGF), of hydrogen-passivated X-graphene nanoribbons cut along four distinct edge geometries: zigzag (zzXGR-H), two armchair variants exposing either pentagonal or heptagonal boundary rings (armXGR-2P and armXGR-2Hep), and a chiral termination (chXGR-Hep2H). Ground-state geometries were relaxed using the SIESTA code with a double-zeta polarized numerical-orbital basis, norm-conserving pseudopotentials, and the PBE exchange-correlation functional, and the TranSIESTA extension was then used to obtain relaxed two-probe device geometries, band structures, and bias-dependent transmission spectra; current-voltage characteristics were computed up to finite bias to classify the transport regime associated with every edge motif.

We find that the identity of the ring exposed at the nanoribbon boundary, more than the crystallographic cutting direction itself, governs the transport response. Zero-bias differential conductance spans more than one order of magnitude across the series, from 2.8 μS in the chiral chXGR-Hep2H, which shows a semimetallic pseudogap, to 78.6 μS in armXGR-2Hep, where a heptagonal-edge resonance dominates transmission near the Fermi level. The pentagon-edged armchair ribbon, armXGR-2P, reaches a comparably high conductance of 73.9 μS through a distinct flat-subband mechanism localized on the pentagonal boundary. Most notably, armXGR-2Hep displays robust, symmetric negative differential resistance, with an onset near 0.77 V and a differential conductance of -12.5 μS at the bias extremes, driven by voltage-induced misalignment of the heptagonal-edge transmission resonance with the electrochemical potentials of the two electrodes. Thermal-broadening estimates at 300 K indicate that this NDR window, roughly seven times wider than the thermal smearing scale, should retain its qualitative peak-to-valley character at room temperature, while the narrower resonances of the chiral termination are more susceptible to thermal averaging.

Benchmarking these results against phagraphene, net-τ, C-57, and PHOTH-G nanoribbons places X-graphene among the most versatile all-carbon platforms reported to date, since a

single parent lattice yields ohmic, resonant, and NDR-active devices depending only on which ring is exposed at the edge, without any change in ribbon width, strain, or chemical doping. These findings identify edge-ring selection as an independent design parameter for non-hexagonal carbon nanoribbons and motivate experimental exploration of X-graphene as a chemically tunable platform for carbon-based interconnects, gate-tunable channels, and negative-differential-resistance switching elements.

References:

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