

论文

有限长Y型碳纳米管结构和性质的第一性原理研究

薛冰纯, 蔡文生, 邵学广

南开大学化学学院, 天津 300071

摘要:

采用密度泛函理论的GGA/PW91方法对有限长Y型碳纳米管的结构和性质进行了研究. 研究表明, 由于缺陷环的影响, Y型碳纳米管与直型管的性质明显不同, 而且, Y型碳纳米管的结构和性质与分支管长度存在一定的关系. 当分支管长度大于1 nm 时, Y型碳纳米管的结构、能隙和电学性质均出现周期性振荡变化的趋势.

关键词: 有限长Y型碳纳米管 几何结构 电子结构和性质

First-principle Theoretical Study of Structures and Properties of Finite-length Y-shaped Carbon Nanotubes

XUE Bing-Chun, CAI Wen-Sheng, SHAO Xue-Guang\*

Department of Chemistry, Nankai University, Tianjin 300071, China

Abstract:

The geometry and electronic structure of finite-length(4,4) Y-shaped carbon nanotubes(CNTs) were investigated using density functional theory with GGA-PW91 method. The results indicate that the difference between the Y-shaped CNT and the pristine one is remarkable due to the influence of the defects in the junctions of the former. Furthermore, the structures and properties of Y-shaped CNTs are found to be related to the length of the CNT branch. By comparing the properties of the Y-shaped CNTs with different lengths, the length-dependent oscillation behavior including structure, energy gap and electronic property were observed when the length is longer than 1 nm.

Keywords: Finite-length Y-shaped carbon nanotube Geometry Electronic structure and property

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作者简介:

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