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From DFT-computed conductivity to full-wave design of γ-graphyne terahertz patch antennas

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Abstract:

Realizing compact terahertz (THz) radiators requires radiating materials whose dispersive electromagnetic response is known with atomistic accuracy, since experimental data for emerging two-dimensional carbon allotropes at THz frequencies remain scarce. We present a first-principles-informed study of THz microstrip patch antennas that use gamma-graphyne as the radiating sheet. The complex surface conductivity of gamma-graphyne was computed from density functional theory, using SIESTA, combined with a Kubo-Greenwood linear-response evaluation, then imported as a dispersive surface boundary into full-wave finite-element simulations in COMSOL. Four patch topologies were compared: a plain patch, a patch with edge gamma-graphyne nanoribbons, a patch on a photonic-bandgap substrate, and a hybrid nanoribbon-plus-photonic-bandgap design, all built around a common substrate width of 40 μm and length of 48 μm.

All four designs operate in the low-THz region and exhibit stable resonances with compact electrical size and competitive radiation performance. The plain and nanoribbon-edged patches resonate near 3.28-3.29 THz, with reflection-coefficient minima of about -33.6 and -34.8 dB and bandwidths of 0.14 THz, a fractional bandwidth near 4.25%, while the photonic-bandgap and hybrid variants resonate higher, at 3.45-3.59 THz, with shallower minima between -22 and -19.2 dB. Peak broadside gains reach 5.9-6.4 dB across the family, and radiation efficiencies at each design's center frequency lie in the 80-83% range. The nanoribbon-edged variant provides the best intrinsic impedance match to 50 ohms, with an input resistance of 51.16 ohms and a voltage standing-wave ratio of 1.03, without any external matching network, whereas the photonic-bandgap variants improve peak gain and efficiency by suppressing substrate-guided modes at the cost of additional feed tuning. Convergence and sensitivity checks confirm that these trends are robust to reasonable variations in mesh parameters, scattering broadening, and substrate permittivity, although lithographic errors of only a few percent in patch length or lattice constant are found to shift the operating frequency by tens to hundreds of gigahertz. Specific absorption rate calculations against a three-layer skin, fat, and muscle phantom confirm that the peak exposure, 2.75×10^{6} W/kg at an input power of 1 W, remains well below permitted whole-body exposure limits.

These findings demonstrate that gamma-graphyne, when characterized from atomistic theory and applied in device-scale design, is a promising two-dimensional material candidate for compact THz radiators, and that edge-nanoribbon shaping and photonic-bandgap substrates offer complementary, independently tunable routes to impedance matching and radiation efficiency in graphyne-family antennas.

References:

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