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A systematic DFT+NEGF map of contact, length, and strain effects in polyacetylene/carbyne junctions

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Abstract:

One-dimensional sp-carbon systems are attractive testbeds for molecular electronics because their electronic structure is controlled almost entirely by chain length, end-group chemistry, and contact geometry, yet a systematic, internally consistent map of these factors, together with mechanical strain, for a single chemical family has been missing. We use density functional theory combined with non-equilibrium Green's-function transport calculations (DFT+NEGF) to study electronic transport across a systematic series of polyacetylene/carbyne junctions, sampling device geometries and contact registries to identify stable configurations and to extract channel-resolved transmission eigenvalues together with transition-voltage spectroscopy, Fowler-Nordheim, and Millikan-Lauritsen diagnostics under both unstrained and axially strained conditions.

Computed cohesion energies cluster tightly around -7.0 eV per atom across the whole series, indicating comparable thermodynamic stability for all ten families regardless of length or contact registry. Eigenchannel analysis and transport diagnostics instead reveal three distinct bias-driven regimes. Short bridges such are essentially non-conducting at zero bias, but develop a near-open resonant channel under bias. Intermediate families show only partial bias activation, with moderate $\tau 1$ growth. Long bridges, remain tunneling-dominated throughout, with $\tau 1$ typically confined to the 10^{-6}-10^{-3} range even at the highest bias studied. Applying uniaxial strain to representative members of each length class shifts the resonance onset bias systematically without changing which of the three regimes a given family occupies, showing that strain acts as a fine control superposed on the coarser, length-set transport class. Because similar cohesive stability across the series does not translate into similar transport, we conclude that conduction is governed primarily by level alignment and electrode coupling rather than by the intrinsic stability of each bridge.

These results supply a coherent design map for 1D sp-carbon devices contacted by sp-carbon electrodes, showing how a single chemical motif evolves from tunneling-dominated transport to bias-activated resonant conduction as length, contact registry, and strain change, and they yield concrete, experimentally testable signatures, including parity oscillations in low-bias conductance, systematic transition-voltage shifts with length and strain, and eigenchannel-resolved spatial fingerprints, that provide direct guidance for scanning tunneling microscopy and mechanically controllable break-junction validation.

References:

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