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Stability and Superconductivity of N-(B-) Doped Graphene JIAN ZHOU, Virginia Commonwealth Univ, QIANG SUN, QIAN WANG, Peking University, PURU JENA, Virginia Commonwealth Univ — Superconductivity of two-dimensional honeycomb lattice has been predicted to possess a wealth of fascinating properties. For example, if graphene is heavily electron/hole doped, it exhibits high-temperature topological superconductivity. However, to achieve this, the carrier concentration will be too high, and graphene will be dynamically unstable. One possible route will be atomic substitution by B or N atoms, which, unfortunately, again is dynamic instability in nature. Using density functional theory combined with a global structural search and phonon dispersion calculations, we show that an ordered 50% N- (B-) doped graphene can be made energetically and dynamically stable by simultaneous doping carriers and applying biaxial tensile strain. By using a simple model, we show that tensile strain reduces the electrostatic interaction and moves imaginary phonon dispersion to be positive. Electron-phonon coupling calculations show that the N- (B-) doped graphene is superconducting with critical temperature reaching 66 K in the case of 50% N-doped graphene.

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