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Ab Initio Study of the Interaction between Dopant Atoms and Point Defects in Graphene TAREK TAWALBEH, IGOR VASILIEV, NMSU — We apply a first-principles computational method based on density functional theory to study the interaction of substitutional boron (B) and nitrogen (N) atoms with Stone-Wales defects and 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 (Spanish Initiative for Electronic Simulations with Thousands of Atoms) electronic structure package. Graphene sheets are modeled by periodic supercells containing up to 160 atoms. The equilibrium geometries, total energies, electronic structures, and densities of states of doped and defective graphene sheets are examined as a function of the separation distance between dopant atoms and point defects in graphene.

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