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Contact-site and ring-topology design rules for carbyne-nanoribbon molecular junctions

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Abstract:

Linear sp-carbon chains, or carbynes, are natural atomic-scale leads for contacting two-dimensional carbon nanoribbons, yet how the ring environment at the point of attachment shapes the resulting junction has remained largely unexplored. We report a first-principles density functional theory and non-equilibrium Green's function (DFT+NEGF) investigation of charge transport across eight molecular-junction configurations formed by graphene and phagraphene nanoribbons, with zigzag and armchair edge topologies, connected to semi-infinite sp-hybridized carbyne electrodes at two geometrically distinct attachment sites. In the edge-proximal geometry the carbyne electrode bonds to an sp^2 carbon atom sharing its ring connectivity with a single adjacent hexagon, while in the extended-conjugation geometry it bonds to an atom whose ring environment includes a pentagonal ring of the 5-6-7 phagraphene network, or an equivalent laterally shifted hexagonal site. Systematically varying ring topology, edge orientation, and contact geometry isolates the individual contribution of each factor to the quantum transport response, using relaxed SIESTA geometries and TranSIESTA transport calculations converged with respect to k-point sampling and real-space mesh cutoff.

The electrode attachment site emerges as the primary qualitative determinant of device behavior: edge-proximal attachment produces weakly conducting, rectifying junctions governed by sharp transmission resonances, whereas extended-conjugation attachment opens high-transmission pathways across the whole series. Ring topology then provides the decisive quantitative modulation on top of this qualitative split. The zigzag phagraphene junction contacted at the extended-conjugation site carries -27.5 to +28.3 μA at ±1.0 V, with a rectification ratio of 1.03 and a zero-bias conductance of 0.37 G0, a 3.3-fold enhancement over its graphene counterpart at the same contact site. The armchair phagraphene device contacted at the edge-proximal site instead exhibits voltage-controlled rectification reaching a ratio of 4.2 at ±0.5 V, which we trace to a near-resonant Fermi-level state, with a density of states up to 356 eV^{-1}, created specifically by the 5-6-7 ring topology of phagraphene; the corresponding graphene devices at either contact site never approach this density of states, confirming that the effect originates in the pentagon-containing ring network rather than in the carbyne electrode itself.

Taken together, these eight junctions establish quantitative, transferable design rules linking ring topology, edge orientation, and contact geometry to conductance and rectification in sp-sp^2 carbon nanoelectronic junctions, and they identify contact-site selection, independent of

the nanoribbon's own edge chemistry, as a practical, synthetically accessible lever for engineering carbyne-contacted nanoribbon devices with a prescribed rectification ratio.

References:

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