Semiconducting tubes derived from a rectangular graphyne: a DFT study

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Proposing new ways to organize carbon in 2D nanomaterials has been a relevant strategy in the search for systems with targeted properties for different applications. One focus is the study of fully sp^2 non-graphitic networks, with successfully synthesized examples [1,2]. Hybrid sp-sp^2 systems of the graphyne family are a related approach, and many systems have the honeycomb lattice as a base model. However, other examples have been inspired by other lattices as the recently proposed rγGY sheet[3], which features a semiconducting behaviour with highly localized quasi-1D states. Here, we investigate how to tune rγGY properties by folding this sheet into nanotube forms. We elucidate mechanisms that determine their electronic structure by means of density functional theory calculations. We also identify the interplay involving chirality, diameter, and the emergence of dispersive/localized frontier states on gap modulation. Alternatively, we explore gap engineering in these systems through controlled mechanical deformation with the application of uniaxial strain. Following DFT-based simulations, we analysed the stress-strain curves, the elastic constants, the mechanical and electronic anisotropy. Our findings also show that strain has revealed as an efficient band gap engineering mechanism, promoting a semiconductor-metallic transition dependent on the deformation direction and the parity of the structural indices. The results presented here reinforce the potential of rγGY as a promising candidate for applications in nanoelectronic devices.

References

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[2] A. G. Vieira, M. L. Pereira, V. Meunier, E. C. Girão. Carbon Trends 16 (2024), 100395.
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Figure

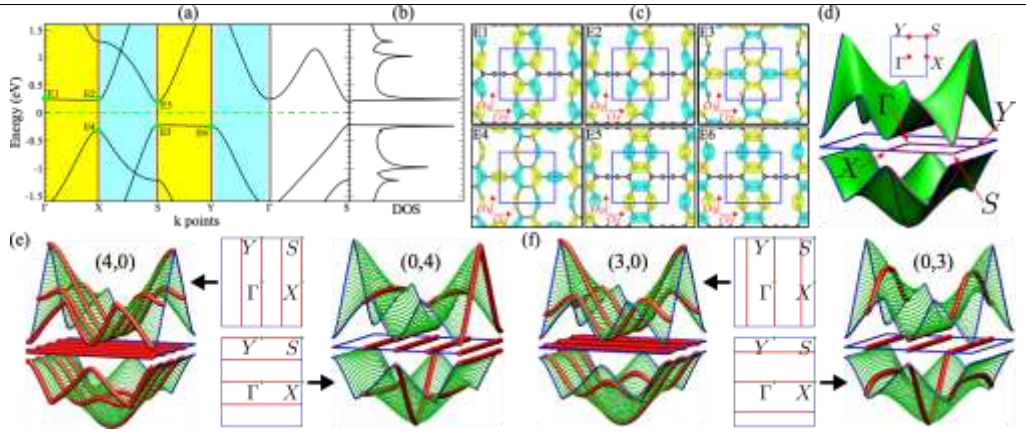

Figure 1: Electronic structure of rγGY represented over high-symmetry lines of the BZ. E1-E6 represent important energy levels from the frontier bands. (b) Density of states of rγGY. (c) Real part of the wavefunction for the E1-E6 energy levels indicated in (a), with cyan and yellow clouds representing portions of the wavefunction with opposite sign. (d) Valence and conduction bands of rγGY are represented by a surface plot over the entire BZ, with the Fermi energy represented by the blue rectangle. (e) Cutting lines for the (4,0) and (0,4) tubes represented over the 2D BZ and over the frontier bands of rγGY. (f) Same as (e), but for the (3,0) and (0,3) tubes.