Abstract Submitted
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First Principles Study of Interactions between Dopant Atoms in Graphene[1] NABIL AL-AQTASH, IGOR VASILIEV, New Mexico State University — We study 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. The interaction energy between the two dopant atoms is found to be inversely proportional to the square of the separation distance. We find the B-B and N-N interactions to be repulsive and the B-N interaction to be attractive. The changes in the density of states observed in B- and N-doped graphene are explained in terms of electronic charge transfer.

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Nabil Al-Aqtash
New Mexico State University

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