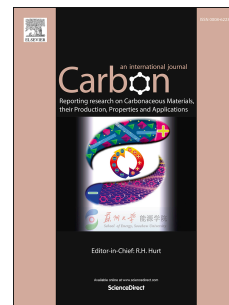


Accepted Manuscript

Band Gap Engineering of Carbon Nanotubes via Regular Addition Patterns of Covalent Functional Groups

Elise Y. Li



PII: S0008-6223(15)30549-2

DOI: [10.1016/j.carbon.2015.12.083](https://doi.org/10.1016/j.carbon.2015.12.083)

Reference: CARBON 10609

To appear in: *Carbon*

Received Date: 19 October 2015

Revised Date: 15 December 2015

Accepted Date: 26 December 2015

Please cite this article as: E.Y. Li, Band Gap Engineering of Carbon Nanotubes via Regular Addition Patterns of Covalent Functional Groups, *Carbon* (2016), doi: 10.1016/j.carbon.2015.12.083.

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.

Band Gap Engineering of Carbon Nanotubes via Regular Addition Patterns of Covalent Functional Groups

Elise Y. Li*

Department of Chemistry, National Taiwan Normal University, Taipei, 11677,
Taiwan

Abstract

We perform comprehensive first-principles calculations to study the addition pattern in multiply functionalized carbon nanotubes. We evaluate the relative strength of the rivaling forces between electronic effect and steric hindrance that determine whether the “cooperative addition” or the “random addition” takes place for monovalent or divalent functionalizations. We find that the electronic effect is the dominating factor and that small functional groups prefer to aggregate during successive functionalizations on CNTs. The aggregation of these functional groups leads to regular addition patterns that may drastically change the electronic properties of the original CNTs and may even result in a metallic to semiconducting transition, or vice versa.

1. Introduction

Chemical functionalization is an important method to manipulate the electrical, optical, and mechanical properties of carbon nanotubes (CNTs).[1-3] While the chemical identity of the functional groups may change from system to system, most functionalization reactions on CNT sidewalls fall into three categories: (1) Monovalent additions, such as hydrogenation, fluorination, alkylation, as well as the

* Corresponding author. Tel: 886 2 7734-6218. E-mail: eliseyli@ntnu.edu.tw (Elise Y. Li)

Download English Version:

<https://daneshyari.com/en/article/7850168>

Download Persian Version:

<https://daneshyari.com/article/7850168>

[Daneshyari.com](https://daneshyari.com)