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Ab Initio Study of the Interactions between Dopant Atoms in Graphene[1] IGOR VASILIEV, NABIL AL-AQTASH, TAREK TAWALBEH, KHALDOUN AL-TARAWNEH, New Mexico State University — We present a first-principles computational study of the interactions between the boron (B) and nitrogen (N) dopant atoms in graphene. Our calculations are carried out using density functional theory combined with the generalized gradient approximation for the exchange-correlation functional. The total energies, equilibrium geometries, electronic charge distributions, and densities of states of doped graphene sheets are examined in cases of B-B, N-N, and B-N co-doped graphene. We find the B-B and N-N interactions to be repulsive and the B-N interaction to be attractive. In all cases studied, dopant-dopant interactions appear to have a relatively short range. The interaction energy between the two dopant atoms is found to be inversely proportional to the square of the separation distance. We interpret these results in terms of structural relaxation and electronic charge transfer.

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