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Diameter Dependence of Band Gap of Single-Walled Boron Nitride Nanotubes

© *B.J. Abdullah*

Department of Physics, College of Science, Salahaddin University-Erbil, Erbil, Kurdistan Region, Iraq

E-mail: botan.abdullah@su.edu.krd

Received: March 19, 2021
Revised: March 19, 2021
Accepted: March 26, 2021

The electronic structure of single-walled boron nitride nanotubes (BNNTs) is investigated by density functional theory within HSE06. Material Studio software is used in the CASTEP code to examine the functional energy gap using various exchange correlation functionals. The band gap energy of the bulk BN is calculated within HSE06 and the results are more accurate compared with those calculated using LDA and GGA. Based on the results, the performance of HSE06 is also applied to study the optical band gaps for BNNTs in armchair and zigzag form. It is found that the energy band gap is a function of the small tube diameter and band gaps decrease with decreased tube size. It is also found that the change in the band gap energy of the zigzag is more sensitive than that of the armchair of the same tube diameters, which results from many factors including chirality, total energy, strain energy, and binding energy that can lead to decreasing energy gap. The calculated results can be useful for experimental verification via HSE06 for BNNTs.

Keywords: boron nitride, nanotubes, energy band gap, density functional theory, HSE06.