### Accepted Manuscript

The structural and Electronic properties of (10,0) zigzag Single-Wall Carbon Nanotubes Modified by Thiophene groups

Masood Hamadanian, Zahra Tavangar, Sara Naseh

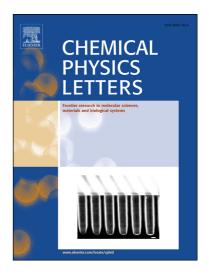
PII: S0009-2614(13)01044-0

DOI: http://dx.doi.org/10.1016/j.cplett.2013.08.034

Reference: CPLETT 31489

To appear in: Chemical Physics Letters

Received Date: 21 July 2013 Accepted Date: 13 August 2013



Please cite this article as: M. Hamadanian, Z. Tavangar, S. Naseh, The structural and Electronic properties of (10,0) zigzag Single-Wall Carbon Nanotubes Modified by Thiophene groups, *Chemical Physics Letters* (2013), doi: http://dx.doi.org/10.1016/j.cplett.2013.08.034

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

## ACCEPTED MANUSCRIPT

# The structural and Electronic properties of (10,0) zigzag Single-Wall Carbon Nanotubes Modified by Thiophene groups

Masood Hamadanian<sup>1,2</sup>\*, Zahra Tavangar<sup>2</sup>, Sara Naseh<sup>2</sup>

<sup>1</sup> Institute of Nano Science and Nano Technology, University of Kashan, I.R. Iran

<sup>2</sup> Department of Physical Chemistry, Faculty of Chemistry, University of Kashan, I.R. Iran

#### **Abstract**

In this work, modifications of (10, 0) functionalized zigzag Single-Wall Carbon Nanotubes in different sites by thiophene groups were studied using density functional theory. Geometric structures and electronic properties were investigated. After modification a significant change was observed in band structure and density of states and metallic properties were obtained. The best result for application in organic photovoltaic cells was achieved when two organic groups were placed on opposite sides of the wall of the SWCNT symmetrically.

*Keywords:* Single Wall Carbon Nanotubes; Density functional theory; Band structure; Density of state; Thiophene group; Organic photovoltaic cell

<sup>\*</sup> Corresponding author; Tel.: +98 361 5912382; Fax: +98 361 5552930; P.O. Box 87317-51167 Email: hamadani@kashanu.ac.ir

#### Download English Version:

## https://daneshyari.com/en/article/5381618

Download Persian Version:

https://daneshyari.com/article/5381618

<u>Daneshyari.com</u>