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Ab-initio investigation of optical absorption spectra properties of doped Graphene GIRIJA DUBEY, Department of Earth & Physical Sciences,York College,CUNY, NY, POOJA RANI, VIJAY JINDAL, Department of Physics, Panjab University Chandigarh-160014 — Ab-initio calculations based on density functional theory(DFT) have been performed to study the changes in the absorption spectrum of graphene substituted with B, N and BN. The dielectric function and hence the absorption spectrum of single layer graphene sheet have been calculated. The present study can be concluded as, the individual B and N doping does not significantly affect the imaginary dielectric function and hence the absorption spectrum.However, red shift in the absorption towards visible range of the radiation at high doping is found to occur in case of B/N co-doping at high doping concentration. It can be inferred the B/N co-doping of graphene can alter the optical properties of graphene to make it reflect in the visible region.

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