A computacional study on the mechanical and eletronic properties of graphenyldiene materials

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Graphene-derived systems demonstrate characteristics that could revolutionize the electronics industry. For example, graphenylene is an effective allotrope of carbon for the separation and storage of hydrogen, promising for many other applications such as highly sensitive gas and ion sensors[1]. Another carbon-based material is graphenyldiene (GPD), a semiconductor monolayer with octadecagonal, hexagonal and tetragonal rings[2]. We performed calculations based on DFT simulations to investigate the mechanical and electronic properties of nanotubes and membranes graphenyldiene's. When strain is applied small fluctuations in the band gap value are observed, indicating that the material retains its electronic characteristics even when stretched. The anisotropic effect is also observed when measuring the Young's modulus obtained through the stress-strain graph.

Key-words: graphenyldiene, electronic properties, mechanical properties, DFT, Young's modulus, stress-strain.

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