Influence of C-Doping on the B-11 and N-14 Quadrupole Coupling Constants in Boron-Nitride Nanotubes: A DFT Study

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A computational study at the level of density functional theory (DFT) was carried out to investigate the influence of carbon doping (C-doping) on the ^{11}B and ^{14}N quadrupole coupling constants (C_Q) in the (6,0) single-walled boron-nitride nanotube (BNNT). To this aim, a 10 Å length of BNNT consisting of 24 B atoms and 24 N atoms was selected where the end atoms are capped by hydrogen atoms. To follow the purpose, six C atoms were doped instead of three B and three N atoms as a central ring in the surface of the C-doped BNNT. The calculated C_Q values for both optimized BNNT systems, raw and C-doped, reveal different electrostatic environments in the mentioned systems. It was also demonstrated that the end nuclei have the largest C_Q values in both considered BNNT systems.

Key words: C-Doping; Boron-Nitride; BNNT; Nanotube; Quadrupole Coupling Constant; DFT.