A semiconducting study to nanotubes based on graphyne family

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The graphyne structures is a theoretical/partially synthesized family of 2D carbon materials. These systems exhibit a network made from $sp + sp^2$ hybridized carbons. The physical properties of these structures include: tunable band gap, high carrier mobility, strong anisotropy, remarkable strain engineering and promising for spintronics[1]. The rγGY (rectangular γ-graphyne) is another proposed semiconductor from this family with hexagonal sp^2 rings connected by acetylenic connections[2]. Here we investigate the electronic properties of rγGY nanotubes using computational simulations with DFT first principles calculations. We identify the interplay involving chirality, diameter, and the emergence of dispersive/localized frontier states on gap modulation through simple extrapolated methods. Furthermore, the DFT and ZF (Zone Folding) approaches reveal an oscillation of the band gap across the nanotube diameter, indicating different electronic behavior even when dealing with nanotubes of the same chirality. This study may lead experimental researchers to understand electronic behavior in similar porous carbon materials with relevant results.

Key-words: rγGY nanotubes, electronic properties, DFT, gap modulation.

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