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Magnetism of substitutional sp-element impurities in graphene and silicene: energetics and concentration dependence[1] J. HERNÁNDEZ-TECORRALCO, L. MEZA-MONTES, IF-BUAP, M.E. CIFUENTES-QUINTAL, R. DE COSS, CINVESTAV-Mérida — It has been predicted from ab-initio calculations that a finite spin magnetic moment may result in sp-element substitutional impurities in two-dimensional materials. Particularly, phosphorus-doped graphene and nitrogen-doped silicene for 3.2% concentrations (supercell 4x4) have been reported to present this effect. In this work, we have performed a structural, electronic, magnetic, and energetics properties systematic study of substitutional impurities for P@graphene and N@silicene as a function of doping concentration, by means of first principles calculations. We have calculated the electronic and magnetic properties for different supercell sizes, from 3x3 to 8x8. The energetics and the magnetic moment for the studied systems were obtained with the Fixed-Spin Moment Method. We found that the magnetic moment in P@graphene practically remains constant for supercell sizes from 3x3 to 8x8, however the exchange energy gained by the spin-polarization is strongly reduced as the concentration decreases. In contrast, N@silicene showed a magnetic moment around 0.8 μ_B for the 3x3 and 4x4 supercells, but for lower concentrations the system becomes non-magnetic. Finally, the results are analyzed in terms of the charge and spin density distributions in the σ and π orbitals.

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