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Magnetism of single and divacancies in graphene nanoflakes[1] SILVIA FERNANDEZ-SABIDO, M.E. CIFUENTES-QUINTAL, CARLOS RAMOS, ROMEO DE COSS, Centro de Investigaciones y de Estudios Avanzados del Instituto Politécnico Nacional - Unidad Mérida — Vacancy-induced magnetism in graphene is a recent topic of great scientific relevance because of the potential applications of spin-polarized graphene-based systems. In this work, we have studied by means of DFT calculations, the structural, electronic and magnetic properties of single and divacancies in hexagonal zigzag graphene nanoflakes $C_{6n^2}H_{6n}(n = 2, \ldots, 7)$. We have found that, when a single carbon atom is removed, the structure undergoes a magnetic 5-9 reconstruction where the interatomic distances depend on the nanoflake size. The charge density distribution suggests that there is not a complete bond reconstruction in the vacancy zone, however, the existence of a partial bond is sufficient to conclude that only two electrons remain unpaired, resulting in the $2\mu_B$ spin moment. The spin moment is equally distributed over the localized-sp^2 and delocalized-p_z orbitals. For a carbon-divacancy, we have varied the distance between the vacancies and we have found magnetic structural reconstructions (9-4-9, 5-9-9-5, 5-9-6-5) which have not been reported for graphene layer with magnetic moments between 2 and $4\mu_B$; although the most stable is the nonmagnetic 5-8-5 reconstruction.

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