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Ab initio study of boron nitride lines on graphene BERENICE MATA-CARRIZAL, RAÚL SANGINÉS-MENDOZA, EDGAR MARTINEZ, Universidad Autónoma de Nuevo León — Graphene has unusual electronic properties which make it a promising material for electronic devices. Neverthless, the absence of a band gap sets limitations on its practical applications. Thus, it is crucial to find methods to create and tune the band gap of systems based on graphene. In this way, we explore the modulation of the electronic properties of graphene through doping with boron nitride lines. In particular, we studied the electronic structure of graphene sheets doped with boron nitride lines armchair and zigzag type. The calculations were performed using the pseudopotential LCAO method with a Generalized Gradient Approximation (GGA) for the exchange-correlation energy functional. We found that both doping lines type induce a bandgap and that the energy gap increases as the length of doping lines increases. Accordingly to our DFT calculations, we found that the energy gap on graphene doped with armchair and zigzag lines is due to a two different mechanisms to drain charge from pi- to sigma- orbitals. Thus, we found that doping graphene with boron nitride lines is a useful way to induce and modulate the bandgap on graphene. This research was supported by Consejo Nacional de Ciencia y Tecnología (Conacyt) under Grant No. 133022.

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