Ti and Mn doped graphene nanoribbons: an *ab initio* study

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The experimental discovery of graphene with one atom thick allows the production of ribbons, called graphene nanoribbons. While these materials share properties with other carbon based materials, such as carbon nanotubes and graphene, other effects arise due to their width and the edge geometries. In this context, this work aims to investigate the zigzag nanoribbons electronic and magnetic properties dependence on the impurity position by *ab intio* calculations. A chemical sensitivity of the ribbon properties is demonstrated, noting different behaviors of the electronic properties with magnetic Mn impurities and non-magnetic Ti impurities doping. It is also shown that the nanoribbons edges are the energetically favorable sites, independent of the impurity type.
Keywords: nanoribbons, chemical doping, DFT.

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