عنوان مقاله:
Tight Binding Study of Armchair CNTs (۱۴, ۱۴) Geometrical Parameters and Energy Sub-Bands

محل انتشار:
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خلاصه مقاله:
Investigating the physical properties of carbon nanotubes is a useful method to recognize their nature and clarify the operation of these nanostructures in nanotechnology market. In this work we have used the tight binding method to simulate the geometrical parameters, the effect of chirality on the number of non-degenerate and degenerate sub-bands, and the sub-bands of armchair (۱۴, ۱۴) carbon nanotubes. The results show that the C–C bond lengths and diameter of CNTs (۱۴, ۱۴) are ۱.۳۹ Å and ۱۸.۵۳ Å, respectively. The other calculated parameters haven't been reported yet to assess the accuracy of the data. The symmetry operations of the infinitely long CNTs (۱۴, ۱۴) can be described via the symmetry groups D۱۴d. The crossing sub-bands at Fermi level suggest that CNTs (۱۴, ۱۴) has metallic behavior. The origin of energy was arbitrarily set to be at the maximum valence band. The band structure shows ۵۶ sub-bands and it is clear that ۱۳ conduction (valence) sub-bands are doubly degenerate, and ۲ conductions and ۲ valence sub-bands are non-degenerate sub-bands.

کلمات کلیدی:
CNTs, Stone-Wales defect, Tight binding, Electronic sub-bands, Geometrical Parameters