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Binary Doping of N-B and N-P into Graphene and Graphene Nanoribbons: Structural, Electronic, and Transport properties

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We apply a density functional theory (DFT) and DFT-based non-equilibrium Green's function approach to study the structures, energetics and charge transport characteristics of nitrogen-doped graphene and graphene nanoribbons (GNRs) with additional doping of phosphorus or boron atoms. Considering graphitic, pyridinic, and porphrin-like N doping sites and increasing N-doping concentration, we analyze the structures of N-P and N-B doped graphene and particularly focus on how they affect the charge transport along the lateral direction. For the GNRs, we also consider the differences between defects formed at the edge and bulk regions. Implications of our findings in the context of electronic and energy device applications will be also discussed.

Keywords: DFT, Graphene, Quantum transport