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Energy gap of Graphene Nanoflakes: Edge Magnetism and Self-Energy Corrections. ROMEO DE COSS GOMEZ, CARLOS MANUEL RAMOS CASTILLO, Departement of applied physics centro de investigacion y de estudios avanzados del instituto politecnico nacional — Previous theoretical works has predicted that graphene nanostructures with zigzag edge exhibit metallic behavior around 6-7 nm, however in such calculations the magnetic nature of zigzag edges was not considered. In this work, the influence of the edge magnetism on the size dependence of energy-gap in hexagonal gaphene nanoflakes (GNFs) with zigzag borders is studied by density functional theory calculations. Thus, we found that meanwhile the calculations without spin polarization predicts that the metallic behaviour for GNFs begin at 6 nm deviating from the trend predicted for effective model of Dirac fermions, spin-polarized calculations predicts semiconducting behavior at 6 nm. This result shows clearly that the origin of metallic behaviour predicted at 6 nm in previous works is not related with the well known band-gap problem of Kohn-Sham scheme, but with neglecting spin polarization. Furthermore, to correct the band-gap problem of Kohn-Sham Scheme, we have calculated the size dependence of fundamental energy-gap using the quasiparticle formalism by adding/removing an electron to/from the system.

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