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Magnetism of single-vacancy defects in graphene and boron-nitride nanoflakes[1] SILVIA FERNANDEZ-SABIDO, CARLOS RAMOS, EDUARDO CIFUENTES-QUINTAL, ROMEO DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico — In this work we have used the hexagonal zigzag graphene and boron-nitride nanoflakes as a simple systems for studying the new class of magnetic materials obtained by structural vacancies in nonmagnetic s-p nanostructures. We have shown that for these systems, it is possible to predict the total spin moment from a electron counting analysis. Employing DFT calculations based on the LCAO approximation and the Fixed Spin Moment method, we have determinate the ground state spin multiplicity and the spin magnetic distribution for these structures. We have found that the ground state multiplicity of graphene nanoflakes is triplet, corresponding to a spin magnetic moment of $M = 2\mu_\beta$. Analyzing the spin orbital distribution we have determinate that the spin-polarized for the graphene nanoflakes is equally distributed in the sp^2 and p_z orbitals. For the boron-nitride nanoflakes we have obtained a quartet state ($M = 3\mu_\beta$) in the case of a boron vacancy, and a doublet state ($M = 1\mu_\beta$) for a nitrogen vacancy. We have found that for the boron-vacancy the spin-polarized is mainly localized on the sp^2 orbitals of nitrogen atoms. In contrast, for the nitrogen-vacancy the spin-polarized is concentrated at the p_z orbitals of boron atoms.

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