عنوان مقاله:

(The Effect of Stone-Wales Defect on the Geometrical Parameters and Electronic Properties of ACNTs (۱۴, ۱۴

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خلاصه مقاله:

In this work, we intend to investigate the effect of Stone–Wales defect (SW defect) in armchair (۱۴, ۱۴) carbon nanotubes (ACNTs (۱۴, ۱۴)) and how it perturbs the energy states near the Fermi level. The SW defect may occur in graphene, carbon nanotubes (CNTs), and similar carbon frameworks, in which the four adjacent six-membered rings of a pyrene-like region turn into two five-membered rings and two seven-membered rings when the bond uniting two of the adjacent rings rotate. Our calculations indicate that ACNTs (۱۴, ۱۴) with SW defect have semiconducting behavior, although the armchair CNTs are expected to be metal. The band-gap of ACNTS (۱۴, ۱۴) with SW defect is ۰.۱۱ eV. In addition, the obtained results show that the density of states of ACNTs (۱۴, ۱۴) with SW defect reaches its zenith at ۱۳ eV. The results show that the C–C bond lengths and diameter of ACNTs (۱۴, ۱۴) with SW defect are ۱.۴۰ Å and ۱۸.۷۴ Å, .respectively

کلمات کلیدی:

Armchair CNTs, Tight-binding, Stone-Wales defect, Electronic properties