Nonlinear Gap Modulation of Graphene Nanoribbon in Infinite Monolayers of Hexagonal Boron Nitride

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Abstract: The possibility of modulating the hexagonal boron nitride gap from carbon doping[1,2], motivates us to study the behavior of these structures with the presence of different families of carbon nanowires. Using the Density Functional Theory (DFT)[3], the nonlinearity was verified in the reduction of the gap of the structure with the lateral growth of the nanotape armchair. The band structures, state density and localized charge density were analyzed. There was a significant increase in the gap in the transition of faze between the three different families studied, 3p, 3p + 1 and 3p + 2, from which we studied 9 systems. It has been found that the states of the valence bands concentrate on the carbon atoms of the nanoribbon, concluding that the material may have a possible application in nanocircuits with the possibility of transporting in carbon trails in mono layers of boron nitride hexagonal.

Key-words: Nanoribbons, band gap and DFT

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References: