Optik - International Journal for Light and Electron Optics 170 (2018) 436–443

Contents lists available at ScienceDirect

Optik

journal homepage: www.elsevier.com/locate/ijleo

Original research article

# Optoelectronic properties of silicon nanotubes with electron–electron interactions in orthogonal tight-binding model

N. Ahmadi

*Department of Basic Sciences, Garmsar Branch, Islamic Azad University, Garmsar, Iran*

ARTICLE INFO

*Keywords:*
Hubbard model
Silicon nanotube
Orthogonal tight-binding
Optical absorption
Band structure

ABSTRACT

We investigate the electron–electron (e–e) interactions effect on the optoelectronic properties of zigzag silicon hexagonal nanotubes (Si h-NTs). Analytic expressions for the band structure and optical absorption of Si h-NTs have been derived based on orthogonal tight-binding (OTB) method. We combine OTB method and Hubbard model and show electron–electron interactions effect on the band structure of metallic and semiconducting zigzag nanotubes for the first and second-nearest neighbor. Moreover, the optical matrix elements and optical absorption are analytically derived for light polarization parallel to the tube axis in low energy for first nearest-neighbor (1NN) and second nearest-neighbor (2NN) approximation. It is found that the electron–electron interactions do not modify the optical absorption spectrum of zigzag Si h-NTs. These results can be beneficial for the explanation of resonant Raman Spectra of nanotube samples.

## 1. Introduction

Due to silicon atoms are similar to carbon atoms many scientists work on silicon nanostructures such as clusters, nanowires and nanotubes. In the recent years, silicon nanotubes have been considered, because of their applications in optoelectronic devices and rechargeable batteries [1,2]. Single walled silicon nanotubes are one dimensional nanostructures which according to their hybridization divided two parts: silicon hexagonal nanotubes (Si h-NTs) and silicon gear-like nanotubes (Si g-NTs) [3].

In recent years there has been strong interest in the e–e interactions on the properties of nanotubes [4–14]. One simple model to study electron–electron interactions was introduced by Hubbard et al. [15]. Accordingly, optoelectronic properties of nanotubes was investigated with considering e–e interactions [16,17,10]. The experimental results on nanotubes have shown that e–e interactions play strong role in optoelectronic properties of low dimensional systems [18–23].

In this work our aims is to provide detailed analytical and computational method of the e–e interactions for metallic and semiconducting zigzag Si h-NTs in orthogonal tight-binding (OTB) method.

We use OTB method and dynamical mean field theory [24] to approximate the extended Hubbard model and we obtain the energy dispersion and optical absorption of zigzag Si h-NTs. Our calculations show a rigid shift in the band structure of metallic and semiconducting nanotubes for both nearest neighbor (1NN) and next-nearest neighbor (2NN) approximations.

In our previous works we have investigated optoelectronic properties of zigzag Si h-NTs under intrinsic curvature effect in low energy regime [25]. We have also obtained the energy dispersion, dipole matrix elements and optical absorption of the Si h-NTs up to the second-nearest neighbors approximation (2NN) for incident light polarized parallel to the tube axis [26]. Furthermore we obtained an analytical expression for optical transitions of zigzag Si h-NT under an axial magnetic field [3].

This article is organized as follow: after a brief introduction in Section 1, we calculate the band structure and optical absorption of

*E-mail address:* ahmadiphysic@gmail.com.

https://doi.org/10.1016/j.ijleo.2018.05.115
Received 8 April 2018; Accepted 24 May 2018

