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Ab Initio Study of the Interactions between Dopant Atoms and Vacancies in Graphene[1] TAREK TAWALBEH, NSMU, IGOR VASILIEV, NMSU — We apply a first-principles computational method based on density functional theory to study the interaction of substitutional boron and nitrogen atoms with single vacancies in graphene. Our calculations are carried out using a pseudopotential technique combined with the generalized gradient approximation for the exchange-correlation functional implemented in the SIESTA electronic structure package. The equilibrium geometries, total energies, electronic structures, magnetization, and spin-polarized densities of states of doped and defective graphene sheets are examined as a function of the separation distance between dopant atoms and vacancies. Our study shows the presence of attractive interaction between dopant atoms and vacancies. Furthermore, we found that boron dopants enhance the magnetism of graphene sheets containing single vacancies, whereas nitrogen dopants reduce it. The influence of dopant site location on both the interaction energy and magnetization is discussed.

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