ELECTRONIC PROPERTIES OF BORON DOPED GRAPHENE NANOWIGGLES.

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RESUMO

Graphene nanoribbons with complex edge structures have been broadly synthesized during the last decade, resulting in a diverse collection of different forms which includes several doping configurations. While most studies of these so-called doped nanowiggles focus on nitrogen doping, understanding how boron doping affects their electronic structure is a fundamental issue, as boron has complementary features relative to nitrogen when compared to carbon. With this motivation, we apply first-principles simulations to investigate the electronic properties of boron doped graphitic nanowiggles (GNWs). In summary, we investigated the electronic properties of boron substituted nanowiggles with doping at different atomic (internal/edge) setups. Our results show that these systems exhibit non trivial spin polarized electronic configurations, which turn these nanowiggles into narrow semiconductors with clear separation between spin-up and -down states in the vicinity of the Fermi energy. Furthermore, we demonstrate that spin polarized states are more robust in internal doping, as they result in a stronger energy lowering mechanism than in edge doping. Such features can potentially result in nontrivial features for spintronic applications, similarly to what happens for other systems studied in the literature. However, the systems here studied have the advantage of corresponding to structures with a more favorable prospect for experimental realization than other systems investigated previously by computational methods.

PALAVRAS-CHAVE: graphene, nanoribbons, First Principles, Electronic Properties, nanowiggles

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