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STRAIN EFFECT IN CARBON NANORIBBONS WITH 5-8-5 CARBON RINGS SYMMETRY

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Resumo

Carbon allotropes are frequently applied in different areas of technology since they have great features like high carrier mobility and mechanical resistance. Among the carbon structures predicted so far, graphene receives special attention, since it has great mechanical, electrical, and thermody namical properties. Motivated by the achievement of graphene by Geim and Novoselov in 2004, several works have proposed new 2D carbon allotropes with different symmetries. In 2018, a the oretical work by Wang et al. predicted a 2D carbon allotrope with a 5-8-5 carbon rings symmetry named POPGraphene, which was proposed as a possible new anode material for Li-ion batteries. As carbon nanoribbons present different properties from their 2D counterpart, in 2021 Mota et al. proposed new carbon nanoribbons based on POPGraphene structures. Carbon nanoribbons are in teresting system because it has a possibility of wide range of applications, since there are a lot of methods that can be performed to tunning there features. In this work we investigated the tensile and compressive strain application effetc on five carbon nanoribbons, with different edges shape, based on POPGraphene (three in zigzag and two in armchair directions). The structural and electronic properties of the nanoribbons were investigated using Density Functional Theory implemented in the SIESTA code. The GGA functional was implemented with a DZP basis set to represent the valence electrons, and normalized pseudopotentials of Kleinmann and Bylander to represent the inner shell. The reults show that the electronic and transport are strongly dependent of the strain application. Therefore, we see that strain application is an excellent method to modulate the electronic properties of carbon nanoribbons, promoting a wide range of applications for these systems.

Palavras chave: Carbon nanoribbons; DFT; Strain Effect