Session: Nanotechnology
Preferred presentation type: Poster

Ribbon width as an independent design parameter for strain-tunable Dodecanophene nanoribbons

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Abstract:

Two-dimensional Dodecanophene, a carbon allotrope built from fused three-, six-, and twelve-membered rings, hosts a single Dirac cone that remains open, that is, ungapped, under uniaxial strain of up to ±10%. Whether this untunable behavior survives lateral confinement into a nanoribbon had not previously been established. Using density functional theory combined with the non-equilibrium Green's function formalism, implemented in SIESTA and TranSIESTA with a double-zeta polarized basis, PseudoDojo norm-conserving pseudopotentials, and a 45×1×1 Monkhorst-Pack k-mesh, we compute the strain-resolved electronic structure, quantum transport, and mechanical response of two hydrogen-passivated Dodecanophene nanoribbons of different widths but identical edge chemistry and ring composition, denoted DDCNR-1H and DDCNR-3H.

At zero strain, both ribbons are metallic. Under uniaxial strain from -5% to +5%, DDCNR-3H remains gapless throughout, reproducing the parent sheet's behavior, while the narrower DDCNR-1H develops a compression-induced gap that grows from 0.238 to 0.579 eV, with a strain-gap slope of -107.0 meV per percent strain and an essentially strain-invariant effective mass of 0.089-0.095 free-electron masses. Within its metallic window, DDCNR-1H's Fermi velocity increases by up to 25% under tension. The zero-strain transmission spectrum of DDCNR-1H shows a sharp antiresonance, dropping more than six orders of magnitude, that is entirely absent in DDCNR-3H; a Shannon-entropy analysis of the transmission spectrum quantifies this contrast on a single, bias-resolved scale that is independent of the underlying chemistry and comparable across ribbons of different width. Young's moduli of 503.8 and 624.2 GPa are obtained for DDCNR-1H and DDCNR-3H respectively, consistent with the anisotropic stiffness already reported for the parent two-dimensional sheet, and confirming that the width dependence seen electronically is mirrored, though less dramatically, in the mechanical response.

Ribbon width alone, independent of edge termination or ring composition, is therefore sufficient to switch Dodecanophene nanoribbons between a featureless metallic conductor and a multiply strain-tunable narrow-gap semiconductor. This identifies width as an independent design parameter for post-graphene carbon nanoribbons, on equal footing with edge termination and strain in other two-ring allotrope families, and motivates experimental

exploration of the Dodecanophene family for flexible, strain-responsive nanoelectronics and for mechanically gated switching elements that require no chemical doping to open a transport gap.

References:

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