Defective BN Nanotubes: A Density Functional Theory Study of B-11 and N-14 NQR Parameters

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A density functional theory (DFT) study is performed to investigate the influence of structural defects on the electronic structure properties of perfect boron nitride nanotubes (BNNTs). To this aim, as representative models, the single-walled (6,0) BNNT consisting of 36 boron, 36 nitrogen, and 12 hydrogen atoms and the single-walled (4,4) BNNT consisting of 36 boron, 36 nitrogen, and 16 hydrogen atoms are considered. The nuclear quadrupole resonance (NQR) parameters are calculated and compared in two perfect and defective models of the considered BNNTs. The results indicate that due to formation of non-hexagonal rings in the defective model because of removing a B – N bond, the NQR parameters at the sites of first neighbouring nuclei are significantly influenced by imposed perturbation, however, the sites of other nuclei, farther from perturbation, remain almost unchanged. The calculations are performed at the level of the BLYP method and 6-31G* standard basis set using the GAUSSIAN 98 package.

Key words: Defect; Boron Nitride; Nanotube; Electric Field Gradient; DFT.