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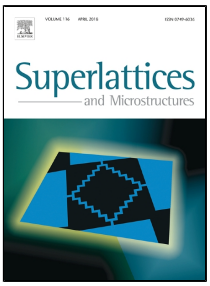

The electron properties of infinite length single-walled silicon nanotubes are studied by density functional theory

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The electron properties of infinite length single-walled silicon nanotubes are studied by density functional theory

Deng-Hui Liu Cheng-Peng Yao* Ming Yang[b] and Heng-Jiang Zhu[a]

Abstract:

In this article, we aim to use LGTO-PBC-DFT calculation method with PBEPBE/ 6–31G(d) basis sets and PBC model to optimize geometric structure, obtain electron characteristics and band gaps of (n, m) chiral (6 ≤n≤16, 2≤m≤8); (n, 0) zigzag (3≤n≤15) and (n, n) armchair (2≤n≤8) pure infinite length single-walled Silicon nanotubes.

We have obtained that the HOCO-LUCO gaps decrease with the radii of the SWSiNTs increase by using the PBEPBE functional and 6–31G(d) basis set. most of the infinite length SWSiNTs which we studied are narrow band gaps semiconductors. perhaps the surface structure is the most important factor affecting the band gap of the nanotubes. there have been a research on the infinite silicon nanotubes and with the increase of the tube radius, an indirectdirect band gap transition has been revealed.

For all the armchair SWSiNTs, the infinite zigzag SiNTs (n,0), (3≤n≤9) and the infinite chiral SWSiNTs (6, 2), (9, 3), (10, 5), (12, 6) are semiconductors with indirect band gaps. While for the infinite zigzag SiNTs (n, 0) 15≥n≥10, and the infinite chiral SWSiNT (12, 4) are semiconductors with direct gaps at X point, the direct gaps open at X point. It is possible that direct band gap will become potential building blocks for electronic and optoelectronic devices.

Keywords Silicon nanotubes; Density functional theory; Periodic boundary conditions; Band gap ; Semiconductor

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Introduction

For almost thirty years, with the development of science and technology, nanomaterials[1-2]have gradually become the focus of researchers.

From graphene[3-4], diamond[5-6], C_{60} fullerene[7-8]to nanowires[9-10], nanobelt[1112], nanotubes[13-14]. the successful synthesis of graphene[15] has attracted widespread attention to carbon-based nanomaterials[1617]. later, people gradually increased their attention from carbon based nanomaterials[1819] to non-carbon nanomaterials[2021], and gradually increased from zero-dimensional nanoparticles[22] to one-dimensional nanotubes[23-24] and nanowires[25-26]to two-dimensional graphene[27-28]and then extended to three-dimensional graphite[29-30].

Nano-materials with its unique physical and chemical properties in lithium batteries[31-32], optoelectronic nanodevices[33-34], industrial areas[35] and even global sustainability[36] have a lot of value. the most famous graphene is a strong material with good electrical conductivity, like rare metals (Rickard Arvidsson and Bjorn Sanden et al[37] Have studied new ways to replace rare metals with carbon nanomaterials. Rare metals are widely found in our daily necessities around us, computers, mobile phones, etc. almost all other electronic devices and around you found in the plastic, our society is highly dependent on rare metals, which ensures a high degree of pursuit of rare metals, but Because rare metals such as tin, silver, tungsten and indium are rare and difficult to extract because their concentration is very small).

In addition to two-dimensional graphene[3839], one-dimensional nanotube[40-41]and nanowires[4243]have also attracted widespread attention from scientists, especially carbon nanotubes[4445] and non-carbon nanotubes[46-47], which exhibit different physical and chemical properties, the application of drugs[48], catalysis[49] and nano-electronic[50] equipment and other fields[51].

There are some articles on the theory and experiment of silicon nanotubes. J Sha et al[52] using nanochannel Al_2O_3 as a template and a chemical vapor deposition（CVD）synthesize silicon nanotubes, SB Fagan et al[53] using first-principles calculations based on density functional theory, RQ Zhang et al[54] using the semiempirical molecular orbital PM3 method, M Zhang