Optical properties and terahertz applications of one-dimensional nanocarbons

R. R. Hartmann[1] and M. E. Portnoi[2]
[1]*Physics Department, De La Salle University, 2401 Taft Avenue, 0922 Manila, Philippines*
[2]*Physics and Astronomy, University of Exeter, Stocker Road, Exeter EX4 4QL, United Kingdom*
m.e.portnoi@exeter.ac.uk

Carbon-based nanostructures are believed to be promising candidates for terahertz (THz) applications [1]. Following our earlier work on narrow-gap carbon nanotubes and graphene nanoribbons [2], as well as graphene bipolar waveguides [3] and double quantum wells [4], we are now considering dipole optical and terahertz transitions in two other types of nanocarbons – carbynes and cyclocarbons.

The technology for synthesizing carbynes (polyyne carbon chains) has rapidly evolved over the last few years, with stable long chains deposited on substrates now a reality [5]. We have recently demonstrated and explained a strong polarization dependence of photoluminescence from highly-aligned carbon chains terminated by gold clusters [6]. A prominent feature of long polyyne chains (chains with two alternating non-equal bonds) is the presence of topologically protected mid-gap edge states. For a finite-length chain, the two edge states form an even and odd combination with the energy gap proportional to the edge-state overlap due to tunneling. These split states of different parity support strong dipole transitions. We have shown [7] that for long enough carbyne chains, the energy separation between the HOMO and LUMO molecular orbitals formed by the edge states corresponds to the THz frequency range. There are several other allowed optical transitions in this system that can be used to maintain the inversion of population required for THz lasing. The frequency of THz transitions can be tuned by an external electric field [8].

Another recent achievement in nanocarbon technology is the demonstration of controlled synthesis of cyclocarbons, particularly the cyclocarbon allotropes C_{18} [9] and more recently C_{16} [10]. The properties of cyclocarbons in an external (lateral in the plane of the molecule) electric field differ drastically depending on the parity of the number of dimers in a polyyne ring. This is a direct consequence of breaking the inversion symmetry in a ring consisting of an odd number of dimers, including the famous C_{18}. Our estimates [11] show that adding just one extra carbon dimer to C_{16} is equivalent to placing this molecule in an external magnetic field of over 1000 T. For an odd-dimer cyclocarbon, as a result of the absence of inversion symmetry, an experimentally attainable electric field should open a tunable gap between otherwise degenerate states, leading to two states with allowed dipole transitions between them in the THz range. Population inversion can be achieved again using optical pumping.

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