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Electronic structures and electron-phonon interactions of boron-doped carbon nanotube TAKASHI KORETSUNE, SUSUMU SAITO, Tokyo Institute of Technology — We study the boron-doped single-walled carbon nanotubes using first-principles method based on the density functional theory. The total energy, band structure and density of states are calculated. From the formation energy of boron-doped nanotubes with different diameter, it is found that the narrower tube needs lower energy to substitute a carbon atom with a boron atom. Using the result of different doping rate in the (10,0) tube, we extrapolate the result to low boron density limit and find that the ionization energy of the acceptor impurity level is approximately 0.2 eV. Furthermore, we discuss the doping rate dependence of the density of states at the Fermi level and the electron-phonon interactions which are important for superconductivity.

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