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Defect-induced magnetism in graphene nanoflakes E. MARTINEZ-GUERRA, M.E. CIFUENTAS-QUINTAL, R. DE COSS, Departamento de Fisica Aplicada, Cinvestav-Merida, Yucatan, Mexico — The interaction between electron spin and the magnetic moments of vacancies in graphene could open new opportunities for spintronic and quantum computation. In that direction, we have studied the magnetic properties of graphene nanoflakes ($C_{6n^2}H_{6n}$) with vacancies within the framework of density functional theory, using the pseudopotential LCAO method with a Generalized Gradient Approximation (GGA) for the exchange-correlation energy functional. In particular, we have calculated the magnetic moment of graphene nanoflakes of different diameters with a simple vacancy. We have found that the total spin-polarization of the graphene nanoflakes with a simple vacancy decreases as the diameter increases. In particular, we show that the vacancy induces the appereance of a midgap state at Fermi level. Thus, the spin degeneracy is broken, being only one of the spin channels of the midgap state occupied, the other being empty. This feature could be exploited for future spintronic applications. This research was supported by Consejo Nacional de Ciencia y Tecnología (Conacyt) under Grant No. 83604.

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