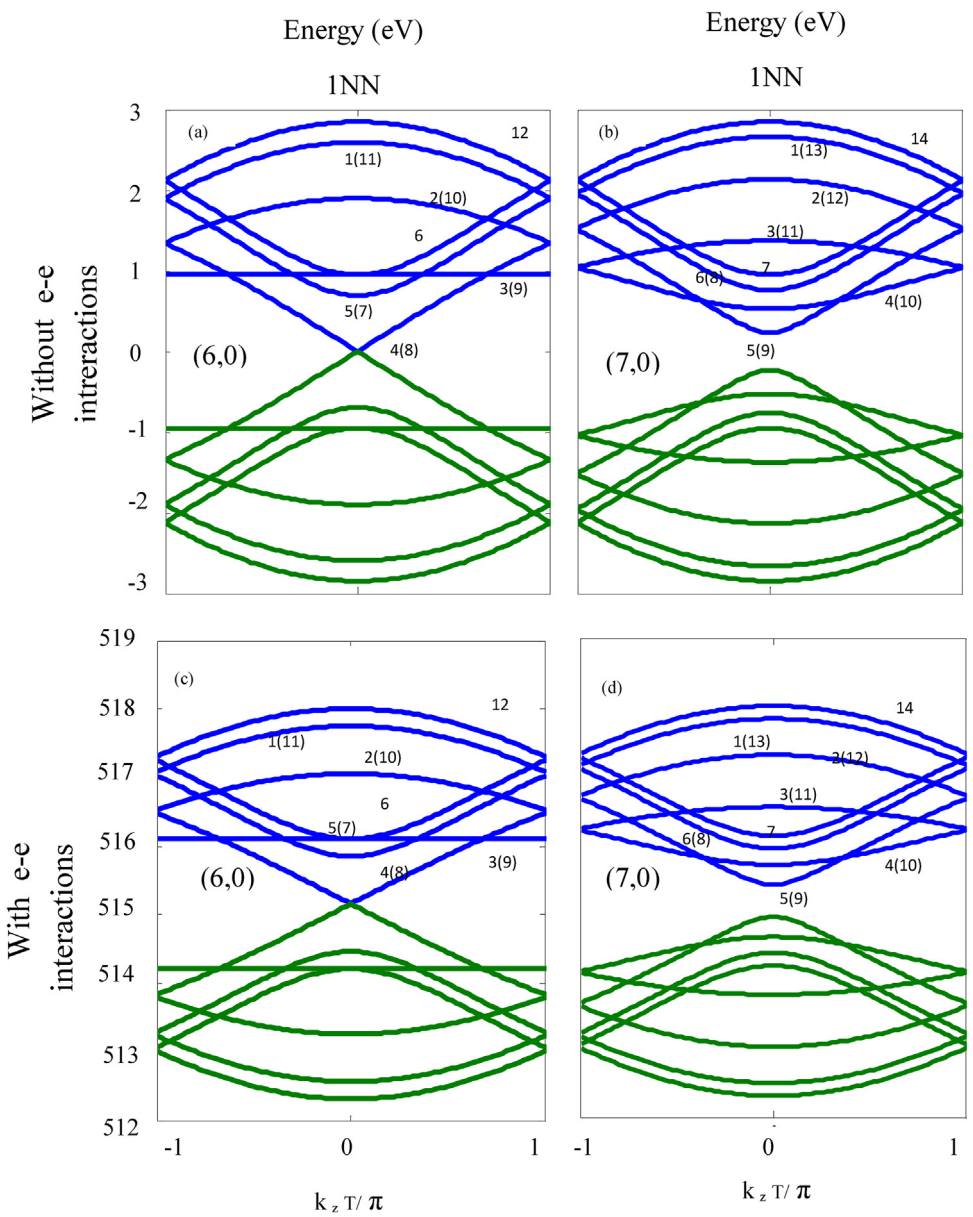


**Fig. 1.** Calculated the band structure of (6,0) and (7,0) Si h-NTs in term of $k_z$ for 1NN approximation, (a) and (b) without considering electron–electron interactions, (c) and (d) with considering electron–electron interactions.

Si h-NTs with considering e–e interactions for 1NN and 2NN approximations in OTB model (Section 2). In Section 3 we present the numerical results. Finally we conclude the study in Section 4.

## 2. Model and formalism

### 2.1. Band structure

In this study we considered the nanotube unit cell as a cylindrical segment with length $T$, which $T$ is the nanotube translation vector. We also considered the nanotube axis in the $Z$-direction and the number of unit cells is $N = 18$. Silicon hexagonal nanotube is formed by rolling up silicene sheets. Due to the similarity of silicene and graphene sheet there are two kinds of atoms in silicene: A- and B-types. Periodic boundary condition along the longitudinal direction causes the wave vector $k_z$ takes values in the first Brillouin zone as $\frac{-\pi}{T} \leq k_z \leq \frac{\pi}{T}$. Zigzag Si h-NTs are specified with a pair of indices $(n, m = 0)$ and $n$ take the values $n = 3s_0$, $n = 3s_0 + 1$ and $n = 3s_0 + 2$ which $s_0$ is integer and $n$ shows the metallic nanotubes and semiconducting types I and II, respectively. The position vectors of the nearest neighbor (1NN) approximation for the three nearest neighbors are [3]